Lecture

WKB approximation

\[ \psi(x) = 1 |\psi(x)| \frac{\psi(x)}{|\psi(x)|} \]

\[ A(x) = 1 |\psi(x)| \]

\[ \frac{i \phi(x)}{e} = \frac{\psi(x)}{|\psi(x)|} \]

This means that the equation above reads

\[ \psi(x) = A(x) e^{i \phi(x)} \]

where \( A(x) \) is real and positive and \( \phi(x) \) is real.

We define

\[ p^2_{cl}(x) = 2m (E - V(x)) \]

This is not necessarily positive, it is positive in the classically allowed region, negative in the classically forbidden region.
The Schrödinger equation can be expressed as

\[-\hbar^2 \frac{d^2}{dx^2} (A(x)e^{i\Phi(x)}) = P_{el}(x) A(x)e^{i\Phi(x)}\]

Note

\[
\frac{d}{dx} A(x)e^{i\Phi(x)} = A'(x)e^{i\Phi(x)} + i A(x) \Phi'(x) e^{i\Phi(x)}
\]

\[
= (A'(x) + i A(x) \Phi'(x)) e^{i\Phi(x)}
\]

\[
\frac{d^2}{dx^2} A(x)e^{i\Phi(x)} = [A''(x) + i A'(x) \Phi'(x) + i A'(x) \Phi'(x)]
\]
\[
+ i A(x) \Phi''(x) - A(x) \Phi'(x)^2 \right] e^{i\Phi(x)}
\]

Using this in the Schrödinger equation gives

\[-\hbar^2 \left[ A''(x) + 2i A'(x) \Phi'(x) + i A(x) \Phi''(x) - A(x) \Phi'(x)^2 \right] e^{i\Phi(x)}
\]

\[= P_{el}(x) A(x)e^{i\Phi(x)}\]

We can cancel \(e^{i\Phi(x)}\) from both sides of this equation.
in the classically allowed region $A(x)$, $\phi(x)$, $P_{\phi}(x)$ are real so we can equate the real and imaginary parts of this equation.

Real part

$$-\hbar^2 (A'' - A(x)\phi'^2(x)) = P_{\phi}(x)A(x)$$

Im part

$$-\hbar^2 (2A'(x)\phi'(x) + A(x)\phi''(x)) = 0$$

These are a pair of coupled non-linear differential equations in $A(x)$ and $\phi(x)$.

The second equation has the form

$$\frac{\phi''}{\phi'} = -2 \frac{A'}{A}$$

$$\frac{d}{dx} \ln \phi' = -2 \frac{d}{dx} \ln A = \frac{d}{dx} \ln \frac{1}{A^2} = -1$$

$$\frac{d}{dx} (\ln \phi' - \ln \frac{1}{A^2}) = \frac{d}{dx} \ln (\phi'/A^2) = 0$$
This means

\[ \phi'(x) A^2(x) = C = \text{constant} \]

\[ A(x) = \frac{1C}{|\phi'(x)|^{1/2}} = \frac{c'}{1 \phi'(x)|^{1/2}} \]

To get an equation for \( \phi \)

\[ \frac{d}{dx} \left( \frac{\phi''}{\phi'} \right) = -2 \frac{d}{dx} \left( \frac{A^1}{A} \right) = -2 \frac{A''}{A} + 2 \frac{A'^2}{A^2} \]

\[ \frac{A''}{A} = \left( \frac{A^1}{A} \right)^2 - \frac{1}{2} \left( \frac{\phi''}{\phi'} \right)' \]

Dividing the first equation by \( A \)

\[ \frac{A''}{A} - \phi'^2 = -\frac{1}{\hbar^2} P_{cl}(x) \]

Using the relation in the box above in this expression gives

\[ \left( \frac{A^1}{A} \right)^2 - \frac{1}{2} \left( \frac{\phi''}{\phi'} \right)' - \phi'^2 = -\frac{1}{\hbar^2} P_{cl}(x) \]

Using

\[ \frac{A^1}{A} = -\frac{1}{2} \left( \frac{\phi''}{\phi'} \right) = 0 \]
\[ -\frac{1}{4}\left(\frac{\phi''}{\phi'}\right)^2 - \frac{1}{2}\left(\frac{\phi''}{\phi'}\right)\phi' - \phi'^2 = -\frac{1}{\hbar}\, P_{cc}(x) \]

It is useful to express this in the form

\[ \phi'^2(x) = \frac{1}{\hbar^2} P_{cc}^2(x) + \frac{1}{4} \left(\frac{\phi''}{\phi'}\right)^2 - \frac{1}{2} \left(\frac{\phi''}{\phi'}\right)' \]

\[ A(x) = \frac{\phi}{|\phi'(x)|^{1/2}} \]

The equation in the phase is a non-linear differential equation involving 3rd derivatives of \( \phi \).

The working assumption about the WKB approximation is that the term

\[ \left(\frac{\phi''}{\phi'}\right)^2 \left(\frac{\phi''}{\phi'}\right)' \]

are small relative to \( \frac{1}{\hbar^2} P_{cc}^2(x) \). This is a classical limit since \( P_{cc}^2(x) \) dominates in the limit \( \hbar^2 \to 0 \).
When these conditions are satisfied one can use iteration to get an approximate solution

\[ \phi_0'(x) = \pm \frac{1}{\hbar} P_{cl}(x) \]

\[ \phi_n(x) = \pm \int_x^x \frac{1}{\hbar} P_{cl}(x')dx' \]

Iteration gives:

\[ \phi_n'(x) = \pm \frac{1}{\hbar} \sqrt{P_{cl}^2(x) + \frac{\hbar^2}{4} \left( \frac{P_{cl}''}{P_{cl}'} \right)^2 - \frac{\hbar^2}{2} \left( \frac{P_{cl}''}{P_{cl}'} \right)^2} \]

Using this,

\[ \phi_1'(x) = \pm \frac{1}{\hbar} \sqrt{P_{cl}^2(x) + \frac{\hbar^2}{4} \left( \frac{P_{cl}'}{P_{cl}} \right)^2 - \frac{\hbar^2}{2} \left( \frac{P_{cl}'}{P_{cl}} \right)^2} \]

= \pm \frac{1}{\hbar} \left( P_{cl}(x) + \frac{1}{2} \frac{\hbar^2}{4} \frac{1}{P_{cl}(x)^2} \left( \frac{P_{cl}'}{P_{cl}} \right)^2 - \frac{\hbar^2}{2} \frac{1}{P_{cl}(x)^2} \left( \frac{P_{cl}'}{P_{cl}} \right)^2 \right) + \ldots

Higher order terms in powers of \( \frac{\hbar}{\hbar} \)

(Here I used \( \sqrt{1+x} = 1 + \frac{1}{2} x + \ldots \))
The lowest order approximation gives a wave function of the form

$$\psi(x) \sim \frac{N}{\sqrt{P_c(x)}} e^{\pm \frac{i}{\hbar} \int_{x'}^x P_c(x') \, dx'}$$

The lower limit of integration can be absorbed into the normalization constant so it can be anything.

This approximation applies to the classically allowed region.

In the classically forbidden region $P_c(x)$ becomes imaginary and the solution becomes

$$\psi(x) \sim \frac{N}{\sqrt{P_c(x)}} e^{\pm \frac{i}{\hbar} \int_{x'}^x |P_c(x')| \, dx}$$
The derivation we used breaks down when $P_{cc}(x)$ is imaginary.

If instead we write

$$\psi(x) = A(x) e^{\frac{i}{\hbar} S(x)}$$

and we separated even and odd powers of $\hbar$ instead of real and imaginary parts we would have the same equations but they would also apply to the case $P_{cc}^2(x) < 0$.

Conditions for the approximation to be valid

$$\frac{\hbar^2}{P_{cc}(x)^2} \left( \frac{P_{cc}'}{P_{cc}} \right)^2 \ll 1$$

$$\frac{\hbar^2}{P_{cc}(x)^2} \left( \frac{P_{cc}'}{P_{cc}} \right) \ll 1$$

To check these
\[ P_\text{el}^2 (x) = 2m \left( E - V(x) \right) \]

\[ \frac{d}{dx} \left( \frac{P_{\text{el}}^2}{P_{\text{el}}(x)} \right) = - \frac{m \frac{dV}{dx}}{P_{\text{el}}^2 (x)} = - \frac{m \frac{dV}{dx}}{2m(E-V(x))} = - \frac{1}{2} \frac{dV}{dx} \frac{1}{E-V(x)} \]

\[ \frac{d}{dt} \left( \frac{p^2}{P} \right) = \frac{d}{dx} \left( - \frac{1}{2} \frac{dV}{dx} \frac{1}{E-V(x)} \right) \]

\[ = - \frac{1}{2} \frac{V''}{E-V} + \frac{1}{2} \frac{V'^2}{(E-V)^2} \]

So the quantities that should be small for the WKB approximation to be valid are

\[ \left| \frac{k^2}{p^2} \left( \frac{p'}{P} \right)^2 \right| = \frac{k^2}{2} \left| \frac{V'}{E-V} \right|^2 \]

\[ \left| \frac{k^2}{p^2} \left( \frac{p'}{P} \right) \right| \leq \frac{k^2}{2} \left| \frac{V''}{E-V} \right| + \frac{k^2}{2} \left| \frac{V'^2}{E-V} \right|^2 \]
This requires that when $P_{CL}(x)$ is not close to 0, that $V'$ and $V''$ are small.

The sense of smallness is made precise by the inequality - the factors of $l$ to set the relevant scale

This simplest case is when the potential is piecewise constant. In that case $V' = V'' = 0$ and the correction terms vanish.

Case 1: Particle of mass $m$ in an infinite square well of width $a$.

$$P_{CL}^2 = 2mE$$

$$\psi(x) = \frac{C_1}{\sqrt{2mE}} x + \frac{C_2}{\sqrt{2mE}} e^{-\frac{x}{\sqrt{2mE}}}$$

$$\Phi = \pm \int \frac{x}{\sqrt{2mE}} = \pm \sqrt{2mE} x$$
boundary conditions require this to vanish at $x=0$ and $x=a$

$$0 = \frac{c_1 + c_1}{\sqrt{2mE}} \quad c_1 = -c_2$$

$$0 = \frac{c_1}{\sqrt{2mE}} \left( e^{\frac{i}{\hbar}\sqrt{2mE}a} - e^{-\frac{i}{\hbar}\sqrt{2mE}a} \right)$$

$$= \frac{2ic_1}{\sqrt{2mE}} \sin\left(\frac{\sqrt{2mE}}{\hbar}a\right)$$

this will vanish when

$$\frac{\sqrt{2mE}}{\hbar}a = n\pi \quad E_n = \frac{1}{2m} \frac{k^2n^2\pi^2}{a^2}$$

which are the exact eigenfunctions for particles in an infinite square well - the wave functions $c_1$

$$c_1 \sin\left(\frac{n\pi x}{\alpha}\right)$$

where normalization requires

$$c_n = \sqrt{\frac{2}{a}}$$
In this case the WKB approximation recovers the exact solution.

 realms $I$, $M$ are classically allowed

\[
\begin{align*}
\frac{i}{\hbar} \sqrt{2mE} x &+ \frac{1}{i\hbar} \sqrt{2mE} x \\
AE &+ BE \\
\frac{i}{\hbar} \sqrt{2m(E-V_2)} x &+ \frac{-i}{\hbar} \sqrt{2m(E+V_1)} x \\
EE &+ EE \\
\frac{i}{\hbar} \sqrt{2m(V_1-E)} x &+ \frac{-i}{\hbar} \sqrt{2m(V-E)} x \\
CE &+ DE
\end{align*}
\]

(The WKB fixe) the $x$ dependence in $ABCDE$, but in this special case the are constant.

The coefficients can be determined by requiring
\[ \int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = 1 \]

\( \psi(x) \), \( \psi'(x) \) continuous at \( x = 0 \)

\( \psi(x) \), \( \psi'(x) \) continuous at \( x = a \)

\[ A + B = C + D \]

\[ i \sqrt{2mE} (A - B) = \sqrt{2m(V_1 - E)} (C - D) \]

\[ E \begin{pmatrix} \frac{i}{\hbar} \sqrt{2m(E-V_3)} a & -\frac{i}{\hbar} \sqrt{2m(E-V_3)} c \\ \frac{i}{\hbar} \sqrt{2m(V_1 - E)} c & -\frac{i}{\hbar} \sqrt{2m(V_1 - E)} a \end{pmatrix} + E \begin{pmatrix} \frac{i}{\hbar} \sqrt{2m(E-V_3)} c & \frac{i}{\hbar} \sqrt{2m(E-V_3)} a \\ \frac{i}{\hbar} \sqrt{2m(V_1 - E)} a & -\frac{i}{\hbar} \sqrt{2m(V_1 - E)} c \end{pmatrix} = \]

\[ i \sqrt{E-V_2} \begin{pmatrix} \frac{i}{\hbar} \sqrt{2m(E-V_3)} a & -\frac{i}{\hbar} \sqrt{2m(E-V_3)} c \\ \frac{i}{\hbar} \sqrt{2m(V_1 - E)} c & -\frac{i}{\hbar} \sqrt{2m(V_1 - E)} a \end{pmatrix} = \]

\[ \sqrt{V_1 - E} \begin{pmatrix} \frac{i}{\hbar} \sqrt{2m(E-V_3)} c & \frac{i}{\hbar} \sqrt{2m(E-V_3)} a \\ \frac{i}{\hbar} \sqrt{2m(V_1 - E)} a & -\frac{i}{\hbar} \sqrt{2m(V_1 - E)} c \end{pmatrix} \]

We can solve this linear system - expressing \( B, C, D, E \) in terms of \( A \) and then fix \( A \) by normalization.

Again - the recovery the known results for piece-wise constant potentials.
In these cases the approximation worked because $V'$ was constant everywhere.

In general

\[ \Psi_{\text{WKB}}(x) = \frac{C}{\sqrt{IP_c(x)}} e^{i \int P_c(x') dx'} \]

\[ P_c(x) = \sqrt{2m (E - V(x))} \]

The problem is that the boundary between the classically allowed and forbidden region is when $E - V(x) = 0$ (the classical turning points). At these points:

1. \[ \frac{1}{\sqrt{IP_c(x)}} = \infty \]

2. The conditions for the validity of the WKB approximation are not satisfied.
mis makes it impossible to match solutions at the turning points.

\[ V(x) \]

It turns out that the region where the approximation breaks down is small for a slowly varying potential. One way to match boundary conditions is to use the exact solution of the Schrödinger equation at the turning point and match to that solution.

Approximate the potential by

\[ V(x) \approx V(x_r) + \frac{dV}{dx}(x_r)(x-x_r) \]

where \( x_r \) is the classical turning point - at that point \( V(x_r) = E \)

\[ E - V(x) \approx -\frac{dV}{dx}(x_r)(x-x_r) \]
In this case

\[ P_{cl} = 2m(E-V) = -2m \frac{dV}{dx}(x_+)(x-x_+) \]

\[ -\hbar^2 \frac{d^2}{dx^2} = -2m \frac{dV}{dx}(x_+)(x-x_+) \]

It is useful to shift the origin to \( x_+ \) \( y = x - x_+ \)

\[ \frac{d}{dx} = \frac{d}{dx} \frac{d}{dy} = 1 \]

\[ \frac{d^2 \psi}{d\eta^2} = \frac{m}{\hbar^2} \frac{dV}{dx}(x_+) \eta \]

It is useful to use dimensionless variables:

\[ z = \alpha y \quad \frac{d}{dw} = \alpha \frac{d}{dz} \]

\[ \frac{d^2 \psi}{dz^2} = \frac{1}{\alpha^3} \left( \frac{m}{\hbar^2} \frac{dV}{dx}(x_+) \right) z \]

Let \( \alpha^3 = \left( \frac{m}{\hbar^2} \frac{dV}{dx}(x_+) \right) \quad \alpha = \sqrt[3]{\frac{m}{\hbar^2} V'(x_+)} \]

(this could be positive or negative)
\[
\Psi(x) = f(x(x-x_1)) \\
\psi''(z) = z \psi(z)
\]

The solutions of the \( \psi(z) \) equation are called Airy functions.

We expect that they oscillate in the classically allowed region and fall off in the classically forbidden region.

\[
\text{Ai}(z) = \frac{1}{\pi} \int_0^\infty ds \cos(sz + \frac{1}{3}s^3)
\]

Is an integral representation of the Airy function.
To demonstrate that this satisfies the differential equation it is useful to write it in the form

\[ Ai = \frac{1}{2\pi} \int_{-\infty}^{\infty} (e^{i(sz + \frac{1}{3}s^3)} + e^{-i(sz + \frac{1}{3}s^3)}) \, ds \]

let \( s' = -s \) in the second term

\[ \frac{1}{2\pi} \int_{0}^{\infty} e^{i(sz + \frac{1}{3}s^3)} \, ds \]

\[ -\frac{1}{2\pi} \int_{0}^{\infty} e^{i(sz + \frac{1}{3}s^3)} \, ds \]

\[ -\frac{1}{2\pi} \int_{-\infty}^{0} e^{i(sz + \frac{1}{3}s^3)} \, ds \]

\[ \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(sz + \frac{1}{3}s^3)} \, ds \]

\[ \frac{d^2}{dz^2} \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(sz + \frac{1}{3}s^3)} \, ds = \]

\[ \frac{1}{2\pi} \int_{-\infty}^{\infty} i(sz + \frac{1}{3}s^3) \, dz \]

\[ \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{is^2} (i \frac{d}{ds}) e^{\frac{1}{3}s^3} \, ds \]

Integrate by parts

\[ \frac{1}{2\pi} \int (e^{iz^2}) e^{\frac{1}{3}s^3} + \text{boundary terms} \]

\[ = Ai(z) + \text{boundary terms} \]
The Airy function is something like a plane wave, when integrated against a nice function of $z$, it falls off - and in that case the boundary terms vanish:

$$\frac{1}{\sqrt{\pi}} \int e^{is^2} f(s) \, ds = \tilde{f}(s) \to 0$$

To use this we need to know the structure of the Airy function in regions that are far from the turning point.