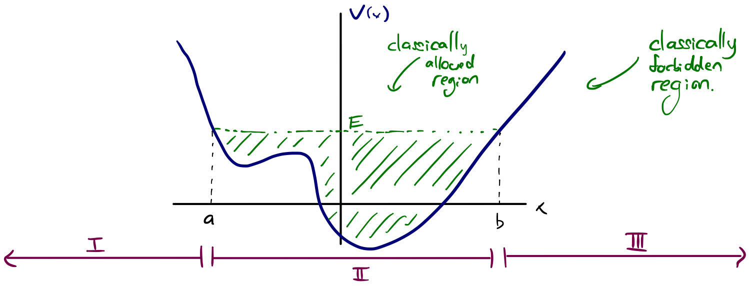
B7.3 Further Quantum Theory Lecture 14

Now we want to consider more realistic applications of the WKB approximation, namely to cases with non-square walls.



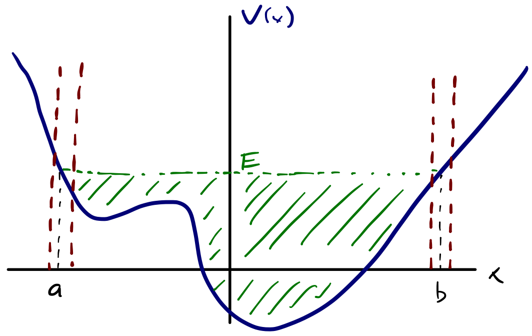
$$\psi^{I} = \frac{C_I}{\sqrt{q(x)}} \exp\left(\frac{-1}{\hbar}\int_x^a q(x)\,dx\right)$$

$$\psi^{II} = \frac{C_-}{\sqrt{p(x)}} \exp\left(\frac{-i}{\hbar}\int_a^x p(x)\,dx\right) + \frac{C_+}{\sqrt{p(x)}} \exp\left(\frac{i}{\hbar}\int_a^x p(x)\,dx\right)$$

$$\psi^{III} = \frac{C_{III}}{\sqrt{q(x)}} \exp\left(\frac{-1}{\hbar}\int_b^x q(x)\,dx\right)$$

How to determine coefficients? Might think to just match ψ and ψ' like in square well, but this doesn't work: $|p|$ and $|q|$ vanish at $x=a,b$, so wavefunctions diverge. In particular, $\frac{A''}{A}\to\infty$, so our approximation definitely breaks down.

We must apply a separate analysis in the neighbourhoods of the classical turning points.



In the vicinity of (say) $x=b$, we approximate the potential by a linear function:

$$V(x) \approx V(b) + (x-b)V'(b)$$

We can solve the time-independent Schrödinger equation in this approximation. Set $y = x-b$; $\tilde{\psi}(y) = \psi(x)$

$$-\frac{\hbar^2}{2m}\tilde{\psi}''(y) = \left(E - V(b) - yV'(b)\right)\tilde{\psi}(y) = -yV'(b)\tilde{\psi}(y)$$

Set $z = \left[\frac{2mV'(b)}{\hbar^2}\right]^{1/3} y$, $\phi(z) = \tilde{\psi}(y)$. Now $\phi''(z) = z\phi(z)$. This is a famous ODE, the "Airy equation".

The Airy functions $Ai(z)$ & $Bi(z)$ are a basis for the space of solutions to the Airy equation.

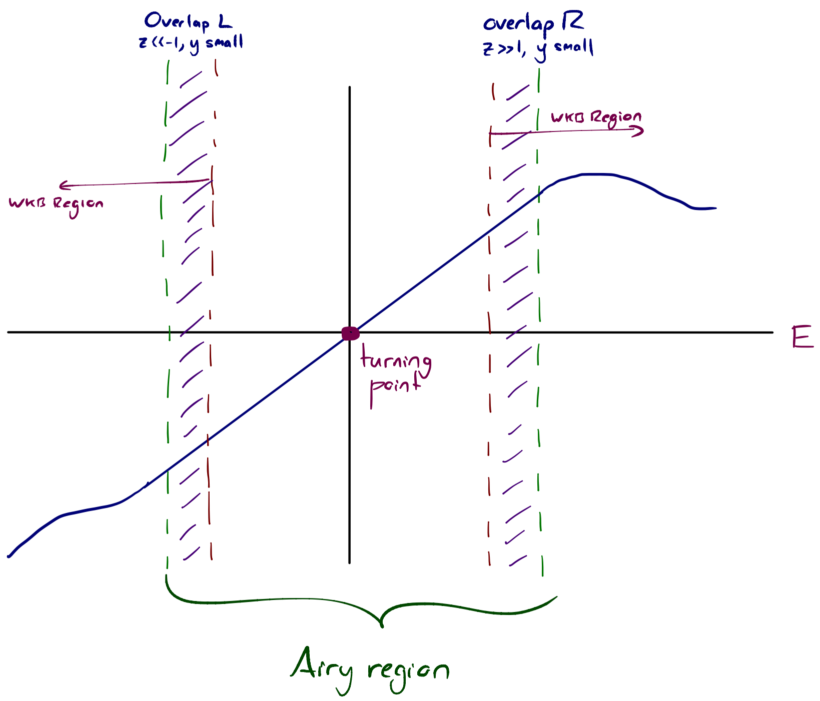
$$Ai(z) = \frac{1}{\pi}\int_0^\infty \cos\left(\frac{t^3}{3} + zt\right) dt \qquad Bi(z) = \frac{1}{\pi}\int_0^\infty \left(\sin\left(\frac{t^3}{3} + zt\right) + e^{-\frac{t^3}{3} + zt}\right) dt$$

The large-$|z|$ asymptotics of these functions can be found:

$$z \gg 1 \qquad Ai(z) \sim \frac{e^{-\frac{2}{3}z^{3/2}}}{2\sqrt{\pi}\, z^{1/4}} \qquad Bi(z) \sim \frac{e^{\frac{2}{3}z^{3/2}}}{\sqrt{\pi}\, z^{1/4}}$$

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

If $\frac{2mV'(b)}{\hbar^2} \gg 1$, then large $|z|$ is compatible with small-ish y. So the idea is to match the Airy functions with the WKB wave-functions away from the turning points.



In the overlaps, we have $p(x) \approx \sqrt{2m(-yV'(y))}$ in region L, $q(x) = \sqrt{2m(yV'(y))}$ in region R. This gives WKB wave-functions as follows:

$$\psi_\pm^{(L)}(y) \approx \frac{1}{(2m(-yV'(y)))^{\frac{1}{4}}} \exp\left(\mp\frac{i}{\hbar}\int_y^0 \sqrt{2m(-y'V'(b))}\, dy'\right) = \frac{1}{(2m(-yV'(b)))^{\frac{1}{4}}} \exp\left(\mp\frac{i}{\hbar}\sqrt{2mV'(b)}\,\frac{2}{3}(-y)^{\frac{3}{2}}\right)$$

$$= \frac{1}{(-z)^{1/4}} \exp\left(\mp\frac{2}{3} i (-z)^{3/2}\right)$$

Airy asymptotics

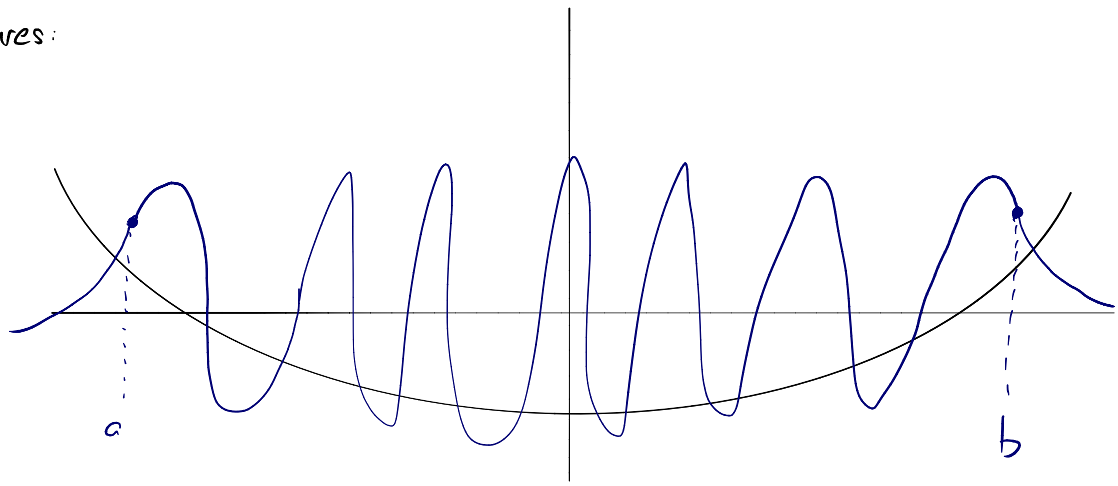
$$\psi_\pm^{(R)}(y) \approx \frac{1}{(2myV'(b))^{\frac{1}{4}}} \exp\left(\pm\frac{1}{\hbar}\int_0^y \sqrt{2my'V'(b)}\, dy'\right) = \frac{1}{z^{1/4}} \exp\left(\pm\frac{2}{3} z^{3/2}\right)$$

To get dying exponential in overlap region $\mathbb{R}$, need $Ai(z)$ in the turning point region, which fixes the combination of $\psi_\pm^{(L)}$ in the classically allowed region. In particular,

$$\frac{1}{q(x)^{1/4}}\exp\left(-\frac{1}{\hbar}\int_b^x q(x')dx'\right) \approx \frac{1}{z^{1/4}}\exp\left(-\frac{2}{3}z^{3/2}\right) \overset{z\ll -1}{\sim} 2\sqrt{\pi}\,Ai(z) \overset{z\gg 1}{\sim} \frac{2\cos\left(\frac{2}{3}(-z)^{3/2}-\frac{\pi}{4}\right)}{(-z)^{1/4}} \approx \frac{2}{\sqrt{p(x)}}\cos\left(\frac{1}{\hbar}\int_x^b p(x')dx' - \frac{\pi}{4}\right)$$

$$\frac{2\cos\left(\frac{2}{3}(-z)^{3/2}-\frac{\pi}{4}\right)}{(-z)^{1/4}} = \frac{e^{-\frac{i\pi}{4}}e^{\frac{2}{3}i(-z)^{3/2}} + e^{\frac{i\pi}{4}}e^{-\frac{2}{3}i(-z)^{3/2}}}{(-z)^{1/4}} \approx \frac{e^{-\frac{i\pi}{4}}e^{\frac{i}{\hbar}\int_x^b p(x')dx'} + e^{\frac{i\pi}{4}}e^{-\frac{i}{\hbar}\int_x^b p(x')dx'}}{\sqrt{p(x)}} = \frac{2}{\sqrt{p(x)}}\cos\left(\frac{1}{\hbar}\int_x^b p(x')dx' - \frac{\pi}{4}\right)$$

In pictures:



More generally, we have matching conditions

$$\frac{C\exp\left(-\frac{1}{\hbar}\int_b^x q(x')dx'\right)}{\sqrt{q(x)}} \longleftrightarrow \frac{2C\cos\left(\frac{1}{\hbar}\int_x^b p(x')dx' - \frac{\pi}{4}\right)}{\sqrt{p(x)}}$$

$$\frac{D\exp\left(\frac{1}{\hbar}\int_b^x q(x')dx'\right)}{\sqrt{q(x)}} \longleftrightarrow \frac{D\cos\left(\frac{1}{\hbar}\int_x^b p(x')dx' + \frac{\pi}{4}\right)}{\sqrt{p(x)}}$$

An analogous treatment at the turning point at $x=a$ gives the matching conditions

$$\frac{C\exp\left(-\frac{1}{\hbar}\int_x^a q(x')dx'\right)}{\sqrt{q(x)}} \longleftrightarrow \frac{2C\cos\left(\frac{1}{\hbar}\int_a^x p(x')dx' - \frac{\pi}{4}\right)}{\sqrt{p(x)}}$$

$$\frac{D\exp\left(\frac{1}{\hbar}\int_x^a q(x')dx'\right)}{\sqrt{q(x)}} \longleftrightarrow \frac{D\cos\left(\frac{1}{\hbar}\int_a^x p(x')dx' + \frac{\pi}{4}\right)}{\sqrt{p(x)}}$$

In our bound state problem, requiring the right exponential behaviour on both sides over determines the problem.

$$\psi^{I} = \frac{C_I}{\sqrt{q(x)}} \exp\left(\frac{-1}{\hbar}\int_x^a q(x)\,dx\right)$$

$$\psi^{II} = \frac{2C_I}{\sqrt{p(x)}} \cos\left(\frac{1}{\hbar}\int_a^x p(x')dx' - \frac{\pi}{4}\right) = \frac{2C_{III}}{\sqrt{p(x)}} \cos\left(\frac{1}{\hbar}\int_x^b p(x')dx' - \frac{\pi}{4}\right)$$

$$\psi^{III} = \frac{C_{III}}{\sqrt{q(x)}} \exp\left(\frac{-1}{\hbar}\int_b^x q(x)\,dx\right)$$

The compatibility condition is that

$$C_I \cos\left(\frac{1}{\hbar}\int_a^x p\,dx' - \frac{\pi}{4}\right) = C_{III} \cos\left(\frac{1}{\hbar}\int_x^b p\,dx' - \frac{\pi}{4}\right) \equiv C_{III} \cos\left(\frac{\pi}{4} - \int_x^b p\,dx'\right)$$

Note that $\frac{\pi}{4} - \frac{1}{\hbar}\int_x^b p\,dx' = \frac{\pi}{4} - \frac{1}{\hbar}\int_a^b p\,dx' + \frac{1}{\hbar}\int_a^x p\,dx'$, so we need

$$\cos\left(\frac{1}{\hbar}\int_a^x p\,dx'\right) = \frac{C_{III}}{C_I} \cos\left(\frac{\pi}{2} - \frac{1}{\hbar}\int_a^b p\,dx' + \frac{1}{\hbar}\int_a^x p\,dx'\right)$$

The two possibilities are

- $C_{III} = C_I, \quad \frac{1}{\hbar}\int_a^b p\,dx' - \frac{\pi}{2} = 2n\pi \quad (n=0,1,2,\ldots)$
- $C_{III} = -C_I, \quad \frac{1}{\hbar}\int_a^b p\,dx' - \frac{\pi}{2} = (2n+1)\pi \quad (n=0,1,2,\ldots)$

These give a "corrected" quantization condition:

"Maslov correction"

$$\int_a^b p\,dx = \left(n + \frac{1}{2}\right)\pi\hbar \qquad (n=0,1,2,\ldots)$$

This can again be rephrased as an integral in phase space

$$\int_{p^2=2m(E-V)} p(x)\,dx = 2\pi\hbar\left(n+\tfrac{1}{2}\right) \qquad \int_{p^2\leq 2m(E-V)} \frac{dp\,dx}{2\pi\hbar} = n + \tfrac{1}{2}$$

"Bohr Sommerfeld quantization condition"

More applications of WKB:

Radial Schrödinger equation in $d>1$ (mostly 3d). In 3d with central potential $V(\underline{r})=V(r)$, we obtain (by standard derivation) the radial equation where $\psi(\underline{r}) = Y_\ell^m(\phi,\theta)R(r)$:

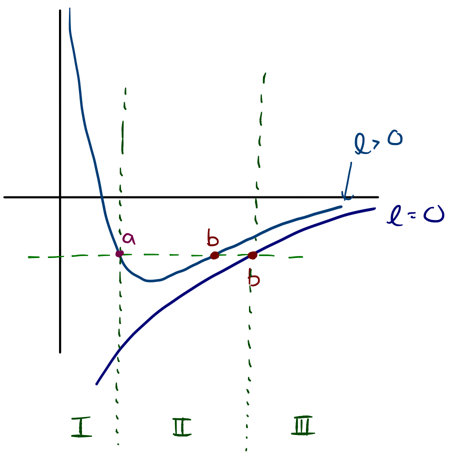
$$\frac{-\hbar^2}{2m}\left[\frac{1}{r}\frac{\partial^2}{\partial r^2}(rR)\right] + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}R(r) = (E-V(r))R(r) \iff \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial r^2}(rR) = \left(E - V(r) - \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right)(rR)$$

This is just the 1-d time-independent equation for $u(r) = rR(r)$ with a potential including the centrifugal term.

$$u_{WKB}(r) = \frac{1}{\sqrt{p(r)}}\exp\left(\frac{\pm i}{\hbar}\int^r p(r')dr'\right) \qquad \text{or} \qquad u_{WKB}(r) = \frac{1}{\sqrt{q(r)}}\exp\left(\frac{\pm 1}{\hbar}\int^r q(r')dr'\right)$$

$$p(r) = \left[2m\left(E - V(r) - \frac{\hbar^2\ell(\ell+1)}{2mr^2}\right)\right]^{\frac{1}{2}} \qquad q(r) = \left[2m\left(V(r) + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2} - E\right)\right]^{\frac{1}{2}}$$

As before, we identify classical turning points and match WKB approximations on either side. Let's look at the example of the Coulomb potential.



$$u_{III}(r) = \frac{C}{\sqrt{q(r)}}\exp\left(\frac{-1}{\hbar}\int_b^r q(r')dr'\right)$$

$$u_{II}(r) = \frac{2C}{\sqrt{p(r)}}\cos\left(\frac{1}{\hbar}\int_r^b p(r')dr' - \frac{\pi}{4}\right)$$

Two different cases on the left:

- $\ell=0$, no region I. Then $u(0) = 0\cdot R(0) = 0$, so this is like an infinite potential barrier at $r=0$.
- $\ell>0$, extra turning point, need to match falling exponential in region I.

This is actually a very subtle problem, because the potential (in both cases) is singular at $r=0$. There is a way to improve the estimate (the "Langer correction") but we will be content with the present level of analysis.

Next week, we will talk about 1d scattering, which is another place where the WKB method can come in handy!