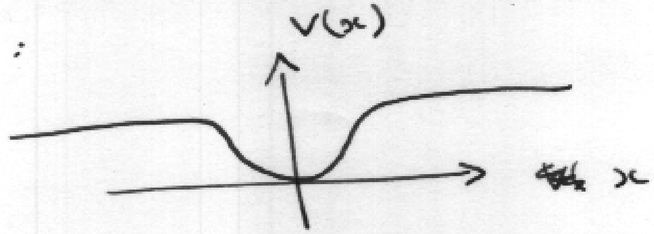
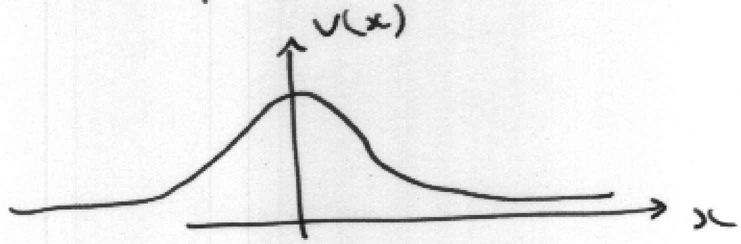
Lecture 8 : WKB approximation

this approximation is useful in finding energy levels for particles in a "generic" well :



as well as for studying barrier penetration at a "hump" :



Importantly the potential does not have to be simple or symmetric or solvable in nature.

The key idea is to consider situations where a particle's trajectory is "quasi-classical" in a sense we will make precise. Roughly this means that away from a "wall" or turning point, the particle propagates like a free particle with wave function

$$\psi(x) \sim e^{ipx/\hbar}$$

At turning points this fails and we bring in some new information to fully determine ψ.

Start with a generic 1d problem:

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + V(x)\Psi(x) = E\Psi(x)$$

and let us make the substitution

$$\Psi(x) = e^{iS(x)/\hbar}$$

Here S can be complex, so this is nothing but a change of variables for the moment.

Then:
$$\Psi' = \frac{iS'}{\hbar} e^{iS/\hbar}$$

$$\Psi'' = \left(\frac{iS''}{\hbar} - \frac{(S')^2}{\hbar^2}\right) e^{iS/\hbar}$$

So
$$-\frac{\hbar^2}{2m}\left(-\frac{(S')^2}{\hbar^2} + \frac{iS''}{\hbar}\right) + V(x) - E = 0$$

$$\Rightarrow \quad S'(x)^2 - i\hbar S''(x) + 2m(V(x) - E) = 0$$

In the limit $\hbar \to 0$ ("classical limit") we have

$$S'(x) = \pm \sqrt{2m(E - V(x))}$$

Compare this with a classical particle undergoing bounded periodic motion between two turning points, for which

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

We see that $S'(x)$ is the classical momentum of the particle in this limit.

Integrating, we get:

$$S(x) = \pm \int^{x} \sqrt{2m(E - V(x'))}\, dx'$$

When is this approximation valid? When

$$\hbar |S''(x)| \ll |(S'(x))^2|$$

i.e.

$$\frac{d}{dx} \left| \frac{\hbar}{S'(x)} \right| \ll 1$$

Now $S'(x) \sim p$, the classical momentum,

so

$$\frac{d}{dx} \left(\frac{\hbar}{p} \right) \ll 1$$

But $\lambda = \frac{2\pi\hbar}{p}$ is the de Broglie wavelength of the particle. So

$$\frac{d}{dx} \lambda(x) \ll 1$$

ie the de Broglie wavelength should be slowly varying.

Near turning points this fails: $p = \sqrt{2m(E - V(x))} \to 0$ at $V(x) = E$: the "classical turning points."

So we need to find <u>corrections</u> to the naive approximation.

Take $S(x) = S_0(x) + \hbar S_1(x) + \cdots$

and keep terms to $O(\hbar)$:

$$S'(x)^2 - i\hbar S''(x) + 2m(V(x) - E) = 0$$

$$\Rightarrow \quad (S_0' + \hbar S_1')^2 - i\hbar(S_0'' + \hbar S_1'') + 2m(V-E) = 0$$

$$\Rightarrow \quad S_0'^2 + 2m(V(x) - E) = 0 \qquad \text{(order 0 in } \hbar)$$

$$2S_0'S_1' - i S_0'' = 0 \qquad \text{(order 1 in } \hbar)$$

Thus $\quad S_0 = \pm \int^x \sqrt{2m(E - V(x'))}\, dx' \equiv \int p(x)\, dx$

$$S_1' = \frac{i}{2}\frac{S_0''}{S_0'} = \frac{i}{2}\frac{d}{dx}(\log S_0')$$

$$\therefore \quad S_1(x) = \frac{i}{2}\log S_0' = \frac{i}{2}\log p(x)$$

Now $\quad \psi_\pm(x) \simeq e^{\frac{i}{\hbar}(S_0 + \hbar S_1)}$

$$= e^{\pm\frac{i}{\hbar}\int p\, dx} \cdot e^{-\frac{1}{2}\log p(x)}$$

$$= \frac{1}{\sqrt{p(x)}}\, e^{\pm\frac{i}{\hbar}\int p\, dx}$$

So a general solution is

$$\psi(x) = \frac{c_1}{\sqrt{p(x)}}\, e^{\frac{i}{\hbar}\int p\, dx} + \frac{c_2}{\sqrt{p(x)}}\, e^{-\frac{i}{\hbar}\int p\, dx}$$

Note that S_0 is real, so

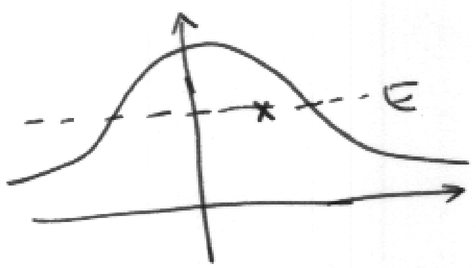
$$|\psi_\pm|^2 \simeq \frac{1}{p(x)}$$

hence for ~~small~~ large momentum $p(x)$ there is a small probability of finding the particle at x (ie between x, $x+dx$).

Near the turning point, $|\psi_\pm|^2 \to \infty$ so the approximation becomes quite poor.

Suppose that instead of being in a classically allowed region (a well) we were in a classically forbidden region (a barrier). The classical momentum is now imaginary.

$$p(x) = \sqrt{2m(E-V(x))} = i\sqrt{2m(V(x)-E)}$$
$$= i\,|p|$$



($E < V(x)$ inside a barrier).

Notation: $k = \frac{p}{\hbar}$, $\kappa = \frac{|p|}{\hbar}$

Then we can still write

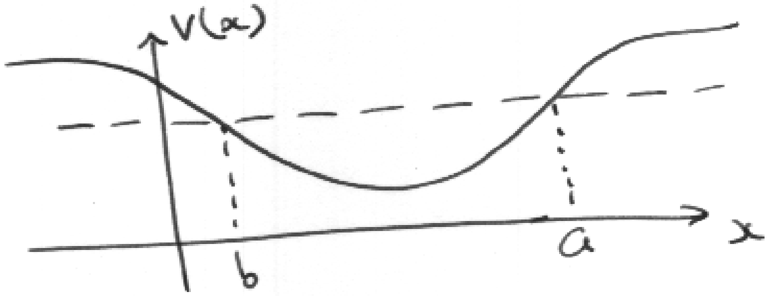
$$\psi(x) = \frac{c_1}{\sqrt{|p(x)|}} e^{-\frac{1}{\hbar}\int |p|\,dx} + \frac{c_2}{\sqrt{|p(x)|}} e^{\frac{1}{\hbar}\int |p|\,dx}$$

(the first term may not be meaningful: being exponentially small, it could be smaller than the error in the second term!)

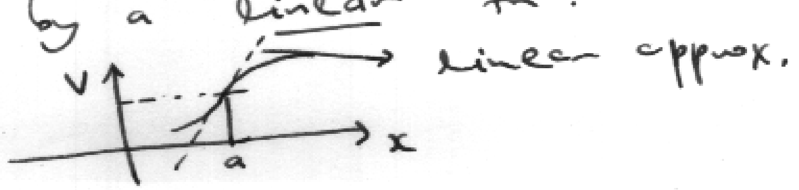
Note that so far we have not achieved very much! Until we match wave functions across regions we will not get correct energy eigenvalues, eigenfunctions & ~~tran~~transmission/reflection coefficients. And this matching is the hard part, since it is done at classical turning points where the WKB wave functions diverge!

~~Also~~

Now let us consider the turning points:



The wave fns we have written down above are reasonably good only for $x \gg a$ or $x \ll a$ or $x \gg b$ or $x \ll b$. Now focus on the $x = a$ turning point. Near this points, assume $V(x) - E = g(x-a)$ where g is a constant. Thus we approximate the potential by a linear fn:



Then, in the region $x \sim a$ we approximate the Schrödinger eqn by:

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + g(x-a)\psi = 0$$

(ie $V(x) - E \simeq g(x-a)$)

Define $z = \left(\frac{2mg}{\hbar^2}\right)^{1/3}(x-a)$, then all the dimensional quantities drop out and we get:

$$\psi(z)'' - z\psi(z) = 0$$

The solutions of this equation are the Airy functions $Ai(z)$, $Bi(z)$. These are special functions whose behaviour is:

$$\left.\begin{aligned} Ai(z) &\simeq \frac{1}{2\sqrt{\pi}} z^{-\frac{1}{4}} e^{-\frac{2}{3}|z|^{3/2}} \\ Bi(z) &\simeq \frac{1}{\sqrt{\pi}} z^{-\frac{1}{4}} e^{\frac{2}{3}|z|^{3/2}} \end{aligned}\right\} \quad z \gg 0$$

$$\left.\begin{aligned} Ai(z) &\simeq \frac{1}{\sqrt{\pi}}|z|^{-\frac{1}{4}} \cos\left(\frac{2}{3}|z|^{3/2} - \frac{\pi}{4}\right) \\ Bi(z) &\simeq \frac{-1}{\sqrt{\pi}}|z|^{-\frac{1}{4}} \sin\left(\frac{2}{3}|z|^{3/2} - \frac{\pi}{4}\right) \end{aligned}\right\} \quad z \ll 0$$

In comparison, the WKB wave functions depend on

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

which for a linear potential is: $\rightarrow$

$$p(x) = \pm\sqrt{2mg(x-a)}$$

$$= \pm\sqrt{2mg}\left(\frac{\hbar^2}{2mg}\right)^{1/6}\sqrt{z} \qquad \text{for } z>0$$

$$= \pm(2mg\hbar)^{1/3}\sqrt{z} \qquad \text{for } z>0$$

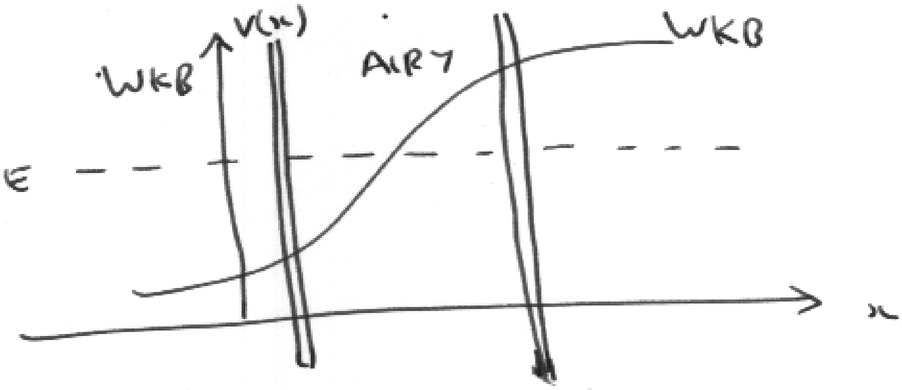
while for $z<0$ we have similarly that

$$p(x) = \pm i(2mg\hbar)^{1/3}\sqrt{|z|}$$

In both cases, $\int p(x)\,dx \sim |z|^{3/2}$.

Thus the asymptotic behaviour of the Airy functions away from the turning point <u>agrees</u> with that of WKB wave fns for a linear potential!

This gives a way to match the WKB wave functions on two sides of a turning point:



The key new insight from Airy functions is a shift of $\pi/4$ in the phase of the oscillating solution. Thus we propose that the solution

$$\frac{A}{\sqrt{\kappa(x)}} e^{-\int \kappa(x)\, dx} + \frac{B}{\sqrt{\kappa(x)}} e^{\int \kappa(x)\, dx}$$

on the RHS of a turning point, matches on to the solution

$$\frac{2A}{\sqrt{k(x)}} \cos\left(\int k\, dx - \frac{\pi}{4} \right) - \frac{B}{\sqrt{k(x)}} \sin\left(\int k\, dx - \frac{\pi}{4} \right)$$

on the LHS of the turning point.

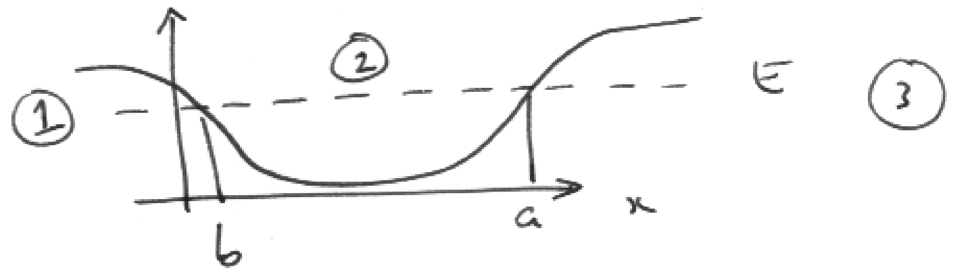
The RHS can be written:

$$\frac{2A}{\sqrt{k(x)}} \left[\frac{1}{2} \left(e^{i\int k\, dx} e^{-i\frac{\pi}{4}} + e^{-i\int k\, dx} e^{i\frac{\pi}{4}} \right) \right]$$

$$- \frac{B}{\sqrt{k(x)}} \left[\frac{1}{2i} \left(e^{i\int k\, dx} e^{-i\frac{\pi}{4}} - e^{-i\int k\, dx} e^{i\frac{\pi}{4}} \right) \right]$$

$$= \frac{\left(A + \frac{iB}{2}\right) e^{-i\frac{\pi}{4}}}{\sqrt{k(x)}} e^{i\int k\, dx} + \frac{\left(A - \frac{iB}{2}\right) e^{i\frac{\pi}{4}}}{\sqrt{k(x)}} e^{-i\int k\, dx}$$

Since we now know the coefficients on the LHS in terms of those on the RHS, we can determine physical quantities like energy eigenvalues & transmission/reflection coefficients. (Clearly for energy eigenvalues we need to also consider the turning point b).



With the configuration shown, there is no transmission or reflection. But there should be quantised energies. Thus, take

$$\psi_1(x) = \frac{1}{\sqrt{\kappa}} e^{-\int_x^b \kappa(x)\,dx}$$

the connection formula then gives

$$\psi_2(x) = \frac{2}{\sqrt{k}} \cos\left(\int_b^x k\,dx - \frac{\pi}{4} \right)$$

Now we need to consider this wave fn near $x = a$ and use the connection formula again to get the wave fn in region 3.

Now $\psi_2(x) = \frac{2}{\sqrt{k}} \cos\left(\int_b^x k\,dx - \frac{\pi}{4} \right)$

$$= \frac{2}{\sqrt{k}} \cos\left(\int_b^a k\,dx - \int_x^a k\,dx - \frac{\pi}{4} \right)$$

$$= \frac{2}{\sqrt{k}} \cos\left(\left[\int_b^a k\,dx - \frac{\pi}{2} \right] - \left[\int_x^a k\,dx - \frac{\pi}{4} \right] \right)$$

$$= \frac{2}{\sqrt{k}} \sin \int_a^b k\,dx \, \cos\left(\int_x^a k\,dx - \frac{\pi}{4} \right)$$

$$- \frac{2}{\sqrt{k}} \cos \int_a^b k\,dx \, \sin\left(\int_x^a k\,dx - \frac{\pi}{4} \right)$$

Now we can match this at $x = a$ onto the exponentially growing/falling terms at $x > a$. But there should be no exponentially growing term (for normalisability). Hence the coefficient of $\sin\left(\int_x^a k\,dx - \frac{\pi}{4} \right)$ must vanish.

This says that

$$\cos \int_a^b k(x)\,dx = 0 \quad \text{ie} \quad \int_a^b k(x)\,dx = (n + \tfrac{1}{2})\pi$$

this gives quantised energies!