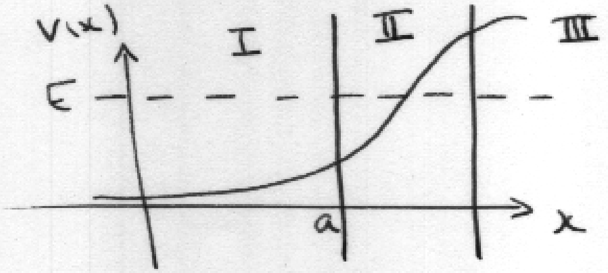
Lecture #9

Let us review what we learned about the WKB approximation.

For a potential of the generic form:



we can identify three regions:

(I) in which the WKB approximation works and gives

$$\psi_I = \frac{C_I}{\sqrt{p(x)}} e^{\frac{i}{\hbar}\int^x p\, dx'} + \frac{D_I}{\sqrt{p(x)}} e^{-\frac{i}{\hbar}\int^x p\, dx'}$$

for some constants C_I, D_I.

(II) in which the WKB approximation fails (too close to the turning point). However hopefully the linear approximation works and hence

$$\psi_{II} = C_{II}\, Ai(z) + D_{II}\, Bi(z)$$

where $z = \left(\frac{2mg}{\hbar^2}\right)^{\frac{1}{3}} (x-a)$ with

$V(x) - E \simeq g(x-a)$, ie $g = V'(a)$.

III in which the WKB approximation again works and

$$\psi_{III} = \frac{C_{III}}{\sqrt{|p|}} e^{-\int^x |p| dx'} + \frac{D_{III}}{\sqrt{|p|}} e^{\int^x |p| dx'}$$

Suppose now that we choose C_{III} and D_{III} to take some values. This must determine the values of C_{II} and D_{II}, and hence the values of C_I and D_I. The way to do this is to note that Airy functions have an asymptotic behaviour, for $z \gg 0$, of:

$$Ai \simeq \frac{1}{2\sqrt{\pi}} z^{-\frac{1}{4}} e^{-\frac{2}{3}|z|^{3/2}}$$

$$Bi \simeq \frac{1}{\sqrt{\pi}} z^{-\frac{1}{4}} e^{\frac{2}{3}|z|^{3/2}}$$

Putting $z = \left(\frac{2mg}{\hbar^2}\right)^{1/3}(x-a)$ this gives:

$$Ai(x) \simeq \frac{1}{2\sqrt{\pi}} \left(\frac{\hbar^2}{2mg}\right)^{1/12} \frac{1}{(x-a)^{\frac{1}{4}}} e^{-\frac{2}{3}\cdot\frac{\sqrt{2mg}}{\hbar}(x-a)^{3/2}}$$

$$Bi(x) \simeq \frac{1}{\sqrt{\pi}} \left(\frac{\hbar^2}{2mg}\right)^{1/12} \frac{1}{(x-a)^{\frac{1}{4}}} e^{+\frac{2}{3}\frac{\sqrt{2mg}}{\hbar}(x-a)^{3/2}}$$

We assume this is the behaviour as we approach the boundary between II and III from the left.

$$\psi_{\mathrm{II}\to\mathrm{III}} = \left(\frac{\hbar^2}{2mg}\right)^{\frac{1}{12}} \frac{1}{(x-a)^{\frac{1}{4}}} \left[\frac{C_{\mathrm{II}}}{2\sqrt{\pi}}\, e^{-\frac{2}{3}\frac{\sqrt{2mg}}{\hbar}(x-a)^{3/2}} + \frac{D_{\mathrm{II}}}{\sqrt{\pi}}\, e^{\frac{2}{3}\frac{\sqrt{2mg}}{\hbar}(x-a)^{3/2}} \right]$$

On the other hand, if we approach the II – III boundary from the RHS, then we may use $|p| = \sqrt{2m(V(x)-E)}$

$$\simeq \sqrt{2mg}\,\sqrt{x-a}$$

So $\frac{1}{\hbar}\int |p|\, dx \simeq \frac{2}{3}\frac{\sqrt{2mg}}{\hbar}(x-a)^{3/2}$

Hence

$$\psi_{\mathrm{III}\to\mathrm{II}} = \frac{1}{(2mg)^{\frac{1}{4}}} \frac{1}{(x-a)^{\frac{1}{4}}} \left[C_{\mathrm{III}}\, e^{-\frac{2}{3}\frac{\sqrt{2mg}}{\hbar}(x-a)^{3/2}} + D_{\mathrm{III}}\, e^{\frac{2}{3}\frac{\sqrt{2mg}}{\hbar}(x-a)^{3/2}} \right]$$

Comparing, we get:

$$C_{\mathrm{II}} = 2\sqrt{\pi}\cdot\left(\frac{2mg}{\hbar^2}\right)^{\frac{1}{12}} \frac{1}{(2mg)^{\frac{1}{4}}}\, C_{\mathrm{III}}$$

$$D_{\mathrm{II}} = \sqrt{\pi}\left(\frac{2mg}{\hbar^2}\right) \frac{1}{(2mg)^{\frac{1}{4}}}\, D_{\mathrm{III}}$$

Note: this matching depends on the potential being smooth enough that both WKB and linear approximation are valid together on the II – III boundary.

Now we repeat the same thing on the I – II boundary, to get:

$$\Psi_{II \to I} = \left(\frac{\hbar^2}{2mg}\right)^{\frac{1}{12}} \frac{1}{|x-a|^{\frac{1}{4}}} \times$$

$$\left\{ \frac{C_{II}}{\sqrt{\pi}} \cos\left(\frac{2}{3} \frac{\sqrt{2mg}}{\hbar} |x-a|^{3/2} - \frac{\pi}{4} \right) - \frac{D_{II}}{\sqrt{\pi}} \sin\left(\frac{2}{3} \frac{\sqrt{2mg}}{\hbar} |x-a|^{3/2} - \frac{\pi}{4} \right) \right\}$$

and $$\Psi_{I \to II} = \frac{1}{(2mg)^{\frac{1}{4}}} \frac{1}{|x-a|^{\frac{1}{4}}} \times$$

$$\left\{ C_I e^{i \frac{2}{3} \frac{\sqrt{2mg}}{\hbar} |x-a|^{3/2}} + D_I e^{-i \frac{2}{3} \frac{\sqrt{2mg}}{\hbar} |x-a|^{3/2}} \right\}$$

~~Hence comparing, we find:~~

This time, to compare we must expand $\Psi_{II \to I}$ to get:

$$\Psi_{II \to I} = \left(\frac{\hbar^2}{2mg}\right)^{\frac{1}{12}} \frac{1}{|x-a|^{\frac{1}{4}}} \times$$

$$\left\{ \frac{C_{II} + iD_{II}}{2\sqrt{\pi}} e^{-i\pi/4} e^{i \frac{2}{3} \frac{\sqrt{2mg}}{\hbar} |x-a|^{3/2}} + \frac{C_{II} - iD_{II}}{2\sqrt{\pi}} e^{i\pi/4} e^{-i \frac{2}{3} \frac{\sqrt{2mg}}{\hbar} |x-a|^{3/2}} \right\}$$

Hence:

$$C_I = (2mg)^{\frac{1}{4}} \cdot \left(\frac{\hbar^2}{2mg}\right)^{\frac{1}{12}} \frac{C_{II} + i D_{II}}{2\sqrt{\pi}} e^{-i\pi/4}$$

$$D_I = (2mg)^{\frac{1}{4}} \left(\frac{\hbar^2}{2mg}\right)^{\frac{1}{12}} \frac{C_{II} - i D_{II}}{2\sqrt{\pi}} e^{i\pi/4}$$

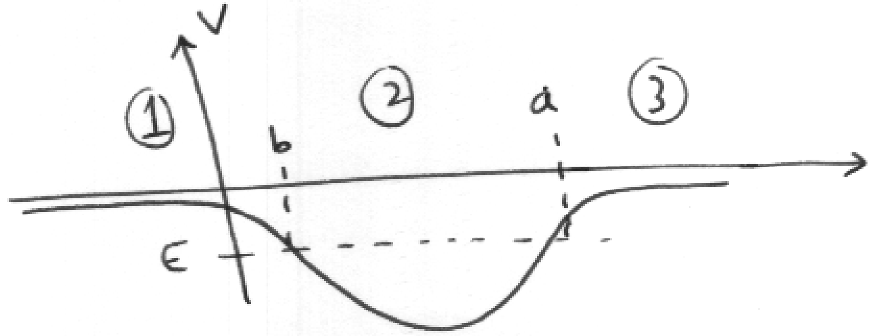
Combining this with the relation between II and III, we can eliminate C_{II} and D_{II} to get:

$$C_I = C_{III} e^{-i\pi/4} + \frac{i}{2} D_{III} e^{-i\pi/4}$$

$$\boxed{\begin{aligned} C_I &= \left(C_{III} + \frac{i D_{III}}{2}\right) e^{-i\pi/4} \\ D_I &= \left(C_{III} - i \frac{D_{III}}{2}\right) e^{i\pi/4} . \end{aligned}}$$

This is the "connection formula" relating WKB wave fns on both sides of the turning point.

Now let's apply this to a well where there are two turning points a and b.



In this situation, it is clear that ψ should be exponentially decaying for $x > a$ or $x < b$.

Thus $\psi_1(x) \sim \frac{1}{\sqrt{|p|}} e^{\frac{1}{\hbar}\int_b^x |p| dx'}$ (note that $x<b$)

$$= \frac{1}{\sqrt{|p|}} e^{-\frac{1}{\hbar}\int_x^b |p| dx'}$$ (so $C_1 = 1$, $D_1 = 0$)

Now using the connection formula, we get in region 2:

$$C_2 = C_1 e^{-i\pi/4} = e^{-i\pi/4}$$

$$D_2 = C_1 e^{i\pi/4} = e^{i\pi/4}$$

So $\psi_2 = \frac{1}{\sqrt{p}}\left(e^{-i\pi/4} e^{\frac{i}{\hbar}\int_b^x p\, dx'} + e^{i\pi/4} e^{-\frac{i}{\hbar}\int_b^x p\, dx'}\right)$

$$= \frac{2}{\sqrt{p}} \cos\left(\frac{1}{\hbar}\int_b^x p\, dx' - \frac{\pi}{4}\right)$$

Next we apply the connection formula at $x = a$.

Then: $$\cos\left(\frac{1}{\hbar}\int_b^x p\,dx' - \frac{\pi}{4}\right)$$

$$= \cos\left(\frac{1}{\hbar}\int_b^a p\,dx' - \frac{1}{\hbar}\int_x^a p\,dx' - \frac{\pi}{4}\right)$$

$$= \cos\left(\left[\frac{1}{\hbar}\int_b^a p\,dx' - \frac{\pi}{2}\right] - \left[\frac{1}{\hbar}\int_x^a p\,dx' - \frac{\pi}{4}\right]\right)$$

$$= \cos\left(\frac{1}{\hbar}\int_b^a p\,dx' - \frac{\pi}{2}\right)\cos\left(\frac{1}{\hbar}\int_x^a p\,dx' - \frac{\pi}{4}\right)$$

$$+ \sin\left(\frac{1}{\hbar}\int_b^a p\,dx' - \frac{\pi}{2}\right)\sin\left(\frac{1}{\hbar}\int_x^a p\,dx' - \frac{\pi}{4}\right)$$

Now we know that the term involving $\cos\left(\frac{1}{\hbar}\int_x^a p\,dx' - \frac{\pi}{4}\right)$ matches onto a decaying exponential, while $\sin(\quad)$ matches to the growing exponential. To have the latter vanish, we must have that the coeff. of $\sin(\quad)$ vanishes:

$$\sin\left(\frac{1}{\hbar}\int_b^a p\,dx' - \frac{\pi}{2}\right) = 0 = \cos\left(\frac{1}{\hbar}\int_b^a p\,dx'\right)$$

Hence $$\int_b^a p\,dx' = \hbar\left(n+\tfrac{1}{2}\right)\pi$$

This can also be written

$$\oint p\,dx = 2\pi\hbar\left(n+\tfrac{1}{2}\right)$$

where $\oint$ is taken over a full orbit $b \to a \to b$.

This reproduces the familiar Bohr-Sommerfeld quantisation rule - which was originally introduced ~~to~~ in an adhoc manner to explain atomic levels!

<u>Example</u>: SHO with $V(x) = \frac{1}{2}m\omega^2 x^2$

Thus $E - V(x) = E - \frac{1}{2}m\omega^2 x^2$

The turning points are at

$$E - \frac{1}{2}m\omega^2 x^2 = 0 \Rightarrow x = \pm\sqrt{\frac{2E}{m\omega^2}}$$

Thus

$$\int_b^a p\,dx' = \int_{-\sqrt{\frac{2E}{m\omega^2}}}^{\sqrt{\frac{2E}{m\omega^2}}} \sqrt{2m(E - \tfrac{1}{2}m\omega^2 x^2)}\,dx$$

$$= \sqrt{2mE}\cdot\sqrt{\frac{2E}{m\omega^2}}\int_{-1}^{+1} dy\,\sqrt{1-y^2}$$

$$= \frac{2E}{\omega}\cdot\frac{\pi}{2} = \frac{E\pi}{\omega}$$

Equating this to $\pi\hbar(n+\frac{1}{2})$, we have

$$E = \hbar\omega(n+\tfrac{1}{2})$$

So for the SHO, WKB gives the <u>exact</u> energy spectrum!

Now lets examine the wave fn:

$$\psi_2 \sim \frac{C}{\sqrt{p}} \cos\left(\frac{1}{\hbar} \int_b^x p\, dx - \frac{\pi}{4} \right) \quad \text{in region 2.}$$

Because ψ decays exponentially in regions 1 and 3, one can approximately normalise it by imposing

$$\int_b^a |\psi_2|^2\, dx = 1$$

Moreover one can estimate the integral by setting $\cos^2(\ ) \simeq \frac{1}{2}$, its average value. Thus

$$\int_b^a |\psi_2|^2 dx = \frac{C^2}{2} \int_b^a \frac{dx}{p(x)}$$

Now $m \frac{dx}{dt} = p \Rightarrow \int \frac{dx}{p} = \frac{1}{m} \int dt = \frac{T}{2m}$

where T is the time period of the periodic trajectory ~~from b to a~~, so $\int_b^a dt = \frac{T}{2}$

Hence $\frac{C^2 T}{4m} = 1$, $\Rightarrow C = 2\sqrt{\frac{m}{T}}$

So $$\psi_2 \simeq 2\sqrt{\frac{m}{T}} \frac{1}{\sqrt{p(x)}} \cos\left(\frac{1}{\hbar} \int_b^x p\, dx - \frac{\pi}{4} \right)$$

Returning to the harmonic oscillator, note fact the wave fn

$$\psi_2(x) \sim \frac{1}{\sqrt{p(x)}} \cos\left(\frac{1}{\hbar}\int_b^x p\,dx - \frac{\pi}{4}\right)$$

does not look like the exact SHO wave fn! In fact,

$$\int_b^x p\,dx = \int_{-\sqrt{\frac{2E}{m\omega^2}}}^{x} \sqrt{2m(E - \tfrac{1}{2}m\omega^2 x'^2)}\,dx'$$

~~Now we put in $E = (n+\frac{1}{2})\hbar\omega$.~~

Let $x' = \sqrt{\frac{2E}{m\omega^2}}\, y'$. Then the limits in y' are:

$$x' = -\sqrt{\frac{2E}{m\omega^2}} \rightarrow y' = -1$$

$$x' = x \rightarrow y' = y$$

where $y = \sqrt{\frac{m\omega^2}{2E}}\, x = \sqrt{\frac{m\omega^2}{2\hbar\omega(n+\frac{1}{2})}}\, x$

$$= \sqrt{\frac{m\omega}{(2n+1)\hbar}}\, x$$

Thus $\displaystyle\int_b^x p\,dx' = \sqrt{2mE}\cdot\sqrt{\frac{2E}{m\omega^2}} \int_{-1}^{y} \sqrt{1-y'^2}\,dy'$

$$= \frac{2E}{\omega}\int_{-1}^{y}\sqrt{1-y'^2}\,dy'$$

Thus $\frac{1}{\hbar}\int_b^x p\,dx' = \frac{2E}{\hbar\omega}\int_{-1}^{y}\sqrt{1-y'^2}\,dy'$

$= (2n+1)\int$ " . (note that $-1 \le y \le 1$)

For the integral, we have:

$$\int_{-1}^{y}\sqrt{1-y'^2}\,dy' = \frac{1}{2}\left(\sin^{-1}y + \frac{\pi}{2}\right) + \frac{y}{2}\sqrt{1-y^2}$$

next we have to put this into the cosine; and multiply by $\frac{1}{\sqrt{p(x)}}$ where:

$$p(x) = \sqrt{2m\left(E - \tfrac{1}{2}m\omega^2x^2\right)}$$

$$= \sqrt{2mE}\,\sqrt{1 - \frac{m\omega^2}{2E}x^2}$$

$$= \sqrt{2mE}\,\sqrt{1-y^2}$$

So $\psi(x) \sim \frac{1}{(1-y^2)^{\frac{1}{4}}}\cos\left((2n+1)\left\{\frac{1}{2}\sin^{-1}y + \frac{y}{2}\sqrt{1-y^2}\right\}\right)$

(keep in mind that ψ depends on the level n through y as well). This is not at all the true SHO wave fn (not even for $n=0$) but it should look numerically similar in the interior, while diverging at the turning points.