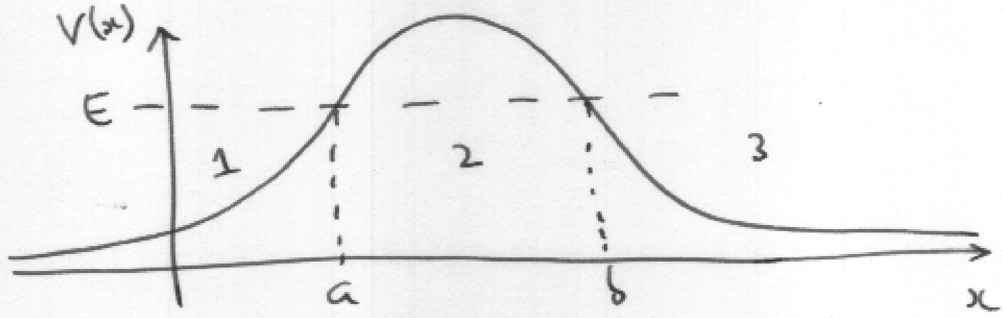
Lecture 10

Transmission through a barrier.

Consider the following type of potential:



From our previous analyses, we know that the wave functions in the three regions are:

$$\psi_1(x) = \frac{C_1}{\sqrt{p(x)}} e^{\frac{i}{\hbar}\int_a^x p\, dx'} + \frac{D_1}{\sqrt{p(x)}} e^{-\frac{i}{\hbar}\int_a^x p\, dx'}$$

$$\psi_2(x) = \frac{C_2}{\sqrt{|p(x)|}} e^{\frac{-1}{\hbar}\int_a^x p\, dx'} + \frac{D_2}{\sqrt{|p(x)|}} e^{\frac{1}{\hbar}\int_a^x p\, dx'}$$

$$\psi_3(x) = \frac{C_3}{\sqrt{p(x)}} e^{\frac{i}{\hbar}\int_b^x p\, dx'} + \frac{D_3}{\sqrt{p(x)}} e^{-\frac{i}{\hbar}\int_b^x p\, dx'}$$

where (C_1, D_1), (C_2, D_2) and (C_3, D_3) can be matched using the connection formulae.

At the first turning point, we have:

$$\frac{C_2}{\sqrt{|p(x)|}} e^{-\int_a^x |p| dx'} + \frac{D_2}{\sqrt{|p(x)|}} e^{\int_a^x |p| dx'} \longleftrightarrow$$

$$\frac{2C_2}{\sqrt{p}} \cos\left(\frac{1}{\hbar}\int_x^a p \, dx' - \frac{\pi}{4}\right) - \frac{D_2}{\sqrt{p}} \sin\left(\frac{1}{\hbar}\int_x^a p \, dx' - \frac{\pi}{4}\right)$$

$$= \frac{1}{\sqrt{p}} \Big\{ \left(C_2 - \frac{D_2}{2i}\right) e^{-i\frac{\pi}{4}} e^{\frac{i}{\hbar}\int_x^a p \, dx'}$$

$$+ \left(C_2 + \frac{D_2}{2i}\right) e^{i\frac{\pi}{4}} e^{-\frac{i}{\hbar}\int_{\cancel{x}}^a p \, dx'} \Big\}$$

Notice that we have $\int_x^a p \, dx'$ which is $-\int_a^x p \, dx'$. Comparing with the original expression, we find

$$C_1 = \left(C_2 + \frac{D_2}{2i}\right) e^{i\frac{\pi}{4}}$$

$$C_2 = \left(C_2 - \frac{D_2}{2i}\right) e^{-i\pi/4}$$

At the second turning point, we ~~have~~ have:

$$\frac{Q}{\sqrt{|p|}} e^{-\frac{1}{\hbar}\int_x^b |p| dx'} + \frac{R}{\sqrt{|p|}} e^{\frac{1}{\hbar}\int_x^b |p| dx'} \longleftrightarrow$$

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

We need a little work to get the relation between (C_2, D_2) and (C_3, D_3).

In the forbidden region 2, we compare

$$\frac{Q}{\sqrt{|p|}} e^{-\frac{1}{\hbar}\int_x^b |p| dx'} \quad \text{with} \quad \frac{D_2}{\sqrt{|p|}} e^{\frac{1}{\hbar}\int_a^x |p| dx'}$$

(both are exponentially increasing to the right).

Since $-\int_x^b = \int_a^x - \int_a^b$, we have:

$$\text{LHS} = \frac{Q}{\sqrt{|p|}} e^{\frac{1}{\hbar}\int_a^x |p| dx'} e^{-\frac{1}{\hbar}\int_a^b |p| dx'}$$

Hence $\quad Q e^{-\frac{1}{\hbar}\int_a^b |p| dx'} = D_2$

Define $\quad \Theta = e^{\frac{1}{\hbar}\int_a^b |p| dx'}$

Then $\quad Q = D_2 \Theta \quad$ and similarly,

$$R = C_2 \Theta^{-1}$$

Now we may apply the connection formulae, to get

$$C_3 = \left(D_2\Theta - \frac{C_2\Theta^{-1}}{2i}\right) e^{-i\pi/4}$$

$$D_3 = \left(D_2\Theta + \frac{C_2\Theta^{-1}}{2i}\right) e^{-i\pi/4}$$

Combining, we find that

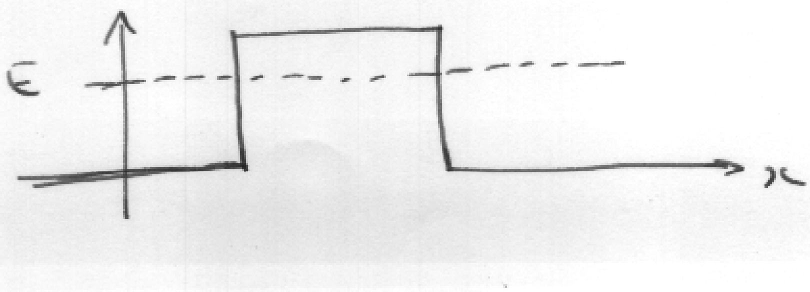
$$\begin{pmatrix} C_1 \\ D_1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2\theta + \frac{1}{2\theta} & i\left(2\theta - \frac{1}{2\theta}\right) \\ -i\left(2\theta - \frac{1}{2\theta}\right) & 2\theta + \frac{1}{2\theta} \end{pmatrix}\begin{pmatrix} C_3 \\ D_3 \end{pmatrix}$$

Now suppose we want to study transmission of an incoming wave from $x = -\infty$, with coefficient C_1. ~~Here C_1 is the~~ Then D_1 represents the reflected wave back to $-\infty$, while C_3 is the transmitted wave to $+\infty$. So D_3 must be zero, since our problem does not involve anything coming in from $+\infty$.

Usually (in simplified square-well problems) we define the transmission probability as

$$\left|\frac{\Psi_{trans}}{\Psi_{incoming}}\right|^2.$$

However in those problems, the velocity of the particle in the allowed region is the same on both sides:



In the potentials we are allowing, the momentum / velocity is not necessarily equal on the two sides, as $p = p(x) = \sqrt{2m(E-V(x))}$. In such a situation it makes sense to define

$$T = \frac{|\psi_{trans}|^2}{|\psi_{in}|^2}\frac{v_{trans}}{v_{in}} = \left[\frac{|\psi_{trans}|\sqrt{p_{trans}}}{|\psi_{in}|\sqrt{p_{in}}}\right]^2$$

This is easily seen to give:

$$T = \left|\frac{C_3}{C_1}\right|^2$$

since the extra momentum factors in the definition of T cancel against the $\frac{1}{\sqrt{p}}$ factors in the wave function.

Now with $D_3 = 0$, $C_1 = \frac{1}{2}\left(2\theta + \frac{1}{2\theta}\right)C_3$

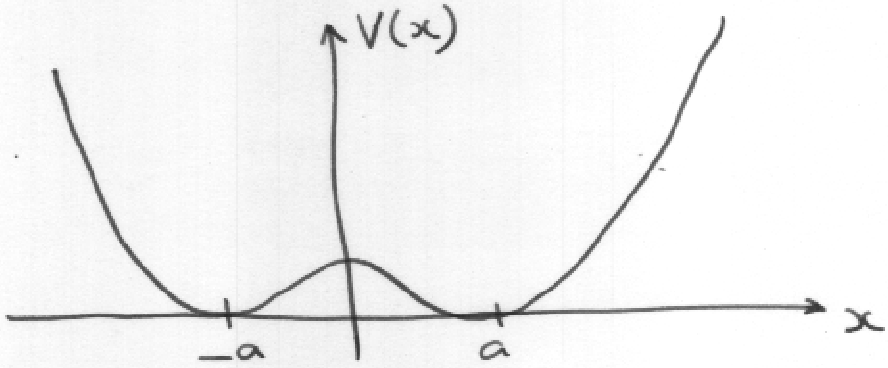
and hence

$$T = \frac{4}{\left(2\theta + \frac{1}{2\theta}\right)^2}$$

Recall that $\theta = e^{\frac{1}{\hbar}\int_a^b |p|\,dx'}$ so usually $\theta^{-1} \ll \theta$ and we have:

$$\boxed{T = e^{-\frac{2}{\hbar}\int_a^b |p(x')|\,dx'}}$$

Now let us consider the interesting special case of a <u>double-well</u> potential:



We take the potential to be symmetric, with minima at $\pm a$. A concrete example of such a potential would be:

$$V(x) = \frac{\lambda}{4!}(x^2-a^2)^2$$

Suppose we neglect ~~the~~ possibility of barrier penetration. In that case a wave fn localised in one well or the other is a reasonable approximation. Thus, let $\psi_a(x)$ be a wave-fn localised around $x = a$, and $\psi_{-a}(x) = \psi_a(-x)$ be the <u>same</u> wave fn localised around $x = -a$. (In the example above with $V \sim (x^2-a^2)^2$, the potential near $x = a$ is $V(x) \sim (x-a)^2$ while near $x = -a$ it is $V(x) \sim (x+a)^2$. Thus in this example the wave fns ψ_a, ψ_{-a} are just harmonic-oscillator wave fns.

Since we take the same wave fn for ψ_a and ψ_{-a}, the corresponding energy E is the same for both. Note also that $\psi_a(x)$ is extremely small near $x=-a$, while $\psi_{-a}(x)$ is very small near $x=+a$.

[Comment: with Coulomb potentials at a and $-a$, this is almost exactly the problem of a H_2^+ molecule that we studied before. Here we will use WKB to extract a more general result].

An argument based on the variational principle would tell us that $\psi_a + \alpha\psi_{-a}$ is the "best" combination of the two, with $\alpha = \pm 1$.

Let us normalise ψ_a, ψ_{-a} independently in their own well:

$$\int_{-\infty}^{+\infty} |\psi_a|^2 \simeq \int_0^{\infty} |\psi_a|^2 = 1$$

$$\int_{-\infty}^{+\infty} |\psi_{-a}|^2 \simeq \int_{-\infty}^{0} |\psi_{-a}|^2 = 1$$

Now consider the norm of $\psi_a + \psi_{-a}$.

We have

$$\int_{-\infty}^{+\infty} |\psi_a + \psi_{-a}|^2 = 1 + 1 + \int_{-\infty}^{+\infty} (\psi_a^* \psi_{-a} + \psi_a \psi_{-a}^*)$$

the last integral is vanishingly small since for $x > 0$, $\Psi_{-a} \simeq 0$ and for $x < 0$, $\Psi_a \sim 0$.

Therefore the RHS $\simeq 2$ and hence

$\Psi_\pm = \frac{1}{\sqrt{2}} (\Psi_a \pm \Psi_{-a})$ are approximately normalized.

Now we use the fact that $\Psi_a, \Psi_{-a}, \Psi_\pm$ are all approximate solutions of the <u>same</u> Schrödinger eqn with ~~all~~ possibly different energies:

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

$$-\frac{\hbar^2}{2m} \frac{d^2 \Psi_\pm}{dx^2} + V(x) \Psi_\pm = E_\pm \Psi_\pm (x)$$

Let us eliminate the potential between the two equations:

$$-\frac{\hbar^2}{2m} \Psi_a'' + V(x) \Psi_a = E \Psi_a$$

$$-\frac{\hbar^2}{2m} \Psi_+'' + V(x) \Psi_+ = E_+ \Psi_+$$

Multiplying the first eqn by Ψ_+ and the second by Ψ_a, ~~[illegible]~~ and subtracting, we get:

$$-\frac{\hbar^2}{2m} \left(\Psi_+'' \Psi_a - \Psi_a'' \Psi_+ \right) = (E_+ - E) \Psi_+ \Psi_a$$

Now integrate both sides in x from 0 to ∞.

On the RHS, we have

$$\int_0^\infty \psi_+ \psi_a = \frac{1}{\sqrt{2}} \int_0^\infty \Big(\underbrace{|\psi_a|^2}_{=\,1} + \underbrace{\psi_{-a}\psi_a}_{=\,0} \Big)$$

$$= \frac{1}{\sqrt{2}}$$

On the LHS,

$$\int_0^\infty \left(\psi_+'' \psi_a - \psi_a'' \psi_+ \right) =$$

$$\frac{1}{\sqrt{2}} \int_0^\infty \left(\cancel{\psi_a'' \psi_a} + \psi_{-a}'' \psi_a - \cancel{\psi_a'' \psi_a} - \psi_a'' \psi_{-a} \right)$$

$$= \frac{1}{\sqrt{2}} \Big\{ \left[\psi_{-a}' \psi_a \right]_0^\infty - \int_0^\infty \cancel{\psi_{-a}' \psi_a'}$$
$$- \left[\psi_a' \psi_{-a} \right]_0^\infty + \int_0^\infty \cancel{\psi_a' \psi_{-a}'} \Big\}$$

$$= \frac{1}{\sqrt{2}} \left(-\psi_{-a}' \psi_a \big|_0 + \psi_a' \psi_{-a} \big|_0 \right)$$

Now $\psi_{-a}\big|_0 = \psi_a\big|_0$, $\psi_{-a}'\big|_0 = -\psi_a'\big|_0$ so:

$$= \sqrt{2} \left(\psi_a \psi_a' \right) \Big|_0$$

Hence $$-\frac{\hbar^2}{2m} \cdot \sqrt{2}\, \psi_a \psi_a' \Big|_0 = \frac{(E_+ - E)}{\sqrt{2}}$$

$$\Rightarrow \quad E_+ - E = -\frac{\hbar^2}{m} \left[\psi_a \psi_a' \right]_0$$

A similar calculation performed with E_- and ψ_- in place of E_+ and ψ_+ gives:

$$E_- - E = \frac{\hbar^2}{m} \left[\psi_a \psi_a' \right]_0$$

[Note: while we threw away $\int_0^\infty \psi_a^* \psi_{-a}$, we could not be sure whether $\int_0^\infty \psi_a'' \psi_{-a}$ is small on the same interval, which is why we carefully kept all terms].

Thus we find the energy splitting to be

$$E_- - E_+ = \frac{2\hbar^2}{m}\left[\psi_a' \psi_a\right]_0$$

Now we can use WKB to estimate the RHS.

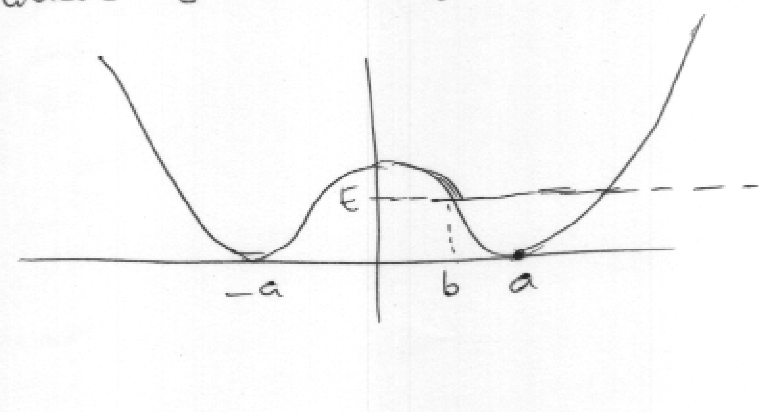
The WKB form of ψ_a is, in the allowed region around $x = a$:

$$\psi_a = \frac{C}{\sqrt{p}} \cos\left(\frac{1}{\hbar}\int p\,dx - \frac{\pi}{4}\right)$$

where we argued last time that $C = 2\sqrt{\frac{m}{T}}$ with T the classical period. This wave function matches in the forbidden region to:

$$\frac{C}{2}\frac{1}{\sqrt{|p|}} e^{-\frac{1}{\hbar}\int_x^b |p|\,dx}$$

where b is the turning point on the left:



Thus $\psi_a(0) = \sqrt{\frac{m}{T}}\,\frac{1}{\sqrt{|p|}}\, e^{-\frac{1}{\hbar}\int_0^b |p|\,dx}$

and $\psi_a'(0) = \frac{|p|}{\hbar}\psi_a(0)$

Hence $\psi_a(0)\psi_a'(0) = \frac{m}{T}\,\frac{1}{|p|}\cdot\frac{|p|}{\hbar}\cdot e^{-\frac{1}{\hbar}\int_0^b |p|\,dx}$

$$= \frac{m}{T\hbar}\, e^{-\frac{1}{\hbar}\int_0^b |p|\,dx}$$

and hence

$$\Delta E = E_- - E_+ \simeq \frac{2\hbar}{T}\, e^{-\frac{2}{\hbar}\int_0^b |p|\,dx}$$

$$\boxed{E_- - E_+ = \frac{2\hbar}{T}\, e^{-\frac{1}{\hbar}\int_{-b}^{+b} |p|\,dx}}$$

This is the WKB formula for energy splitting.

<u>Validity of WKB</u> Note that the WKB approximation is a "semi-classical" approximation and therefore holds better and better as $\hbar \to 0$, which really means that $\frac{E}{\hbar\omega} \to \infty$. where E is the typical energy. This means that the semi-classical quantisation rule $\oint p\,dx = 2\pi\hbar(n+\frac{1}{2})$ is valid for $n \gg 1$. So it should <u>not</u> really be applied to estimate the ground-state energy ($n=0$)!

In fact, in examples one can check that it gives a fairly poor estimate for E_0 but a much better estimate for E_n with n large.