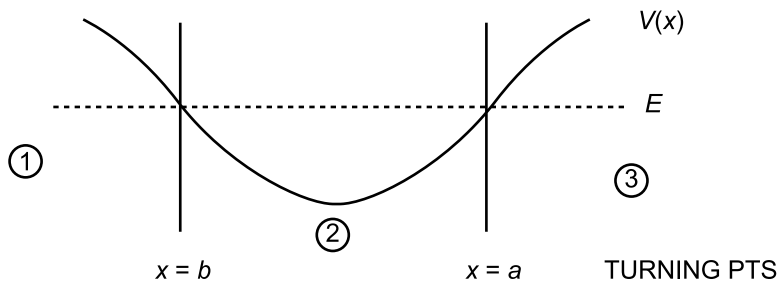
November 26, 2007

APPLICATION OF WKB TO BOUND STATES (1)POTENTIAL WELL WITH NO RIGID WALLS



Region (1) spans $x = -\infty \to b$. The WKB solution must remain finite. Hence,

$$\psi_1(x) \simeq \frac{1}{\sqrt{q(x)}} e^{-\int_x^b q(x)dx} \tag{3.22}$$

Region 3 spans $x = a \to +\infty$, and, for the same reason, the WKB solution must take the form:

$$\psi_3(x) \simeq \frac{1}{\sqrt{q(x)}} e^{-\int_a^x q(x)dx} \tag{3.23}$$

ie ψ_1, ψ_3 both correspond to exponentially decaying solutions which remain finite asymptotically.

From C.3, the solution in region 2 which connects with ψ_1 is:

$$\psi_2(x) \simeq \frac{2}{\sqrt{k(x)}} \cos\left(\int_b^x k(x')dx' - \frac{\pi}{4}\right) \quad \text{for } b < x < a$$

We can re-write the above as follows:

$$\psi_2(x) \simeq \frac{2}{\sqrt{k(x)}} \cos\left(\underbrace{\int_b^a k(x')dx'}_{A} - \underbrace{\int_x^a k(x')dx' - \frac{\pi}{4}}_{B}\right) \tag{3.24}$$

ie this is in the form

$$\psi_2(x) \simeq \frac{2}{\sqrt{k(x)}}\cos\left[A - \left(B + \frac{\pi}{4}\right)\right] \tag{3.25}$$

$$= \frac{2}{\sqrt{k(x)}}\sin\left[A - \left(B - \frac{\pi}{4}\right)\right]$$

$$= \frac{2}{\sqrt{k(x)}}\sin A\cos\left(B - \frac{\pi}{4}\right) - \cos A\sin\left(B - \frac{\pi}{4}\right) \tag{3.26}$$

WE NOTE THAT the term:

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

$$= \frac{2}{\sqrt{k(x)}}\text{Cst}\ \ \cos\int_x^a k(x')dx' - \frac{\pi}{4} \tag{3.27}$$

is the term which connects with the region 3 wavefunction

$$\psi_3 \simeq \frac{1}{\sqrt{q(x)}}e^{-\int_a^x q(x)dx}.$$

so the other term in (3.26) must $= 0$
ie

$$\cos A\sin\left(B - \frac{\pi}{4}\right) = 0$$

ie

$$\cos A = \cos\int_b^a k(x)dx = 0 \quad \text{since } B(x) \text{ is arbitrary} \tag{3.28}$$

$$= \int_b^a k(x)dx = \int_b^a \left\{\frac{2m}{\hbar^2}[E - V(x)]\right\}^{\frac{1}{2}} dx$$

$$= \left(n + \frac{1}{2}\right)\pi \quad n = 0, 1, 2\ldots \tag{3.29}$$

This imposes a quantisation condition on the energy. Only the eigenenergies $\{E_n\}$ for which Eq (3.29) is satisfied yield a quantum state.

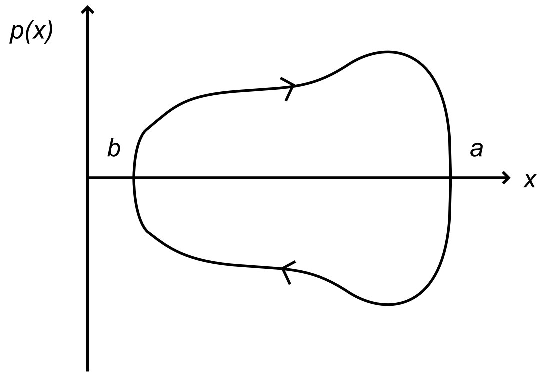
Note also that the turning points are fixed by energy: $V(a) = V(b) = E$.

Written in terms of momentum, we have

$$2\int_b^a k(x)dx = 2\pi\left(n + \frac{1}{2}\right)$$

$$= 2\int_b^a p \cdot dx = \left(n + \frac{1}{2}\right)h \tag{3.30}$$

The 'action' of a closed trajectory in phase space.



This is almost the same as the Bohr-Sommerfeld quantisation rule

$$\oint p \cdot dx = nh$$

seen in the Bohr atom model, for example in 1st year, where the action around circular orbits in electron of hydrogen atom was quantised)

EXAMPLE 1 The Harmonic oscillator

$$\begin{aligned} \hat{H} &= \frac{\hat{p}^2}{2m} + \frac{1}{2}mw^2x^2 \\ \Rightarrow p(x) &= \left[2m\left(E - \frac{1}{2}mw^2x^2\right)\right]^{\frac{1}{2}} \end{aligned}$$

the turning-points are where $x = a$ and also where

$$\begin{aligned} E &= \frac{1}{2}mw^2x^2 \\ \Rightarrow a &= \pm\sqrt{\frac{2E}{mw^2}} \end{aligned}$$

The WKB quantisation condition:

$$\int p.dx = \left(n + \frac{1}{2}\right)h$$

$$2 \cdot \int_{-a}^{+a} \left[2m\left(E - \frac{1}{2}mw^2x^2\right)\right]^{\frac{1}{2}} dx = \left(n + \frac{1}{2}\right)h$$

$$\Rightarrow \frac{E_n\pi}{w} = \left(n + \frac{1}{2}\right)\frac{h}{2}$$

$$E_n = \left(n + \frac{1}{2}\right)\hbar w \text{ which is,}$$

in fact exactly right for all n. In this regard, the harmonic oscillator is special: we might have expected WKB to only give the right result only for n large, ie for high energies.

Integral 1

$$I = \int_{-a}^{a} \left[2m \left(E - \frac{1}{2} m w^2 x^2 \right) \right]^{\frac{1}{2}} dx$$

$$\text{Let } \cos\theta = \sqrt{\frac{m w^2}{2E}} x$$

Then,

$$-\sin\theta \, d\theta = \sqrt{\frac{m w^2}{2E}} dx$$

and

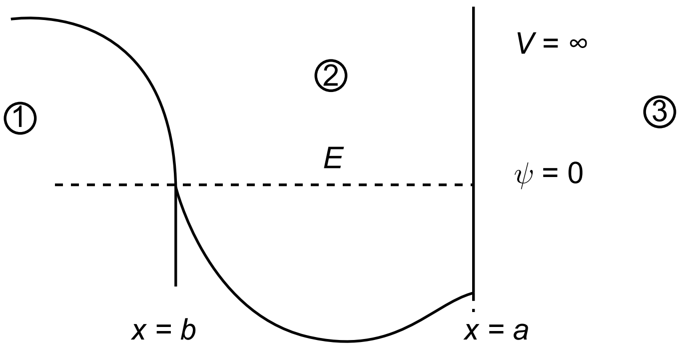
$$I = -\int_{-a}^{a} [2mE(1 - \cos^2\theta)]^{\frac{1}{2}} \sqrt{\frac{2E}{m w^2}} \sin\theta \, d\theta$$

$$\begin{aligned} \text{if } x = a, &\quad \cos\theta = +1 \quad \theta = 0 \\ x = -a, &\quad \cos\theta = -1 \quad \theta = -\pi \end{aligned}$$

so

$$\begin{aligned} I = \frac{-2E}{w} \int_{-\pi}^{0} \sin^2\theta \, d\theta \quad &= \quad \frac{2E}{w} \int_{0}^{\pi} \sin^2\theta d\theta \\ &= \quad \frac{\cancel{2}E\pi}{\cancel{2}w} \end{aligned}$$

(2) POTENTIALS WITH ONE RIGID WALL



If there is an impenetrable wall at $x = a$ ie $V(x) = \infty$ for $x \gtrsim a$, then $\psi_3(x) = 0$.

In region (2) we still have

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

for similar reason to previous section: it must be a *cosine* term since it connects with an exponentially decaying solution $e^{-\int}$ in region (1).

Inside the well, $b < x < a$.

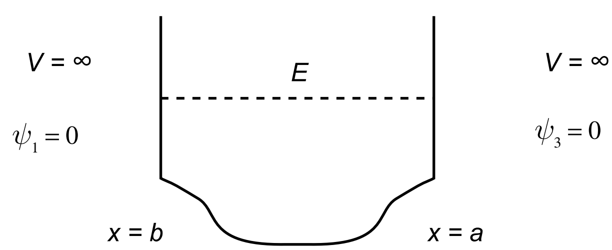
$\psi_2(x = a) = 0$, hence

$$\cos\left(\int_b^a k(x')\, dx' - \frac{\pi}{4}\right) = 0$$

$$\Rightarrow \int_b^a k(x')\, dx' - \frac{\pi}{4} = \left(n + \frac{1}{2}\right)\pi$$

$$\int_b^a k(x')dx' = \left(n + \frac{3}{4}\right)\pi \quad n = 0, 1, 2, \ldots \tag{3.31}$$

(3) POTENTIALS WITH TWO RIGID WALLS



Now

$$\psi_2 \simeq \frac{2}{\sqrt{k(x)}} \cos\left[\int_b^x (k(x')\,dx' + \alpha)\right]$$

where α is a phase factor since $\psi_2(x=b) = 0$
ie

$$\int_b^{x=b} k(x')dx' + \alpha$$

$\Rightarrow \alpha = \pm\pi/2$; take $\alpha = -\pi/2$

At $x = a$ we have (as in previous example)

$$\begin{aligned} \psi_2(a) \quad &\simeq \quad \frac{2}{\sqrt{k(x)}} \cos\left(\int_b^a k(x')\,dx' - \frac{\pi}{2}\right) = 0 \\ &\Rightarrow \int_b^a k(x')dx' - \frac{\pi}{2} = \left(n + \frac{1}{2}\right)\pi \\ &\Rightarrow \int_b^a k(x')dx' = (n+1)\pi \quad n = 0, 1, 2, \ldots \end{aligned} \tag{3.32}$$

BOUND STATE

Example

Calculate the energy levels of an electron, in an s-state, bound to a nucleus. Radially, the particle moves in a potential

$$V(r) = \frac{-Ze^2}{4\pi\varepsilon_o r}$$

It may be viewed as moving between a rigid wall at $r = 0$ and $r = a$, where a is the turning point, and the energy of the electron $E < 0$.

FIRST, FIND TURNING POINT:
there

$$\begin{aligned} V(a) \quad &= \quad E \\ \Rightarrow a \quad &= \quad \frac{-Ze^2}{4\pi\varepsilon_o E} \end{aligned}$$

SECONDLY, APPLY QUANTISATION CONDITION:
HERE, ONE RIGID WALL, SO:

$$\begin{aligned} &\Rightarrow \quad \int_a^b k(x)dx = \left(n + \frac{3}{4}\right)\pi \\ &\Rightarrow \quad \int_0^a \sqrt{2m\left(E + \frac{Ze^2}{4\pi\varepsilon_o r}\right)}dr = \left(n + \frac{3}{4}\right)\pi\hbar \\ &\Rightarrow \quad \int_0^a \sqrt{2mE\left(1 - \frac{a}{r}\right)}dr = \sqrt{-2mE}\int_0^a \sqrt{\left(\frac{a}{r} - 1\right)}dr \\ &= \quad \sqrt{-2mE}\frac{a\pi}{2} = \left(n + \frac{3}{4}\right)\pi\hbar \end{aligned}$$

Hence

$$E_n = -\frac{m}{2\hbar^2}\left(\frac{Ze^2}{4\pi\varepsilon_0}\right)^2 \frac{1}{(n+\frac{3}{4})^2}; \quad n = 0, 1, 2, \ldots$$

while the exact result has the same form, but

$$\frac{1}{(n+\frac{3}{4})^2} \to \frac{1}{n^2}$$

WE RECAP:

WKB Quantisation: 3 possibilities

Soft potential $\to$ $(n+\frac{1}{2})\pi$

1 Hard Wall $\to$ $(n+\frac{3}{4})\pi$

2 Hard Walls $\to$ $n\pi$

Integral 2

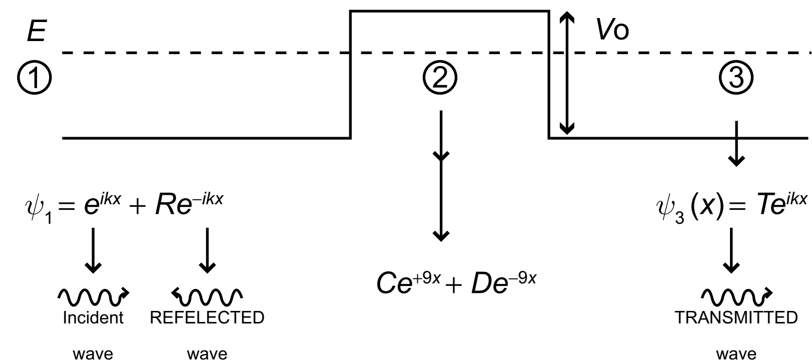
$$\int \sqrt{\frac{a}{r} - 1}\ dr = I$$

use substitution $r = a\cos^2\theta$

$$\begin{aligned}
I &= -\int_{\frac{\pi}{2}}^{0} \left(\sqrt{\frac{a}{a\cos^2\theta} - 1}\right)\ 2a\cos\theta\sin\theta\, d\theta \\
&= 2a\int_0^{\frac{\pi}{2}} \frac{\sin\theta}{\cos\theta}\cos\theta\sin\theta d\theta \\
&= 2a\int_0^{a} \sin^2\theta d\theta \\
&= a\int_0^{\frac{\pi}{2}} (1 - \cos 2\theta) d\theta = a[\theta]_0^{\frac{\pi}{2}} \\
&= \frac{a\pi}{2}
\end{aligned}$$

TUNNELLING THROUGH A BARRIER

REVISION OF CONSTANT BARRIER



Current operator:

$$\hat{J}(x) = \frac{\hbar}{2im}\left(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right)$$

Hence:

$$\begin{aligned} \text{incident current} &= \hbar\frac{k}{m} = J_I \\ \text{Transmitted current} &= |T|^2 \hbar\frac{k}{m} = J_T \\ \text{Reflected current} &= |R|^2 \hbar\frac{k}{m} = J_R \end{aligned}$$

$$k = \sqrt{\frac{2mE}{\hbar^2}} q = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}.$$

We match wavefunction and derivatives to obtain

$$\frac{J_T}{J_I} = |T|^2$$

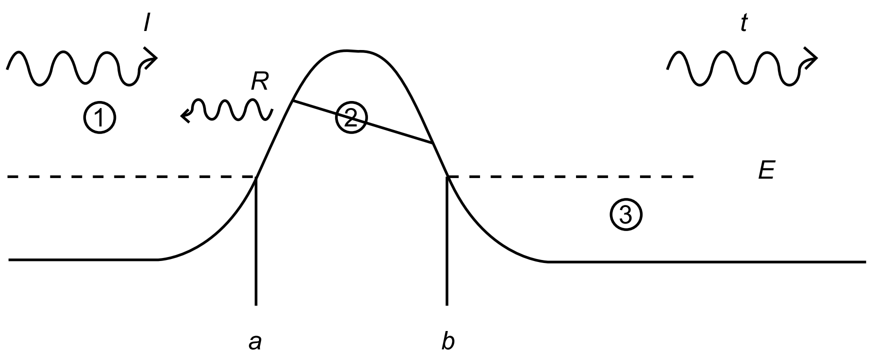
in terms of V_0 and E (ie in terms of k and g) and

$$\frac{J_R}{J_I} = |R|^2$$

in terms of V_0 and E (ie in terms of k and g).

The classical turning points are at $V(a) = E$ and $V(b) = E$, the points where a classical particle would stop.

The transmitted wave here has only one component (corresponding to motion $\rightarrow$ to right, if incident particles approach from left)



$$\psi_3(x) = \frac{A}{\sqrt{k(x)}}\ e^{i\left[\int_b^x k(x')dx' - \frac{\pi}{4}\right]} \tag{3.33}$$

factor $e^{\frac{-i\pi}{4}}$ could be absorbed into the A.

WKB procedure

1) decompose $\psi_3(x)$ into cos / sin functions so as to connect with region 2.

2) Having found ψ_2 connect with region 1.

3) Decompose ψ_1 into incident and reflected parts

4) Calculate currents, transmitted/incident

Rewrite

$$\psi_3(x) = \frac{A}{\sqrt{k(x)}}\{\cos\Phi + i\sin\Phi\}$$

where

$$\phi = \int_b^x k(x')dx' - \frac{\pi}{4}$$

which connect with:

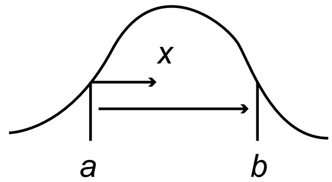
$$\psi_2(x) = \frac{A}{2\sqrt{q(x)}}\ e^{-\int_x^b q(x')dx'}\ - \frac{iA}{\sqrt{q(x)}}\ e^{\int_x^b q(x')dx'} \tag{3.34}$$

now, sin:

$$\int_x^b q(x')dx' = \int_a^b q(x')dx' - \int_a^x q(x')dx'$$

$\Rightarrow$ 2nd term of (3.34)

$$\Rightarrow e^{\int_x^b q(x')dx'} = re^{-\int_a^x q(x')dx'} \tag{3.35}$$



where

$$r = e^{\int_a^b q(x')dx'}$$

and similarly (1st term of 3.34)

$$e^{-\int_x^b q(x')dx'} = r^{-1} e^{\int_a^x q(x')dx'} \tag{3.36}$$

So, combine (3.35) and (3.36) in (3.34)

$$\psi_2 = \frac{A}{\sqrt{q(x)}} \left[\frac{1}{2r} e^{\theta} - ire^{-\theta} \right] \tag{3.37}$$

$$\theta = \int_a^x q(x')dx'$$

Finally, This can be connected to region 1: (using connection formulae)

$$\Psi_1 \simeq \frac{A}{\sqrt{k(x)}} \left[\frac{-1}{2r} \sin\phi - 2ir\cos\phi \right] \tag{3.38}$$

$$\phi = \int_x^a k(x')dx' - \frac{\pi}{4}$$

To calculate currents, we must 'turn full circle' and re-express ψ_1 as plane waves $e^{\pm i\phi}$, so as to compare with ψ_3:

$$\psi_1 = \frac{Ai}{\sqrt{k(x)}} \left[\underbrace{\left(\frac{1}{4r} - r \right)}_{\text{TERM 1}} e^{i\phi} - \underbrace{\left(\frac{1}{4r} + r \right)}_{\text{TERM 2}} e^{-i\phi} \right] \tag{3.39}$$

far from the boundary, as $x \to -\infty$, $V(x) \to 0$, $k \sim$ constant. and:

$$\phi \simeq ka - kx - \frac{\pi}{4}.$$

ie as $x \to -\infty$, term 2 becomes $\propto e^{ikx}\ e^{i\alpha}$ where $\alpha =$ constant phase
so *term 2 is incident wave.*
For a wave of form Ce^{ikx}, $J = |C|^2 \frac{\hbar k}{m}$
Transmitted wave, $\psi_3(x) \to \frac{A}{\sqrt{k_{trans}}} e^{ik_{trans}x}$ as $x \to \infty$

Incident component in (3.39)

$$\psi_{inc} \to \frac{iA}{\sqrt{k_{inc}}}\left(\frac{1}{4r}+r\right)e^{ik_{inc}x}$$

as $x \to -\infty$

hence $\frac{J_{\text{TRANS}}}{J_I}$= Transmission coefficient J = tunnelling probability

$$= \frac{\left|\frac{A}{\sqrt{k_{trans}}}\right|^2 k_{trans}}{\left|\frac{A}{\sqrt{k_{inc}}}\left(\frac{1}{4r}+r\right)\right|^2 k_{inc}}$$

hence:

$$J = \frac{1}{\left(\frac{1}{4r}+r\right)^2} = \frac{1}{\left(\frac{1}{16r^2}+r^2+\frac{1}{2}\right)}$$

now, in WKB regime, r is *large* ie a high wide barrier (see below):

$$\Rightarrow J \simeq \frac{1}{r^2} = \exp - 2\int_a^b q(x')dx'$$
$$= e^{-2\lambda},$$

where

$$\lambda = \int_a^b \left[\frac{2m}{\hbar^2}(V(x')-E)\right]^{\frac{1}{2}} dx'$$

r large $\Rightarrow \Lambda$ large

$$r = e^{+\Lambda} \sim e^{+(b-a)\langle q \rangle}$$

big$\langle q \rangle$ = average $q \propto \langle (V(x)-E)^{\frac{1}{2}} \rangle \Rightarrow$ high barrier big $b-a$ = width large.