Phys 521 Fall 2023

Semiclassical WKB

Expansion in powers of $\hbar$ (Schiff, Shankar)

$$\psi(x) = \exp\left(\frac{i}{\hbar}\phi(x)\right)$$

Schrödinger time independent

$$-\frac{\hbar^2}{2m}\psi'' + V\psi = E\psi$$

$$\psi'' = \frac{-2m(E-V)}{\hbar^2}\psi \equiv -\left(\frac{P(x)}{\hbar}\right)^2\psi$$

$P(x)$ momentum function

$$\psi' = \frac{i\phi'}{\hbar}\psi \quad ; \quad \psi'' = \left(\frac{i\phi'}{\hbar}\right)^2\psi + \frac{i\phi''}{\hbar}\psi$$

equation for ϕ:

$$-\frac{\phi'^2}{\hbar^2} + \frac{i}{\hbar}\phi'' + \frac{p^2}{\hbar^2} = 0$$

expand $\phi = \phi_0 + \hbar\phi_1 + \hbar^2\phi_2 + \cdots$

$$-(\phi_0' + \hbar\phi_1')^2 + i\hbar(\phi_0'' + \hbar\phi_1'') = -p^2$$

$\mathcal{O}(\hbar^0)$ $\quad -(\phi_0')^2 = -p^2$

$\mathcal{O}(\hbar)$ $\quad -2\phi_0'\phi_1' + i\phi_0'' = 0$

$O(\hbar)$ $\quad \phi_0' = \pm p(x)$

$$\phi_0 = \pm \int^x p\, dx'$$

$O(\hbar)$ $\quad \phi_0'' = -i2\phi_0'\phi_1'$

$$\frac{\phi_0''}{\phi_0'} = -2i\phi_1'$$

$$\ln(\phi_0') = -2i\phi_1 + C$$

$$\ln(p) = -2i\phi_1 + C$$

$$\phi_1' = i \ln\sqrt{p} + C'$$

$$\psi(x) = \exp\left(\frac{i}{\hbar}(\phi_0 + \hbar\phi_1)\right)$$

$$= \frac{A}{\sqrt{p}} \exp\left(\frac{\pm i}{\hbar}\int^x p(x')dx'\right)$$

note probability |Ψ |^2 goes like 1/(velocity)

Valid when $O(\hbar) \ll O(\hbar^0)$ terms

$$\left|\frac{\phi_0''}{\hbar}\right| \ll \left|\frac{\phi_0'}{\hbar}\right|^2 \qquad \phi_0' = \pm p(x)$$

$$|p'| = \left|p^2 \frac{d}{dx}\frac{1}{p}\right| \ll \frac{p^2}{\hbar}$$

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

or in terms of de Broglie $\lambda\!\!\!^{-} = \frac{\hbar}{p}$

$$\left|\frac{d}{dx}\lambda\!\!\!^{-}\right| \ll 1$$

with $F = -\frac{dV}{dx}$ classical force

$$\frac{dp}{dx} = \frac{d}{dx}\sqrt{2m(E-V)} = -\frac{m}{p}\frac{dV}{dx} = \frac{mF}{p}$$

then validity condition

$$\hbar\left|\frac{d}{dx}\frac{1}{p}\right| = \hbar\,\frac{1}{p^2}\left|\frac{dp}{dx}\right| = \frac{m\hbar^2 |F|}{p^3} << 1$$

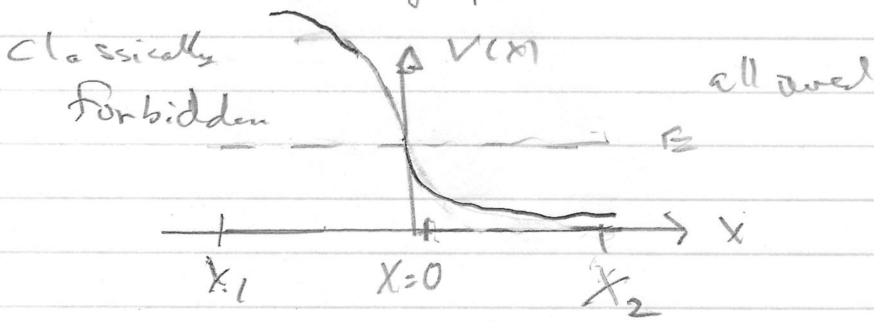
invalid for small p, in particular near classical turning point.

In classically forbidden region, p(x) is pure imaginary so solution is

$$\psi = \frac{C_1}{\sqrt{|p|}}\, e^{-\frac{1}{\hbar}\int |p|\,dx} + \frac{C_2}{\sqrt{|p|}}\, e^{+\frac{1}{\hbar}\int |p|\,dx}$$

approximation says ignore smaller of two terms.

Consider turning point at $x=0$



$$P(x) = 2m\left(E - V(x)\right)\Big|_{x=0} = 0$$

Approximate $V(x)$ linearly near $x=0$,

$$V(x) = V(0) + x\frac{dV}{dx}\Big|_0 = E - F_0 x$$

$F_0 \equiv -\frac{dV}{dx} > 0$, $P(x) = 2m(E-V(x)) = 2mF_0 x$

define $\beta = \left(\frac{2mF_0}{\hbar^2}\right)^{1/3}$ and let $z = \beta x$

Schrodinger equation becomes

$$\frac{d^2\psi}{dz^2} + z\psi = 0$$ solutions are airy functions

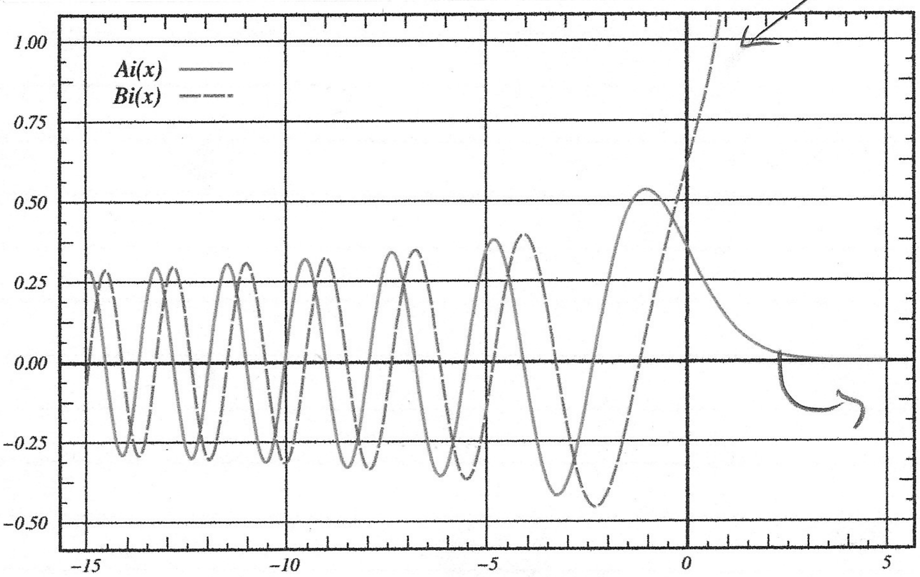
Consider wave function $x > 0$; $\psi_-(x)$

From Wikipedia;

Two linearly independent solutions, $A_i(x)$; $B_i(x)$

exponentially increasing

asymptotic phase shift



exponentially decreasing

$x = -z$

Asymtotic solutions in allowed region to B_i

$$\psi(z) = \frac{\text{const}}{z^{1/4}} \sin\left(\frac{2}{3} z^{3/2} - \frac{\pi}{4}\right)$$

$$\frac{2}{3} z^{3/2} = \int_0^{x_2} z^{1/2}\, dz = \int_0^{x_2} p(x)\, dx$$

So solution with exponential increasing in forbidden region,

$$\psi_+ = \frac{A}{2\sqrt{|p(x)|}} \exp\left(+\frac{1}{\hbar}\int_{x_1}^{0} |p(x)|\, dx\right) \qquad x < 0$$

$$\psi_+ = \frac{A}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar}\int_0^{x_2} p(x)\, dx - \frac{\pi}{4}\right)$$

Tunneling through square barrier

Recall exact solution for plane wave incident on finite square barrier. In classically forbidden region ($E < V_0$), there are two linearly independent solutions which must both be included to get exact solution.

$$\Psi_{\text{forbidden}} = \text{C}e^{-\text{qx}} + \text{D}e^{\text{qx}}$$

Where $\hbar q = \sqrt{2m(V - E)}$

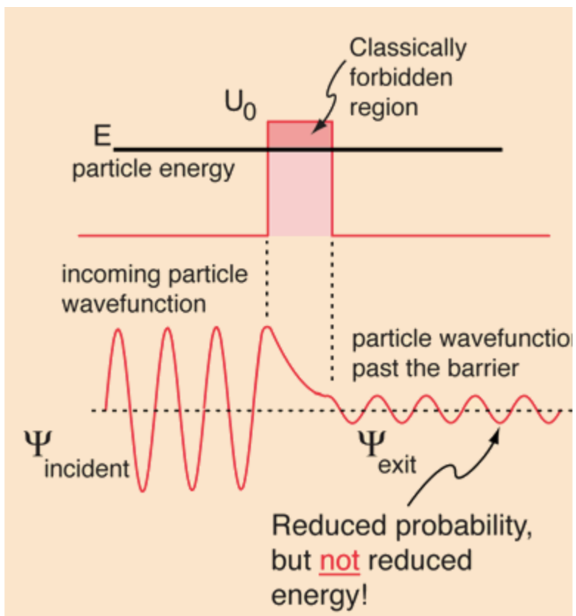


Figure 1: Tunneling through square barrier solution, from hyperphysics. Inside the barrier, the solution initially decays exponentially but must increase exponentially leaving the barrier in order to fit smoothly with the wave after the barrier.

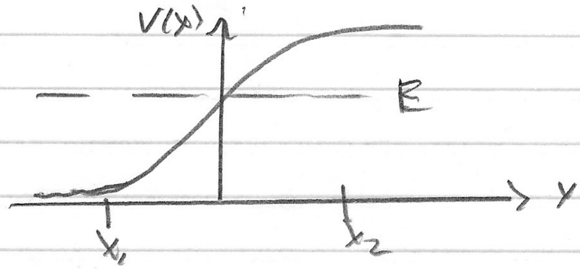
Asymptotic solutions of Airy function are, going into exponentially decaying in forbidden region,

$$\text{Ai}(-\text{z}) = \frac{1}{\sqrt{\pi}}\left(\frac{1}{|\text{z}|}\right)^{1/4}\cos\left(\frac{2}{3}\text{z}^{3/2} - \pi/4\right) = \frac{-1}{\sqrt{\pi}}\left(\frac{1}{|\text{z}|}\right)^{1/4}\sin\left(\frac{2}{3}\text{z}^{3/2} + \pi/4\right) \sim \psi_-$$

And for solutions exiting exponentially increasing in forbidden region,

$$\text{Bi}(-\text{z}) = \frac{1}{\sqrt{\pi}}\left(\frac{1}{|\text{z}|}\right)^{1/4}\sin\left(\frac{2}{3}\text{z}^{3/2} - \pi/4\right) \sim \psi_+$$

for other turning point,

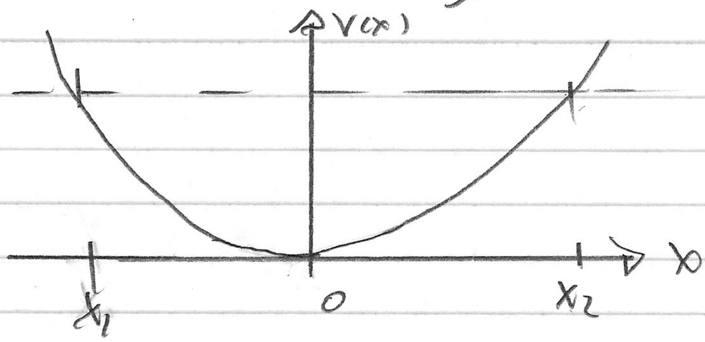


$$\psi_- = \frac{A}{2\sqrt{p(x)}} \exp\left(-\frac{1}{\hbar}\int_0^{x_2} |p(x)|\,dx\right) \qquad x>0$$

$$\psi_- = \frac{A}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar}\int_{x_1}^{0} |p(x)|\,dx + \frac{\pi}{4}\right)$$

exponential decay for plane wave entering forbidden region.

<u>Born-Sommerfeld quantization rule</u>



for $x_1 < x < 0$

$$\psi(x) = \psi_-(x) = \frac{A}{\sqrt{p}} \sin\left(\int_{x_1}^{x} p(x)\,dx + \frac{\pi}{4}\right)$$

for $0 < x < x_2$

$$\psi(x) = \psi\_(x) = \frac{A'}{\sqrt{p}} \sin\left(\int_{x}^{x_2} p(x)\,dx + \frac{\pi}{4}\right)$$

phase difference now absorbed in A'

then $\int_{x}^{x_2} p\,dx = \int_{x_1}^{x_2} p\,dx - \int_{x_1}^{x} p\,dx$

giving

$$\psi_- = \frac{A'}{\sqrt{p}} \sin\left(-\frac{1}{\hbar}\int_{x_1}^{x} p\,dx + \frac{1}{\hbar}\int_{x_1}^{x_2} p\,dx + \frac{\pi}{4} \right)$$

matching gives

$$A = (-1)^m A' \quad \text{using}$$

$$\sin\left(-\theta + \left(m+\tfrac{1}{2}\right)\pi + \tfrac{\pi}{4}\right) = (-1)^m \sin\left(\theta + \tfrac{\pi}{4}\right)$$

giving quantization rule

$$\frac{1}{\hbar}\int_{x_1}^{x_2} p(x)\,dx = \left(m + \tfrac{1}{2}\right)\pi \quad \text{in 1 dimension}$$

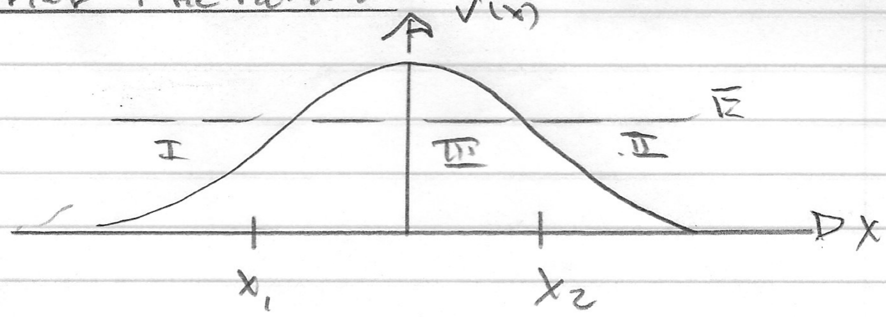
Note: WKB energy for hydrogen with $l=0$ (Weinberg, Lectures on Q.M.) 3 dimensions,

$$E_{WKB} = -\frac{mc^2\alpha^2}{2\left(n+\frac{3}{4}\right)^2} \quad \text{correct for } n \gg 1$$

Whereas, Born quantization rule $mvr = n\hbar$ gives correct energy with

$$E = \frac{mv^2}{2} - \frac{e^2}{r}$$

Barrier Penetration



incident wave (ψ_-)

$$\psi_I = \frac{A}{\sqrt{p}} \sin\left(\frac{1}{\hbar}\int_x^{x_1} p(x)\,dx + \frac{\pi}{4}\right)$$

probagates into barrier

$$\psi_{III} = \frac{A}{2\sqrt{|p|}} \exp\left(-\frac{1}{\hbar}\int_{x_1}^{x} |p|\,dx\right)$$

general form for wave exiting barrier region III

$$\psi'_{III} = \frac{C}{2\sqrt{|p|}} \exp\left(\frac{1}{\hbar}\int_x^{x_2} |p|\,dx\right)$$

connects to outgoing wave region II

$$\psi'_{II} = \frac{C}{\sqrt{p}} \sin\left(\frac{1}{\hbar}\int_{x_2}^{x} p(x)\,dx - \frac{\pi}{4}\right)$$

with $\int_{x_1}^{x} + \int_{x}^{x_2} = \int_{x_1}^{x_2}$ rewrite ψ'_{III}

$$\psi'_{III} = \frac{C}{2\sqrt{|p|}} \exp\left(\frac{1}{\hbar}\int_{x_1}^{x_2} |p|\,dx\right) \exp\left(-\frac{1}{\hbar}\int_{x_1}^{x} p\,dx\right)$$

then $C \exp\left(\frac{1}{\hbar}\int_{x_1}^{x_2} |p|\,dx\right) = A$

then the transmission coefficent is

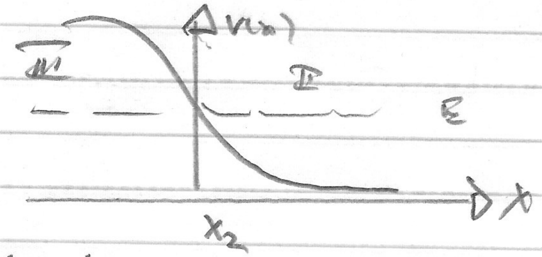
$$T = \left| \frac{C}{A} \right|^2 = \exp\left(-2I\right)$$

with $I \equiv \exp\left(\frac{1}{\hbar} \int_{x_1}^{x_2} |p| \, dx \right)$

integrate over forbidden region

Another way to see connection formula
Landau, Lifshitz, QM 3rd ed.
Also Carrier, Krook, Pearson, Functions of a complex variable

Airy functions are analytic



$x_1 > x_2$, right traveling wave

right traveling wave

$$\psi_+ = \frac{1}{\sqrt{p}} \sin\left(\xi - \pi/4\right) = -\frac{1}{\sqrt{p}} \cos\left(\xi + \pi/4\right) \to \frac{1}{2} e^{(i\xi + i\pi/4)}$$

$$\psi_{II} = \frac{C}{2\sqrt{p}} \exp\left(\frac{i}{\hbar}\int_{x_2}^{x} p(x)\,dx + \frac{i\pi}{4}\right)$$

linear approximation of V

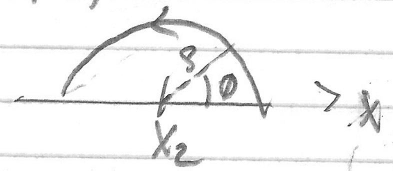
$$V(x) = E + \frac{dV}{dx}\Big|_{x_2} x = E - F_0 x \qquad F_0 > 0$$

$$p(x) = \sqrt{2mF_0 x}$$

$$\int_{x_2}^{x} p(x)\,dx = \sqrt{2mF_0}\int_{x_2}^{x} (x - x_2)^{1/2}\,dx$$

$$x - x_2 \equiv z = \rho e^{i\theta} \qquad \rho = |x - x_2|$$

in complex plane,



Choice of direction around x_2 chooses one of Airy linear independent solutions

$$\int_{x_2}^{x} \sqrt{x - x_2} = \frac{2}{3} z^{3/2}\Big|_{\theta=\pi} = -i\left(\frac{2}{3}\right)\rho^{3/2}$$

So $\sqrt{2mF_0}\int_{x_2}^{x}\sqrt{x-x_2}\,dx = -i\sqrt{2mF_0}\int_{x}^{x_2}(x_2-x)^{1/2}\,dx$

$$= -i\int_{x}^{x_2}|p(x)|\,dx$$

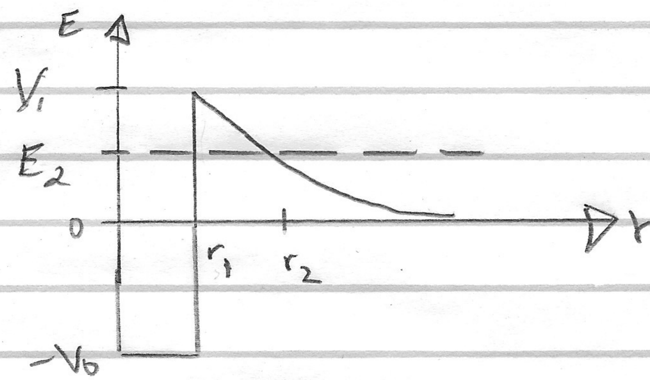
and $p(x)$ becomes $\sqrt{2mF_0}\, z^{1/2} = 2mF_0|x-x_2|e^{i\pi/2}$
for $x<x_2$

$$= e^{i\pi/2}\,|p(x)|$$

giving $\psi_{III} = \frac{C}{2}\frac{1}{e^{i\pi/4}\sqrt{|p(x)|}}\exp\left(\frac{1}{\hbar}\int_{x}^{x_2}|p|\,dx + i\frac{\pi}{4}\right)$

$$= \frac{C}{2\sqrt{|p(x)|}}\exp\left(\frac{1}{\hbar}\int_{x}^{x_2}|p(x)|\,dx\right.$$

Gamov's Theory of α-decay



$$\tau = (f T)^{-1}$$

f = semi-classical barrier collision frequency

transmission coefficient

$$T = e^{-2I} \quad \text{where } I = \exp\left(-\frac{1}{\hbar}\int_{r_1}^{r_2} |p(x)|\,dx\right)$$

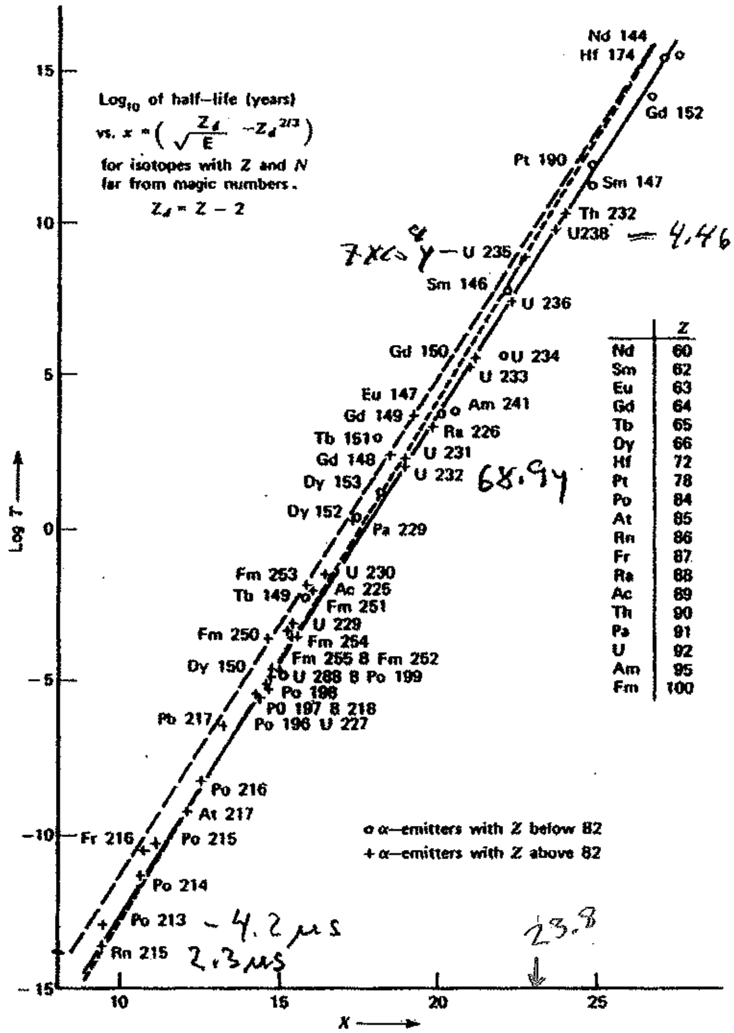
On homework you will show that $I = K X$ where X depends only on decay energy E_α and daughter nucleus $Z_d = Z - 2$ as

$$X = \frac{Z_d}{\sqrt{E_\alpha[\text{MeV}]}} - Z_d^{2/3}$$

WKB-12

α-decay data: Log_{10} of $\frac{1}{2}$ life (years) vs

$x = \frac{Z_d}{\sqrt{E}} - Z_d^{2/3}$ where $Z_d = Z-2$ (daughter)



$X_{U238} = 23.8\ \text{MeV}^{-1/2}$

<u>From</u>: Hyde, Perlman and Seaborg
<u>The Nuclear Properties of Heavy Elements, Vol. I</u>
Prentice-Hall, Englewood Cliffs, NJ (1964)

From PDG:

	$T_{1/2}$
U^{238}	4.47 Gy
Po^{212}	0.299 μs $= 3\times10^{-7}$ s