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

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

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

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

$O(\hbar^0)$ $\qquad \phi_0' = \pm p(x)$

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

$O(\hbar)$ $\qquad \phi_0'' = -i 2 \phi_0' \phi_1'$

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

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

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

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

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

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

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

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

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

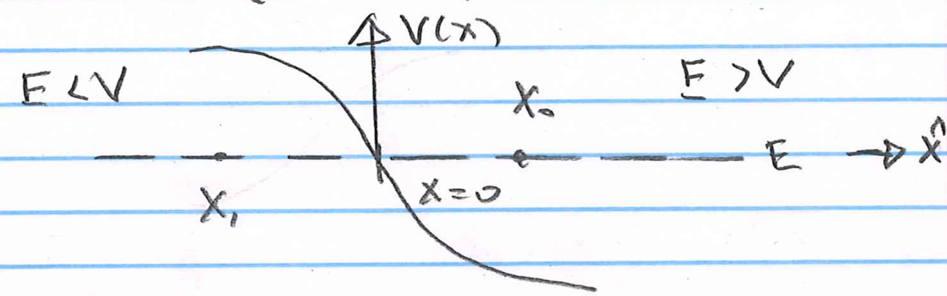
$$\hbar\left|\frac{d}{dx}\frac{1}{p}\right| \ll 1$$

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

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

so valid for slowly varying in x
de Broglie wavelength.

Near classical turning point, WKB is invalid: (Following Commins here)



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

For $E < V$ $(x<0)$ bound state wave function is non-degenerate and real (up to overall phase).

Proof is in Commins, but for bound state $\vec{j} = \frac{\hbar}{m}\,\mathrm{Im}(\psi^* \vec{\nabla}\psi) = 0$ implying ψ real.

Then for $x > 0$, solution is also non-degenerate and real. Take linear superposition of WKB solutions

$$\psi_+(x_0) = \frac{A}{\sqrt{p}} \sin\left(\frac{1}{\hbar}\int_0^{x_0} p\,dx + \alpha\right)$$

Make linear approximation near $x = 0$,

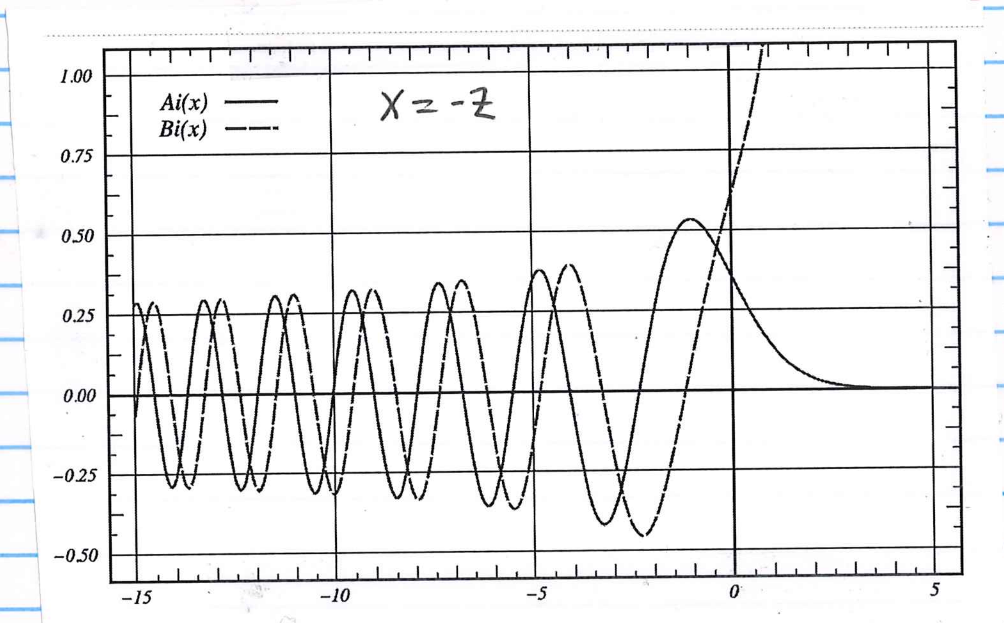
$$V_0(x) = E - F_0 x \quad , \quad F_0 = -\frac{\partial V}{\partial x}\Big|_{x=0}$$

with constant $\beta = \left(\frac{2 m F_0}{\hbar^2}\right)^{1/3}$

substitute $z = \beta X$ to get

$$\frac{d^2\psi}{dz^2} + z\psi = 0$$

solution: Airy function



note! $+z \longleftarrow | \longrightarrow -z$

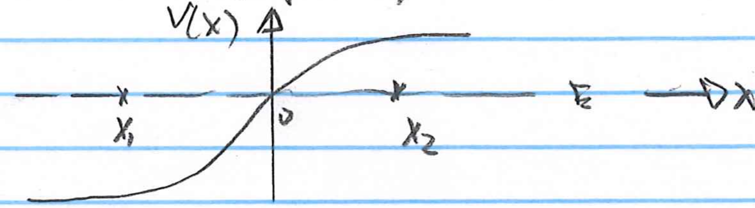
Only need asymptotic:

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

then at x_0, $\frac{2}{3} z^{3/2} = \frac{1}{\hbar} \sqrt{2m(E - V_0)}$

$$\psi(x_0) = \frac{\text{const}}{\sqrt{p(x_0)}} \sin\left(\frac{1}{\hbar}\int_0^{x_0} p\, dx + \frac{\pi}{4}\right)$$

For other turning point,

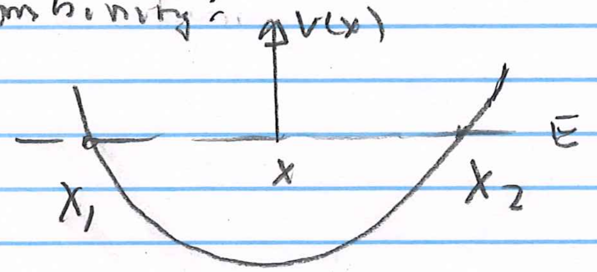


$$\psi(x_1) = \frac{A}{\sqrt{p(x_1)}} \sin\left(\frac{1}{\hbar}\int_{x_1}^{0} p(x)\,dx + \frac{\pi}{4}\right)$$

In classically forbidden region

$$\psi(x_2) = \frac{A}{2\sqrt{|p(x_2)|}} \exp\left(-\frac{1}{\hbar}\int_{0}^{x_2} |p|\,dx\right)$$

Then combining:



x_1, x_2 turning points

for $x_1 < x < x_2$

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

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

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

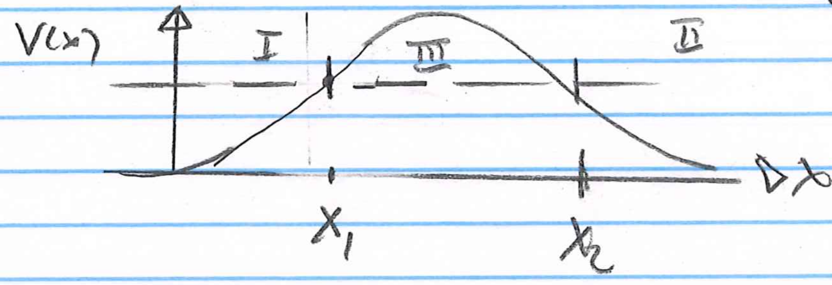
$$\psi(x) = \frac{A'}{\sqrt{p}} \sin\left[\frac{1}{\hbar}\int_{x_1}^{x_2} p\,dx - \int_{x_1}^{x} p\,dx + \frac{\pi}{4}\right]$$

the equality then requires:

$$\int_{x_1}^{x_2} p(x)\,dx = \left(m+\frac{1}{2}\right)\pi\hbar \quad ; \quad A = (-1)^m A'$$

Bohr-Sommerfeld quantization rule

Barrier penetration
simplified from Commins (consult for details)



incident wave

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

propagated into barrier

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

General form of wave heading toward barrier from $x < x_2$,

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

connects to outgoing wave as

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

transmission is $\quad T = \left|\frac{C}{A}\right|^2$

with $\int_{x_1}^{x} + \int_{x_2}^{x} = \int_{x_1}^{x_2}$

rewrite $\phi_{III}(x)$ as

$$\phi_{III}(x) = \frac{C}{\sqrt[?]{|p|}} \exp\left(\frac{1}{\hbar}\int_{x_1}^{x_2}|p(x)|dx\right) \exp\left(-\frac{1}{\hbar}\int_{x_1}^{x}|p(x)|dx\right)$$

$$= \psi_{III}(x)$$

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

giving $T = \left|\frac{C}{A}\right|^2 = \exp\left(-\frac{2}{\hbar}\int_{x_1}^{x_2}|p|dx\right)$