WKB Approximation

- Approximate solution to the Time-Independent S. eqn. (Eigenvalues of $\hat{H}$).

- <u>Key Idea:</u>

Consider a particle of Energy E moving through a region where the potential is a Constant. $V(x) = V$.
If $E > V$, then we have already seen that

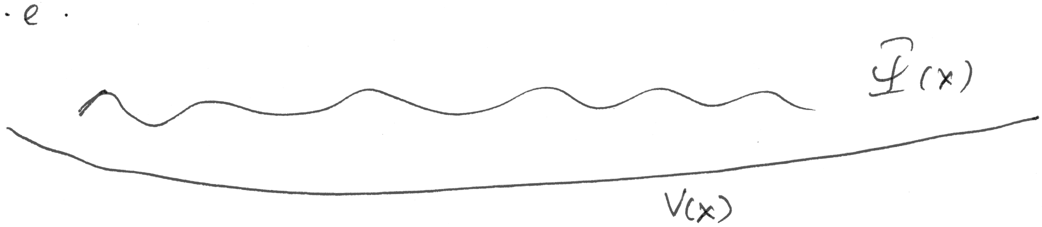
$$\Psi(x) = A e^{\pm ikx} \quad \text{where} \quad k = \frac{\sqrt{2m(E-V)}}{\hbar}$$

ikx: particle traveling in ~~one~~ direction (say left to right)
$-ikx$ Opposite direction.

- The wavefunction is oscillatory with fixed wavelength $\lambda = \frac{2\pi}{k}$ and a fixed amplitude A.

- If $V(x) \neq$ constant, but varies slowly compared to $\lambda = \frac{2\pi}{k}$

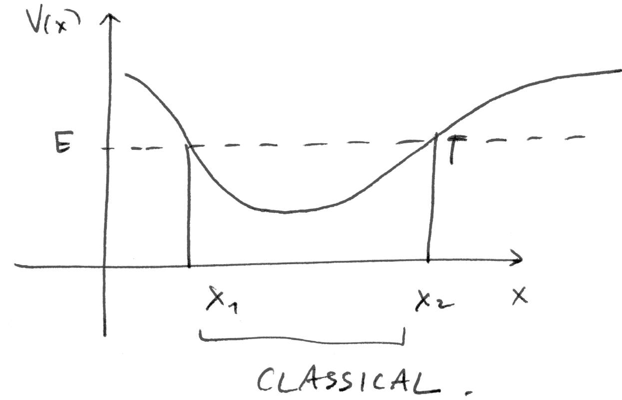
i.e.



In this case it is reasonable to suppose that $\Psi(x)$ remains ~~approxi~~ sinusoidal, except that the wavelength and amplitude have x dependence. - This guess leads to the WKB approximation.

The same argument can be applied to the non-classical case where $E < V$.

The place where the entire argument fails ~~is~~ are the turning points where $k \to 0$, $\lambda \to \infty$. $V(x)$ no longer varies slowly in the vicinity of turning points.



(i) <u>Classical Region:</u>

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} + V(x)\,\Psi(x) = E\,\Psi(x)$$

Then:

$$\frac{d^2\Psi(x)}{dx^2} = -\frac{p^2}{\hbar^2}\,\Psi(x)$$

where $\underbrace{p(x) = \sqrt{2m(E - V(x))}}$

Classical formula for the momentum of a particle of mass 'm', with Energy E and p.E = V(x).

Classical Region $\Rightarrow$ $p(x)$ is real.

The solution $\Psi(x)$ is some complex function

$$\Psi(x) = A(x)\, e^{i\phi(x)}$$

$$\therefore \frac{d\Psi(x)}{dx} = A'(x)\, e^{i\phi(x)} + A(x)\, i\phi'(x)\, e^{i\phi(x)}$$

$$= \left[A'(x) + i\, A(x)\, \phi'(x)\right] e^{i\phi(x)}$$

and

$$\frac{d^2\Psi(x)}{dx^2} = \left[A''(x) + i\, A'(x)\, \phi'(x) + i\, A(x)\, \phi''(x)\right] e^{i\phi(x)}$$

$$+ \left[A'(x) + i\, A(x)\, \phi'(x)\right] i\phi'(x)\, e^{i\phi(x)}$$

$$= \left[A''(x) + 2i\, A'(x)\, \phi'(x) + i\, A(x)\phi''(x) - A(x)\left[\phi'(x)\right]^2\right] e^{i\phi(x)}$$

$\therefore$ Substituting for $\frac{d^2\Psi}{dx^2}$ and $\frac{d\Psi}{dx}$ into the eqn:

$$\frac{d^2\Psi(x)}{dx^2} = -\frac{p^2}{\hbar^2}\Psi(x)$$

we get:

$$A''(x) + 2i\, A'(x)\, \phi'(x) + i\, A(x)\, \phi''(x) - A(x)\, (\phi'(x))^2 = -\frac{p^2}{\hbar^2} A(x)$$

Equating real and imaginary parts:

$$A''(x) - A(x)\, (\phi'(x))^2 = -\frac{p^2}{\hbar^2} A(x) \qquad \text{—— (i)}$$

$$2\, A'(x)\, \phi'(x) + A(x)\, \phi''(x) = 0$$

From the 1^{st} eqn:

$$A''(x) = A(x)\left[(\phi'(x))^2 - P^2/\hbar^2\right]$$

and from the second:

$$\frac{d}{dx}\left(A^2(x)\,\phi'(x)\right) = 0$$

Equivalent to the original S. eqn.

from:

$$\frac{d}{dx}\left(A^2(x)\,\phi'(x)\right) = 0$$ we see that:

$$A^2(x)\,\phi'(x) = c^2 = \text{Const}$$ (Square is for convenience).

$$\Rightarrow \boxed{A(x) = \frac{c}{\sqrt{\phi(x)}}}.$$

In order to solve the 1^{st} eqn, let us do an approximation:

- Assume that $A(x)$ varies slowly so that $A''(x)$ term is small.

$$\Rightarrow (\phi'(x))^2 = P^2/\hbar^2$$

$$\therefore \frac{d\phi(x)}{dx} = \pm P/\hbar \quad \Rightarrow \quad \phi(x) = \pm\frac{1}{\hbar}\int P(x)\,dx$$

Then the solution

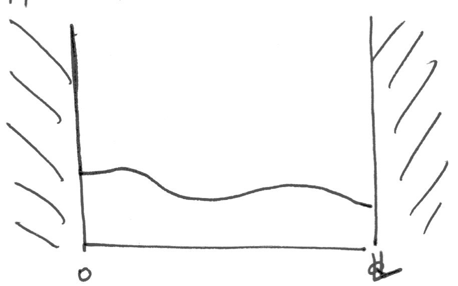
$$\Psi(x) = \frac{c}{\sqrt{P(x)}} \, e^{\pm \frac{i}{\hbar} \int p(x)\, dx}$$

$$|\Psi(x)|^2 = \frac{|c|^2}{P(x)} .$$

i) the prob. of finding a particle at a point x is inversely proportional to its momentum. (classical momentum).

→ This is what we would expect classically!

Application:



$$V(x) = \begin{cases} f(x) & \text{if } 0 < x < L \\ \infty & \text{otherwise.} \end{cases}$$

Inside the well: (If $E > V(x)$)

$$\Psi(x) = \frac{1}{\sqrt{P(x)}} \left[C_+ e^{i\phi(x)} + C_- e^{-i\phi(x)} \right]$$

$$= \frac{1}{P(x)} \left[C_1 \sin\phi(x) + C_2 \cos\phi(x) \right]$$

$$\phi(x) = \frac{1}{\hbar} \int_0^x p(x')\, dx'$$ (gives you a fn of x).

Can leave it as an indefinite integral and ~~these~~ fix a const. which will be absorbed into C_1, C_2.

At $x=0$ $\Psi(0)=0$ (infinitely high walls).

$\Rightarrow \phi(0)=0$ or $C_2=0$

At $x=\cancel{L}$, $C_1 \sin\phi(a)=0$

$$\Rightarrow \phi(a)=n\pi$$

$$\Rightarrow \boxed{\int_0^a p(x)\,dx = n\pi\hbar} \rightarrow \text{leads to Energy quantization.}$$

If the well has a flat bottom: $V(x)=0$,

then: we trivially get $\sqrt{2mE}\,(L) = n\pi\hbar$

$$\therefore E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

<u>Interesting application is to the H.O!</u>

Before that we need to see what happens if the walls are not rigid. We seek a solution in the classically forbidden region. $E<V(x)$. By an analogous argument where $V(x)$ is slowly varying compared to the wavelength,

$$\cancel{2m} \quad \cancel{E_n} \quad p(x) = \frac{\sqrt{2m(V(x)-E)}}{\hbar}$$

$$\therefore \quad \psi(x) = \frac{C}{(V(x)-E)^{1/4}} \exp\left[\pm \frac{1}{\hbar}\int^{x} dx' \sqrt{2m(V(x')-E)}\right]$$

$$E < V(x).$$

The point where the approximation has trouble is the place where

$$V(x) = E \quad \text{(turning points)}.$$

Fortunately there is a standard procedure to match the solution at the ~~this~~ turning point.

(i) Make a linear approximation for the potential near the turning point by expanding the solution in the classically forbidden region about the turning point (say x_0).

(ii) Plug the solution into the differential eqn. (S. eqn). This usually leads to a Bessel fn of order $\pm 1/3$ near x_0.

(iii) Match this solution to the 2 other solutions by choosing appropriately the constants of integration.