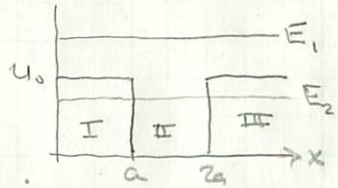
Classical / Quantum Comparison



For a particle w/ energy E_1, speed is larger in region II than in I or III

$$p_I = \pm\sqrt{2m(E_1 - U_0)} \quad \text{(momentum)}$$

$$p_{II} = \pm\sqrt{2mE_1}$$

For a particle w/ energy E_2, motion does not occur in regions I or III – the particle bounces back & forth between a & 2a w/ momentum

$$p_{II} = \pm\sqrt{2mE_2}$$

Quantum story – in region II, we have

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E_1\psi \qquad \text{(time-independent)}$$

so $\psi_{II} = A e^{\pm i\sqrt{\frac{2mE_1}{\hbar^2}}x}$

an oscillatory function w/ wavelength:

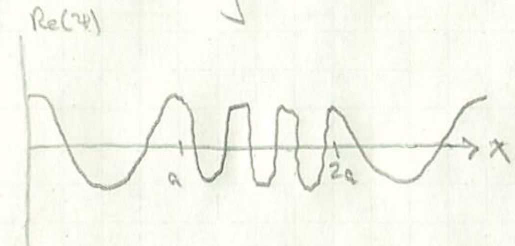
$$\sqrt{\frac{2mE_1}{\hbar^2}}\lambda_{II} = 2\pi \Rightarrow \lambda_{II} = \frac{2\pi\hbar}{\sqrt{2mE_1}}$$

In region I: $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U_0\psi = E_1\psi$

and $\psi_I = F e^{\pm i\sqrt{\frac{2m(E_1 - U_0)}{\hbar^2}}x}$

w/ $\lambda_I = \frac{2\pi\hbar}{\sqrt{2m(E_1 - U_0)}}$

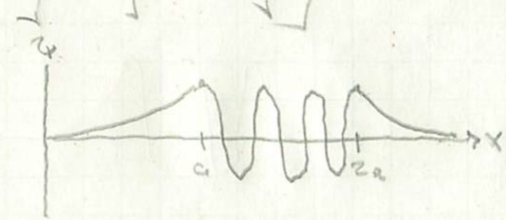
$\lambda_I > \lambda_{II}$, so the rough sketch looks like:



What changes for E_2? We still have:

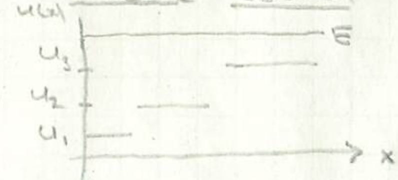
$$\psi_I = F e^{\pm i\sqrt{\frac{2m(E_2 - U_0)}{\hbar^2}}x}$$

but now, w/ $E_2 - U_0 < 0$, the oscillation has become growing + decaying exponentials:



unlike the classical case, there is non-zero probability of finding the particle at $x < a$ + $x > 2a$.

Piecewise Solution



in each region,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U_j\psi = E\psi \qquad j = 1, 2, 3, \ldots$$

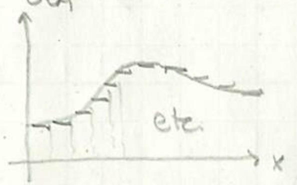
has:

$$\psi_j(x) = A_j e^{\pm i\sqrt{2m(E - U_j)}\,x/\hbar}$$

let $p_j = \sqrt{2m(E-U_j)}$ (the classical momentum)

$\psi_j(x) = A_j e^{\pm i p_j x/\hbar}$

a continuous potential can be thought of as infinitesimally piecewise:



→ we could imagine a solution of the form:

$$\psi(x) = A(x)\, e^{i p(x) x/\hbar}$$

<u>Wentzel</u>- <u>Kramers</u>- <u>Brillouin</u> <u>Approximation</u>

Motivated by the above, take:

$$\psi(x) = e^{i f(x)/\hbar}$$

w/ $\psi'(x) = \dfrac{i f'(x)}{\hbar}\psi(x)$

$$\psi''(x) = \frac{i f''(x)}{\hbar}\psi(x) + \frac{i f'(x)}{\hbar}\psi'(x)$$

$$= \frac{1}{\hbar}\left[i f''(x) - \frac{(f'(x))^2}{\hbar}\right]\psi(x)$$

then: $-\dfrac{\hbar^2}{2m}\psi''(x) + U(x)\psi(x) = E\psi(x)$

written as: $\dfrac{d^2\psi(x)}{dx^2} = -\dfrac{1}{\hbar^2}\cdot \underbrace{2m(E-U(x))}_{\equiv p(x)^2}\psi(x)$

$$= -\left(\frac{p(x)}{\hbar}\right)^2 \psi(x)$$

becomes: $i\hbar f''(x) - (f'(x))^2 = -p(x)^2$ $\quad(*)$

now for the approximation:

$$f(x) = f_0(x) + \hbar f_1(x) + \hbar^2 f_2(x) + \cdots$$

putting this in to $(*)$:

$$i\hbar\left(f_0''(x) + \hbar f_1''(x) + \hbar^2 f_2''(x) + \cdots\right) - \left(f_0'(x) + \hbar f_1'(x) + \hbar^2 f_2'(x) + \cdots\right)^2 = -p(x)^2$$

and collecting in powers of $\hbar$:

$$\hbar^0\left[-f_0'(x)\right]^2 + \hbar^1\left[i f_0''(x) - 2 f_0'(x) f_1'(x)\right] + \hbar^2 + \cdots = -p(x)^2$$

then: $-f_0'(x)^2 = -p(x)^2 \Rightarrow f_0'(x) = \pm p(x) \Rightarrow f_0(x) = \pm\int p(x)\,dx$

$$i f_0''(x) - 2 f_0'(x) f_1'(x) = 0$$

$$\Downarrow$$

$$\frac{i}{2}\frac{f_0''(x)}{f_0'(x)} = f_1'(x)$$

or $\frac{i}{2}\frac{d}{dx}\left(\log p(x)\right) = f_1'(x)$

$$i\frac{d}{dx}\log\left(\sqrt{p(x)}\right) = f_1'(x) \Rightarrow f_1(x) = i\log\left(\sqrt{p(x)}\right)$$

$$\to f(x) \cong f_0(x) + \hbar f_1(x)$$

$$= \pm\int p(x)dx + i\hbar\log\left(\sqrt{p(x)}\right)$$

then

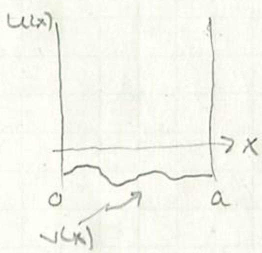
$$\psi(x) = e^{if(x)/\hbar} = e^{\pm\frac{i}{\hbar}\int p(x)dx}\, e^{-\log\left(\sqrt{p(x)}\right)}$$

$$= \frac{A}{\sqrt{p(x)}}\, e^{\pm\frac{i}{\hbar}\int_0^x p(\bar{x})d\bar{x}}$$

note that: $\psi^*\psi = \frac{|A|^2}{p(x)}$

the faster the particle goes (classically), the less likely it is to be found at x.

Example



$$U(x) = \begin{cases} \infty & x<0 \;\&\; x>a \\ V(x) & 0<x<a \end{cases}$$

the b.c. are $\psi(0) = 0 = \psi(a)$

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

$$\psi(x) = \frac{A e^{\frac{i}{\hbar}\int_0^x p(\bar{x})d\bar{x}}}{\sqrt{p(x)}} + \frac{B e^{-\frac{i}{\hbar}\int_0^x p(\bar{x})d\bar{x}}}{\sqrt{p(x)}}$$

or, using cosine & sine:

$$\psi(x) = \frac{1}{\sqrt{p(x)}}\left[\bar{A}\cos\left(\frac{1}{\hbar}\int_0^x p(\bar{x})d\bar{x}\right) + \bar{B}\sin\left(\frac{1}{\hbar}\int_0^x p(\bar{x})d\bar{x}\right)\right]$$

$$\psi(0) = \frac{\bar{A}}{\sqrt{p(0)}} = 0$$

$$\psi(a) = \frac{\bar{B}}{\sqrt{p(a)}}\sin\left[\frac{1}{\hbar}\int_0^a p(\bar{x})d\bar{x}\right] = 0$$

giving $\frac{1}{\hbar}\int_0^a p(\bar{x})d\bar{x} = n\hbar$ for integer n.

for $V(x) = 0$, we recover:

$$\frac{1}{\hbar}\int_0^a \sqrt{2mE}\, d\bar{x} = n\pi$$

or $2mEa^2 = n^2\pi^2\hbar^2 \Rightarrow E = \frac{n^2\pi^2\hbar^2}{2ma^2}$