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WKB

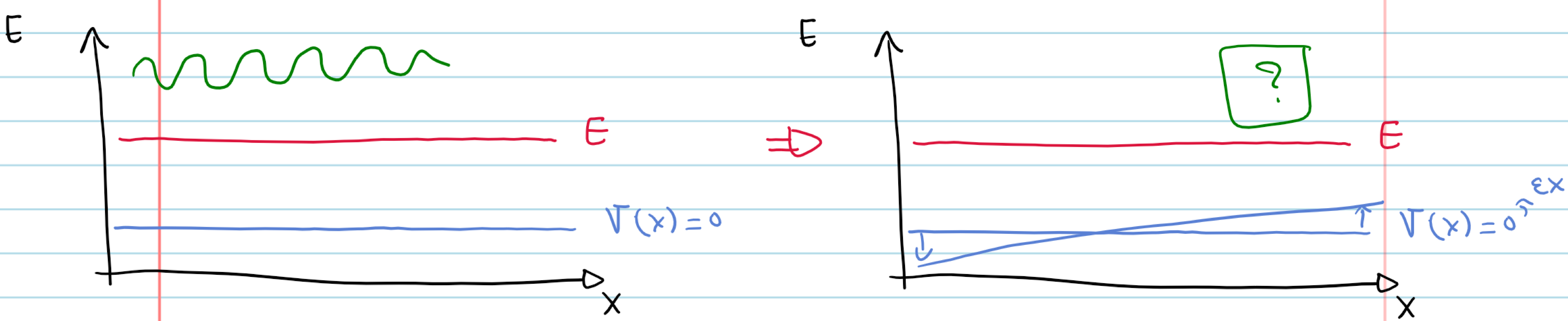
Consider the situation where $V(x) = V_0$.

The Sch. eq. gives

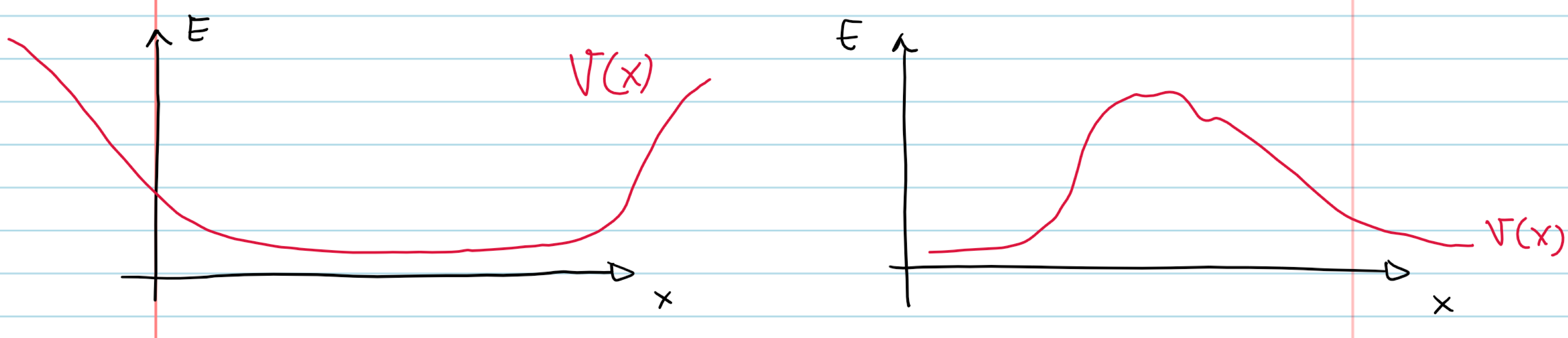
$$\underbrace{-\hbar^2 \frac{d^2\psi(x)}{dx^2}} = 2m(E - V_0)\,\psi(x)$$

$$p^2\psi(x) = q^2\psi(x) \Rightarrow \text{An eigenvalue eq.}$$

Now, we want to see how this can be generalized to a situation where $V(x) \neq V_0$.



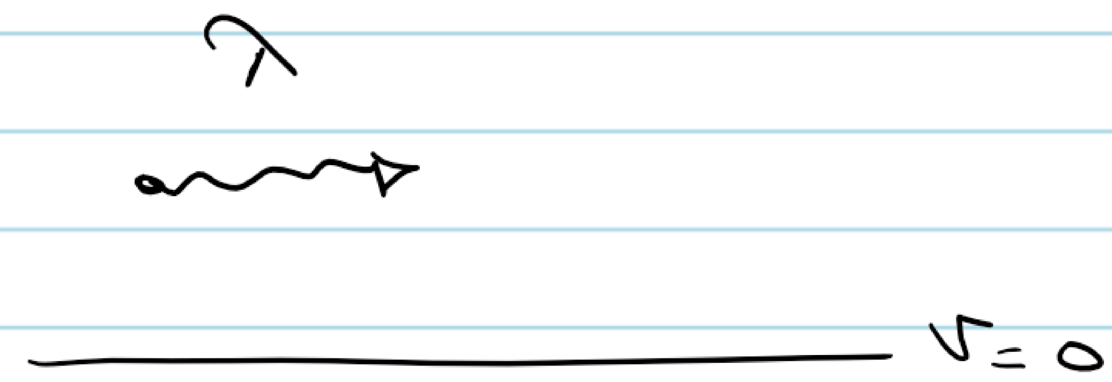
What happens?



Basically, for an arbitrary potential, is there sth. we can say based on our solution for the $V(x) = V_0$?

WKB

For a free particle



A wave with wavelength $\lambda = \frac{h}{p}$.

Now, let's imagine that $V(x) \neq 0$

An extention of the deBroglie wave-length is $\lambda(x) = \frac{h}{P(x)}$

S.E.: $$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = (E - V(x))\psi(x)$$

$$p^2 \psi(x) = \underbrace{2m(E - V(x))}_{P^2(x)} \psi(x) \qquad P(x) = \sqrt{2m(E-V)}$$

$\Rightarrow p^2 \psi(x) = P^2(x)\, \psi(x) \rightsquigarrow ?$ Is this an eigen-value eq.?

Are $\psi(x)$ the eigen vecs?

Note that $P = P(x)$. For eigenvectors,

p should be constant.

Reminder: $V=0 \Rightarrow \psi(x) = A e^{\pm i 2\pi \frac{x}{\lambda}}$

$\lambda = h/p \rightarrow$ de Broglie wave length (Solution to $P^2\psi(x) = p^2\psi(x)$)

Now, if $V(x) \neq V_0$, then

$$p \rightarrow p(x) = \sqrt{2m(E - V(x))} \Rightarrow P^2\psi(x) = p(x)^2\psi(x).$$

↳ Sort of: $\lambda \rightarrow \lambda(x) = \frac{h}{p(x)}$.

But: This is not an eigen value, since it depends on x.
So, $e^{ip \cdot x/\hbar}$ is not exactly a solution. However, we want to construct a solution based on that.

Take the solution to be:

$$\psi(x,t) = \sqrt{\rho(x,t)}\; e^{iS(x,t)/\hbar}$$

$$P(x,t) = |\psi(x,t)|^2 = \rho(x,t)$$

$$J(x,t) = \frac{\hbar}{m}(\psi^* \nabla \psi) = \dots = \frac{\rho(x,t)\, \nabla S(x,t)}{m}$$

We want to make a major assumption:

$$\left| \frac{d}{dx} \lambda(x) \right| \ll 1 \longrightarrow \lambda(x) \text{ is almost constant.}$$

↳ This is equivalent to $\left| \frac{dV(x)}{dx} \right| \ll P^2/2m$ ← Show this!

Let's rewrite $\psi(x) = e^{iS(x)/\hbar}$ with complex S.

↳ Now, plug this into the Sch. eq.

$$-\hbar^2 \frac{d^2}{dx^2} e^{i/\hbar \, S(x)} = p^2(x)\, e^{i/\hbar \, S(x)} \quad , \quad P(x) = \sqrt{2m(E-V(x))}$$

$$-\hbar^2 \left[\left(\frac{i}{\hbar} S'(x)\right)^2 + \frac{i}{\hbar} S''(x) \right] e^{i/\hbar \, S(x)} = P^2(x)\, e^{\frac{i}{\hbar} S(x)}$$

$$S'(x)^2 \underbrace{- i\hbar S''(x)}_{\text{This term has } \hbar \rightarrow \text{ We want to drop this.}} = P^2(x)$$

For that we need to say that S'' is small enough.

<u>Example</u>: $V(x) = V_0$

$$\psi(x) = e^{iqx/\hbar} \quad , \quad q = \sqrt{2m(E-V_0)}$$

$$S(x) = qx/\hbar \quad , \quad S'(x) = q \quad , \quad S'' = 0$$

$$\Rightarrow q^2 = P^2(x) = \sqrt{2m(E-V_0)} \quad \rightarrow \text{Which is fine.}$$

For arbitrary $V(x)$, we can do

$$S(x) = S_0(x) + \hbar S_1(x) + \hbar^2 S_2(x) + \dots$$

Then

$$\Rightarrow S'(x)^2 + i\hbar S''(x) = P^2(x) \qquad \text{gives:}$$

$$\left(S_0'(x) + \hbar S_1'(x) + O(\hbar^2)\right)^2 - i\hbar\left(S_0''(x) + O(\hbar)\right) = P(x)^2$$

$\hbar^0$: $S_0'(x)^2 = P(x)^2 \Rightarrow S_0'(x) = \pm P(x) \Rightarrow S_0(x) = \pm\int P(x)\,dx$

$\hbar^{(1)}$: $2S_1'(x)S_0'(x) - iS_0''(x) = 0$

$$\Rightarrow S_1'(x) = \frac{i\,S_0''(x)}{2S_0'(x)} = \frac{i\,P'(x)}{2\,P(x)} = i/2\left(\log P(x)\right)'$$

$$\Rightarrow S_1(x) = i/2 \log(P(x)) + C$$

Global phase

$$\psi(x) = e^{iS(x)/\hbar} = e^{i/\hbar(S_0(x) + \hbar S_1(x))} = e^{\frac{i}{\hbar}\int P(x)dx - \log\sqrt{P} + iC}$$

$$= \frac{1}{\sqrt{P(x)}}\, e^{i/\hbar\int p(x)dx}$$

We would need a normalization factor A too.

$$\psi(x) = \frac{A}{\sqrt{P(x)}}\, e^{\frac{i}{\hbar}\int P(x)dx} + \frac{B}{\sqrt{P(x)}}\, e^{-i/\hbar\int P(x)\,dx}$$

Validity:

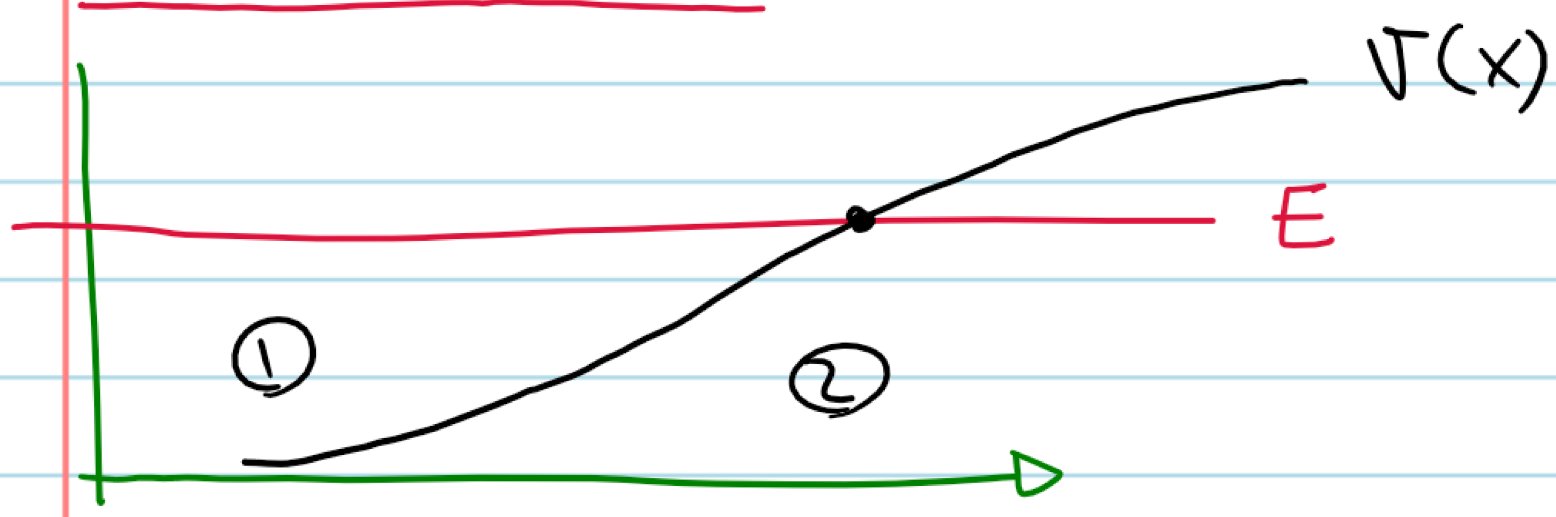
We wanted to say that $|S''(x)\hbar| \ll |S'(x)|^2$.

To the first order, that is:

$$\hbar P'(x) \ll P(x)^2 \quad : \quad \hbar\frac{1}{P(x)^2}\frac{dP(x)}{dx} = -\frac{d}{dx}\frac{\hbar}{P(x)}$$

So: $\equiv \left|\frac{d}{dx}\lambda(x)\right| \ll 1 \longrightarrow$ Which is the assumption that this is a slow varying $V(x)$.

WKB solutions :



$$\psi_1(x) = \frac{A}{\sqrt{P(x)}} e^{\frac{i}{\hbar}\int P(x)\,dx} + \frac{B}{\sqrt{P(x)}} e^{-i/\hbar \int P(x)\,dx}$$

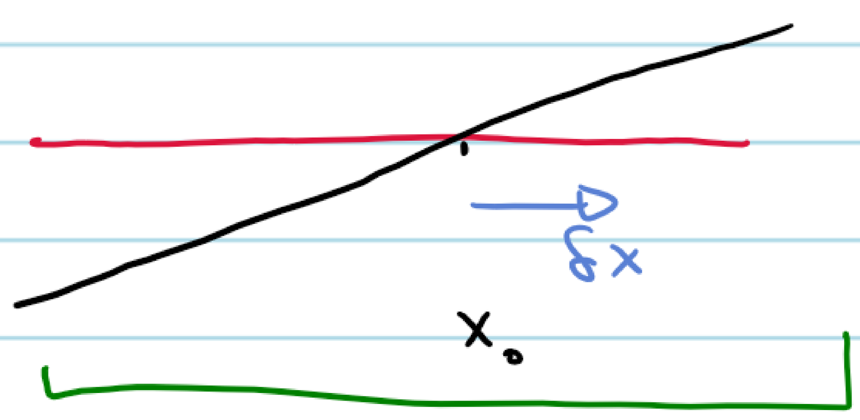
For (2): $\sqrt{2m(E-V)} = i\sqrt{2m(V-E)} \rightarrow q(x) = \sqrt{2m(V(x)-E)}$

$$\psi_2(x) = \frac{A'}{\sqrt{q(x)}} e^{\frac{1}{\hbar}\int q(x)\,dx} + \frac{B'}{\sqrt{q(x)}} e^{-1/\hbar \int q(x)\,dx}$$

Question: Are these solutions valid close to the point where $V(x_0) = E$?

Question: How do we relate ψ_1 & ψ_2 ?

The turning point



Close to the crossing, we can approximate $V(x)$ with a linear function:

$$V(\delta x) = \underbrace{V(x_0)}_{E} + \delta x \underbrace{\frac{dV(x)}{dx}\Big|_{x=x_0}}_{F_0}$$

$$V(\delta x) = E + F_0 \bar{x}$$

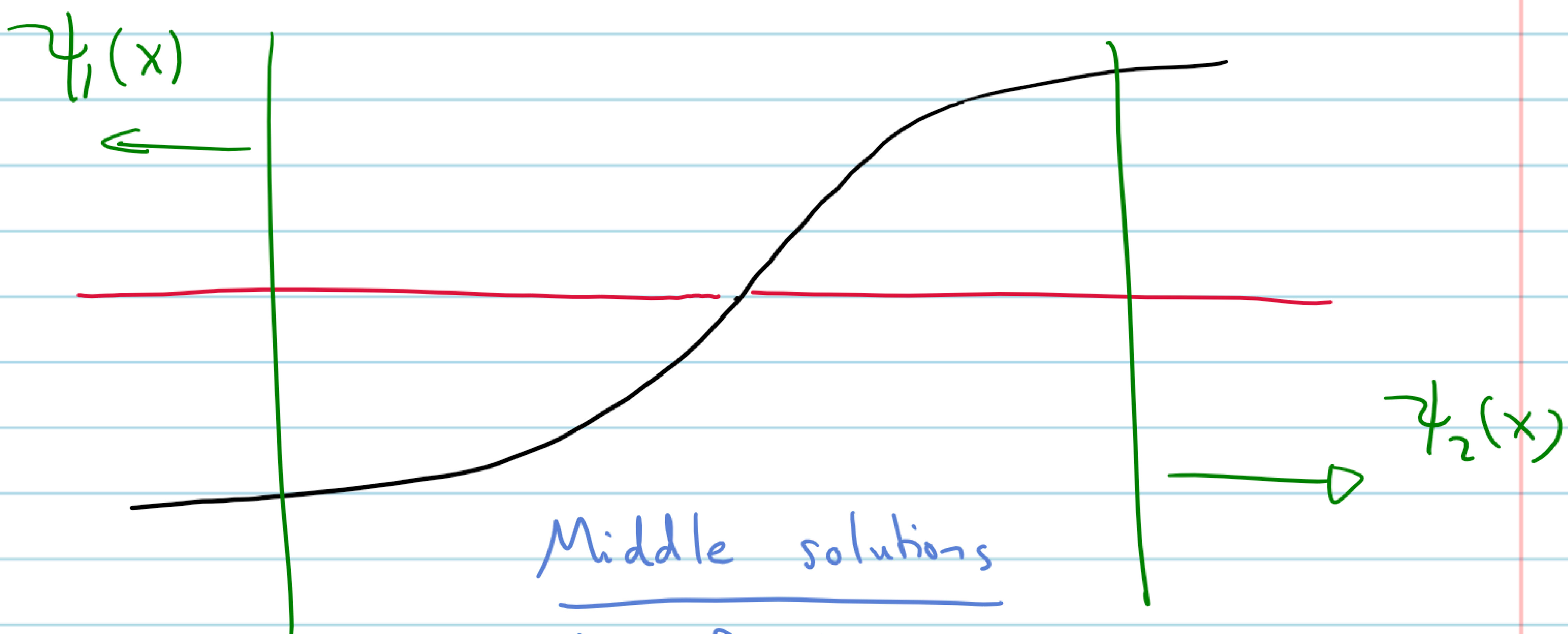
$$\bar{x} = x - x_0$$

$\Rightarrow$ Sch. eq.: $$-\hbar^2 \frac{d^2\psi(x)}{dx^2} = 2m \underbrace{(E-V)}_{F_0 x} \psi(x)$$

$$y = \left(\frac{2mF_0}{\hbar^2}\right)^{1/3} \bar{x}$$

$$\Rightarrow \frac{d^2\psi(y)}{dy^2} = y\psi(y) \longrightarrow \text{Airy diff. eq.}$$

Solutions are the Airy functions: $$\psi(y) = \frac{A'}{\pi} \int_0^\infty \cos\left(\frac{z^3}{3} + yz\right) dz$$



Middle solutions

Airy function $y \gg 0$
$y \ll 0$

$\rightarrow$ Connection equations.

From matching the asymptotic behaviours.

Connection Formulas:

$$\psi_{Middle}(x) = \begin{cases} \frac{1}{\pi |y|^{1/4}} \sin\left(\frac{2}{3}(-y)^{3/2} + \pi/4\right) & y \gg 0 \\ \frac{1}{2\pi |y|^{1/4}} \exp\left(\frac{-2}{3} y^{3/2}\right) & y \ll 0 \end{cases}$$

There's a region where $y \gg 0$ or $y \ll 0$ yet $V(x)$ is still linear (enough) partly b/c $\left|\frac{dV}{dx}\right| \ll \left|\frac{p^2(x)}{2m}\right|$.

So, the asymptotic $\psi_1(x \to x_0)$ should match $\psi_M(y \gg 0)$ and $\psi_2(x \to x_0)$ should match $\psi_M(y \ll 0)$.

For this case, we get

$$\psi_2(x) = \frac{A}{2\sqrt{q(x)}} \exp\left(\frac{-1}{\hbar}\int_{x_0}^{x} |q(x')| \, dx'\right)$$

$$\psi_1(x) = \frac{A}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar}\int_{x}^{x_0} p(x') \, dx' + \pi/4\right)$$

→ Double Check with the eq. in the text book.

I leave it to you to check this for different kinds of potential.