Wentzel–Kramers–Brillouin (WKB) Approximation
(semiclassical)

– Useful for slowly varying potentials (that remain constant over ~ de Broglie wavelength).

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\,\psi(\vec{r}) \qquad \text{Schrödinger equation.}$$

If $V(\vec{r}) =$ constant, then solution is of form: $\psi(\vec{r}) = A\,e^{\pm i\vec{p}\cdot\vec{r}/\hbar}$.

If $V(\vec{r}) \sim$ slowly varying, then WKB says try:

$$\psi(\vec{r}) = A(\vec{r})\,e^{iS(\vec{r})/\hbar} \qquad S(\vec{r}) \equiv \text{"Eikonal"}$$

Amplitude and phase are
(real) functions of $\vec{r}$.

Substitute into Schrödinger equation:

$$-\frac{\hbar^2}{2m}\nabla^2\left(A(\vec{r})\,e^{iS(\vec{r})/\hbar}\right) + V(\vec{r})A(\vec{r})\,e^{iS(\vec{r})/\hbar} = E\,A(\vec{r})\,e^{iS(\vec{r})/\hbar}.$$

$$\underbrace{\nabla^2\left(A(\vec{r})\,e^{iS(\vec{r})/\hbar}\right)}_{\text{Look at this}} + \frac{2m}{\hbar^2}\left(E - V(\vec{r})\right)A(\vec{r})\,e^{iS(\vec{r})/\hbar} = 0.$$

$$\begin{aligned}\nabla^2\left(A\,e^{iS/\hbar}\right) &= \vec{\nabla}\cdot\left(\vec{\nabla}A\,e^{iS/\hbar} + \frac{i}{\hbar}A\,\vec{\nabla}S\,e^{iS/\hbar}\right)\\ &= \nabla^2A\,e^{iS/\hbar} + (\vec{\nabla}A)\cdot\frac{i}{\hbar}(\vec{\nabla}S)\,e^{iS/\hbar} + \frac{i}{\hbar}(\vec{\nabla}A)\cdot(\vec{\nabla}S)\,e^{iS/\hbar}\\ &\quad + \frac{i}{\hbar}A\,\nabla^2S\,e^{iS/\hbar} + \left(\frac{i}{\hbar}\right)^2A\,(\vec{\nabla}S)^2\,e^{iS/\hbar}\\ &= \Big(\underbrace{\nabla^2A + \left(\frac{i}{\hbar}\right)^2A(\vec{\nabla}S)^2}_{\text{Factor out an } A(\vec{r})/\hbar^2} + \frac{2i}{\hbar}(\vec{\nabla}A)\cdot(\vec{\nabla}S) + \frac{i}{\hbar}A\,\nabla^2S\Big)\,e^{iS/\hbar}\end{aligned}$$

Schrödinger eqn becomes:

$$\frac{A}{\hbar^2}\left(\frac{\hbar^2}{A}\nabla^2A - (\vec{\nabla}S)^2 + 2m\left(E - V(\vec{r})\right)\right)e^{iS(\vec{r})/\hbar} + \frac{i}{\hbar}\left(2(\vec{\nabla}A)\cdot(\vec{\nabla}S) + A\,\nabla^2S\right)e^{iS/\hbar} = 0.$$

or $$A\left(\frac{\hbar^2}{A}\nabla^2A - (\vec{\nabla}S)^2 + 2m(E-V)\right) + i\hbar\left(2(\vec{\nabla}A)\cdot(\vec{\nabla}S) + A\,\nabla^2S\right) = 0.$$

WKB Approx: Drop $O(\hbar^2)$ term since it is small in semi-classical approx.
represents a quantum correction to classical Hamilton–Jacobi equation

Real and imaginary parts vanish independently:

$$\Rightarrow \begin{cases} ① \quad (\vec\nabla S)^2 = 2m(E - V(\vec r)) & \text{(classical) Hamilton–Jacobi equation} \\ ② \quad 2(\vec\nabla A)\cdot(\vec\nabla S) + A\,\nabla^2 S = 0 \end{cases}$$

Can explicitly solve this $\underline{\text{in one-dimension}}$: $\frac{1}{2m}\left(\frac{dS}{dx}\right)^2 + V(x) = E$

$$①: \quad \left(\frac{dS}{dx}\right)^2 = 2m(E - V(x)) \quad \text{or} \quad \frac{dS}{dx} = \pm\sqrt{2m(E-V)} \equiv \pm p_{clas.}(x)$$

$$\Rightarrow \boxed{S(x) = \pm \int dx\, \sqrt{2m(E - V(x))}} \qquad \text{(becomes imaginary if } V > E)$$

$$②: \quad 2\,\frac{dA}{dx}\frac{dS}{dx} + A\,\frac{d^2S}{dx^2} = 0 \qquad \text{divide by } A$$

$$\underbrace{2\,\frac{1}{A}\frac{dA}{dx}}_{\frac{d}{dx}\ln A(x)}\left(\pm\sqrt{2m(E-V)}\right) + \frac{d}{dx}\left(\pm\sqrt{2m(E-V)}\right) = 0. \qquad \text{divide by } \pm\sqrt{2m(E-V)}$$

$$2\,\frac{d}{dx}\ln A(x) + \underbrace{\frac{1}{\sqrt{2m(E-V)}}\frac{d}{dx}\left(\sqrt{2m(E-V)}\right)}_{\frac{d}{dx}\ln\left(\sqrt{2m(E-V)}\right)} = 0.$$

Hence, $$\frac{d}{dx}\left(2\ln A(x) + \ln\sqrt{2m(E-V)}\right) \equiv \frac{d}{dx}\ln\left[A^2(x)\sqrt{2m(E-V(x))}\right] = 0.$$

$$\Rightarrow \ln A^2(x)\sqrt{2m(E-V(x))} = C \quad \text{or} \quad \boxed{A(x) = \frac{C}{|2m(E-V(x))|^{1/4}}}$$

↖ integration constant

There are two solutions:

$$\psi_\pm(x) = \frac{C_\pm}{|2m(E-V(x))|^{1/4}}\exp\left[\pm\frac{i}{\hbar}\int dx\,\sqrt{2m(E-V(x))}\right]$$

↖ absolute phase is unobservable
$\Rightarrow$ integration const. is irrelevant.
(one can define a "phase shift" relative to a reference "free" wavefunc)

- Amplitude $\sim \dfrac{1}{|2m(E-V)|^{1/4}} = \dfrac{1}{\sqrt{p}}$
- Becomes exponential decay (growth) for $E < V(x)$ (classically forbidden regions).

Solution in classically allowed region: $p(x) = \sqrt{2m(E-V(x))}$ (semiclassical) WKB momentum.

$$\psi(x) = \frac{C_+}{|p(x)|^{1/2}} \exp\left[\frac{+i}{\hbar}\int dx\, p(x)\right] + \frac{C_-}{|p(x)|^{1/2}} \exp\left[\frac{-i}{\hbar}\int dx\, p(x)\right]$$

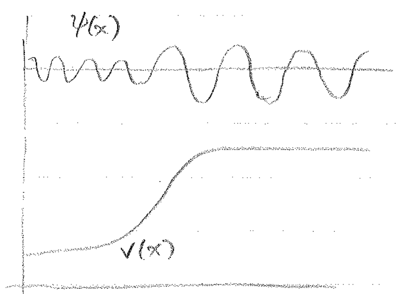
Solution in classically forbidden region:

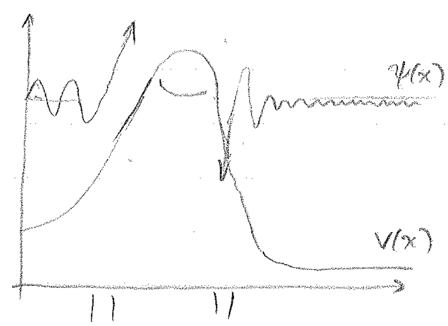
$$\psi(x) = \frac{C_-}{|p(x)|^{1/2}} \exp\left[-\frac{1}{\hbar}\int dx\, |p(x)|\right] + \frac{C_+}{|p(x)|^{1/2}} \exp\left[+\frac{1}{\hbar}\int dx\, |p(x)|\right]$$

Summary:

The WKB approximation gives an approximate form of the wavefunction that matches the expected qualitative behavior.

eg:





WKB approx. breaks down close to turning points. —see below.

Validity of WKB approx:

Recall we dropped $O(\hbar^2)$ claiming it to be small:

$$\text{valid if} \quad \begin{pmatrix} O(\hbar) \\ \text{terms}\end{pmatrix} \ll \begin{pmatrix} O(\hbar^0) \\ \text{terms}\end{pmatrix} \quad \text{or} \quad |\hbar \nabla^2 S| \ll (\vec{\nabla} S)^2$$

$$\underline{\text{in 1D:}} \quad \hbar \left| \frac{S''(x)}{(S'(x))^2} \right| \ll 1$$

Then using $S'(x) = \sqrt{2m(E-V(x))} = p(x)$, $\quad \hbar \left| \dfrac{p'(x)}{p^2(x)} \right| \ll 1$

Then, using $\lambda(x) = \dfrac{2\pi\hbar}{p(x)}$, $\longrightarrow \quad \left| \dfrac{d\bar{\lambda}(x)}{dx} \right| = \left| \dfrac{d}{dx}\left(\dfrac{\hbar}{p(x)}\right) \right| \ll 1$

Fixing WKB at classical turning points is difficult, but doable.