

WKB Approximation (Semiclassical)

identify regions in which wavelength is much shorter than typical distance over which potential energy varies

1D:
$$\frac{d^2 u_E}{dx^2} + \frac{2m}{\hbar^2} (E - V(x)) u_E(x) = 0$$



define:
$$k(x) = \sqrt{\frac{2m}{\hbar^2} (E - V(x))} \quad E > V(x) \quad \text{"allowed region"}$$

$$k(x) = -i \sqrt{\frac{2m}{\hbar^2} (V(x) - E)} \quad E < V(x) \quad \text{"forbidden region"}$$

$$= -i \kappa(x)$$

$$\rightarrow \frac{d^2 u_E}{dx^2} + [k(x)]^2 u_E(x) = 0$$

if $V(x)$ does not change with x (is constant) $\rightarrow k(x)$ constant

$$\rightarrow u_E(x) \propto e^{\pm ikx}$$

if $V(x)$ varies slowly with $x \rightarrow$ try solution of form

$$u_E(x) = e^{\frac{i}{\hbar} W(x)}$$

$$\rightarrow i \hbar \frac{d^2 W}{dx^2} - \left(\frac{dW}{dx}\right)^2 + \hbar^2 [k(x)]^2 = 0 \quad \text{Schrödinger-like equation}$$

Make approximation (expansion etc.)

$$\hbar \left| \frac{d^2 W}{dx^2} \right| \ll \left| \frac{dW}{dx} \right|^2$$

$$\rightarrow$$
 lowest order approximation $W_0'(x) = \pm \hbar k(x)$

$$\rightarrow$$
 1st order approximation:
$$\left(\frac{dW_1}{dx}\right)^2 = \hbar^2 [k(x)]^2 + i \hbar W_0''(x)$$

$$= \hbar^2 [k(x)]^2 \pm i \hbar^2 k'(x)$$

term #1 \gg term #2

$$\rightarrow W(x) \approx W_1(x) = \pm \hbar \int^x dx' [k^2(x') \pm i k'(x')]^{\frac{1}{2}}$$

$$\approx \pm \hbar \int^x dx' k(x') \left[1 \pm \frac{i}{2} \frac{k'(x')}{k^2(x')} \right]$$

$$\sqrt{1-\epsilon^2} = 1 - \frac{1}{2}\epsilon^2$$

$$= \pm \hbar \int^x dx' k(x') + \frac{i}{2} \hbar \ln[k(x)']$$

\rightarrow wavefunction in WKB limit to first order

$$u_\epsilon(x) \approx e^{\frac{i}{\hbar} W(x)} = \frac{1}{\sqrt{k(x)}} \exp\left[\pm i \int^x dx' k(x')\right]$$

\rightarrow specifies two solutions (\pm)

1. for region $E > V(x)$

2. for region $E < V(x)$

\rightarrow we need to join them: at classical turning point

$$\lambda = \frac{1}{k} \rightarrow \infty \text{ potential cannot}$$

be thought of as slowly varying

\rightarrow approximate region around $E \approx V$ with linear potential

$$\left[\begin{array}{l} \rightarrow SE \text{ in appropriately scaled units: } \frac{d^2 u_\epsilon}{dz^2} - z u_\epsilon(z) = 0 \\ \rightarrow \text{solutions are Airy functions} \end{array} \right]$$

Asymptotic dependences of Airy functions:

$$Ai(z) \rightarrow \frac{1}{2\sqrt{\pi}} z^{-\frac{1}{4}} \exp\left[-\frac{2}{3} z^{\frac{3}{2}}\right] \quad z \rightarrow \infty$$

$$Ai(z) \rightarrow \frac{1}{\sqrt{\pi}} |z|^{-\frac{1}{4}} \cos\left(\frac{2}{3} |z|^{\frac{3}{2}} - \frac{\pi}{4}\right) \quad z \rightarrow -\infty$$

$$I \rightarrow II \quad \frac{1}{(V(x)-E)^{\frac{1}{4}}} \exp\left[-\frac{1}{\hbar} \int_x^{x_1} dx' \sqrt{2m[V(x')-E]}\right] \rightarrow \frac{2}{(E-V(x))^{\frac{1}{4}}} \cos\left[\frac{1}{\hbar} \int_{x_1}^x dx' \sqrt{2m(E-V(x'))} - \frac{\pi}{4}\right]$$

$$III \rightarrow II \quad \left\{ \frac{1}{(V(x)-E)^{\frac{1}{4}}} \right\} \exp\left[-\frac{1}{\hbar} \int_{x_2}^x dx' \sqrt{2m[V(x')-E]}\right] \rightarrow \left\{ \frac{2}{(E-V(x))^{\frac{1}{4}}} \right\} \cos\left[-\frac{1}{\hbar} \int_x^{x_2} dx' \sqrt{2m(E-V(x'))} + \frac{\pi}{4}\right]$$

matching two solutions across turning point very difficult

1. Make linear approximation of V potential around turning point
2. find solutions to SE in this region
3. match solutions to other solutions choosing appropriate integration constants.

class \rightarrow I \rightarrow II ...

III \rightarrow II ...

\rightarrow note that form in region II must be identical

\rightarrow argument differ by integer multiple of π (Amplitude, Phase)
Solve yourself

\rightarrow consistency condition

$$\int_{x_1}^{x_2} dx \sqrt{2m[E - V(x)]} = (n + \frac{1}{2})\pi \hbar \quad (*)$$

\rightarrow fixed energy spectrum

Example: Sourcing Ball (Sourcing neutron)

$$V = \begin{cases} mgx & \text{for } x > 0 \\ 0 & \text{for } x < 0 \end{cases} \quad \begin{array}{c} \circ \\ \downarrow x \end{array}$$

1st idea: use (*) with $x_1 = 0$, $x_2 = \frac{E}{mg}$

\rightarrow but does not work since no leaking into surface!

2nd idea: find odd-parity solutions for $V(x) = mg|x|$

\rightarrow turning points $x_1 = -\frac{E}{mg}$, $x_2 = \frac{E}{mg}$

$$\rightarrow \int_{-E/mg}^{E/mg} dx \sqrt{2m(E - mg|x|)} = (n_{\text{odd}} + \frac{1}{2})\pi \hbar \quad (n_{\text{odd}} = 1, 3, 5, \dots)$$

or equivalently

$$\int_0^{E/mg} dx \sqrt{2m(E - mgx)} = (n - \frac{1}{4}) \pi \hbar \quad n = 1, 2, 3, 4, \dots$$

→ $E_n = \frac{3(n - \frac{1}{4})^2}{2} (mg^2 \hbar^2)^{\frac{1}{3}}$ quantised energy levels of
 bouncing ball

compare to exact numerical solutions:

n	WKB	Exact	Example: quarkonium bound state of quark-antiquark mg ⇔ force between quarks 1.6 · 10 ⁵ N (16 tons) 100 μ ball: 0.98 N
1	2.320	2.338	
2	4.082	4.088	
⋮			
10	12.828	12.827	

← almost perfect

Outstanding: interpretation of $\hbar \left| \frac{d^2 W}{dx^2} \right| \ll \left| \frac{dW}{dx} \right|^2$

becomes exact in limit $\hbar \rightarrow 0$ (classical limit)

time dependent w.f.:

$$\psi(x,t) \propto u_E(x) e^{-\frac{i}{\hbar} E t} = e^{i W(x) - \frac{i}{\hbar} E t}$$

in Hamilton Jacobi formalism: $W \hat{=}$ Hamilton's characteristic function

→ condition describes classical limit

also: condition the same as $|k'(x)| \ll |k^2(x)|$ (see lowest order WKB)

$$\frac{\lambda}{2\pi} = \frac{\hbar}{\sqrt{2m(E - V(x))}} \ll \frac{2(E - V(x))}{dV/dx}$$

de Broglie wavelength must be small compared to characteristic distance over which potential varies