The Wentzel-Kramers-Brillouin (WKB) Method.

* The premise: Not all ~~(well, most~~ quantum mechanical problems are exactly (analytically) solvable (well, most realistic problems are not analytically solvable!).

→ Consider the Schroedinger equation:

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

For examples if $\underbrace{V(x) \propto \frac{1}{x^2}}_{\text{Very difficult to solve exactly!}}$ ~ H-atom problem

Now imagine: $V(x) \propto \frac{1}{x^2} + \frac{1}{x^3}$!!

or

$\propto \frac{1}{x^n}$, $n>2$!!

or

some other non-trivial fn.!!

→ Clearly, there is a need to find approximate methods of solving the Sch. eq.

* Our goal: $\boxed{\text{WKB method of semi-classical approximation.}}$

→ The basis for WKB method:

Consider a particle in 1D moving in a constant potential V.

⇒ TISE is exactly solvable.

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

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

$$\Rightarrow \boxed{\psi(x) = \psi(\cancel{x_0})\, e^{\pm ipx/\hbar}}, \quad p \equiv \sqrt{2m(E-V)}$$

(*) Note: ± indicates forward and backward moving plane waves.

→ From our knowledge of the wave equations,

$$\frac{p}{\hbar} \longleftrightarrow k = \frac{2\pi}{\lambda}$$

$$\Rightarrow \boxed{\lambda = \frac{2\pi\hbar}{p}} \leftarrow \text{de-Broglie wavelength!}$$

→ Suppose now, that $\boxed{V = V(x)}$ ← Not a constant

But, let's assume that V(x) varies sufficiently slowly such that over a region of interest, $\boxed{V = V(x) \approx V_0 \text{ (const.)}}$

$$\Rightarrow \boxed{\lambda(x) \approx \frac{2\pi\hbar}{p(x)} \approx \frac{2\pi\hbar}{[2m(E-V(x))]^{1/2}}}$$

← s.t. $\psi(x)$ can still be approximated as a plain wave.

The logic of WKB!! →

(*) Therefore, WKB approximation is a semi-classical approximation valid in cases where V(x) varies sufficiently slowly to allow $\psi(x)$ to be approximated as a plain wave.

→ If $p = p(x)$, then over $x = 0$ to $x = x$:

$$\psi(x) = \psi(0) \exp\left[\pm \frac{i}{\hbar} \int_0^x p(x')\,dx'\right] \leftarrow \text{expected}$$

$$\Rightarrow \boxed{\psi(x) = \psi(x_0) \exp\left[\pm \frac{i}{\hbar} \int_{x_0}^x p(x')\,dx'\right]}$$

[Q] What does position-dependent $\lambda(x)$ mean?
— Does it make sense to define $\lambda = \lambda(x)$?
[By definition, λ is a quantity defined over a range of distance !!]

→ For $\lambda(x)$ to be sensible, ~~to~~ and therefore for V(x) to be "slowly varying", — how slowly?

we must require that

$$\boxed{\delta\lambda << \lambda}$$

$$\Rightarrow \left|\frac{\delta\lambda}{\lambda}\right| << 1 \Rightarrow \left|\cancel{\frac{1}{\lambda}} \frac{d\lambda}{dx} \cancel{\frac{\delta x}{\lambda}}^{\sim 1}\right| << 1$$

$$\Rightarrow \boxed{\left|\frac{d\lambda}{dx}\right| << 1}$$

Formal derivation of the WKB approximation.

→ So far, we arrived at the approximate $\psi(x)$ using semi-classical "logic". Let's now derive mathematically to validate the correctness of our logic.

→ <u>The problem:</u>

To solve the TISE:

$$\left\{\frac{d^2}{dx^2} + \frac{2m}{\hbar^2}\left[E - V(x)\right]\right\}\psi(x) = 0$$

$$\Rightarrow \boxed{\left[\frac{d^2}{dx^2} + \frac{1}{\hbar^2}p^2(x)\right]\psi(x) = 0}$$

→ The desired solution / <u>"ansatz"</u>:

$$\psi(x) = \exp\left[i/\hbar\, \phi(x)\right]$$

Substituting in the TISE:

$$\frac{d\psi}{dx} = \frac{i}{\hbar}\frac{d\phi}{dx}\psi(x)$$

$$\frac{d^2\psi}{dx^2} = \frac{i}{\hbar}\frac{d^2\phi}{dx^2}\psi(x) - \frac{1}{\hbar^2}\left(\frac{d\phi}{dx}\right)^2\psi(x)$$

$$\Rightarrow \left[-\frac{1}{\hbar^2}(\phi'(x))^2 + \frac{i}{\hbar}\phi''(x) + \frac{1}{\hbar^2}p^2(x)\right]\psi(x) = 0$$

$$\Rightarrow \boxed{-\left(\frac{\phi'}{\hbar}\right)^2 + \frac{i\phi''}{\hbar} + \frac{p^2(x)}{\hbar^2} = 0}$$

To solve this differential equation,
Let's take power series ~~ansat~~ soln. of $\phi(x)$:

$$\phi = \phi_0 + \hbar \phi_1 + \hbar^2 \phi_2 + \cdots$$

where $\hbar$ is the parameter that characterizes deviation from constant V solution.

* Note: when $\hbar \to 0 \Rightarrow \phi \to \phi_0$

$$\Rightarrow \psi \to e^{i\phi_0/\hbar}$$

also the classical limit

Plain wave!!

→ In the WKB method, we only consider upto $O(\hbar)$ terms i.e $O(\hbar^2)$ terms are ignored.

$$\therefore \boxed{\phi \approx \phi_0 + \hbar \phi_1} + O(\hbar^2)$$

$\boxed{H/W}$ Substitute this ϕ into the differential eq. and obtain $O(\hbar^0)$ & $O(\hbar)$ equations.

Ans: upto ~~At~~ $\hbar^0$ order:

$$-\frac{(\phi_0')^2 + p^2(x)}{\hbar^2} + \frac{i\phi_0'' - 2\phi_1'\phi_0'}{\hbar} + O(\hbar^0) = 0$$

As a first approximation, if we only consider the first term $O(\hbar^{-2})$:

$$-(\phi_0')^2 + p^2(x) \approx 0$$

$$\Rightarrow \boxed{\phi_0' = \pm p(x)}$$

$$\Rightarrow \quad \phi_0(x) = \pm \int^x dx' \, p(x')$$

$$\Rightarrow \quad \psi(x) = A \exp\left[\pm \frac{i}{\hbar} \int^x p(x') dx'\right]$$

A → normalization factor

Considering some given initial condition:

$$\boxed{\psi(x) = \psi(x_0) \exp\left[\pm \frac{i}{\hbar} \int_{x_0}^x p(x') dx'\right]}$$

→ Now, considering upto $O(\hbar^{-1})$ terms:

$$\frac{-(\phi_0')^2 + p^2(x)}{\hbar^2} + \frac{i\phi_0'' - 2\phi_1'\phi_0'}{\hbar} \approx 0$$

Here we introduce a constraint:

i.e Let's demand that ϕ_0' is such that s.t. $\boxed{\phi_0' = \pm p(x)}$

$$i\phi_0'' - 2\phi_1'\phi_0' = 0$$

$$\Rightarrow \quad \frac{\phi_0''}{\phi_0'} = -2i\phi_1'$$

$$\Rightarrow \quad \int \frac{d\phi_0'}{\phi_0'} = -2i \int d\phi_1$$

$$\Rightarrow \quad \ln \phi_0' = -2i\phi_1 + c$$

$$\Rightarrow \quad -i\frac{1}{2} \ln \phi_0' = \phi_1 + i\frac{c}{2}$$

$$\Rightarrow \quad \boxed{\phi_1 = i \ln (\phi_0')^{1/2} + \frac{c}{2i}}$$

Using $\phi_0' = p$:

$$\Rightarrow \quad \boxed{\phi_1 = i \ln p^{1/2} + \tilde{c}}$$

$\left[\because \ln[(-p)^{1/2}] \text{ would be undefined}\right]$

Therefore,

$$\psi(x) = \exp\left[\frac{i}{\hbar}\phi(x)\right] = \exp\left[\frac{i}{\hbar}\left\{\phi_0(x) + \hbar\phi_1(x)\right\}\right]$$

$$\Rightarrow \psi(x) = A e^{-\ln[p(x)]^{1/2}} \exp\left[\pm\left(\frac{i}{\hbar}\right)\int^x p(x')\,dx'\right]$$

$$\Rightarrow \boxed{\psi(x) = \frac{A}{[p(x)]^{1/2}} \exp\left[\pm\left(\frac{i}{\hbar}\right)\int^x p(x')\,dx'\right]}$$

H/W: Using the initial conditions $\psi(x_0)$, $p(x_0)$ at $x = x_0$, show that

$$\psi(x) = \psi(x_0)\left[\frac{p(x_0)}{p(x)}\right]^{1/2} \exp\left[\pm\frac{i}{\hbar}\int_{x_0}^{x} p(x')\,dx'\right]$$

Q What are the conditions for validity of above calc.?

→ Note: We are assuming $\boxed{O(\hbar^{-2}) \gg O(\hbar^{-1}) \gg O(\hbar^0) \ldots}$

$\Rightarrow$ We require the fns. $\phi'(x)$, $\phi''(x)\ldots$ in the numerator to be s.t:

$$\boxed{\left|\frac{\phi_0''}{\hbar}\right| \ll \left|\frac{\phi_0'}{\hbar}\right|^2} \leftarrow \text{Condition for WKB approx.}$$

$$\Rightarrow \hbar\left|\frac{1}{\phi_0'^2}\frac{d\phi_0'}{dx}\right| \ll 1$$

$$\Rightarrow \hbar\left|\frac{d}{dx}\left(\frac{1}{\phi_0'}\right)\right| \ll 1$$

$$\Rightarrow \left|\frac{d}{dx}\left(\frac{\hbar}{p(x)}\right)\right| \ll 1 \quad \Rightarrow \boxed{\frac{1}{2\pi}\left|\frac{d\lambda}{dx}\right| \ll 1} \leftarrow \text{Matches our earlier expectation!!}$$

explicit proof of WKB

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Bound state energies using WKB approximation:

So far, we have derived the WKB wavefn:

$$\psi(x) = \psi(x_0)\left[\frac{p(x_0)}{p(x)}\right]^{1/2} \exp\left[\pm\frac{i}{\hbar}\int_{x_0}^{x} p(x')\,dx'\right]$$

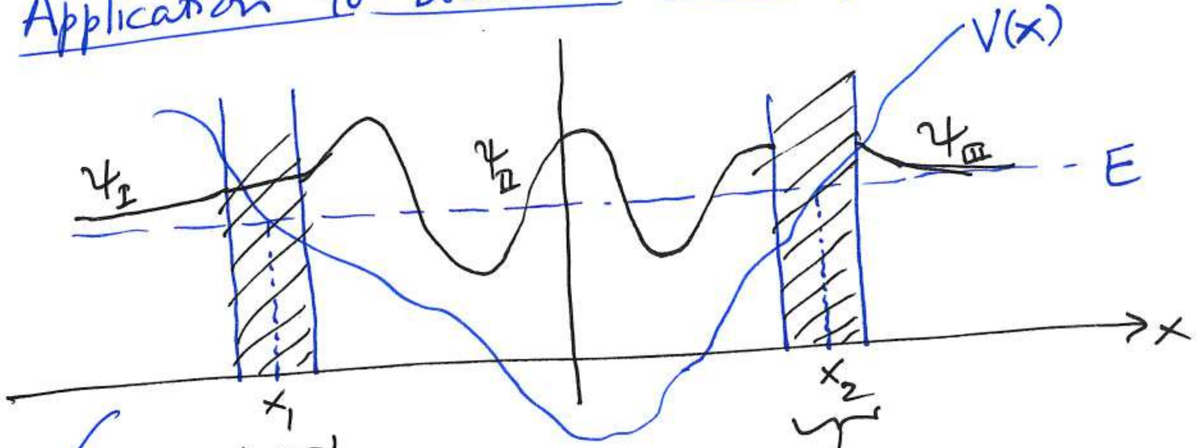
where,

$p(x) \approx \sqrt{2m(E-V(x))}$ due to the semi-classical approximation

and the condition for WKB validity:

$$\frac{1}{2\pi}\left|\frac{d\lambda}{dx}\right| << 1$$

Application to bound state energies & wavefn:



The finite potential well problem

Classical turning points → $\boxed{V(x) \approx E}$

→ point of rebound/reversal of motion classically.

→ Difficult to solve exactly!!

→ $p(x) \to 0$ near the turning points.

→ Using the WKB result in region III / I (~~forbidden~~ classically forbidden):

Taking, $p(x) = \sqrt{2m(E - V(x))}$, $x \in (-\infty, x_1)$

$= i\sqrt{2m(V(x) - E)}$ or $\in (x_2, \infty)$

Taking, $p(x_0) = p(x_0 \to \pm\infty)$ such that

$\psi(x_0)\, p(x_0) \sim \mathbb{1}$ (after taking into account any i factor)

We have,

$$\psi_{III}(x) \sim \frac{1}{(2m[V(x) - E])^{1/2}} \underbrace{\exp\left(-\frac{1}{\hbar}\int^{x} [2m(V(x') - E)]^{1/2} dx'\right)}_{\text{damped particle.}}$$

Illy in region II :

$$\psi_{II}(x) = \frac{A}{[p(x)]^{1/2}} \underbrace{\cos\left[\frac{1}{\hbar}\int p(x')dx' + B\right]}_{\text{oscillating particle}}$$

where we assume two parameters A & B in place of $\psi(x_0)$

→ ~~A~~ Near the turning points : x_1 & x_2, $\psi_{I, II, III}$ are invalid !!

$\because \; p(x) \approx \sqrt{2m(V(x) - E)} \longrightarrow 0 \Rightarrow \frac{1}{[p(x)]^{1/2}} \longrightarrow \infty$!!

$$\Downarrow$$

No longer satisfies the semi-classical requirement that V(x) must be slowly varying.

Therefore, we define transition regions near x_1 & x_2:

→ Assuming slowly varying $V(x)$:

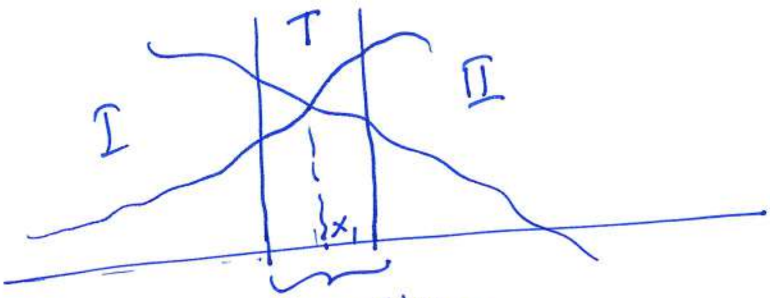
$$V(x) \simeq V(x_1) + V' \cdot (x - x_1) \leftarrow \text{linear approximation.}$$

$$\Rightarrow \boxed{V(x) \simeq E + V' \cdot (x - x_1)}$$

→ With this $V(x)$, the transition region wavefn is found by solving Schroedinger eq.

<u>followed by</u>

matching the boundary conditions b/w transition region(s) and region III/II/I.



$\boxed{\text{H/W}}$ (1) Find the exact soln. $\psi_T(x)$ in this transition region.

(2) Find $\psi_{II}(x)$ by applying the boundary conditions with $\psi_T(x)$.

→ Derived soln:

$$\psi_{II}(x) = \frac{A}{[p(x)]^{1/2}} \cos\left[\frac{1}{\hbar}\int_{x_1}^{x} p(x')\,dx' - \frac{\pi}{4}\right]$$

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Ily at x_2 boundary:

$$\psi_{II}(x) = \frac{A'}{[p(x)]^{1/2}} \cos\left[\frac{1}{\hbar}\int_{x_2}^{x} p(x')\,dx' + \frac{\pi}{4}\right]$$

$$\Rightarrow \quad \boxed{|A| = |A'|}$$

& For the $\cos[\cdots]$ to have the same phase:

$$\frac{1}{\hbar}\int_{x_1}^{x} p(x')\,dx' - \frac{1}{\hbar}\int_{x_2}^{x} p(x')\,dx' - \frac{\pi}{2} = n\pi, \; n=0,1,2,\ldots$$

$$\Rightarrow \frac{1}{\hbar}\left[\left(\int_{x_1}^{x} + \int_{x}^{x_2}\right) p(x')\,dx'\right] = \left(n+\frac{1}{2}\right)\pi, \; n=0,1,2,\ldots$$

$\Rightarrow$

Quantization condition.

$$\boxed{\int_{x_1}^{x_2} p(x')\,dx' = \left(n+\frac{1}{2}\right)\pi\hbar, \; n=0,1,2,\ldots}$$

Or

$$\boxed{\oint p(x')\,dx' = \left(n+\frac{1}{2}\right)2\pi\hbar, \; n=0,1,2,\ldots}$$

$n \to$ even $\Rightarrow A = A'$; $n \to$ odd $\Rightarrow A = -A'$.

→ Energies from WKB method:

Consider a particle moving in $V(x) = k|x|$.

Turning points: $\boxed{x_{1,2} = \pm\frac{E}{k}}$

Quantization condition:

$$\int_{-E/k}^{E/k} [2m(E-k|x|)]^{1/2}\,dx = \left(n+\frac{1}{2}\right)\pi\hbar$$

$$\Rightarrow 2\int_0^{E/k} [2m(E-kx)]^{1/2}\, dx = \left(n+\tfrac{1}{2}\right)\pi\hbar$$

→ Introducing a change of variables:

$$x = \frac{E}{k}y \Rightarrow dx = \frac{E}{k}dy$$

$$\cancel{\Rightarrow 2\int_0^1 (2mE)^{1/2}}$$

$$\Rightarrow 2\int_0^1 (2mE)^{1/2}(1-y)^{1/2}\left(\frac{E}{k}\right) dy = \left(n+\tfrac{1}{2}\right)\hbar\pi$$

$$\Rightarrow (2m)^{1/2}\cdot\frac{1}{k}\cdot E^{3/2}\cdot 2\int_0^1 dy\,(1-y)^{1/2} = \left(n+\tfrac{1}{2}\right)\hbar\pi$$

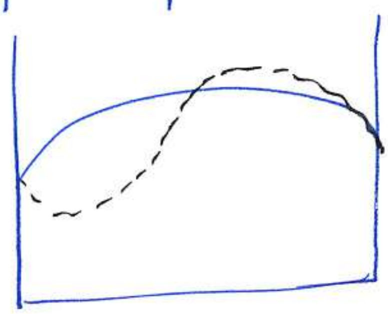
$$\Rightarrow \boxed{E \propto (k)^{2/3}\, m^{-1/3}\left(n+\tfrac{1}{2}\right)^{2/3}\hbar^{2/3}}$$

$$\Rightarrow \boxed{E_n = \left[\frac{3k\hbar\pi}{4(2m)^{1/2}}\left(n+\tfrac{1}{2}\right)\right]^{2/3}}$$

→ Bohr-Sommerfeld quantization rule:

If finite potential wall → infinite potential wall.

⇒ The phase must be s.t.



$$\boxed{\int_{x_1}^{x_2} p(x)\,dx = (n+1)\hbar\pi}$$

Bohr-Sommerfeld quantization rule