W.K.B . Method

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Introduction:

- Generally, the **WKB approximation** or **WKB method** is a method for finding approximate solutions to linear differential equations with spatially varying coefficients.
- In Quantum Mechanics it is used to obtain approximate solutions to the time-independent Schrödinger equation in one dimension.

Applications in Quantum Mechanics

In quantum mechanics it is useful in

1. Calculating bound state energies (Whenever the particle cannot move to infinity)
2. Transmission probability through potential barriers.

These are given in next slides.

Main idea:

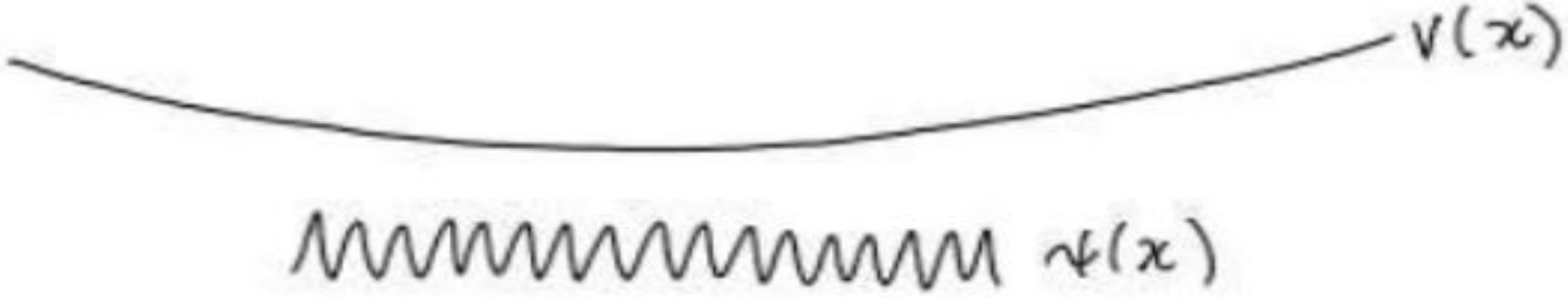
- If **potential $V(x)$ is constant** and energy E of the particle is $\boldsymbol{E > V}$, then the particle wave function has the form
  $\psi(x) = Ae^{\pm ikx}$ where $k = \sqrt{(2m(E-V))}/\hbar$
  (+) sign indicates : particle travelling to right
  (-) sign indicates : particle travelling to left

- General solution : Linear superposition of the two.

- The wave function is oscillatory, with fixed wavelength, $\lambda = \frac{2\pi}{k}$.

- The amplitude (A) is fixed.

- If **V (x) is not constant**, but varies slow in comparison with the wavelength λ in a way that it is essentially constant over many λ, then the wave function is practically sinusoidal, but wavelength and amplitude slowly change with x. **This is the inspiration behind WKB approximation**. In effect, it identifies two different levels of x-dependence :- rapid oscillations, modulated by gradual variation in amplitude and wavelength.



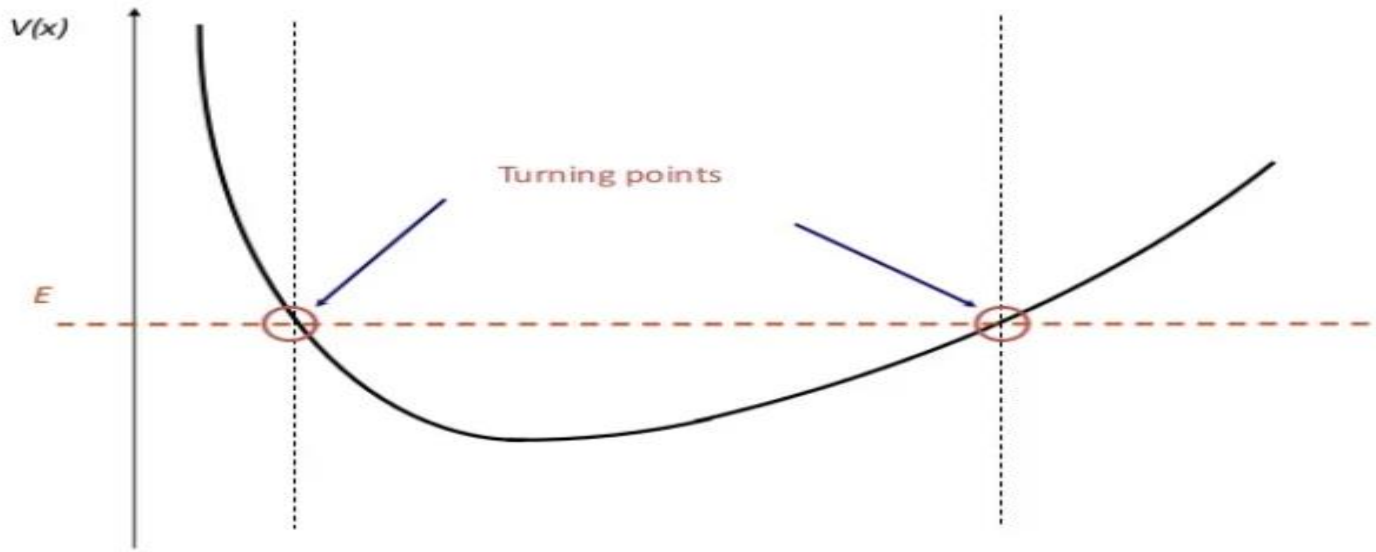
- If **<u>E<V and V is constant</u>**, then wave function is $\psi(x) = Ae^{\pm\kappa x}$ where $\kappa = \sqrt{(2m(V-E))}/\hbar$

If ***<u>V(x) is not constant</u>***, but varies slowly in comparison with $1/\kappa$, the solution remain practically exponential, except that A and κ are now slowly-varying function of x.

Failure of this idea

There is one place where this whole program is bound to fail, and that is in the immediate vicinity of a **classical turning point**, where $E \approx V$. For here $\lambda(or\ ^1/_{\kappa)})$ goes to infinity and $V(x)$ can hardly be said to vary "slowly" in comparison. A proper handling of the turning points is the most difficult aspect of the WKB approximation, though the final results are simple to state and easy to implement. The diagram showing turning points is given in next slide.

The WKB approximation



The Classical Region

- Let's now solve the Schrödinger equation using WKB approximation

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$ can be rewritten in the following way:

$$\frac{d^2\psi}{dx^2} = -\frac{p^2}{\hbar^2}\psi\ ;\quad p(x) = \sqrt{2m(E - V(x))}$$ is the classical formula for the momentum of a particle with total energy E and potential energy $V(x)$. Let’s assume $E > V(x)$, so that $p(x)$ is real. This is the classical region , as classically the particle is confined to this range of x. The classical and non-classical region is shown in the diagram on the next slide.

The WKB approximation

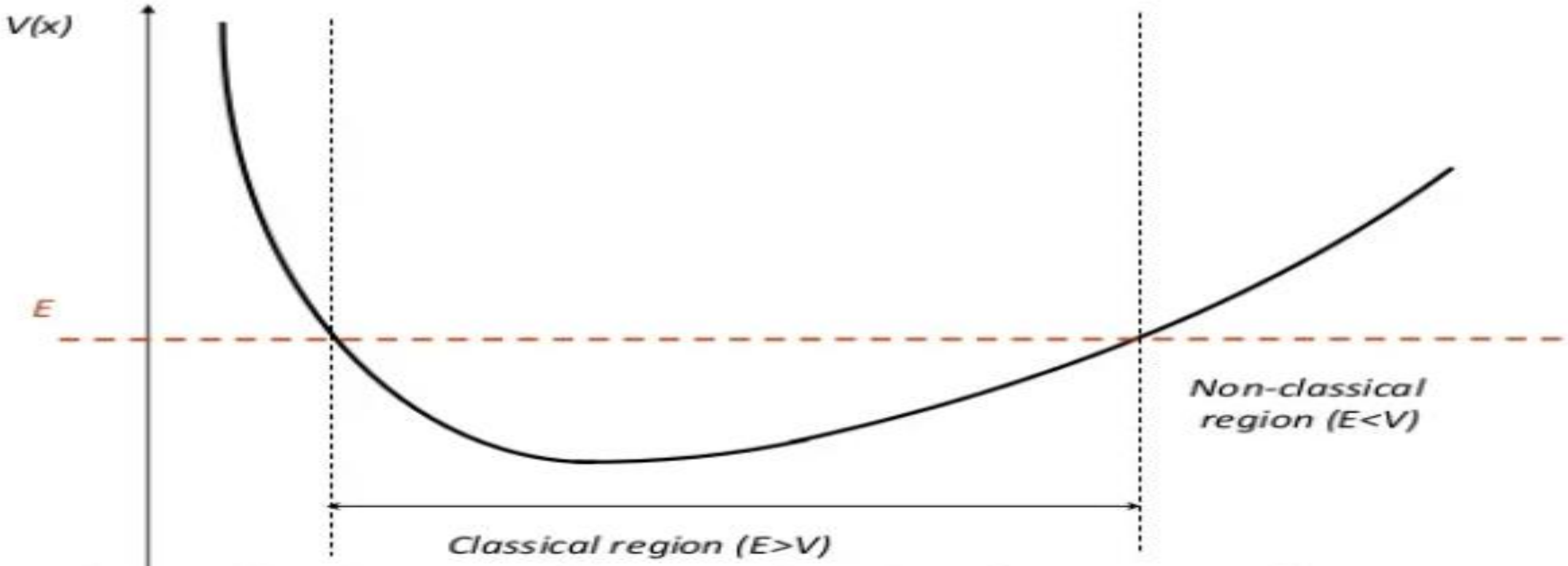


Fig: Classically, the particle is confined to the region where $E \geq V(x)$

The function ψ

In general, ψ is some complex function; we can express it in terms of its amplitude $A(x)$, and its phase, $\phi(x)$ – both of which are real :

$$\psi(x) = A(x)e^{i\phi(x)}$$

Solving the Schrödinger equation

$$\psi(x) = A(x)e^{i\phi(x)}$$

Using prime to denote the derivative with respect to x, we find:

$$\frac{d\psi}{dx} = (A' + iA\phi')e^{i\phi}$$

and

$$\frac{d^2\psi}{dx^2} = [A'' + 2iA'\phi' + iA\phi'' - A(\phi')^2]e^{i\phi}$$

Putting all these into $\frac{d^2\psi}{dx^2} = -\frac{p^2}{\hbar^2}\psi$ (From Schrödinger equation) , we get

$$A'' + 2iA'\phi' + iA\phi'' - A(\phi')^2 = -\frac{p^2}{\hbar^2}A$$

Solving for real and imaginary parts we get,

$$A'' - A(\phi')^2 = -\frac{p^2}{\hbar^2}A$$

$$\Longrightarrow \quad A'' = A\left[(\emptyset')^2 - \frac{p^2}{\hbar^2}\right]$$

$$\Longrightarrow \quad \frac{A''}{A} = \left[(\emptyset')^2 - \frac{p^2}{\hbar^2}\right]$$

The above equation cannot be solved in general, so we use WKB approximation: we assume amplitude A varies slowly, so that the A'' term is negligible. We assume that $A''/_A << [(\emptyset')^2 - \frac{p^2}{\hbar^2}]$.

Therefore, we drop that part and we get

$$\phi(x) = \pm\frac{1}{\hbar}\int p(x)dx$$

And from second equation, we get

$$2A'\phi' + A\phi'' = 0$$

$$\implies \quad (A^2\phi')' = 0$$

$$\implies \quad A = \frac{C}{\sqrt{\phi'}}$$

Where C is real constant.

Thus from the previous slides from the equations and making 'C' a complex constant, we get

$$\psi(x) \cong \frac{C}{\sqrt{p(x)}} e^{\pm\frac{i}{\hbar}\int p(x)dx}$$

And the general solution can be written as

$$\psi(x) \cong \frac{1}{\sqrt{p(x)}}\left[C_1 e^{\frac{i}{\hbar}\int p(x)dx} + C_2 e^{\frac{-i}{\hbar}\int p(x)dx}\right]$$

where C_1 and C_2 are constants.