WKB Approximation

The WKB approximation is a method for obtaining approximate solution of one - dimensional schrodinger equation or wave equation which can be separated into equations of each of which contains only single independent variable. It is based on the expansion of wave function in powers of $\hbar$. This method is applicable especially when the potential is slowly varying.

The WKB Method

The one - dimensional Schrodinger equation of a particle moving in a region of constant potential V_0 is

$$\frac{d^2\Psi}{dx^2} + k^2\Psi = 0 \quad \rightarrow (1)$$

Where $k^2 = 2m\,\frac{E-V_0}{\hbar^2}$

Its solution is $\Psi = e^{\pm ikx} \quad \rightarrow (2)$

If the potential is not constant, k in equ (1) is a function of x given by

$$k^2 = 2m\,\frac{E-V(x)}{\hbar^2} \quad \rightarrow (3)$$

For convenience we shall assume that E > V(x). Writing the solution of Schrodinger equation in the following form and substituting in Equ (1)

We get

$$\Psi = \exp\left(\frac{i}{\hbar}\,S(x)\right) \quad \rightarrow (4)$$

$$\left(\frac{ds}{dx}\right)^2 - i\hbar\,\frac{d^2s}{dx^2} - k^2\hbar^2 = 0 \quad \rightarrow (5)$$

The solution of the equation gives the form of the function S(x). Expanding S(x) in powers of $\hbar$, we get

$$S(x) = S_0(x) + S_1(x)\hbar + S_2(x)\frac{\hbar^2}{2} + \ldots \rightarrow (6)$$

Substituting (6) in Equ (5) and retaining terms up to $\hbar$, we get

$$\left(\frac{ds_0}{dx}\right)^2 - k^2\hbar^2 + \left(2\frac{dS_0}{dx}\frac{dS_1}{dx} - i\frac{d^2s_0}{dx^2}\right)\hbar = 0 \quad \rightarrow (7)$$

The term $-k^2\hbar^2$ is included with the term independent of $\hbar$, since

$$k^2\hbar^2 = 2m\frac{[E-V(x)]\hbar^2}{\hbar^2} = 2m[\text{ E-V(x) }]$$

For Equ (7) to be valid, the coefficient of each power of $\hbar$ must vanish separately. Then

$$\left(\frac{ds_0}{dx}\right)^2 - k^2\hbar^2 = 0 \quad \text{or} \quad \frac{ds_0}{dx} = \pm k\hbar \quad \rightarrow (8)$$

And

$$2\frac{dS_0}{dx}\frac{dS_1}{dx} - i\frac{d^2s_0}{dx^2} = 0 \quad \rightarrow (9)$$

For better results one has to include the terms in $\hbar$ also. Integration of Equ (8) and (9) gives $S_0(x)$ and $S_1(x)$. It follows from Equ (8)

$$S_0(x) = \pm \int k\hbar \, dx = \pm \int (2m[\text{ E} - \text{V(x) }])^{1/2} \, dx \quad \rightarrow (10)$$

With this value of $S_0(x)$. Equ (9) becomes

$$\frac{dS_1}{dx} = \frac{i}{2k}\frac{dk}{dx} \quad \rightarrow (11)$$

Integrating, we get

$$S_1 = \frac{i}{2}\ln k \text{ or } i\,s_1 = \ln k^{-1/2} \text{ or } \exp(iS_1) = k^{-1/2} \rightarrow (12)$$

Restricting to two terms in Equ (6) , it follows Eqs (4), (6) and (12) that

$$\Psi = A\exp\left(\frac{i}{\hbar}S_0\right)\exp(iS_1) = \frac{A}{K^{1/2}}\exp\left(\pm i\int k dx\right) \rightarrow (13)$$

Where A is a constant and k is given by (13). The general solution will be linear combination of two terms, one with each sign. The wavevector k is real and therefore the solution is oscillatory. The probability density.

$$\Psi\Psi^* = \frac{|A|^2}{k}\exp\left(\pm i\int k dx\right)\exp\left(\mp i\int k dx\right) = \frac{|A|^2}{k} \quad \rightarrow (14)$$

As p = kℏ, the probability density is inversely proportional to the velocity . This is understandable because classically the time spent by a particle in a region is inversely proportional to the velocity.

In quantum mechanics, particles can even penetrate classically disallowed regions and therefore we have to consider the case E < V(x).

For E < V(x), the basic equation is

$$\frac{d^2\Psi}{dx^2} - \gamma^2\Psi = 0 , \qquad \gamma^2 = 2m\frac{[E-V(x)]}{\hbar^2} \rightarrow (15)$$

Proceeding in the same fashion, the solution of Equ (15) can be written as

$$\Psi = \frac{B}{\gamma^{1/2}} \exp\left(\pm \int \gamma dx\right)$$

Where B is a constant. The most general solution is a linear combination of the two terms, one with each sign. One term is an exponentially decreasing one. At this stage, we cannot leave E < V(x) is usually finite extent. When E ≅ V(x), both the quantities k and γ tens zero. Consequently Ψ goes to infinity and the approximation fails. The point at which E = V(x) is called classical turning point, since at this point a classical particle would stop and begin to move in the opposite direction.