WKB Approximation Explained

- The Wentzel-Kramers-Brillouin (WKB) approximation is a “semiclassical calculation” in quantum mechanics in which the wavefunction is assumed an exponential function with amplitude and phase that slowly varies compared to the de Broglie wavelength, λ, and is then semiclassically expanded
- While Wentzel, Kramers and Brillouin developed this approach in 1926, earlier in 1923 Harold Jeffreys had already developed a more general method of approximating linear, second-order differential equations (the Schrodinger equation is a linear second order differential equation)

WKB Approximation Explained, Cont'd

- While technically this is an "Approximate Method" not an "Exact solution" to the Schrodinger equation, it is very close to simple plane wave solutions that we discussed thile describing transmission coefficient calculation in piece-wise constant potential barriers
- The WKB method is most often applied to 1D problems but can be applied to 3D Spherically Symmetric problems as well (see Bohm 1951)
- The WKB approximation is especially useful in deriving the tunnel current in a tunnel diode

Basic Idea of the Method

- The WKB approximation states that since in a constant potential, the wavefunction solutions of the Schrodinger equation are of the form of simple plane waves, then

$$\psi(x) = Ae^{\pm ikx}, \quad k = 2\pi / \lambda = \sqrt{\frac{2m(E-U)}{\hbar^2}}$$

- Now, if the potential U=U(x) changes slowly with x, the solution of the Schrodinger equation can also be written of the general form

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

where $\phi(x)=xk(x)$.

\- For the **constant potential case**, $\phi(x)=\pm kx$ so the phase changes linearly with x

\- In a **slowly varying potential** $\phi(x)$ should vary slowly from the linear case $\pm kx$

Basic Idea of the Method, Cont'd

- For the two cases, E>U and E<U, let k(x) be defined as (so we only have to solve the problem once)

$$k(x) = \sqrt{\frac{2m(E - U(x))}{\hbar^2}}, \qquad E > U(x)$$

$$k(x) = -i\sqrt{\frac{2m(U(x) - E)}{\hbar^2}} = -i\kappa(x), \quad E < U(x)$$

Wentzel-Kramers-Brillouin (WKB) Approximation

- Starting from the 1D Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x)+U(x)\psi(x)=E\psi(x)$$

- And substituting the general solution for slowly-varying potentials, one gets the following differential equation

$$i\frac{\partial^2\phi}{\partial x^2}-\left(\frac{\partial\phi}{\partial x}\right)^2+k^2(x)=0$$

Wentzel-Kramers-Brillouin (WKB) Approximation

- The WKB approximation assumes that the potentials are slowly varying in space
- Then the 0^{th} order approximation assumes

$$\frac{\partial^2 \phi}{\partial x^2} = 0, \quad \frac{\partial \phi_0}{\partial x} = \pm k(x) \rightarrow \phi_0(x) = \pm \int k(x)dx + C_0$$

$$\rightarrow \psi(x) = \exp\left[\pm i \int k(x)dx + C_0 \right]$$

Wentzel-Kramers-Brillouin (WKB) Approximation

- If a higher order solution is required, then we solve

$$i\frac{\partial^2\phi}{\partial x^2}-\left(\frac{\partial\phi}{\partial x}\right)^2+k^2(x)=0\rightarrow\frac{\partial\phi}{\partial x}=\pm\sqrt{k^2(x)+i\frac{\partial^2\phi}{\partial x^2}}$$

- Then the 1th order approximation assumes

$$\frac{\partial\phi}{\partial x}=\pm\sqrt{k^2(x)\pm i\frac{\partial k}{\partial x}}$$

$$\rightarrow\psi(x)=\exp\left[\pm i\int\sqrt{k^2(x)\pm i\frac{\partial k}{\partial x}}dx+C_1\right]$$

Wentzel-Kramers-Brillouin (WKB) Approximation

1. In order to apply the WKB approximation we only need to know the shape of the potential since

$$U(x) \to k(x) \to \phi(x) \to \psi(x) = \exp\left[\pm \int \sqrt{k^2(x) \pm i \frac{\partial k}{\partial x}} dx + C_1 \right]$$

2. For slowly varying $U(x)$ the first order and the zero order approximation give almost the same result as

$$\left| \frac{\partial}{\partial x} k(x) \right| << \left| k^2(x) \right|$$

Wentzel-Kramers-Brillouin (WKB) Approximation

3. The WKB approximation breaks down where E~U (classical turning points) in which case the wavevector k(x) approaches zero but the derivative does not and there in fact the argument in (2) does not hold

$$\left|\frac{\partial}{\partial x} k(x)\right| << \left|k^2(x)\right|$$

Under these circumstances, connection formulas must be applied to tie together regions on each side of the classical turning point.

Example 1: Tunneling probability of potential barrier with length L and height U

We consider the case E<U for tunneling to occur.

$$k(x) = -i\sqrt{\frac{2m(U-E)}{\hbar^2}} \rightarrow \psi(x) = \exp\left[\mp i^2\sqrt{\frac{2m(U-E)}{\hbar^2}}x\right] = \exp\left[-\sqrt{\frac{2m(U-E)}{\hbar^2}}x\right]$$

$$T = \frac{\psi^*(L)\psi(L)}{\psi^*(0)\psi(0)} = \exp\left[-2L\sqrt{\frac{2m(U-E)}{\hbar^2}}\right]$$