III.5 The WKB APPROXIMATION

* Recall: If a wave fct. $\psi(\vec{r},t) = C e^{\frac{i}{\hbar} S_{qu}(\vec{r},t)}$ is entirely written in terms of a quantum phase S_{qu} this phase obeys a "quantum" Hamilton - Jacobi equation

$$\frac{\partial S_{qu}}{\partial t} + \frac{1}{2m}\left[(\nabla S_{qu})^2 - i\hbar \Delta S_{qu}\right] + V = 0$$

(see I.5.4)

* For stationary states (energy eigenstates) with energy E we can make the ansatz $\qquad S_{qu}(\vec{r},t) = \hbar u(\vec{r}) - Et$

The phase $u(\vec{r})$ then satisfies the equation

$$i\Delta u - (\nabla u)^2 + k^2(\vec{r}) = 0 \qquad (*)$$

where the real or imaginary wave vector function is

$$k(\vec{r}) = \begin{cases} \sqrt{\frac{2m}{\hbar^2}(E - V(\vec{r}))} & \text{if } E > V(\vec{r}) \\ -i\sqrt{\frac{2m}{\hbar^2}(V(\vec{r}) - E)} & \text{if } E < V(\vec{r}) \end{cases}$$

* We now find approximate solutions to $(*)$

Here: 1-D version.

* If the potential $V(x)$ is varying slowly we expect the second derivative of u to be small:

$$iu'' - (u')^2 + k^2 = 0 \xrightarrow[0^{th}\text{ order}]{} (u_0')^2 = k^2$$

$$\Rightarrow \quad u_0(x) = \pm \int^x k(x')\,dx' + C$$

Recursion: use u_0 in approximation for u'': $u'' \to u_0'' = \pm k'$

$$iu'' - (u')^2 + k^2 = 0 \xrightarrow[1^{st}\text{ order}]{} (u_1')^2 = k^2 \pm ik'$$

$$\Rightarrow \quad u_1(x) = \pm \int^x \sqrt{k(x')^2 \pm ik'(x')}\,dx' + C' \qquad (***)$$

* The recursion step only makes sense if $|k'(x)| \ll k^2(x)$ $\qquad (**)$

Physically: the change of wave length $\frac{d\lambda}{dx} \ll 1$ has to be small over a distance λ $\quad \left(\lambda(x) = \frac{2\pi}{k(x)}\right)$

But if $(**)$ is true we can expand the square root in $(***)$:

$$u_1(x) \approx \pm \int^x k(x')\,dx' + \frac{i}{2} \ln k(x) + C$$

$\Rightarrow$ The approximate wave fct given by this phase is

$$\psi(x) \approx \frac{1}{\sqrt{k(x)}}\, e^{\pm \int^x k(x')\,dx'} \qquad \text{(modulo normalization)}$$

This is called the WKB (Wentzel, Kramers, Brillouin) approximation.

for $E > V(x)$ the approx. solutions correspond to left-/right travelling waves.

For $E < V(x)$, the classically forbidden region

$$\psi(x) = \frac{1}{\sqrt{\kappa(x)}} \, e^{\pm \int^x \kappa(x')dx'}$$

with $\kappa(x) = \sqrt{\frac{2m}{\hbar^2}(V-E)}$

* Interestingly the condition (**) excludes classical turning points $V(x) \approx E$, i.e. WKB is not valid in their vicinity.

~~(The WKB solutions mathematically diverge)~~

One can however merge solutions valid for $E \gg V(x)$ and $E \ll V(x)$ with a matching technique.

See Merzbacher pp116 or HW

* Examples and applications: Merzbacher or HW