THE WENTZEL, KRAMERS, BRILLOUIN APPROXIMATION

Let us now move back to 1-D quantum mechanics to investigate a very useful approximation scheme: the WKB approximation.

The basic idea is the following: let us imagine to have a particle of energy E moving in a region where the potential $V(x)$ is constant. The solution is easy:

$$\psi(x) = Ae^{\pm i\kappa x} \quad , \quad \kappa = \sqrt{2m(E-V)/\hbar^2}$$

If $V(x)$ is almost constant, we can reasonably suppose that ψ remains a sinusoidal function, but its amplitude and wavelength may change.

This approximation works in the so-called semi-classical limit. Let us take a quantum oscillator. For small values of n, we cannot neglect the quantum nature of the $|n\rangle$ wavefunctions. As n increases, though, the De Broglie wavelength of a particle becomes so small that we can neglect it: we reach the classical limit (as opposed to the quantum limit, when n is small).

In the semi-classical limit, we have a bit of both quantum and classical aspects.

The WKB approximation is good for:

1) estimating eigenenergies in the semi-classical limit for complicate 1-D potential functions $V(x)$
2) estimating tunnelling rates though complicate barriers

Then, the basic idea is to find solutions of Schroedinger equation in the form of modulated waves:

$$\psi(x) = A(x)\, e^{i\phi(x)} \qquad \phi(x) = \kappa(x)\cdot x$$

we are assuming that $V(x)$ does not change much over the wavelength $\dfrac{2\pi}{\kappa(x)}$ of the particle.

Let us put this ansatz in Schroedinger equation, after making a small substitution:

$$p(x) = \sqrt{2m(E - V(x))} \Longrightarrow \text{Schroedinger equation becomes } \frac{d^2\psi}{dx^2} = -\frac{p^2}{\hbar^2}\psi$$

$$\frac{d^2\left(A(x)e^{i\phi(x)}\right)}{dx^2} = A''(x)e^{i\phi(x)} + 2iA'\phi'e^{i\phi} + iA\phi''e^{i\phi} - A(\phi')^2e^{i\phi} \underset{\uparrow}{=} -\frac{p^2}{\hbar}Ae^{i\phi}$$

$$\parallel \quad \frac{d}{dx}\left(A'e^{i\phi(x)} + iA\phi'e^{i\phi}\right) \qquad \qquad \text{Schroedinger equation}$$

This is equivalent to two real equations:

$$\begin{cases} A'' - A\phi'^2 = -\frac{p^2}{\hbar}A \\ 2A'\phi' + A\phi'' = 0 \end{cases} \quad \text{rewritten:} \quad \begin{cases} A'' = A\phi'^2 - \frac{p^2}{\hbar^2}A & (1) \\ \frac{d}{dx}\left(A^2\phi'\right) = 0 & (2) \end{cases}$$

(2) is easy to solve:

$$A(x) = \frac{\text{constant}}{\sqrt{\phi'(x)}} \quad \leftarrow \text{note: } \phi'(x) = \frac{d\phi}{dx}$$

(1) is not easy. In fact, in general it cannot be solved. But we can use the fact that $V(x)$ changes slowly, and therefore also $A(x)$ changes slowly over the scale of a wavelength. Then, after dividing by A, (1) becomes:

$$\phi'^2 = +\frac{p^2}{\hbar^2} \Longrightarrow \phi' = \frac{d\phi}{dx} = \pm\frac{p}{\hbar} \Rightarrow \phi(x) = \pm\frac{1}{\hbar}\int p(x)\,dx$$

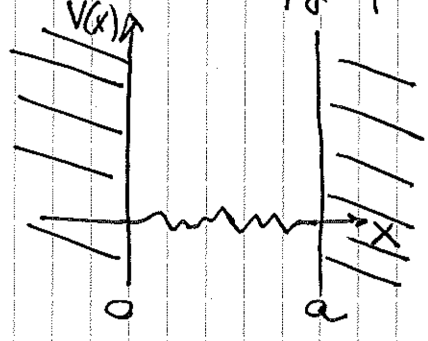
My wavefunction, in the WKB approximation, becomes:

$$\boxed{\psi(x) \simeq \frac{C}{\sqrt{p(x)}}\, e^{\pm\frac{i}{\hbar}\int^x p(x')dx'}} \qquad (C \text{ could be complex number})$$

Note that $|\psi(x)|^2 \simeq \frac{|C|^2}{p(x)}$, where $p(x)$ is the classical momentum. This makes sense: the particle spends less time where it moves fast, so the probability of being found in those points is small.

Therefore, in the semi-classical limit, the probability density is maximal at the classical <u>turning points</u>, where $p = \sqrt{2m(E - V(x))} = 0$. The fact that $|\psi(x)|^2 \to \infty$ at those points suggests that we have some work to do...

Let us first look at an easy, classical (pardon the pun) example: particle in a 1-D bumpy quantum well.



semi-classical limit:
assume $E > V(x)$
everywhere in well

$$\psi_{WKB}(x) = \frac{C_+}{\sqrt{p(x)}} e^{i\phi(x)} + \frac{C_-}{\sqrt{p(x)}} e^{-i\phi(x)} \overset{\text{more convenient}}{=} \frac{1}{\sqrt{p(x)}}\left[C_1 \sin\phi(x) + C_2 \cos\phi(x)\right]$$

The boundary conditions require $\psi_{WKB}(0) = \psi_{WKB}(a) = 0$. In other words:

$$C_2 = 0$$

$$\sin(\phi(a)) = 0 \implies \phi(a) = \frac{1}{\hbar}\int_0^a \sqrt{2m(E_n - V(x))}\, dx = n\pi$$

I replaced E with E_n because its value depend on n, on the right-hand side of the equation. It shall be noted that there exist a minimum value that n can assume: n should start at the first eigennumber that enters the semi-classical limit. This value depends on the problem. Let us consider the case $V(x) = 0$. The integral becomes easy:

$$\frac{1}{\hbar}\underbrace{\int_0^a dx \sqrt{2mE}}_{\sqrt{2mE}\cdot a/\hbar} = n\pi \implies E_n = \frac{\pi^2 \hbar^2 n^2}{2ma^2}$$

This is our good old result. It is reasonable, albeit not too elegant, to consider it valid also for very small n, pointing out that $V(x) = 0$ means that the potential changes on an infinite length scale.