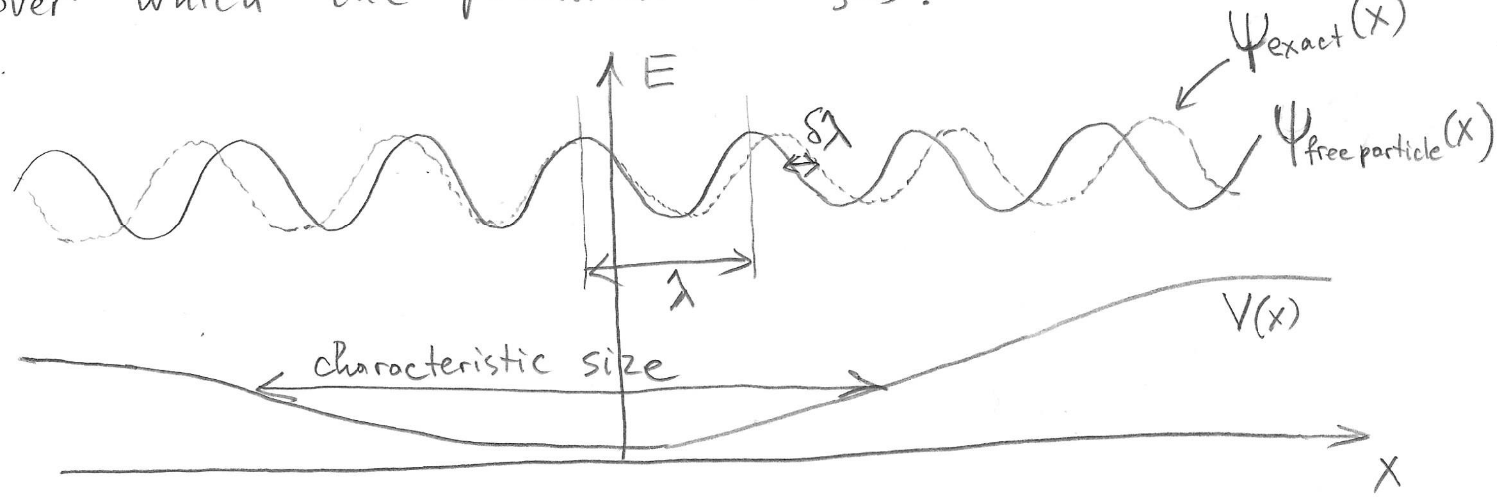
The WKB (Wentzel-Kramers-Brilloin) approximation

Quantum probability density approaches the classical one in the limit of large quantum numbers (recall the harmonic oscillator, for which we solved for the classical probability density and compared it with the quantum one for large n). The states that correspond to large quantum numbers have many rapid spatial oscillations. Equivalently, we may say that in this classical domain the local quantum (de Broglie) wavelength is small compared to the characteristic size of the system (or the size of its "features"). For example, in the case of a harmonic oscillator the characteristic distance may be taken as typical length over which the potential changes.



The change in wavelength accumulated over distance δx is:

$$\delta\lambda = \frac{d\lambda}{dx}\delta x$$

The change in wavelength over one oscillation period (i.e. over the distance of one wavelength) is

$$\delta\lambda = \frac{d\lambda}{dx}\lambda$$

In the classical limit $\delta\lambda \ll \lambda$, so

$$\left|\frac{\delta\lambda}{\lambda}\right| = \left|\frac{d\lambda}{dx}\right| \ll 1$$

If we now consider the classical momentum we find

$$\frac{p^2}{2m} + V(x) = E \qquad p = \sqrt{2m(E-V)}$$

$$\lambda = \frac{\hbar}{p} = \frac{\hbar}{\sqrt{2m(E-V)}} \qquad \frac{d\lambda}{dx} = -\frac{1}{2}\frac{\hbar}{[2m(E-V)]^{3/2}}\left(-2m\frac{dV}{dx}\right) = \frac{\hbar m}{p^3}\frac{dV}{dx}$$

Thus, the condition for nearly classical behavior becomes

$$\left|\frac{\delta\lambda}{\lambda}\right| = \left|\frac{m\hbar}{p^3}\frac{dV}{dx}\right| \ll 1$$

The WKB method provides a recipe for an approximate solution of the Schrödinger equation that is valid in the near-classical domain (defined above). It should be noted that the WKB method is a general mathematical approach that can be applied to any ordinary differential equation of order n with spatially varying coefficients and where the highest derivative is multiplied by a small parameter, ε:

$$\varepsilon\frac{d^n f}{dx^n} + a(x)\frac{d^{n-1}f}{dx^{n-1}} + b(x)\frac{d^{n-2}f}{dx^{n-2}} + \dots + c(x)f = 0$$

The solution is sought in the form

$$f \approx \exp\left[\frac{1}{\delta}\sum_{n=0}^{\infty}\delta^n S_n(x)\right] \qquad \text{where } \delta \to 0$$

By substituting this expression into the original equation we can solve (in principle) for an arbitrary number of terms $S_n(x)$ in the expansion

The WKB method is often used for semi-classical calculations in quantum mechanics. In the case of the Schrödinger equation the WKB expansion is introduced as follows.

Suppose $V(x)$ is slowly varying. Then we expect the wave function to be closely approximated by the free-particle solution:

$$\varphi(x) = Ae^{ikx} = Ae^{\frac{ipx}{\hbar}}$$

So we may look for the solution in the form

$$\varphi(x) = Ae^{\frac{iS(x)}{\hbar}}$$

Substituting $\varphi(x)$ into the Schrödinger equation yields

$$\frac{d\varphi}{dx} = Ai\frac{dS}{dx}e^{\frac{iS}{\hbar}} \qquad \frac{d^2\varphi}{dx^2} = A\left[\frac{i}{\hbar}\frac{d^2S}{dx^2}e^{\frac{iS}{\hbar}} - \frac{1}{\hbar^2}\left(\frac{dS}{dx}\right)^2 e^{\frac{iS}{\hbar}}\right]$$

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2} + V(x)\varphi = E\varphi \Rightarrow -\hbar^2\frac{d^2\varphi}{dx^2} = \underbrace{2m\left[E - V(x)\right]}_{p^2(x)}\varphi$$

$$-i\hbar\frac{d^2S}{dx^2} + \left(\frac{dS}{dx}\right)^2 = p^2(x)$$

Let us now examine the solutions to the last (nonlinear) equation in the limit $\hbar \to 0$. We represent $S(x)$ by a power series:

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

$$-i\hbar\left(\frac{d^2S_0}{dx^2} + \hbar\frac{d^2S_1}{dx^2} + \frac{\hbar^2}{2}\frac{d^2S_2}{dx^2} + \dots\right) + \left(\frac{dS_0}{dx} + \hbar\frac{dS_1}{dx} + \frac{\hbar^2}{2}\frac{dS_2}{dx} + \dots\right)^2 - p^2(x) = 0$$

Collecting terms by the same power of $\hbar$ gives:

$$\left[\left(\frac{dS_0}{dx}\right)^2 - p^2\right] + \hbar\left[2\frac{dS_0}{dx}\frac{dS_1}{dx} - i\frac{d^2S_0}{dx^2}\right] + \hbar^2\left[\frac{dS_0}{dx}\frac{dS_2}{dx} + \left(\frac{dS_1}{dx}\right)^2 - i\frac{d^2S_1}{dx^2}\right] + O(\hbar^3) = 0$$

Since this equation must be satisfied for small but otherwise arbitrary $\hbar$, it is necessary that the coefficient by each power of $\hbar$ vanishes. With that we get:

$$\hbar^0 : \quad \left(\frac{dS_0}{dx}\right)^2 = p^2$$

$$\hbar^1 : \quad \frac{dS_0}{dx}\frac{dS_1}{dx} = \frac{i}{2}\frac{d^2S_0}{dx^2}$$

$$\hbar^2 : \quad \frac{dS_0}{dx}\frac{dS_2}{dx} + \left(\frac{dS_1}{dx}\right)^2 - i\frac{d^2S_1}{dx^2} = 0$$

$$\vdots$$

Integrating the first equation above gives:

$$\frac{dS_0}{dx} = \pm p \qquad S_0 = \pm\int_{x_0}^{x} p(x)\,dx$$

or

$$\frac{S_0}{\hbar} = \pm\int_{x_0}^{x} k(x)\,dx \qquad k = \frac{p(x)}{\hbar}$$

Then we can solve the second equation:

$$k\frac{dS_1}{dx} = \frac{i}{2}\frac{dk}{dx} \qquad \frac{dS_1}{dx} = \frac{i}{2}\frac{d}{dx}\ln k \qquad S_1 = \frac{i}{2}\ln\frac{k}{\varkappa}$$

where $\varkappa$ is an integration constant. We can also write that

$$e^{iS_1} = \frac{\varkappa^{1/2}}{k^{1/2}}$$

Next we can proceed to the equation for S_2 if we need to. However in the near-classical domain the contribution of terms proportional to $\hbar^2, \hbar^3, \hbar^4, \ldots$ to $S(x)$ is progressively smaller. Hence if we limit ourselves with S_0 and S_1 only we end up with

$$\varphi(x) = \frac{A}{[k(x)]^{1/2}}\exp\left[i\int k(x)\,dx\right] + \frac{B}{[k(x)]^{1/2}}\exp\left[-i\int k(x)\,dx\right]$$

or

$$\varphi(x) = \frac{C_+ \exp\left[\frac{\sqrt{2m}}{\hbar}\int\sqrt{V(x)-E}\,dx\right] + C_- \exp\left[-\frac{\sqrt{2m}}{\hbar}\int\sqrt{V(x)-E}\right]}{\left[V(x)-E\right]^{1/4}}$$

In order to see how the above solution approximates classical behavior we will consider the probability density $|\varphi(x)|^2$. More specifically, let us consider the case when the momentum of the particle is specified and the particle moves in the positive x-direction. Then the WKB solution becomes

$$\varphi = \frac{A}{k^{1/2}} \exp\left[i\int k(x)\,dx\right]$$

and

$$|\varphi|^2 = \frac{|A|^2}{k} = \frac{|A|^2 \frac{\hbar}{m}}{v} \qquad \text{where} \quad v = \frac{p}{m}$$

This result, apart from a multiplicative constant, is the same as the classical probability density, which is inversely proportional to the velocity. Thus, as we can see, the lowest order WKB solution reproduces the classical probability.