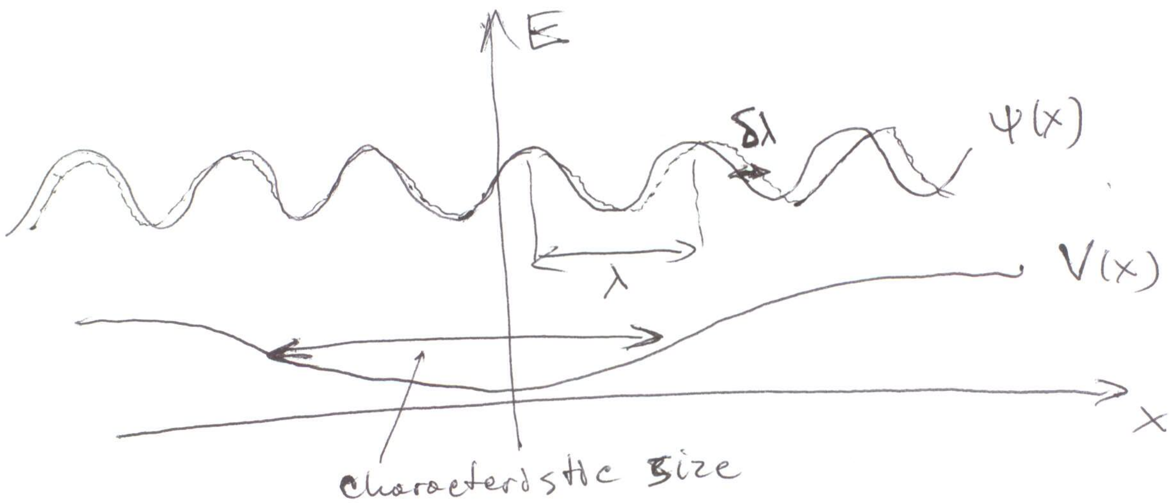
The WKB (Wentzel-Kramers-Brilloin) approximation

Quantum probability density approaches the classical probability density in the limit of large quantum numbers (recall the harmonic oscillator, for which we solved for classical probability density last semester). 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 it "features"). For example, for the harmonic oscillator the characteristic lenght scale is given by the maximum displacement (or amplitude). More generally, this characteristic distance may be taken as the typical length over which the potential changes



$$\delta\lambda = \frac{d\lambda}{dx}\delta x$$ ← the charge in wavelength over distance x

$$\delta\lambda = \frac{d\lambda}{dx}\lambda$$ ← the charge in wavelength over one wavelength

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 momentum we find

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

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

$$= \frac{hm}{p^3}\frac{dV}{dx}$$

Thus, the condition for nearly classical behavior becomes

$$\left|\frac{\delta\lambda}{\lambda}\right| = \left|\frac{mh}{p^3}\frac{dV}{dx}\right| << 1$$

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 shoud be noted that the WKB method is a general mathematical approach that can be applied to any differential equation of order n with spatially varying coefficients and where the highest derivative is multiplied by a small parameter, ε:

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

The solution is sought in the form

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

By sustituting this expression into the original equation we can in principle solve 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 closely approximate the free-particle solution:

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

So we may look for solutions in the form

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

Substitution of $\varphi(x)$ into the Schrödinger equation yields

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

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

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

Let us now examine the solutions to the last (nonlinear) equation in the limit $\hbar \to 0$. We repre-sent $S(x)$ as 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 $\hbar$:

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

Since this equation must be satisfied for small but otherwise arbitrary $\hbar$ it is necessary that the coeffi-cient by each power of $\hbar$ vanish. With that we set:

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

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

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

and so on. Integrating the first equation above gives:

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

Plugging this solution into the equation for $\hbar^1$ and integrating gives:

$$S_1 = \frac{i}{2}\ln\left(\frac{dS_0}{dx}\right) = \frac{i}{2}\ln \hbar k$$

or

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

Substituting S_0 and S_1 into the equation for $\hbar^2$ gives (after integration)

$$S_2 = \frac{1}{2}\frac{m}{p^3}\frac{dV}{dx} - \frac{1}{4}\int\frac{m^2}{p^5}\left(\frac{dV}{dx}\right)^2 dx$$

Comparison of S_2 with the criterion established previously, $\left|\frac{m\hbar}{p^3}\frac{dV}{dx}\right| \ll 1$, shows that in near-classical domain the contribution of $\frac{\hbar^2 S_2}{2}$ to the phase of function φ is small compared to unity. The same takes place to higher-order contributions to $S(x)$. Thus, we can limit ourselves with S_0 and S_1 only, in which case

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

or

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

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

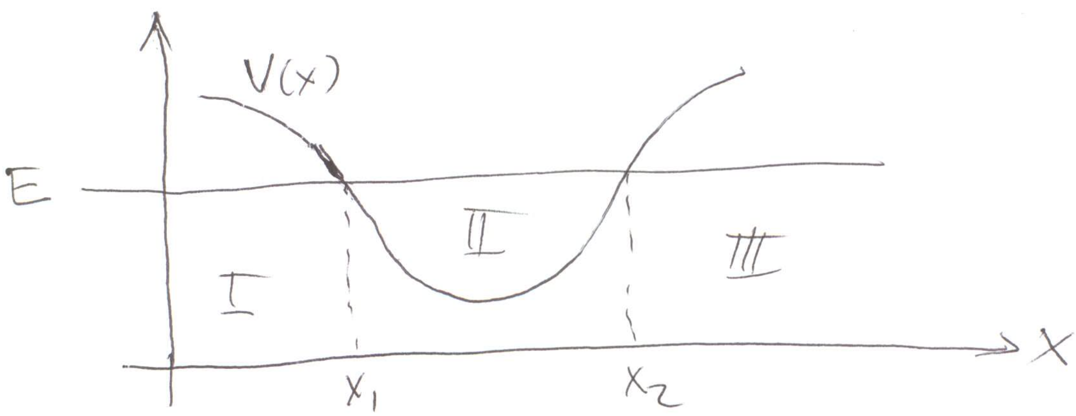
$$\varphi = \frac{A}{k^{1/2}} \exp\left[i\int k(x)\,dx\right]$$

and

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

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

Now let us investigate how we can apply the WKB solution to the bound states



The WKB solution is invalid at the classical turning points x_1 and x_2 for at these points $E=V$ and $\hbar k=0$. Hence, the criterion $\left|\frac{m\hbar}{p^3}\frac{dV}{dx}\right| \ll 1$ is violated. The WKB solution becomes valid in regions far from x_1 and x_2, where $|E-V|$ is large

$$\mathrm{I}: \quad \varphi_{\mathrm{I}} = \frac{A}{\sqrt{k}} \exp\left[\int_{x_1}^{x} \varkappa \, dx \right] \qquad \frac{\hbar^2 \varkappa^2}{2m} = V-E > 0$$

$$\mathrm{III}: \quad \varphi_{\mathrm{III}} = \frac{A}{\sqrt{k}} \exp\left[-\int_{x_2}^{x} \varkappa \, dx \right] \qquad \frac{\hbar^2 \varkappa^2}{2m} = V-E > 0$$

In the classically allowed region the WKB solution is not exponentially decaying, but oscillatory. We separate φ_{II} into two cases:

$$\varphi_{\mathrm{II}}^{-}(x) = \frac{C}{\sqrt{k}} \sin\left[\int_{x_1}^{x} k \, dx + \delta \right] \qquad x_1 < x$$

$$\varphi_{\mathrm{II}}^{+}(x) = \frac{C}{\sqrt{k}} \sin\left[\int_{x}^{x_2} k \, dx + \delta \right] \qquad x < x_2$$