The Semiclassical Approximation

We will now examine in detail the behaviour of a quantum system in a regime in which the quantum effects are "small". Formally, the "strength" of quantum fluctuations is controlled by the Planck constant. This argument, although appealing, can be misleading. The reason is that it has units (of action) and hence its magnitude depends on the choice of units. In practice, it may be regarded as being large or small depending on physical circumstances.

Consider for example the problem of a particle of energy $E$ moving in a constant potential $V$, for simplicity in one dimension. The wave function is

$$\Psi(x) = \begin{cases} \psi_0 e^{iPx/h} & (x \text{ right and } \text{left}) \\ \sqrt{2m(E-V)} & \end{cases}$$

This is a plane wave state with well defined momentum $p$. For a general state
is thus a linear superposition of both types of states. A generic state \( \psi(x) \) has real and imaginary parts which oscililate in space with a wavelength, \( \lambda = \frac{2\pi \hbar}{p} \), i.e., the phase change per unit length is \( p/\hbar \), which is constant.

Imagine that we have a system prepared in such a state but that the potential \( V(x) \) is slowly varying instead of being constant. How slowly? The quantity \( \frac{1}{V(x)} \frac{dV}{dx} \) has units of \((\text{length})^{-1}\) and it represents the rate of change of \( V(x) \) in space. If \( \xi \gg \lambda \) the potential is slowly varying on the scale of \( \lambda \).

Then, in the neighborhood of \( x \) the wave function will be almost a plane wave with a wavelength

\[
\frac{2\pi \hbar}{\sqrt{2m(E-V(x))}} \approx \frac{2\pi \hbar}{p(\xi)} = \lambda(\xi)
\]

in the sense that
\[ \psi(x) = \psi(0) e^{\pm \frac{i}{\hbar} \int_0^x dx' \, p(x')} \]

or more generally

\[ \psi(x) = \psi(x_0) e^{\pm \frac{i}{\hbar} \int_{x_0}^x dx' \, p(x')} \]

However, while this approximation should be accurate for \( x \) close enough to \( x_0 \), it is not clear a-priori how good the approximation actually is.

To investigate this question in detail let us look at the Schrödinger equation

\[ i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V(x) \psi \]

and write \( \psi = e^{\frac{i}{\hbar} \phi} \)

Here \( \phi(x,t) \) is in general a complex function.

By direct substitution we find that \( \phi \)

is the solution of the PDE

\[ \frac{\partial \phi}{\partial t} + \frac{1}{2m} (\nabla \phi)^2 + V(x) \phi = 0 \]

Formally, if we set \( \hbar \to 0 \), we get

\[ \frac{\partial \phi}{\partial t} + \frac{1}{2m} (\nabla \phi)^2 + V(x) \phi = 0 \]

Hamiltonian
In a stationary state, \( \psi(x,t) = e^{i \frac{Et}{\hbar} + \frac{2}{\hbar} \phi(x)} \)

The equation for \( \phi(x) \) is

\[
- \frac{i}{\hbar^2} \left( \nabla^2 \phi \right) + \left( \frac{1}{\hbar^2} \right) \nabla^2 \phi + \frac{1}{\hbar} p^2(x) = 0
\]

where \( p^2(x) = 2m(E - V(x)) \)

If we expand \( \phi(x) = \phi_0 + \hbar \phi_1 + \hbar^2 \phi_2 + \cdots \)

This expansion is known as the semiclassical expansion: the approximation obtained by retaining just the first two terms is known as the WKB approximation (Wentzel-Kramers-Brillouin).

Explicitly \((\text{in } d = 1)\), we get

\[
\frac{1}{\hbar} \left[ -\left( \phi_0' \right)^2 + p^2(x) \right] + \frac{1}{\hbar} \left[ \epsilon \phi_0'' - 2 \phi_0' \phi_0' \right] + O(\hbar^0) = 0
\]

\( \Rightarrow \) \( \phi_0' = \pm |p(x)| \)

\( \Rightarrow \) \( \phi_0 = \pm \int p(x) \, dx \) (up to constants of integration)

\( \Rightarrow \) to leading order, we find
\[ \Rightarrow \Phi(x) = e^{i \frac{\chi}{\hbar} \int_{x_0}^{x} |P(x')| \, dx'} + \text{const} \]

\[ \Rightarrow \Psi(x) = \Phi(x_0) e^{i \frac{\chi}{\hbar} \int_{x_0}^{x} |P(x')| \, dx'} \]

which is the desired result.

How good is this? Let us examine the correction term.

Since \( i \Phi_0'' = 2 \Phi_0' \Phi_0' \)

\[ \Rightarrow \Phi_1 = \frac{i}{2} \frac{\Phi_0''}{\Phi_0'} = \frac{i}{2} \left( \log \Phi_0' \right)' \]

\[ \Rightarrow \Phi_1 = \frac{i}{2} \log \left( \Phi_0'(x) \right) + \text{const} \]

\[ = \frac{i}{2} \log |P(x)| + \text{const} \]

\[ \Rightarrow \Phi_1 = i \log \sqrt{|P(x)|} + \text{const} \quad (\text{we have assumed } |P| > 0) \]

\[ e^{i \Phi_1} = e^{\frac{i}{2} \log \sqrt{|P(x)|} + \text{const}} \]

\[ e^{i \Phi_1} = e^{\frac{i}{2} \log |P(x)|} \]

\[ \Rightarrow \Phi(x) = \frac{A}{\sqrt{|P(x)|}} e^{i \frac{\chi}{\hbar} \int_{x_0}^{x} |P(x')| \, dx'} \]
or

\[ \psi(x) = \psi(x_0) \sqrt{\frac{|p(x)|}{|p(x_0)|}} e^{\pm \frac{i}{\hbar} \int_{x_0}^{x} dx' |p(x')|} \]

Higher order corrections have the form

\[ e^{\frac{i}{\hbar} \delta^2 \phi_2 + \ldots} \]

\[ e^{\frac{i}{\hbar} \delta \phi_2 + \ldots} = e^{\frac{i}{\hbar} \phi_2 + O(\hbar^2)} \]

Hence, the wave function \( \psi \), within the WKB approximation in region I (see figure) is

\[ \psi(x) = \psi(x_0) \sqrt{\frac{|p(x)|}{|p(x_0)|}} e^{\frac{i}{\hbar} \int_{x_0}^{x} dx' |p(x')|} \left\{ 1 + O(\hbar) \right\}^{\text{classical}} \]

Note: \( p(x) = \sqrt{2m(E-V(x))} \) is the momentum of the particle at \( x \).

On the other hand, in the classically forbidden region (III) the wave function now becomes

\[ \psi(x) = \psi(x_0) \sqrt{\frac{|\tilde{p}(x)|}{|\tilde{p}(x_0)|}} e^{\frac{i}{\hbar} \int_{x_0}^{x} dx' |\tilde{p}(x')|} \left( 1 + O(\hbar) \right) \]

where \( \tilde{p}(x) = \sqrt{2m(V(x)-E)} \)

Notice that we have only kept the identity which vanishes as \( |x| \to \infty \)
These approximations fail for \( x \to a \), where \( p \to 0 \). We also need to determine the boundary condition for the wave function at \( x = a \).

There are two ways to do this: (a) we can compute the exact form of the wave function \( \psi(x) \) as \( x \to a \). In this limit, the potential is

\[
V(x) \approx V'(a)(x-a) + O((x-a)^2)
\]

and the wave function is just the wave function for a uniform field \( E = -V'(a) \). This problem is solved in Landau & Lifshitz in terms of Airy functions. (b) we can change (deform) the integration contour so as to remove the singularities at \( x = a \). This last approach turns out to give...
the same result as (a). We will use the second approach.

Consider then a potential \( V(x) \) which is smooth in the neighborhood of \( x = a \), the classical turning point. To the right of \( x = a \), the wave function is

\[
\Psi(x) = \frac{C}{\sqrt{2|p|}} e^{-\frac{i}{\hbar} \int_a^x p(x') dx'} \quad x > a
\]

To the left of \( x = a \), the WKB wave function is

\[
\Psi(x) = \frac{C_1}{\sqrt{p}} e^{\frac{i}{\hbar} \int_a^x p(x') dx'} + \frac{C_2}{\sqrt{p}} e^{-\frac{i}{\hbar} \int_a^x p(x') dx'} \quad x < a
\]

We will also write

\[
E - V(x) = \gamma_0 (x - a) + O((x - a)^2)
\]

where \( \gamma_0 = -\frac{dV}{dx} \) is the force at \( x = a \).

Hence for \( x > a \), we have

\[
\Psi(x) = \frac{C}{\sqrt{2|p|}} e^{-\frac{i}{\hbar} \int_a^x dx' \sqrt{2mE_0 (x-a)^{1/4}}} \quad \frac{2mF_0 (x-a)}{1/4}
\]
Let us regard $x$ as a complex number which obeys

to $x = a$ as

$$x - a = \rho \ e^{i\phi}$$

with $0 < \phi < \pi$ (i.e., \( x \) is positive)

(i.e. as \( x - a > 0 \) to \( x < a \)).

$$\int_a^x \frac{dx'}{\sqrt{x-a}} = \frac{\rho}{3} \left[ \frac{\cos(\frac{3}{2} \phi)}{i} + i \sin(\frac{3}{2} \phi) \right]$$

and

$$\frac{1}{\sqrt{x-a}} = \rho^{-\frac{1}{4}} \ e^{i\phi/4}$$

hence, as $\phi$ increases from 0 to $\pi$, the exponent goes from purely real to purely imaginary.

Thus, $p(x') dx'$ goes from purely real to purely imaginary.

$$-\frac{1}{\pi} \int_a^x p(x') dx' = -\frac{i}{\pi} \int_a^x p(x') \ dx'$$
as we rotate

the exponent of the integrand

The prefactor has the behavior

$$(x-a)^{-\frac{1}{4}} \rightarrow (a-x)^{-\frac{1}{4}} \ e^{-i\pi/4}$$

hence the wave function for $x > a$ becomes $f(x-a)$.

The second term of the linear combination will

be

$$C_1 = \frac{1}{\sqrt{2}} \ e^{-i\pi/4}$$

If we now repeat the argument by rotating on the lower half plane we get the first term with

\[ \ldots \]
\[ c_1 = \frac{c}{2} e^{\frac{\pi}{4}} \]

Hence we find a connection formula between the wave function for \( x > a \)

\[ \psi(x) = \frac{c}{\sqrt{\pi}} e^{-\frac{x}{\hbar}} \int_{a}^{x} \rho(x') \, dx' \quad V(x) > E \]

(which obeys a vanishing B.C. as \( x \to \infty \))

with the wave function for \( x < a \)

\[ \psi(x) = \frac{c}{\sqrt{\pi}} e^{\frac{x}{\hbar}} \cos \left( \frac{1}{\hbar} \int_{a}^{x} \rho(x') \, dx' \right) \quad V(x) < E \]

Conversely, if the wave function is to be exponentially increasing for \( x > a \)

\[ \psi(x) = \frac{c}{2\sqrt{\pi}} e^{\frac{x}{\hbar}} \int_{a}^{x} \rho(x') \, dx' \quad V(x) > E \]

the wave function to the left of \( x = a \) is

\[ \psi(x) = \frac{c}{\sqrt{\pi}} \sin \left( \frac{1}{\hbar} \int_{a}^{x} \rho(x') \, dx' \right) - \frac{\pi}{\hbar} \]
Conversely, for a decreasing potential \( v(x) \)

the correction formulas are

\[
\frac{C}{\sqrt{p}} \cos \left( \frac{1}{\hbar} \int_a^x p(x') \left( -\frac{\pi}{4} \right) \right) \rightarrow \frac{C}{\cos \left( \frac{1}{\hbar} \int_a^x p(x') \right)} \left( \frac{1}{\hbar} \int_a^x p(x') \right) \rightarrow \frac{C}{\cos \left( \frac{1}{\hbar} \int_a^x p(x') \right)} \left( \frac{1}{\hbar} \int_a^x p(x') \right)
\]

We will apply these ideas to two problems:

1. Bohr-Sommerfeld quantization formula
2. Tunneling
The Bohr-Sommerfeld Quantization Formula

Early on in the development of Quantum Mechanics, N. Bohr and A. Sommerfeld argued that if two classical observables are canonically conjugated to each other, e.g., \( \{ \mathbf{q}, \mathbf{p} \} = 1 \),

\[
\Rightarrow \text{the quantity } \frac{1}{2\pi} \int_{2\pi} p \, dq \text{ over a cloud orbit of phase space, must be "quantized" in order to obtain the desired energy levels:}
\]

\[
\frac{1}{2\pi} \int_{2\pi} p \, dq = n \hbar
\]

However, they also found that, again in order to obtain the correct levels, in a number of cases, the rule had to be modified as follows

\[ n \rightarrow n + \nu \]

where \( \nu = 1 \) in many cases. These ad-hoc rules remained mysterious until QM was fully developed. We will see how this works now.
Consider a potential of the form,

\[ V(x) \]

and a particle with energy \( E \). Clearly, \( a \rightarrow b \) are the classical turning points. Let us apply the WKB rules to this case. Let us proceed from left to right. In the region \( x < b \), the wave function is

\[ \psi(x) = \frac{c}{2 \pi |p|} e^{-\frac{1}{\hbar} \int_{b}^{x} |p(x')| dx'} \]

The associated W.F. for \( x > b \) is

\[ \psi(x) = \frac{c}{\sqrt{p}} \cos \left( \frac{\int_{b}^{x} p(x') dx'}{\hbar} \right) \]

On the other hand, for \( x > a \) we have

\[ \psi(x) = \frac{c}{2 \pi |p|} e^{-\frac{1}{\hbar} \int_{a}^{x} \tilde{p}(x') dx'} \]

which requires the W.F. for \( x < a \) to be...
\[ \psi(x) = \frac{C}{\sqrt{p}} \cos \left( \frac{1}{\hbar} \int_{x}^{a} p(x) \, dx - \frac{\pi}{4} \right) \]

However, if \( b < x < a \), these W.F.'s must agree identically. There can only be true if the function of their phases is \( \psi = n\pi \), where \( n \in \mathbb{Z} \).

\[ \Rightarrow \frac{1}{\hbar} \int_{b}^{a} p(x) \, dx - \frac{\pi}{2} = n\pi \]

\[ \Rightarrow \int_{b}^{a} p(x) \, dx = (n+\frac{1}{2})\pi \]

or

\[ \frac{1}{\hbar} \oint p \, dx = (n+\frac{1}{2}) \]

Bohr-Sommerfeld formula:

\[ \oint p \, dx = 2 \int_{b}^{a} p \, dx \] over a whole period of the classical motion of the particle.

Example:

\[ V(x) = -F \frac{1}{|x|} \]

Turning points: \( a = \frac{E}{F} \), \( b = -\frac{E}{F} \).
\[ \int_{b}^{a} dx \ p(x) = \left( n + \frac{1}{2} \right) \pi \ h \]

\[ \int \frac{E}{F} \ dx \ \sqrt{2mE} \ \sqrt{E-F} \left| x \right| = \]

\[ = \frac{E}{F} \]

\[ = 2 \int_{0}^{E/F} \ dx \ \sqrt{2m} \ \sqrt{E-F} \ x \]

\[ x = \frac{E}{F} \ y \]

\[ = 2 \sqrt{2mE} \ \int_{0}^{1} \ y \ \sqrt{1-y} \]

\[ = \frac{4}{3} \left( \frac{2mE^{3/2}}{F^{2}} \right)^{1/2} \]

\[ \Rightarrow E_{n} = \left( \frac{9}{64} \ \frac{F^{2}}{m} \right)^{2/3} \left( \frac{N + \frac{1}{2}}{2\pi \ h} \right)^{2/3} \text{ energy quantization formula for the energy levels} \]
Tunneling and the WKB approximation

Consider a barrier of the form

\[ V(x) \]

\[ E \quad \text{energy of } \]

\[ \text{Kupradoli.} \]

\[ b > a \]

we will construct WKB wave function corresponding to a travelling wave for \( x > b \)

\[ \psi = \sqrt{\frac{k}{2\pi}} e^{\frac{i}{\hbar} \int_a^b p(w) \, dw} e^{-\frac{i}{\hbar} \int_a^b \frac{1}{2m} V(x) \, dx} \]

where \( D \) is the (probability) current density

and \( n = p/m = \frac{p(x)}{m} \)

\[ \Rightarrow \text{for } x < b \text{ we must have} \]

\[ \psi(x) = \frac{1}{\sqrt{2\pi}} e^{\frac{i}{\hbar} \int_a^b p(x') \, dx'} \left[ e^{\frac{i}{\hbar} \int_a^x \frac{1}{2m} V(x) \, dx} - e^{\frac{i}{\hbar} \int_x^b \frac{1}{2m} V(x) \, dx} \right] \]

\[ = \frac{1}{\sqrt{2\pi}} e^{\frac{i}{\hbar} \int_a^b p(x') \, dx'} \left[ e^{\frac{i}{\hbar} \int_a^x \frac{1}{2m} V(x) \, dx} - e^{\frac{i}{\hbar} \int_x^b \frac{1}{2m} V(x) \, dx} \right] \]
The corresponding wave function for \( x < a \) is:

\[
\psi = 2 \sqrt{\frac{b}{v}} \cos \left( \frac{\hbar}{\hbar} \int_{a}^{b} \tilde{p}(x') \, dx' \right) \cos \left( \frac{\hbar}{\hbar} \int_{a}^{b} \tilde{p}(x') \, dx' \right) - \frac{\pi}{2}
\]

Incident and reflected waves:

If the incident wave has the form \(( x < a )\):

\[
\psi = \frac{2}{\sqrt{v}} \cos \left( \frac{\hbar}{\hbar} \int_{a}^{b} \tilde{p}(x') \, dx' + \frac{\pi}{4} \right) \quad \text{(i.e. a plane wave for } x \to \infty) \]

\[
D = -\frac{2}{\hbar} \int_{a}^{b} \tilde{p}(x') \, dx' \quad \text{(is the current density of the transmitted wave)}
\]

(usually called \( T \), the transmission coefficient)

\[
(\text{Here } \tilde{p}(x) = \sqrt{2m(V(x) - E)} \]

(Note: Adjustments may be necessary for clarity and formatting in a digital representation.)