The Semiclassical Approximation

We will now consider in detail the behavior of a quantum system in a regime ~~in~~ 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 $\hbar$ has units (of action) and hence its magnitude depends on the choice of units. In practice $\hbar$ 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

$$\psi(x) = \psi(0)\, e^{\pm i p x/\hbar} \qquad (\pm \text{ right and left})$$

$$p = \sqrt{2m(E-V)}$$

This is a plane wave state with well defined momentum p. ~~The~~ A general state is thus a linear superposition of both types of states. A generic state $\psi(x)$ has real and imaginary parts which oscillate in space with a wavelength $\lambda = 2\pi\hbar/p$, 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 $\frac{1}{V(x)}\frac{dV}{dx} = \frac{1}{\xi}$ 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 λ.

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

$$\frac{2\pi\hbar}{\sqrt{2m(E-V(x))}} = \frac{2\pi\hbar}{p(x)} \equiv \lambda(x)$$

in the sense that

$$\psi(x) \approx \psi(0)\, e^{\pm \frac{i}{\hbar} \int_0^x dx'\, p(x')}$$

or more generally

$$\psi(x) \approx \psi(x_0)\, e^{\pm \frac{i}{\hbar} \int_{x_0}^x dx'\, p(x')}$$

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 ϕ is the solution of the PDE

$$\frac{\partial \phi}{\partial t} + \frac{1}{2m}(\nabla\phi)^2 + V(x) + \frac{i\hbar}{2m}\nabla^2\phi = 0$$

Formally, if we set $\hbar \to 0$, we get

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

Hamilton Jacobi!

For a stationary state $\Psi(x,t) = e^{i\frac{Et}{\hbar} + \frac{i}{\hbar}\phi(x)}$

The equation for $\phi(x)$ is

$$-\frac{1}{\hbar^2}(\nabla\phi)^2 + \frac{i}{\hbar}\nabla^2\phi + \frac{1}{\hbar^2}p^2(x) = 0$$

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

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-~~Bracha~~ Brillouin

Explicitly (in $d=1$) we get

$$\frac{1}{\hbar^2}\left[-(\phi_0')^2 + p^2(x)\right] + \frac{1}{\hbar}\left[i\phi_0'' - 2\phi_1'\phi_0'\right] + O(\hbar^0) = 0$$

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

$$\Rightarrow \quad \phi_0 = \pm\int^x |p(x')|\,dx' \qquad \text{(up to constants of integration)}$$

$\Rightarrow$ to leading order we find

$$\Rightarrow \psi(x) = e^{\pm \frac{i}{\hbar} \int^x |p(x')| dx' + \text{const}}$$

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

which is the desired result.

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

Since $\quad i \phi_0'' = 2 \phi_0' \phi_1'$

$$\Rightarrow \phi_1' = \frac{i}{2} \frac{\phi_0''}{\phi_0'} = \frac{i}{2} (\log \phi_0')'$$

$$\Rightarrow \phi_1 = \frac{i}{2} \log(\phi_0'(x)) + \text{const}$$

$$= \frac{i}{2} \log |p(x)| + \text{const}$$

$$\Rightarrow \phi_1 = i \log \sqrt{p(x)} + \text{const}$$ (we have assumed $p > 0$)

$$e^{\frac{i}{\cancel{\hbar}} \cancel{\hbar} \phi_1} = e^{i \left(i \log \sqrt{|p(x)|} + c \right)}$$

$$= \frac{A}{\sqrt{p(x)}}$$

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

or

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

Higher order corrections have the form

$$e^{\frac{i}{\hbar}\hbar^2 \phi_2 + \cdots} = e^{i\hbar\phi_2 + \cdots} = 1 + i\hbar\phi_2 + O(\hbar^2)$$

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

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

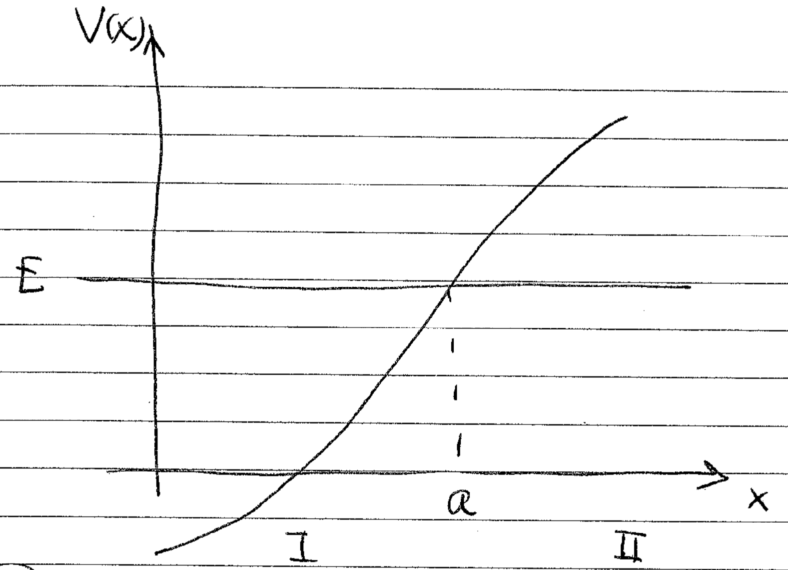
Note: $p(x) = \sqrt{2m(E - V(x))}$ is the classical momentum of the particle at x.

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

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

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

Notice that we have only kept the solution which vanishes as $|x| \to \infty$



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These approximations fail for $x \to a$, where $p \to 0$. We also need to determine the boundary condition for the wave function as $x \to \pm$

There are two ways to do this: (a) we can compute the exact form of the wave function 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 $F = -V'(a)$. 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 singularity 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 WKB wave function is

$$\psi(x) = \frac{C}{2\sqrt{|p|}}\, e^{-\frac{1}{\hbar}\left|\int_a^x p(x')\,dx'\right|} \qquad x>a$$

To the left of $x=a$, the WKB wavefunction is

$$\psi(x) = \frac{C_1}{\sqrt{p}}\, e^{\frac{i}{\hbar}\int_a^x p(x')\,dx'} + \frac{C_2}{\sqrt{p}}\, e^{-\frac{i}{\hbar}\int_a^x p(x')\,dx'} \qquad x<a$$

We will ~~also~~ also write

$$E - V(x) = F_0\,(x-a) + O((x-a)^2)$$

where $F_0 = -\frac{dV}{dx}$ is the force at $x=a$

Hence for $x>a$ we have

$$\psi(x) = \frac{C}{2\left[2m|F_0|(x-a)\right]^{1/4}}\, e^{-\frac{1}{\hbar}\int_a^x dx'\,\sqrt{2m|F_0|(x-a)}}$$

Let us regard x as a complex number which close to $x = a$ as

$$x - a = \rho\, e^{i\phi} \qquad \text{with} \quad 0 < \phi < \pi \quad (\text{i.e. a semicircle})$$

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

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

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

Thus, as ϕ increases from 0 to π, the exponent goes from purely real to purely imaginary

$$-\frac{1}{\hbar}\int_a^x p(x')\,dx' \longrightarrow -\frac{i}{\hbar}\int_a^x p(x')\,dx' \quad \text{as we rotate}$$

The prefactor of the exponential has the behavior $(x-a)^{-1/4}$

$$\Rightarrow (x-a)^{-1/4} \longrightarrow (a-x)^{-1/4}\, e^{-i\pi/4}$$

$\Rightarrow$ the wave function for $x > a$ becomes for $x < a$ the second term of the linear combination with

$$C_2 = \frac{1}{2} C\, e^{-i\pi/4}$$

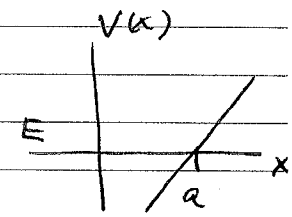
If we now repeat the argument by rotating on the lower half plane we get the first term with

$$C_1 = \frac{c}{2} e^{i\pi/4}$$

Hence we find a connection formula between the wave function for $x > a$

$$\psi(x) = \frac{c}{2\sqrt{|p|}} e^{-\frac{1}{\hbar}\left|\int_a^x \tilde{p}(x')\,dx'\right|} \qquad V(x) > E$$

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



with the wave function for $x < a$

$$\psi(x) = \frac{c}{\sqrt{|p|}} \cos\left(\frac{1}{\hbar}\left|\int_a^x dx'\, p(x')\right| - \frac{\pi}{4}\right)$$

$V(x) < E$

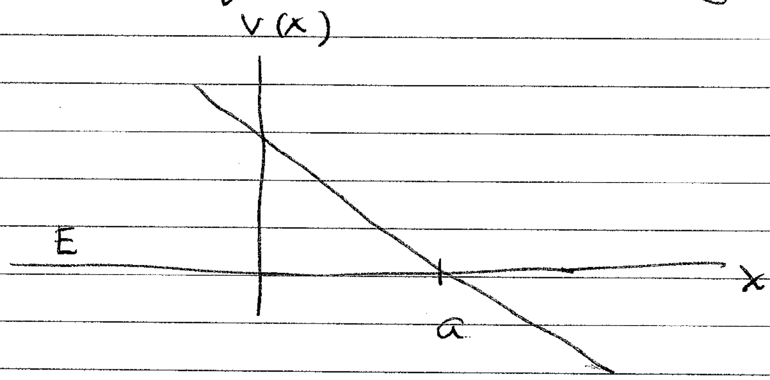
Conversely if the wave function is to be exponentially increasing for $x > a$

$$\psi(x) = \frac{c}{2\sqrt{|p|}} e^{\frac{1}{\hbar}\left|\int_a^x \tilde{p}(x')\,dx'\right|} \qquad V(x) > E$$

the wave function to the left of $x = a$ is

$$\psi(x) = \frac{c}{\cancel{2}\sqrt{p}} \sin\left(\frac{1}{\hbar}\left|\int_a^x dx'\, p(x')\right| - \frac{\pi}{4}\right)$$

Conversely for a decreasing potential



the connection formulas are

$$\frac{C}{\sqrt{p}} \cos\left(\frac{1}{\hbar}\int_a^x dx'\, p(x') - \frac{\pi}{4}\right) \longleftrightarrow \frac{C}{2\sqrt{|p|}}\, e^{-\frac{1}{\hbar}\int_x^a \tilde{p}(x')dx'}$$

$$\frac{C}{\sqrt{p}} \sin\left(\frac{1}{\hbar}\int_a^x dx'\, p(x') - \frac{\pi}{4}\right) \longrightarrow \frac{C}{2\sqrt{|p|}}\, e^{\mp\frac{1}{\hbar}\int_x^a \tilde{p}(x')dx'}$$

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. $\{q, p\}_{PB} = 1$

$\Rightarrow$ the quantity $\frac{1}{2\pi}\oint_\gamma p\, dq$, calculated over a closed orbit γ of phase space, must be "quantized" in order to obtain the desired energy levels:

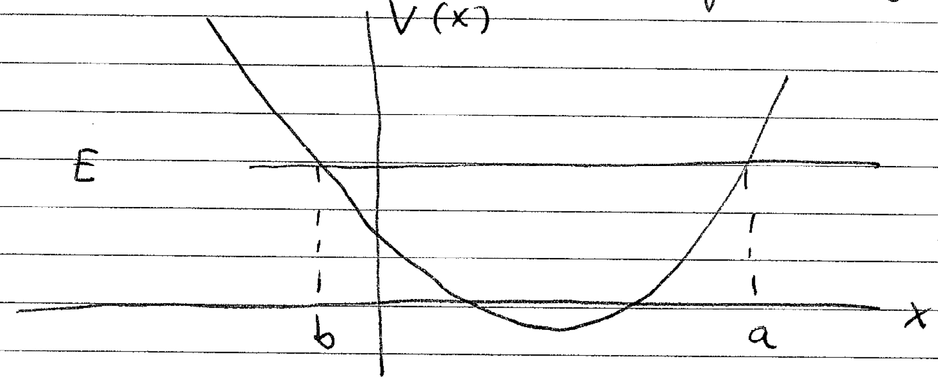
$$\frac{1}{2\pi}\oint_\gamma p\, dq = n\hbar$$

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

$$n \to n+\nu$$

where $\nu = \frac{1}{2}$ in many cases. These ad-hoc rules ~~were~~ remained mysterious until QM was fully developed. We will see how this works now.

Consider a potential of the form



and a particle with energy E. Clearly, a, 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

$$\psi(x) = \frac{C}{2\sqrt{|p|}} e^{-\frac{1}{\hbar}\left|\int_b^x \tilde{p}(x')dx'\right|}$$

The associated w.f. for $x>b$ is

$$\psi(x) \quad \frac{C}{\sqrt{p}} \cos\left(\frac{1}{\hbar}\int_b^x dx'\, p(x') - \frac{\pi}{4}\right)$$

On the other hand, for $x>a$ we have

$$\psi(x) = \frac{C}{2\sqrt{|p|}} e^{-\frac{1}{\hbar}\left|\int_a^x dx'\,\tilde{p}(x')\right|}$$

which requires the w.f. for $x<a$ to be

$$\psi(x) = \frac{C}{\sqrt{p}} \cos\left(\frac{1}{\hbar}\int_x^a dx'\, p(x') - \frac{\pi}{4}\right)$$

However for $b < x < a$ these w.f.'s must agree identically. These can only be true if the sum of their phases $\underbrace{\text{is}}_{\text{(which is a constant)}} = n\pi$, where $n \in \mathbb{Z}$

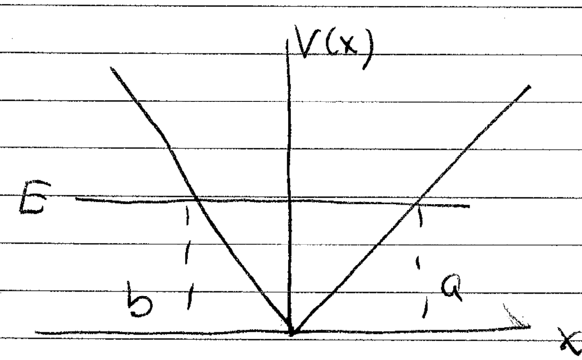
$$\Rightarrow \quad \frac{1}{\hbar}\int_b^a p(x)\, dx - \frac{\pi}{2} = n\pi$$

$$\Rightarrow \quad \int_b^a p(x)\, dx = \left(n + \frac{1}{2}\right)\pi$$

or $\boxed{\dfrac{1}{2\pi}\oint_\gamma p\, dx = \left(n + \frac{1}{2}\right)}$ <u>Bohr-Sommerfeld formula</u>

$\oint_\gamma p\,dx = 2\int_b^a p\, dx$ over a whole period of the classical motion of the ~~partic~~ particle.

<u>Example:</u>



$V(x) = F|x|$

Turning points: $a = \frac{E}{F}$, $b = -\frac{E}{F}$

$$\int_b^a dx \; p(x) = \left(n+\frac{1}{2}\right)\pi\hbar$$

$$\int_{-\frac{E}{F}}^{\frac{E}{F}} dx \; \sqrt{2m} \; \sqrt{E - F|x|} =$$

$$= 2\int_0^{\frac{E}{F}} dx \; \sqrt{2m} \; \sqrt{E - Fx}$$

$$x = \frac{E}{F} y$$

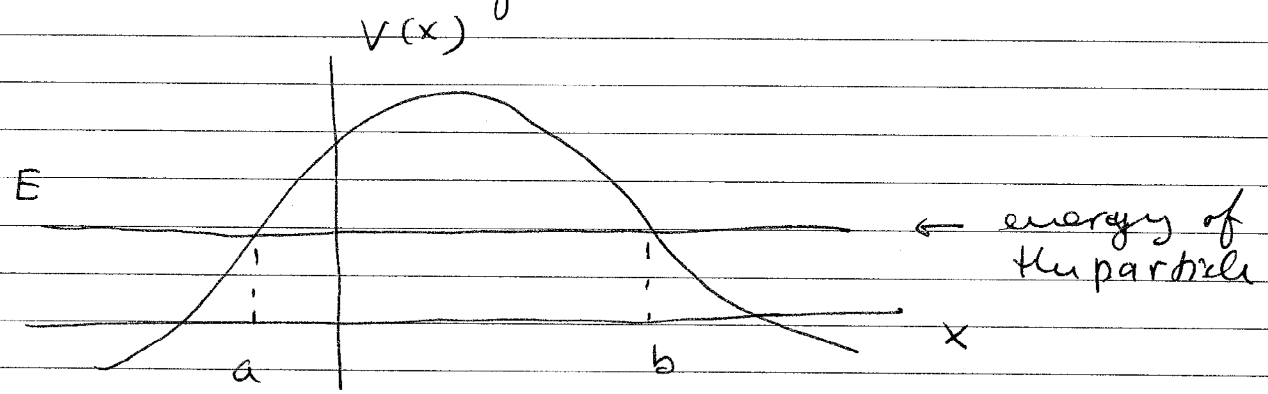
$$= 2\sqrt{2mE} \; \frac{E}{F} \int_0^1 dy \; \sqrt{1-y}$$

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

$$\Rightarrow \quad E_n = \left(\frac{9}{64}\frac{F^2}{m}\right)^{2/3}\left[\left(n+\frac{1}{2}\right)2\pi\hbar\right]^{2/3}$$ is the quantization formula for the energy levels.

Tunneling and the WKB approximation

Consider a barrier of the form



$b > a$

We will construct WKB wave functions corresponding to a travelling wave for $x > b$

$$\psi = \sqrt{\frac{D}{v}}\; e^{\frac{i}{\hbar}\int_b^x p(x')\,dx' + i\frac{\pi}{4}}$$

where D is the (probability) current density

and $v = P/m \equiv \frac{p(x)}{m}$

$\Rightarrow$ for $x < b$ we must have

$$\psi(x) = \sqrt{\frac{D}{|v|}}\; e^{+\frac{1}{\hbar}\left|\int_x^b \tilde{p}(x')\,dx'\right|}$$

$$= \sqrt{\frac{D}{|v|}}\; e^{\frac{1}{\hbar}\left|\int_a^b \tilde{p}(x')\,dx'\right| - \frac{1}{\hbar}\left|\int_a^x \tilde{p}(x')\,dx'\right|}$$

The corresponding wave function for $x < a$ is

$$\psi = 2\sqrt{\frac{D}{v}}\; e^{\frac{1}{\hbar}\int_a^b \tilde{p}(x)\,dx'} \cos\left(\frac{1}{\hbar}\int_x^a p(x')\,dx' - \frac{\pi}{4}\right)$$

↑ incident + reflected waves!

If the incident wave has the form $(x < a)$

$$\psi = \frac{2}{\sqrt{v}} \cos\left(\frac{1}{\hbar}\int_a^x p(x')\,dx' + \frac{\pi}{4}\right)$$ (i.e. a plane wave for $x \to -\infty$)

$$\Rightarrow \quad D = e^{-\frac{2}{\hbar}\int_a^b \tilde{p}(x')\,dx'}$$ is the current density of the transmitted wave

(usually called T, the transmission coefficient)

(Here $\tilde{p}(x) = \sqrt{2m\,(V(x) - E)}$)