Quantum Mechanics: WKB Method

The Semi-Classical (WKB) Approximation

Quantum mechanics is believed to be the ultimate theory to describe nonrelativistic particles. However, in order to describe any arbitrary system using quantum laws, one needs to solved the Schrödinger equation, which may not be an easy task in all situations. One then looks for ways in which one can get an approximate solution, which might be the result of the peculiarity of a situation. For example, if we understand the system in a particular situation, and there is an additional *weak* modification of that situation, it can be treated as a perturbation. The weakness of this perturbation allows one to use the specialized method called *perturbation theory* to understand the system.

We believe that the systems which look classical, should also be describable by quantum laws. However, in that situation the quantum dyanamics would look closer to classical dynamics. However this distinction between quantum behavior and classical behavior cannot be abrupt, it should be gradual. Electrons and protons are well described by quantum mechanics, whereas colloidal particles are well described by classical laws. But there would be intermediate situations where particles will behave partially quantum mechanically and partially classically. We would like to formulate an approximate way of studying such systems within the quantum formalism, exploiting the knowledge that the system behaves in a semi-classical way. This approximation was formulated by Wentzel, Kramers and Brillouin, hence the name WKB approximation.

The Classical Limit

Let us suppose that the wave-function of a particle, in a potential can be written in the form

$$\psi(x) = \exp[\frac{i}{\hbar}S(x)], \tag{1}$$

where $S(x)$ may be some simple or complicated function. This form may occur either naturally, for example for a free particle energy eigenstate $\psi(x) = e^{\frac{i}{\hbar}(px)}$, may be forced by us by introducing a suitable $S(x)$. One would notice that the $S(x)$ for a free particle, $S(x) = px$, is just the classical *action*.

The classical limit is understood to be the limit where $\hbar$ is effectively zero. Of course $\hbar$ being a universal constant, it's value cannot change, but what we means by saying it is effectively zero is that the magnitude of action S of the system is so large that $\hbar$ (which has the dimensions of action) is negligible in comparison. So the semiclassical limit should be the one where $\hbar$ is not effectively zero, but effectively small. Let us then write $S(x)$ in (1) as a series in powers of $\hbar$

$$S(x) = S_0(x) + \hbar S_1(x) + \hbar^2 S_2(x) + \hbar^3 S_3(x) + \ldots \tag{2}$$

We first substitute the form (1) in the time-dependent Schrödinger equation

$$i\hbar\frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V(x)\psi \tag{3}$$

to get

$$-\frac{\partial S}{\partial t}e^{iS/\hbar} = \frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 e^{iS/\hbar} - \frac{i\hbar}{2m}\frac{\partial^2 S}{\partial x^2}e^{iS/\hbar} + V(x)e^{iS/\hbar}. \tag{4}$$

Cancelling out the exponential term on both sides, one gets

$$\frac{\partial S}{\partial t} = -\frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 + \frac{i\hbar}{2m}\frac{\partial^2 S}{\partial x^2} - V(x). \tag{5}$$

If we take the classical limit by putting $\hbar$ equal to zero, the second term on the right hand side goes to zero and, by virtue of (2), the function $S(x)$ is reduced to $S_0(x)$. The Schrödinger equation is now reduced to

$$\frac{\partial S_0}{\partial t} + \frac{1}{2m}\left(\frac{\partial S_0}{\partial x}\right)^2 + V(x) = 0. \tag{6}$$

But this is just the classical Hamilton-Jacobi equation, with $S_0(x)$ being the classical action. Thus we see a remarkable result that in the classical limit, the Schrödinger equation is reduced to the classical Hamilton-Jacobi equation. The limit $\hbar \to 0$ may then be seen as describing the quantum to classical transition, just as $1/c \to 0$ is understood to describe relativistic to non-relativistic transition.

The Quasi Classical Approximation

From the preceding argument, the function $S(x)$ in (2) should be understood to reduce to the classical action in the limit $\hbar \to 0$. However, if $\hbar$ is assumed to be small, but not zero, we should be able to describe the semi-classical regime.

We start by substitution the form of the wave-function (1) in the time-independent Schrödinger equation

$$\frac{-\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V(x)\psi = E\psi \tag{7}$$

to get

$$\frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 e^{iS/\hbar} - \frac{i\hbar}{2m}\frac{\partial^2 S}{\partial x^2}e^{iS/\hbar} + V(x)e^{iS/\hbar} = Ee^{iS/\hbar}. \tag{8}$$

Cancelling out the exponential term from both sides, the above reduces to

$$\left(\frac{\partial S}{\partial x}\right)^2 - i\hbar\frac{\partial^2 S}{\partial x^2} = 2m(E - V(x)) \tag{9}$$

Assuming that $\hbar$ is effectively small, we approximate $S(x)$ by $S(x) \approx S_0(x) + \hbar S_1(x)$. Substituting it in the above equation, and recognizing $2m(E - V(x))$ as p^2, we get

$$\left(\frac{\partial S_0}{\partial x} + \hbar\frac{\partial S_1}{\partial x}\right)^2 - i\hbar\frac{\partial^2 S_0}{\partial x^2} - i\hbar^2\frac{\partial^2 S_1}{\partial x^2} = p^2. \tag{10}$$

Equating like powers of $\hbar$ on both sides, we get

$$\frac{\partial S_0}{\partial x} = \pm p$$
$$2\frac{\partial S_0}{\partial x}\frac{\partial S_1}{\partial x} = i\frac{\partial^2 S_0}{\partial x^2} \tag{11}$$

where we ignore $\hbar^2$ and higher powers with the understanding that $\hbar$ is effectively small. First of the above two relations gives

$$S_0(x) = \pm \int p \, dx \tag{12}$$

and the second one gives

$$\frac{\partial S_1}{\partial x} = \frac{i}{2p}\frac{\partial p}{\partial x}$$

$$S_1 = i\log(\sqrt{|p|}) \tag{13}$$

The wave-function in the semi-classical limit may now be written simply by substituting the above in (1) and (2). The semi-classical energy eigenfunction assumes the following form

$$\psi(x) = \exp\left(\pm\frac{i}{\hbar}\int p\,dx - \log(\sqrt{|p|})\right)$$

$$= \frac{1}{\sqrt{|p|}}\exp\left(\pm\frac{i}{\hbar}\int p\,dx\right) \tag{14}$$

Particle in a bound potential

Let us how to apply the WKB approximation to the case of a particle bound by a one-dimensional potential, as shown the figure alongside. The particle is under the influence of a potential $V(x)$, and its energy $E = \frac{p^2}{2m} + V(x)$ is fixed. Notice that at the two positions x_1 and x_2, the following is true, $V(x_1) = V(x_2) = E$. At these two points, the classical momentum is zero: these are the *classical turning points*, points where the kinetic energy of the particle becomes zero. Taking these points as guides, we can divide the position space into three regions, I, II and III. In region II, $V(x) \leq E$ is true and $p = \sqrt{E - V(x)}$ is real. This is the *classically allowed region*. In regions I, and III, $V(x) \geq E$ is true and $p = \sqrt{E - V(x)}$ is real. This is the *classically forbidden region*, and classically the particle cannot exist here. However, we know that in quantum mechanics, phenomena like tunneling are possible, and the particle can exist in this region too, although with an attenuated probability. In all the three regions, the wave-function (14), with both $\pm$ signs, should be taken into account.
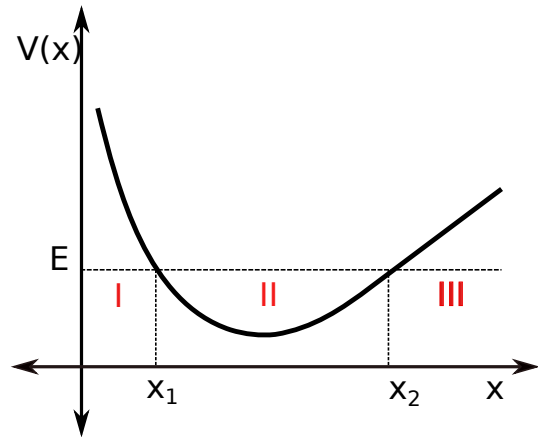
The most general states in the three regions can be written as

$$\psi_I(x) = \frac{A}{\sqrt{|p|}}\exp\left(-\frac{1}{\hbar}\int_x^{x_1}|p|\,dx\right)$$

$$\psi_{II}(x) = \frac{B}{\sqrt{p}}\exp\left(\frac{i}{\hbar}\int p\,dx\right) + \frac{C}{\sqrt{p}}\exp\left(-\frac{i}{\hbar}\int p\,dx\right)$$

$$\psi_{III}(x) = \frac{D}{\sqrt{|p|}}\exp\left(-\frac{1}{\hbar}\int_{x_2}^x|p|\,dx\right), \tag{15}$$

where A, B, C are constants to be determined, and the exponentially increasing terms have been dropped because the wave-function should go to zero as $x \to \pm\infty$. The constants

can be determined by applying the condition that the wave-function is continuous across the three regions:

$$\psi_I(x_1) = \psi_{II}(x_1), \qquad \psi_{II}(x_2) = \psi_{III}(x_2). \tag{16}$$

The problem is that precisely at these two points, the wave-function (14) breaks down because when p becomes zero, the term $1/\sqrt{|p|}$ diverges.

The remedy for this problem is that close to a point (say) x_1, the potential $V(x)$ can be approximated by $V(x) \approx V(x_1) + (x - x_0) \frac{dV}{dx}\big|_{x=x_0}$, which is a linear potential and exactly solvable. The exact wave-function for this potential can expressed in terms of *Airy functions*, and can be used to match $\psi_I(x_1)$ with $\psi_{II}(x_1)$. We skip the derivation of these connection formulas, as excellent analysis of these widely exist in the literature. We just present the final *connection formulas*:

$$\psi_I(x) = \frac{A}{\sqrt{|p|}} \exp\left(-\frac{1}{\hbar} \int_x^{x_1} |p|\, dx\right) \iff \psi_{II}(x) = \frac{A}{\sqrt{p}} \sin\left(\frac{1}{\hbar} \int_{x_1}^{x} p\, dx + \frac{\pi}{4}\right)$$

$$\psi_{II}(x) = \frac{D}{\sqrt{p}} \sin\left(\frac{1}{\hbar} \int_x^{x_2} p\, dx + \frac{\pi}{4}\right) \iff \psi_{III}(x) = \frac{D}{\sqrt{|p|}} \exp\left(-\frac{1}{\hbar} \int_{x_2}^{x} |p|\, dx\right). \tag{17}$$

Now the two expression for $\psi_{II}(x)$, in the two formulas, should be identical, becuase they represent the same wave-function in the same region:

$$\psi_{II}(x) = \frac{A}{\sqrt{p}} \sin\left(\frac{1}{\hbar} \int_{x_1}^{x} p\, dx + \frac{\pi}{4}\right) = \frac{D}{\sqrt{p}} \sin\left(\frac{1}{\hbar} \int_x^{x_2} p\, dx + \frac{\pi}{4}\right) \tag{18}$$

The above equation of the form $A \sin\theta_1 = D \sin\theta_2$, which can be satisfied if

$$\theta_1 + \theta_2 = (n+1)\pi \quad \text{and} \quad A = (-1)^n D.$$

This condition implies

$$\frac{1}{\hbar} \int_{x_1}^{x} p\, dx + \frac{\pi}{4} + \frac{1}{\hbar} \int_x^{x_2} p\, dx + \frac{\pi}{4} = (n+1)\pi$$

$$\frac{1}{\hbar} \int_{x_1}^{x_2} p\, dx = (n + \tfrac{1}{2})\pi \tag{19}$$

Now the phase-space integral from x_1 to x_2 can be written as half the integral over the complete loop $x_1 \to x_2 \to x_1$: $\int_{x_1}^{x_2} p\, dx = \frac{1}{2} \oint p\, dx$. Thus, the above condition simplifies to:

$$\boxed{\oint p\, dx = (n + \tfrac{1}{2})h} \tag{20}$$

The above relation looks deceptively simple, but it's usefulness cannot be overstated. Basically what it says is that if one calculates the *classical* phase-space integral over the complete loop, or the area of phase-space enclosed by the two turning points, it should just be equal to $(n + \frac{1}{2})h$. Notice that no further quantum mechanical analysis required to solve a specific problem. Only the area of phase space needs to be calculated.

Specific examples

Particle in a box

Consider a particle of mass m enclosed in a box whose two walls are at $x = 0$ and $x = L$. The energy is just the kinetic energy, and is given by $E = p^2/2m$. The particle switched between the two momenta values $p = \sqrt{2mE}$ and $p = -\sqrt{2mE}$, as it bounces between the two walls. The phase trajectory is a rectangle whose x-dimension is L and y-dimension is $2\sqrt{2mE}$. So, area of phase-space enclosed inside the phase trajectory is

$$\oint p\, dx = 2\sqrt{2mE} \times L = (n + \tfrac{1}{2})h$$

Squaring both sides, we find the WKB energy as

$$E = \frac{(n + \tfrac{1}{2})^2 h^2}{8mL^2}.$$

As one can see, this energy is very close to the exact energy eigenvalues of the Hamiltonian, given by $E_n = \frac{n^2 h^2}{8mL^2}$.

Harmonic oscillator

Consider a particle of mass m in a harmonic oscillator potential, such that the classical energy is given by

$$E = p^2/2m + \tfrac{1}{2}m\omega^2 x^2.$$

This equation can be recast as

$$\frac{p^2}{2mE} + \frac{x^2}{2E/m\omega^2} = 1,$$

which is immediately recognized as the equation of an ellipse, which has two axes equal to $\sqrt{2mE}$ and $\sqrt{2E/m}/\omega$. The area enclosed by this ellipse is

$$\oint p\, dx = \pi\sqrt{2mE}\sqrt{2E/m}/\omega = (n + \tfrac{1}{2})h,$$

which gives the WKB energy as

$$E = (n + \tfrac{1}{2})\hbar\omega.$$

The above is equal to the exact energy eigenvalues of a quantum harmonic oscillator.