WKB Approximation

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In quantum mechanics, we do not always get to solve the Schrödinger equation exactly, and we need to solve them approximately. One of these powerful approximation methods is the WKB Approximation.

General idea

Consider the Schrödinger equation

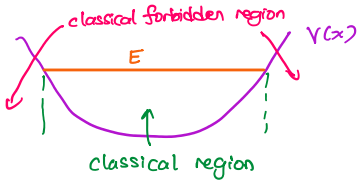
$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right]\psi(x)=E\psi(x)$$

$$\frac{\partial^2}{\partial x^2}\psi(x)=-\underbrace{\frac{2m}{\hbar^2}\left[E-V(x)\right]}_{\equiv\frac{p(x)^2}{\hbar^2}}\psi(x)$$

where $p(x)^2=2m\left[E-V(x)\right]$

If $V(x)$ changes slow enough and we can view $p(x)$ as locally constant, we might recognise the differential equation and guess that, approximately

$$\psi(x)\sim e^{\pm\frac{i}{\hbar}p(x)}$$



We see that within the classical region, $\psi(x)$ oscillates trigonometrically, while outside it, $\psi(x)$ decays exponentially.

The idea of WKB approximation is then to approximate $\psi(x)$ in the form of $\psi(x)\sim A(x)e^{\frac{i}{\hbar}S(x)}\sim e^{\frac{S_0(x)}{\hbar}+S_1(x)}$

Mathematical Detail

Using the Ansatz: $\psi(x)\sim e^{\frac{S_0(x)}{\hbar}+S_1(x)}$

$$\psi'(x)\sim\left(\frac{S_0'(x)}{\hbar}+S_1'(x)\right)e^{\frac{S_0(x)}{\hbar}+S_1(x)}$$

$$\psi''(x)\sim\left[\left(\frac{S_0'}{\hbar}+S_1'\right)^2+\left(\frac{S_0''}{\hbar}+S_1''\right)\right]e^{\frac{S_0}{\hbar}+S_1}$$

$$\therefore\quad\left[\left(\frac{S_0'}{\hbar}+S_1'\right)^2+\left(\frac{S_0''}{\hbar}+S_1''\right)\right]=-\frac{p(x)^2}{\hbar^2}$$

We match the terms by order of $\hbar$:

$$S_1'^2+S_1''=0 \quad\text{——}\ ③$$

$$2S_0'S_1'+S_0''=0 \quad\text{——}\ ②$$

$$S_0'^2=-p(x)^2 \quad\text{——}\ ①$$

From ①: $S_0'=\pm ip(x)\Rightarrow S_0(x)=\pm i\int^x dx'\,p(x')$

From ②:

$$2S_0'S_1'+S_0''=0$$

$$\pm 2ip(x)S_1'=\mp ip'(x)$$

$$S_1'=-\frac{p'(x)}{2p(x)}$$

$$=-\frac{1}{2}\frac{d}{dx}\left(\ln p(x)\right)$$

$$S_1=-\frac{1}{2}\ln p(x)$$

Hence: $\psi(x) \sim C_1\, p(x)^{-1/2}\, e^{\frac{i}{\hbar}\int^x dx' p(x')} + C_2\, p(x)^{-1/2}\, e^{-\frac{i}{\hbar}\int^x dx' p(x')}$

This is the WKB approximation

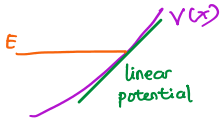
PIs: What about ②? ③ is important for higher order corrections to WKB approximation, with the general expansion $\psi(x) \sim \exp\left\{\frac{1}{\hbar}\sum_{n=0}^{\infty} \hbar^n S_n(x)\right\}$,

where we see that it is an expansion in orders of $\hbar$. Since $\hbar$ is small, higher order corrections will become smaller.

PIs: The WKB approximation works for when $V(x)$ does not change much. In other words, $\psi(x)$ oscillates multiple times before its amplitude changes appreciably. The important point is then when $\hbar$ is considered small

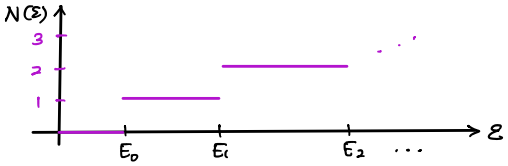
WKB Quantisation Rule

In the WKB approximation above, there is a singularity at the turning points when $E = V(x)$, because of $p(x)^{-1/2}$. Mathematically, what we should do is to treat the turning point differently. We approximate the region around the turning point by a linear potential, whose solution is given by special functions called Airy function. We then match the coefficients between the 3 regions: classical region, linear potential region, and forbidden region. We then further match the conditions at both turning points, and we obtain the WKB quantisation rule.



We will not do it here, because the math can be quite involved. Instead, we derive this by considering the counting function

$N(\varepsilon)$ = number of states below energy ε



Below E_0, there are no states, so $N(\varepsilon < E_0) = 0$

Subsequently, $N(E_0 < \varepsilon < E_1) = 1$

$$N(E_1 < \varepsilon < E_2) = 2$$

and so on. We observe that this is just a sum of the step function:

$$N(\varepsilon) = \sum_n \eta(\varepsilon - E_n)$$

$$= \sum_n \langle E_n | \eta(\varepsilon - \mathcal{H}) | E_n \rangle$$

$$= \mathrm{tr}\{\eta(\varepsilon - \mathcal{H})\}$$

We can approximate this trace by a classical integration. First, trace sums over all states, which in classical mechanics is an integration over the phase space. But in quantum mechanics, because of uncertainty principle, they must be cells of size $2\pi\hbar$.

Hence: $N(\varepsilon) \sim \int \frac{dx\, dp}{2\pi\hbar}\, \eta\left(\varepsilon - \frac{p^2}{2m} - V(x)\right)$

$$= \int \frac{dx}{2\pi\hbar} \int_{-\infty}^{\infty} dp\, \eta\left(\varepsilon - V(x) - \frac{p^2}{2m}\right)$$

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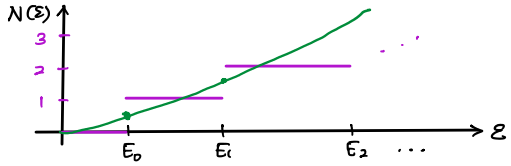
$$\varepsilon - V(x) > \frac{p^2}{2m}$$

$$\Rightarrow 2m(\varepsilon - V(x)) > p^2$$

$$= \int \frac{dx}{2\pi\hbar}\, 2\sqrt{2m(\varepsilon - V(x))}$$

$$= \frac{1}{\pi\hbar} \int_{x_-}^{x_+} dx\, \sqrt{2m(\varepsilon - V(x))}$$

In classical approximation, we smooth over the $N(\varepsilon)$ function



We notice that at the eigenvalues, when smoothing the step function, we have $N(E_n) = \left(n + \frac{1}{2}\right)$.

Hence, we have the WKB quantisation rule:

$$\left(n + \frac{1}{2}\right)\pi\hbar = \int_{x_-}^{x_+} dx\, \sqrt{2m(\varepsilon - V(x))}$$

PS: Compare this with the Sommerfeld quantisation rule that was guessed at the early stages of quantum theory

$$\oint p\, dx = nh$$

for allowed energy states.