The WKB Approximation

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Introduction

The WKB (Wentzel, Kramers, Brillouin) approximation is, in sense to be made clear below, a quasi-classical method for solving the one-dimensional (and effectively one-dimensional, such as radial) time-independent Schrödinger equation. The nontrivial step in the method is the connection formulas (see below), that problem was first solved by Lord Rayleigh (Proc. Roy. Soc. A, 86, 1912, 207) and as Jeffries notes (*Mathematical Physics*, p 526) "it has been rediscovered by several later writers" presumable referring to W, K and B. By the way, the English call it the Jeffries approximation, or, if feeling sufficiently ecumenical, the WKBJ approximation. (In this lecture, we only consider bound states: the most famous application of WKB, α-decay, was covered in detail in the undergraduate quantum mechanics course based on Griffiths' book.)

We'll follow the development in Landau and Lifshitz, who consider this all sufficiently obvious that they don't mention any of these people. In fact, they call it

The Semiclassical Approximation to Leading Order

Consider a particle moving along in a slowly varying one-dimensional potential. By "slowly varying" we mean here that in any small region the wave function is well approximated by a plane wave, and that the wavelength only changes over distances long compared with a wavelength. We're also assuming for the moment that the particle has positive kinetic energy in the region. Under these conditions, it's easy to see the general form of the solution to the time independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x).$$

Very approximately, $\psi(x)$ will look like $A(x)e^{\pm ip(x)x/\hbar}$ where $p(x)$ is the "local momentum" we define classically by

$$p(x)^2/2m+V(x)=E,$$

and $A(x)$ is slowly varying compared with the phase factor.

Clearly this is a *semiclassical* limit: $\hbar$ has to be sufficiently small that there are many oscillations in the typical distance over which the potential varies.

To handle this a little more precisely, we emphasize the rapid *phase* variation in this semiclassical limit by writing the wave function

$$\psi(x)=e^{(i/\hbar)\sigma(x)}$$

and writing Schrödinger 's equation for $\sigma(x)$.

So from

$$i\hbar\psi'(x) = -\sigma'(x)e^{(i/\hbar)\sigma(x)},$$

and

$$-\hbar^2\psi''(x) = -i\hbar\sigma''(x)e^{(i/\hbar)\sigma(x)} + \left(\sigma'(x)\right)^2 e^{(i/\hbar)\sigma(x)},$$

Schrödinger's equation written for the phase function is:

$$-i\hbar\sigma''(x) + \left(\sigma'(x)\right)^2 = \left(p(x)\right)^2.$$

And, since we're assuming the system is close to classical, it makes sense to expand σ as a series in $\hbar$ (following Landau and Lifshitz):

$$\sigma = \sigma_0 + (\hbar/i)\sigma_1 + (\hbar/i)^2\sigma_2 + \ldots$$

The zeroth order approximation is

$$(\sigma_0')^2 = p^2$$

and fixing the sign of p by

$$p(x) = +\sqrt{2m\left(E - V(x)\right)}$$

we conclude that

$$\sigma_0 = \pm\int p(x)\,dx.$$

(As we discussed in the lecture on path integrals, in the classical limit one path dominates, and the phase of the wave function is $(i/\hbar)$ times the classical action *S* along that path. In the present case, $S = -Et \pm \int p dx$, we've already factored out the *Et* since we're dealing here with the time-independent wave function.)

Region of Validity of the Approximation

From the Schrödinger equation $-i\hbar\sigma''(x) + \left(\sigma'(x)\right)^2 = \left(p(x)\right)^2$, it is evident that this approximate solution is *only valid if we can ignore that first term*. That is to say, we must have

$$\left|\hbar\sigma''(x)/\left(\sigma'(x)\right)^2\right| \ll 1,$$

or

$$\left|\frac{d\left(\hbar/\sigma'\right)}{dx}\right| \ll 1.$$

But in leading approximation $\sigma' = p,$ and $p = 2\pi\hbar/\lambda$, so the condition is

$$\frac{1}{2\pi}\left|\frac{d\lambda}{dx}\right| \ll 1.$$

This just means the change in wavelength over a distance of one wavelength must be small.

Obviously, this cannot always be the case: if the particle is confined by an attractive potential, at the edge of the classically allowed region, that is, where $E = V(x)$, p is zero and the wavelength is infinite. The approximation is only good well away from that point, to which we shall return shortly.

Next to Leading Order Correction

The second term in the $\hbar$ expansion of the phase, $\sigma = \sigma_0 + (\hbar/i)\sigma_1 + \ldots$ satisfies

$$-i\hbar\sigma_0'' + 2\sigma_0'(\hbar/i)\sigma_1' = 0$$

so

$$\sigma_1' = -\sigma_0''/2\sigma_0' = -p'/2p,$$

and

$$\sigma_1 = -\tfrac{1}{2}\ln p.$$

So the wave function to this order is:

$$\psi(x) = \frac{C_1}{\sqrt{p(x)}}e^{(i/\hbar)\int p dx} + \frac{C_2}{\sqrt{p(x)}}e^{-(i/\hbar)\int p dx}.$$

(Recall we fixed the sign of p to be positive.)

To interpret the $\sqrt{p(x)}$ factor, consider the first term, a wave moving to the right. Since p is real, the exponential has modulus unity, and the local amplitude squared is proportional to $1/p$, that is, $1/v$, where v is the velocity of the particle. This is simple to understand physically: the probability of finding the particle in any given small interval is proportional to the time it spends there, hence inversely proportional to its speed.

We turn now to the wave function in the classically forbidden region,

$$p(x)^2/2m = E - V(x) < 0.$$

Here p is of course pure imaginary, but the same formal phase solution of the Schrodinger equation works, again provided that the particle is well away from the points where $E = V(x)$.

The wave function is:

$$\psi(x) = \frac{C_1'}{\sqrt{|p(x)|}} e^{-(1/\hbar)\int |p|dx} + \frac{C_2'}{\sqrt{|p(x)|}} e^{(1/\hbar)\int |p|dx}.$$

Connection Formulas, Boundary Conditions and Quantization Rules

Let us assume we're dealing with a one-dimensional potential, and the classically allowed region is $b \le x \le a$. (I'm just following Landau's notation here.) Clearly, in the forbidden region to the right, $x > a$, only the first term in the above equation for $\psi(x)$ appears, and for $x < b$ only the second term. Furthermore, in the "inside" (classically allowed) region, $b \le x \le a$, the wave function has the oscillating form discussed earlier.

But how do we connect the three regions together? We make an assumption: we take it that the potential varies sufficiently smoothly that it's a good approximation to take it to be linear in the vicinity of the classical turning points. That is to say, we assume that a linear potential is a sufficiently good approximation out to the point where the short wavelength (or decay length for tunneling regions) description is adequate.

Therefore, near $x = a$, we take the potential to be

$$E - V(x) \cong F_0(x - a)$$

(so F_0 would be the force) and then approximate the wave function by the known exact solution for a linear everywhere potential: the Airy function.

It is known that for the Airy function, the solution having the form

$$\psi(x) = \frac{C}{2\sqrt{|p(x)|}} e^{-(1/\hbar)\int_a^x |p|dx}$$

to the right becomes

$$\psi(x) = \frac{C}{\sqrt{|p(x)|}} \cos\left((1/h)\int_a^x p dx + \tfrac{1}{4}\pi \right)$$

$$= \frac{C}{\sqrt{|p(x)|}} \sin\left((1/h)\int_x^a p dx + \tfrac{1}{4}\pi \right)$$

for $x < a$. (The derivation of this "connection" is given in my notes here.)

At *b*, the same argument gives

$$\psi(x) = \frac{C}{\sqrt{|p(x)|}} \sin\left((1/h) \int_b^x p dx + \tfrac{1}{4}\pi \right).$$

For these two expressions to be consistent, we must have

$$\frac{1}{\hbar} \int_b^a p dx + \tfrac{1}{2}\pi = (n+1)\pi, \text{ or } \oint p dx = 2\pi\hbar\left(n + \tfrac{1}{2}\right).$$

where the latter integral is over a complete cycle of the classical motion.

Here *n* is the number of zeros of the wave function: this is the *quantization condition*.

Relating Classical Circuit time to Quantized Energy Levels

The time for a complete classical circuit is

$$T = 2\int_b^a dx / v = 2m \int_b^a dx / p.$$

Note that $\oint p dx$ is the area of the classical path in phase space, so we see each state has an element of phase space $2\pi\hbar$. From this, we can figure out the approximate energy splitting between levels in the quasi-classical limit: the change in the integral with energy ΔE corresponding to one level must be $2\pi\hbar$. That is,

$$\Delta E \oint (\partial p / \partial E) dx = 2\pi\hbar.$$

Now $(\partial E / \partial p) = v$, so $\oint (\partial p / \partial E) dx = \oint dx / v = T$.

Therefore, $\Delta E = 2\pi\hbar / T = \hbar\omega$.

This is just saying that if the particle emits one photon and drops to the next level, the frequency of the photon emitted is just the orbital frequency of the particle, a very natural conclusion in the quasi-classical limit.

The Radial Case

In the above analysis for a particle confined to one dimension, the connection formulas can be understood with a simple picture: the wave function "spills over" into the forbidden regime, and its twisting there counts as an extra $\frac{1}{4}\pi$ of phase change, so in the lowest state the total phase

change in the allowed region need only be $\frac{1}{2}\pi$. In the radial case, assuming the potential is well behaved at the origin, the wave function goes to zero there. A bound state will still spill over beyond the classical turning point at r_0, say, but clearly there must be a total phase change of $\frac{3}{4}\pi$ in the allowed region for the lowest state, since there can be no spill over to negative *r*.

The general formula will be

$$\frac{1}{\hbar}\int_0^{r_0} p(r)\,dr = \left(n+\tfrac{3}{4}\right)\pi, \quad n = 0,1,2,\ldots,$$

the series terminating if and when the turning point reaches infinity.

Warning: actually, some potentials, including the Coulomb potential and the centrifugal barrier for $l \neq 0$, are in fact singular at $r = 0$. These cases require special treatment.