The WKB Approximation

Lecture Eleven   Turning Point

As we have mentioned, the WKB approximation is useful in problems of wave propagation. In this section we demonstrate this by applying it to the wave equation which governs the quantum mechanical behavior of a particle.

Consider the time-independent Schrodinger equation of one spatial dimension discussed at the end of Chapter 5. We will write this equation in the form

$$\frac{d^2\phi}{dx^2} + \lambda^2[E - V(x)]\phi = 0, \tag{7.50}$$

where λ is equal to $\sqrt{2m}$ divided by the Planck constant, with m the mass of the particle. We shall consider λ as a very large number.

As we have mentioned, $|\phi|^2$ is the probability density of the particle, E is the energy of the particle, and $V(x)$ is the potential. We note that $E - V$ is equal to the kinetic energy of the particle.

In the region where

$$E > V(x),$$

the kinetic energy of the particle is positive. Comparing with (7.1), we identify $p(x)$ with

$$\lambda\sqrt{E - V(x)}\,.$$

The WKB solutions are

$$p^{-1/2}e^{i\int p\,dx} \text{ and } p^{-1/2}e^{-i\int p\,dx}. \tag{7.51}$$

These solutions are oscillatory as a function of x.

In the region where

$$E < V(x),$$

the kinetic energy of the particle is negative, and the momentum of the particle is imaginary. In classical mechanics, this region is inaccessible to the particle. The WKB solutions are

$$\eta^{-1/2}e^{\int \eta\,dx} \text{ and } \eta^{-1/2}e^{-\int \eta\,dx}, \tag{7.52}$$

where

$$\eta = \lambda\sqrt{V(x) - E}\,.$$

The first solution above is exponentially increasing as x increases, and the second solution above is exponentially decreasing as x increases. Since a particle is rarely observed in the classically inaccessible region, we require the solution to be the one which decreases more and more as x goes deeper and deeper into the classically inaccessble region.

Let there be a point x_0 at which
$E - V(x_0) = 0$.

Note that the point x_0 is the point at which the momentum of the particle vanishes. By (7.4), the WKB approximation fails at x_0. Indeed, (7.4) is not satisfied in a small neighborhood around x_0, and the WKB approximation fails in this small neighborhood.

Let us study the behavior of the wavefunction near x_0. We shall assume that the derivative of $V(x)$ at x_0 is different from zero, hence $E - V(x)$ is negative at one side of x_0 and positive at the other side of x_0. The point x_0 is the dividing point between a classically accessible region and a classically inaccessible region. In classical mechanics, the particle cannot move into the region where its kinetic energy is negative, and must turn back as it arrives at x_0. That is why the point x_0 is called a turning point of the equation. As we may expect, the qualitative behavior of the quantum wavefunction goes through a transition near x_0. More precisely, the WKB solution changes from an oscillatory behavior from one side of x_0 to an exponential behavior at the other side of x_0. However, we cannot continue the solution from one side of x_0 to the other side of x_0 with the WKB approximation alone. This is because the WKB solutions fail in a small neighborhood around x_0.

Fortunately, another approximation is available when x is close to x_0, where we may make the approximation

$$[E - V(x)] \approx -\alpha(x - x_0),$$

with α equal to $V'(x_0)$. This approximation is valid for

$$|x - x_0| \ll 1. \tag{7.53}$$

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Therefore, in the region of (7.53), the Schrodinger equation is approximately equal to

$$\frac{d^2\phi}{dx^2} - \alpha\lambda^2(x - x_0)\phi = 0, \tag{7.54}$$

which is related to the Air equation

$$\frac{d^2 u}{d\rho^2} - \rho u = 0$$

by a linear transformation of the independent variable. Thus the Schrodinger equation in the region near the turning point is approximately a linear superposition of the solutions of the Airy functions. The constants of superposition are determined by the conditions imposed on the solution.

By (7.4), the WKB approximation is valid in the region

$$|x - x_0| \gg \Lambda^{-2/3}, \tag{7.55}$$

where

$\Lambda^2 = |\alpha|\lambda^2$.

By (7.53) and (7.55), there are two overlapping regions in which both the WKB solutions and the Airy function solutions are good approximations of the solution of (7.50). The first overlapping region is

$$1 \gg x - x_0 \gg \Lambda^{-2/3}, \qquad (7.56a) \qquad\qquad \#$$

where x is to the right of x_0, and the second overlapping region is $\qquad\qquad \#$

$$1 \gg x_0 - x \gg \Lambda^{-2/3}, \qquad (7.56b) \qquad\qquad \#$$

where x is to the left of x_0. The existence of such overlapping regions is crucial, as it enables us to join the WKB solutions from one side of the turning point to the other side of the turning point, using the Airy functions to interpolate through the region in which the WKB approximation fails.

We first demonstrate how this is done when (7.50) has only one turning point. We shall assume that α is positive. In such a case, the kinetic energy of the particle is negative in the region $x > x_0$. In classical mechanics, this is the region inaccessible to the particle. Thus we require the solution ϕ of the Schrodinger equation to vanish rapidly as x increases in this region. The WKB solution satisfying this requirement is

$$\phi_{WKB}(x) = \frac{e^{-\int_{x_0}^{x} \eta(x')dx'}}{\sqrt{\eta(x)}}. \tag{7.57}$$

We may choose the solution to be a constant times the right side of (7.57), but this affects only the overall normalization of the wavefunction and we will leave it the way it is. The WKB solution fails as we continue it to the neighborhood of the turning point x_0. When x is close to x_0, we approximate (7.50) by (7.54). The two independent solutions of (7.54) are the Airy functions denoted by $Ai(\rho)$ and $Bi(\rho)$, where

$$\rho = \Lambda^{2/3}(x - x_0). \tag{7.58}$$

Note that a region of x with width unity corresponds to a region of ρ with the width $\Lambda^{2/3}$. Since $\Lambda^{2/3}$ is a very large number, this region of ρ is a very large region. When we study the function in the variable ρ, it is like studying the function with a magnifier. Therefore, the small region in x given by (7.54), in which the Airy function solution is valid, is a large region in ρ.

As we will discuss in the next chapter, the asymptotic form of $Ai(\rho)$ when the magnitude of ρ is large is given by

$$Ai(\rho) \sim \frac{e^{-2\rho^{3/2}/3}}{2\sqrt{\pi}\,\rho^{1/4}}, \rho \to \infty, \tag{7.59}$$

$$\frac{\sin\left[\frac{2}{3}(-\rho)^{3/2} + \frac{\pi}{4}\right]}{\sqrt{\pi}\,(-\rho)^{1/4}}, \rho \to -\infty. \tag{7.60}$$

Since $Ai(\rho)$ vanishes exponentially when ρ is large and positive, it satisfies the requirement we impose on the wavefunction. Thus the wavefunction in the neighborhood of the turning point x_0 is

$$\phi(x) = cAi(\rho), \tag{7.61}$$

where c is a constant. To determine c, we match the solution (7.61) with the solution (7.57) in the overlapping region (7.56a) on the right side of x_0. We will not give the details of the matching

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process here. The result is that the solution in the neighborhood of the turning point x_0 is given by

$$\phi(x) = \frac{2\sqrt{\pi}}{\Lambda^{1/3}} Ai(\rho). \tag{7.62}$$

We use (7.62) to continue the solution to negative values of ρ. By (7.60), the solution (7.62) as ρ is negative and large is

$$\phi(x) \approx \frac{2}{\Lambda^{1/3}} \frac{\sin\left[\frac{2}{3}(-\rho)^{3/2} + \frac{\pi}{4}\right]}{(-\rho)^{1/4}}. \tag{7.63}$$

We find the WKB solution in the region $x < x_0$ by matching it with the solution (7.63). The matching is done in the overlapping region (7.56b). We find that the WKB solution valid for $x < x_0$ is

$$\frac{2\sin\left[\int_x^{x_0} p(x')dx' + \frac{\pi}{4}\right]}{\sqrt{p(x)}}. \tag{7.64}$$

With (7.57), (7.62) and (7.64), we have an approximate solution of the Schrodinger equation covering all values of x, when the equation has one turning point with $\alpha > 0$.

$$\frac{2\sin\left[\int_{x_1}^x p(x')dx' + \frac{\pi}{4}\right]}{\sqrt{p(x)}}, \tag{7.68}$$

which holds in the region $x > x_1$.