

Chapter 14

The WKB Method

The WKB method is useful to obtain approximate eigenenergies of bound states and approximate transmission coefficients for tunneling problems. Interestingly, eigenenergies and transmission coefficients are calculated without reference to a wave function or the Schrodinger equation for most applications. Using an assumed form of the wave function in the Schrodinger equation, the WKB method provides results which are independent of these.

The letters WKB stand for Wentzel of the U.S.A., Kramers of Holland, and Brillouin of France. In Holland, it is known as the KWB method, it is known as the BWK method in France¹, and in England, it is known as the JWKB method because Jeffries used a similar technique at an earlier time². The WKB method relates the Bohr-Sommerfeld quantization rules of old quantum theory with an approximate treatment of the Schrodinger equation. It is thus occasionally called the semi-classical approximation. The general mathematical technique dates back to Liouville in 1837, and was furthered by Lord Rayleigh in 1912.

The WKB method assumes a wave function of the form

$$\psi(x) = A(x)e^{iS(x)/\hbar} = A(x)e^{i\phi(x)},$$

where $A(x)$ is an amplitude and the quotient $S(x)/\hbar = \phi(x)$ is a phase. The quantity $S(x)$ is action which is the time integral of the Lagrangian. Action has dimensions of angular momentum. Where appropriate, using $\phi(x)$ simplifies notation and strengthens the association with phase. The functions $A(x)$ and $\phi(x)$ must be smooth functions of x .

In regions where the potential varies slowly with respect to the de Broglie wavelength, the approximation is very good. Said another way, when there are many oscillations of the wave function over a region where the potential is nearly constant, the WKB approximation is nearly exact. In still other words, the WKB approximation is good for higher excited states but generally lacks precision for the ground state and lower excited states.

The Schrodinger equation can be written

$$\begin{aligned} \mathcal{H}|\psi\rangle = E|\psi\rangle &\Rightarrow \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi = E\psi \\ &\Rightarrow \left[\frac{d^2}{dx^2} + \frac{2m(E - V(x))}{\hbar^2} \right] \psi = 0 \\ &\Rightarrow \left[\frac{d^2}{dx^2} + \frac{p^2}{\hbar^2} \right] \psi = 0, \end{aligned}$$

¹ Griffiths, *Introduction to Quantum Mechanics* (Prentice-Hall, Englewoods Cliffs, New Jersey, 1995), p. 274.

² Sakurai, *Modern Quantum Mechanics* (Addison-Wesley Publishing Company, Reading, Massachusetts, 1994), revised ed., p. 105.

where $p = p(x) = \sqrt{2m(E - V(x))}$. Using the assumed form of the wave function in this form of the Schrodinger equation,

$$\begin{aligned}
& \left[\frac{d^2}{dx^2} + \frac{p^2}{\hbar^2} \right] A(x) e^{iS(x)/\hbar} = 0 \\
\Rightarrow & \left[\frac{d^2}{dx^2} + \frac{p^2}{\hbar^2} \right] e^{iS(x)/\hbar} = 0 \\
\Rightarrow & \frac{d^2}{dx^2} e^{iS(x)/\hbar} + \frac{p^2}{\hbar^2} e^{iS(x)/\hbar} = 0.
\end{aligned} \tag{1}$$

The second derivative in the first term is

$$\begin{aligned}
\frac{d^2}{dx^2} e^{iS(x)/\hbar} &= \frac{d}{dx} e^{iS(x)/\hbar} \left(\frac{i}{\hbar} S'(x) \right) \\
&= e^{iS(x)/\hbar} \left(\frac{i}{\hbar} S'(x) \right)^2 + e^{iS(x)/\hbar} \left(\frac{i}{\hbar} S''(x) \right) \\
&= -\frac{[S'(x)]^2}{\hbar^2} e^{iS(x)/\hbar} + \frac{i}{\hbar} S''(x) e^{iS(x)/\hbar}.
\end{aligned}$$

Using this in equation (1),

$$\begin{aligned}
-\frac{[S'(x)]^2}{\hbar^2} e^{iS(x)/\hbar} + \frac{i}{\hbar} S''(x) e^{iS(x)/\hbar} + \frac{p^2}{\hbar^2} e^{iS(x)/\hbar} &= 0 \\
\Rightarrow -\frac{[S'(x)]^2}{\hbar^2} + \frac{i}{\hbar} S''(x) + \frac{p^2}{\hbar^2} &= 0.
\end{aligned} \tag{2}$$

We are now going to expand $S(x)$ in a power series in \hbar , *i.e.*,

$$S(x) = S_0(x) + \hbar S_1(x) + \frac{1}{2} \hbar^2 S_2(x) + \dots,$$

and keep only the first two terms, so

$$S(x) \approx S_0(x) + \hbar S_1(x).$$

Using this in equation (2),

$$\begin{aligned}
& -\frac{[(S_0(x) + \hbar S_1(x))']^2}{\hbar^2} + \frac{i}{\hbar} [S_0(x) + \hbar S_1(x)]'' + \frac{p^2}{\hbar^2} = 0 \\
\Rightarrow & -\frac{[S_0'(x) + \hbar S_1'(x)]^2}{\hbar^2} + \frac{i}{\hbar} [S_0''(x) + \hbar S_1''(x)] + \frac{p^2}{\hbar^2} = 0 \\
\Rightarrow & -\frac{(S_0')^2}{\hbar^2} - \frac{2\hbar S_1' S_0'}{\hbar^2} - \frac{\hbar^2 (S_1')^2}{\hbar^2} + \frac{i S_0''}{\hbar} + \frac{i \hbar S_1''}{\hbar} + \frac{p^2}{\hbar^2} = 0,
\end{aligned}$$

where both S_0 and S_1 are understood to be functions of x , and

$$\Rightarrow -\frac{(S_0')^2}{\hbar^2} - \frac{2S_1' S_0'}{\hbar} - (S_1')^2 + \frac{i S_0''}{\hbar} + i S_1'' + \frac{p^2}{\hbar^2} = 0$$

$$\Rightarrow \frac{iS_1'' - (S_1')^2}{\hbar^0} + \frac{iS_0'' - 2S_1'S_0'}{\hbar^1} + \frac{p^2 - (S_0')^2}{\hbar^2} = 0.$$

In order for the equation to be zero, the coefficient of each like power of \hbar must be zero, so

$$iS_1'' - (S_1')^2, \quad iS_0'' - 2S_1'S_0', \quad \text{and} \quad p^2 - (S_0')^2.$$

The last of these three equations tells us

$$\begin{aligned} (S_0')^2 = p^2 &\Rightarrow \frac{d}{dx}S_0 = \pm p \Rightarrow S_0 = \pm \int p(x) dx \\ &\Rightarrow S_0 = \pm \int \sqrt{2m(E - V(x))} dx, \end{aligned}$$

and this is the approximation of the action we will use in the assumed form of the wave function, *i.e.*,

$$\psi(x) = A(x)e^{\pm \frac{i}{\hbar} \int p(x) dx} = A(x)e^{\pm \frac{i}{\hbar} \int \sqrt{2m(E - V(x))} dx}.$$

We could use the center equation to solve for S_1 in terms of S_0' and thus express S_1 in terms of the momentum. It would tell us the wave function is inversely proportional to the square root of the momentum, which is interesting, but not particularly useful to us.

Of greater interest are the two primary applications of tunneling and bound states. Both are boundary value problems. Schiff,³ Griffiths,⁴ Bohm,⁵ and Mathews and Walker⁶ and others provide foundation for the results discussed here.

Result for Tunneling

Consider the three regions $x < 0$, $0 < x < L$, and $x > L$ as seen in figure 1. Figure 1 represents a rectangular potential barrier. Any potential barrier can similarly be divided into three regions. The wave functions may be written

$$\psi(x) = \begin{cases} A(x)e^{ikx} + B(x)e^{-ikx}, & \text{for } x < 0, \\ C(x)e^{\kappa x} + D(x)e^{-\kappa x}, & \text{for } 0 < x < L, \\ F(x)e^{ikx}, & \text{for } x > L, \end{cases}$$

where $k = \sqrt{2mE}/\hbar$ and $\kappa = \sqrt{2m(V_0 - E)}/\hbar$. We could write $\psi(x) = F(x)e^{ikx} + G(x)e^{-ikx}$, for $x > L$, but we would immediately recognize $G(x) = 0$ since it is the coefficient of an oppositely directed incident wave which is not physical. In terms of the WKB approximation, the wave functions are

$$\psi(x) = \begin{cases} A(x)e^{\frac{i}{\hbar} \int_{-\infty}^0 p(x) dx} + B(x)e^{-\frac{i}{\hbar} \int_{-\infty}^0 p(x) dx}, & \text{for } x < 0, \\ C(x)e^{\frac{i}{\hbar} \int_0^L p(x) dx} + D(x)e^{-\frac{i}{\hbar} \int_0^L p(x) dx}, & \text{for } 0 < x < L, \\ F(x)e^{\frac{i}{\hbar} \int_l^\infty p(x) dx}, & \text{for } x > L, \end{cases}$$

³ Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, New York, 1968), 3rd ed., pp. 268-279.

⁴ Griffiths, *Introduction to Quantum Mechanics* (Prentice-Hall, Englewood Cliffs, New Jersey, 1995), 3rd ed., pp. 280-291.

⁵ Bohm, *Quantum Theory* (Dover Publications, New York, 1979), pp. 264-295.

⁶ Mathews and Walker, *Mathematical Methods of Physics* (Benjamin/Cummings Publishing Company, Menlo Park, California, 1970), 3rd ed., pp. 27-37.

The amplitude of the incoming incident wave is $A(x)$ and the amplitude of the portion which tunnels through the barrier is $F(x)$. The transmission coefficient is

$$T = \frac{|F|^2}{|A|^2}.$$

If the barrier was infinite, a step function, $C(x) = 0$, the exponentially increasing portion of the wave function would be unbounded, so would be non-physical. Similarly, if we expect a small transmission, then the ratio of the incident wave and the transmitted wave would be dominated by the decreasing exponential, or

$$\frac{|F|}{|A|} \approx e^{-\frac{1}{\hbar} \int_0^L p(x) dx} \quad \text{so}$$

$$T = \frac{|F|^2}{|A|^2} \approx e^{-\frac{2}{\hbar} \int_0^L p(x) dx} = e^{-2\gamma} \quad \text{where} \quad \gamma = -\frac{1}{\hbar} \int_0^L p(x) dx. \quad (3)$$

This is simply a feasibility argument. To solve the problem properly, we would have to use the fact the wave functions and their first derivatives must be equal at the boundaries. Problem 19-1 is similar to this. Exceptions are to solve this problem, we would need to retain the integral form of the WKB wave function, and consider that the wave function is inversely proportional to the square root of the momentum. At this point, we are interested solely in the result denoted in equation (3),

$$T \approx e^{-2\gamma}.$$

Incidentally,

$$\gamma = \frac{1}{\hbar} \int_{x_1}^{x_2} |p(x')| dx'$$

where x_1 and x_2 define the boundaries of the barrier, is called the integral of the action under the barrier.

Bound States

Figure 2 illustrates an excited state in an arbitrary potential. Notice in the central region, the wave function oscillates rapidly compared to the variation in the potential. In this region, the wave function is nearly exactly that provided by the WKB approximation. The wave function must go to zero outside the walls of the potential, so we can ascertain the wave function by its asymptotic behavior in those regions. In the regions near the boundaries of the potential, near the classical turning points, the WKB approximation is poor. Where the wave functions have the least oscillation compared to the variation of the potential, the WKB approximation is poorest. Ground states

and low quantum number excited states have little oscillation, so the WKB approximation works least well with them.

We can, nevertheless, obtain an approximation by connecting the wave function inside the well with the asymptotic wave forms outside the well, which is still a good approximation for excited states. Though it is often a good approximation for all energies, we expect increasing inaccuracy as the ground state is approached.

Connection formulas are based on an approximation to the potential function at the classical turning points. Near the classical turning point x_1 ,

$$V(x) \approx V(x_1) + V'(x_1)(x - x_1).$$

The calculation is simplified if we let the location of the classical turning point be zero, *i.e.*, $x_1 = 0$, so

$$\begin{aligned} V(x) &\approx V(0) + V'(0)x \\ &= E + V'(0)x. \end{aligned}$$

where $V(0) = E$ precisely at the boundary; the energy associated with the wave function is the same as the potential where the wave function intersects it. The Schrodinger equation for this potential is

$$\begin{aligned} &\left[\frac{d^2}{dx^2} + \frac{2m}{\hbar^2}[E - V(0)] \right] \psi = 0 \\ \Rightarrow &\left[\frac{d^2}{dx^2} + \frac{2m}{\hbar^2}[E - E - V'(0)x] \right] \psi = 0 \\ \Rightarrow &\left[\frac{d^2}{dx^2} - \frac{2m}{\hbar^2}[V'(0)x] \right] \psi = 0 \\ \Rightarrow &\left[\frac{d^2}{dx^2} - \alpha^3 x \right] \psi = 0 \quad \text{where} \quad \alpha = \left(\frac{2m}{\hbar^2} V'(0) \right)^{1/3}. \end{aligned}$$

Changing variables where $y = \alpha x \Rightarrow x = \frac{1}{\alpha}y$, so

$$\begin{aligned} \frac{d^2}{dx^2} &= \left(\frac{d}{dy} \frac{dy}{dx} \right) \left(\frac{d}{dy} \frac{dy}{dx} \right) = \left(\frac{d}{dy} \alpha \right) \left(\frac{d}{dy} \alpha \right) = \alpha^2 \frac{d^2}{dy^2} \\ \Rightarrow &\left[\alpha^2 \frac{d^2}{dy^2} - \alpha^3 \frac{1}{\alpha} y \right] \psi = 0 \\ \Rightarrow &\left[\frac{d^2}{dy^2} - y \right] \psi = 0. \end{aligned}$$

This is Airy's equation and its solutions are Airy functions $Ai(y)$ and $Bi(y)$. The $Bi(y)$ are unbounded for large y , so are often not useful to describe a physical system. The Airy functions are the basis for general connection formulas. Abramowitz and Stegun⁷ provide both commentary on Airy functions and tabular data.

⁷ Abramowitz and Stegun, *Handbook of Mathematical Functions* (Dover Publications, inc., New York, 1972), pp. 446-454 and 475-478.

The WKB wave function at the right potential wall is

$$\psi(x) = \begin{cases} A(x)e^{\frac{i}{\hbar} \int_0^{x_2} p(x') dx'} + B(x)e^{-\frac{i}{\hbar} \int_0^{x_2} p(x') dx'}, & \text{for } x < x_2, \\ C(x)e^{-\frac{i}{\hbar} \int_{x_2}^{\infty} p(x') dx'}, & \text{for } x > x_2 \end{cases}$$

where x_2 is now defined as the classical turning point. The top case is inside the potential. We could refine the form of the wave function outside the potential by examining its asymptotic form, and equate the two at x_2 , the right boundary wall. We could then repeat the procedure for the left boundary wall, and have two equations with three unknowns, the unknowns being $A(x)$, $B(x)$, and $C(x)$. We could solve these in terms of $C(x)$ and obtain

$$A(x) = -ie^{i\pi/4}C(x), \quad B(x) = ie^{-i\pi/4}C(x).$$

We could use these in the equations for the wave function inside the right potential wall and obtain

$$\psi(x) = \begin{cases} 2C(x) \sin \left[\frac{1}{\hbar} \int_0^{x_2} p(x') dx' + \frac{\pi}{4} \right], & \text{for } x < x_2, \\ C(x)e^{-\frac{i}{\hbar} \int_{x_2}^{\infty} p(x') dx'}, & \text{for } x > x_2 \end{cases}$$

Now suppose the potential had a vertical wall, an impermeable barrier, at $x = 0$, and a soft or permeable non-vertical wall at the right boundary $x = x_2$. The boundary condition at $x = 0$ dictates that $\psi(0) = 0$,

$$\begin{aligned} \Rightarrow \sin \left[\frac{1}{\hbar} \int_0^{x_2} p(x') dx' + \frac{\pi}{4} \right] &= 0 \\ \Rightarrow \frac{1}{\hbar} \int_0^{x_2} p(x') dx' + \frac{\pi}{4} &= n\pi, \quad n = 1, 2, 3, \dots \end{aligned}$$

$$\Rightarrow \int_0^{x_2} p(x') dx' = \left(n - \frac{1}{4} \right) \pi \hbar \quad \text{for one permeable wall.}$$

Examples of systems with one permeable wall are the half harmonic oscillator and the quantum mechanical bouncing ball.

If the potential has two non-vertical walls, two soft or permeable walls as would most real potentials, we would still expect the sine function to be zero at the center, $x = 0$. This is equivalent to having two adjacent potentials with one permeable wall with their vertical walls in the center, so

$$\int_{x_1}^{x_2} p(x') dx' = \left(n - \frac{1}{2} \right) \pi \hbar \quad \text{for two permeable walls,}$$

where x_1 and x_2 are the classical turning points.

If neither wall is permeable, for instance in an infinite square well,

$$\int_{x_1}^{x_2} p(x') dx' = n\pi\hbar \quad \text{for two impermeable walls,}$$

As promised, notice there is no reference to a wave function or the Schrodinger equation in any of the boxed equations; the equations you will actually use.

The Bohr-Sommerfeld (on occasion the Bohr-Wilson or Wilson-Sommerfeld) quantization condition is

$$\oint p dq = nh.$$

The difference in this and the WKB results is the phase change in the action by the amount $\pi/4$ at a boundary. Landau and Lifshitz⁸ considers this difference so cosmetic that they include the appropriate phase changes in their discussion of the Bohr-Sommerfeld quantization condition.

A roadmap for using the WKB approximation for bound states is
 step 1) determine the classical turning points,
 step 2) evaluate the integral

$$\int_{x_1}^{x_2} p(x') dx' = \int_{x_1}^{x_2} \sqrt{2m(E - V(x'))} dx',$$

step 3) equate the result to the correct quantization condition.

Applying the WKB method to a particle in a one dimensional box of width $2L$, (step 1) the turning points are at $-L$ and L , (step 2) the integral of interest is

$$\int_{-L}^L p(x') dx' = \int_{-L}^L \sqrt{2m(E - V(x'))} dx' = \int_{-L}^L \sqrt{2m(E)} dx'$$

if we define the floor of the box to be $V(x) = 0$. Then

$$\int_{-L}^L p(x') dx' = \sqrt{2m(E)} \int_{-L}^L dx' = \sqrt{2m(E)} \Big|_{-L}^L = 2L\sqrt{2m(E)}.$$

(step 3) Equate this result to the quantization condition for two impermeable walls,

$$2L\sqrt{2m(E)} = n\pi\hbar \Rightarrow \sqrt{2m(E)} = \frac{n\pi\hbar}{2L} \Rightarrow 2mE = \frac{n^2\pi^2\hbar^2}{4L^2}$$

$$\Rightarrow E = \frac{n^2\pi^2\hbar^2}{8mL^2}$$

which are the same eigenenergies as we obtained in chapter 6. The WKB method gives exact eigenenergies here because the exponential WKB wave function models sinusoidal waves, as exist for the particle in a box, exactly.

⁸ Landau and Lifshitz, *Quantum Mechanics* (Pergamon Press, Oxford, 1977), pp 170-175.