

WKB

The WKB method solves the Schrödinger equation by a series of successive approximations. It is named after Wentzel, Kramers, and Brillouin who all three developed the method in 1926, also the year that Schrödinger debuted his equation.

The method is motivated by the simple general oscillating wave solution

$$\psi(x) = a_+ e^{\frac{i}{\hbar} \sqrt{2m(E-V)}x} + a_- e^{-\frac{i}{\hbar} \sqrt{2m(E-V)}x},$$

to

$$-\frac{\hbar^2}{2m} \psi'' + V\psi = E\psi,$$

for V constant. When V is not constant, one looks for solutions having roughly the same form, with the expectation that these will be more accurate when V is slowly varying relative to the oscillations of the waves. In modern mathematical semiclassical analysis it is common to put $\hbar = \hbar/\sqrt{2m}$ to simplify notation, while keeping track of the parameter $\hbar$. We generally suppose $\hbar$ to be small, although we will see that this is not always a must.

We thus take the ansatz

$$\psi_{approx}(x) = a(x) e^{i\varphi(x)/\hbar},$$

which leads to

$$\left(-\hbar^2 \frac{d^2}{dx^2} + V - E \right) a e^{i\varphi/\hbar} = \left(((\varphi')^2 + V - E)a - i\hbar(2\varphi'a' + \varphi''a) - \hbar^2 a'' \right) e^{i\varphi/\hbar},$$

where we have grouped the terms according to powers of $\hbar$. We eliminate the leading term by defining the phase φ to be

$$\varphi = \int \sqrt{E - V}.$$

(We do not worry about the choice of antiderivative, as any two differ by a constant, which just leads to an overall constant factor in front of ψ , but note that the two choices of square root lead to genuinely different solutions.) We eliminate the second term by putting $a = 1/\sqrt{\varphi'}$. Writing in terms of the classical momentum $p(x) = \sqrt{E - V(x)}$, we have obtained that

$$\psi_{approx}(x) = \frac{1}{\sqrt{p(x)}} e^{\frac{i}{\hbar} \int^x \sqrt{p}} e^{i\varphi/\hbar}$$

obeys

$$\left(-\hbar^2 \frac{d^2}{dx^2} + V - E \right) \psi_{approx} = -\hbar^2 \frac{a''}{a} \psi_{approx}.$$

The above calculation was motivated in the setting where $E > V(x)$, but works just as well if $E < V(x)$. Then it is more natural to use $a e^{\varphi/\hbar}$, with $(\varphi'(x))^2 = V(x) - E$, and still $a = 1/\sqrt{\varphi'}$.

1. Remainders in the forbidden region. To deal with the remainders we use Olver's technique, from Chapter 6 of *Asymptotics and Special Functions*. The method is the same in the forbidden and allowed regions, but we focus on the former for definiteness and because this is what we will mainly use later. Suppose V is twice continuously differentiable, and we wish to get a good formula, with control of the remainder, for appropriate particular solutions of

$$-h^2\psi'' + V\psi = E\psi$$

in a (possibly infinite) interval (A_1, A_2) in which $V(x) > E$. Motivated by the above calculation, define a function u by

$$\psi = au, \text{ where } a(x) = (V(x) - E)^{-1/4}, \quad \varphi(x) = \int_{x_0}^x \sqrt{V - E},$$

and where u is a function of the variable φ , i.e. $u = u(\varphi(x))$; this variable is legitimate because φ' is always positive. Let (B_1, B_2) be the interval in φ corresponding to (A_1, A_2) in x . The point is to make the most important part of the solution, the exponential part, as simple as possible. Using prime to continue to denote differentiation with respect to x , and a subscript φ to denote differentiation with respect to φ , we have

$$\psi' = a'u + au_\varphi\varphi', \quad \psi'' = a''u + 2a'u_\varphi\varphi' + au_{\varphi\varphi}(\varphi')^2 + au_\varphi\varphi''.$$

Since $a^2\varphi' = 1$, we have $2aa'\varphi' + a^2\varphi'' = 0$ and the u_φ terms on the right cancel, giving

$$\psi'' = a''u + au_{\varphi\varphi}(\varphi')^2.$$

Hence, rearranging terms shows that

$$-h^2\psi'' + V\psi = E\psi \quad \Longleftrightarrow \quad u_{\varphi\varphi} - h^{-2}u = -a^3a''u.$$

Now define r by

$$u(\varphi) = e^{\varphi/h}(1 + r(\varphi)),$$

which leads to

$$u_{\varphi\varphi} - h^{-2}u = -a^3a''u \quad \Longleftrightarrow \quad r_{\varphi\varphi} + 2h^{-1}r_\varphi = -a^3a''(1 + r),$$

or, using an integrating factor,

$$(e^{2\varphi/h}r_\varphi)_\varphi = -e^{2\varphi/h}a^3a''(1 + r). \quad (1.1)$$

We now integrate, choosing endpoints to make the integrand as small as possible:

$$e^{2\varphi/h}r_\varphi = \int_{B_1}^\varphi e^{2\alpha/h}[-a^3a''(1 + r)](\alpha) d\alpha,$$

and

$$r(\varphi) = \int_{B_1}^\varphi e^{-2\beta/h} \int_{B_1}^\beta e^{2\alpha/h}[-a^3a''(1 + r)](\alpha) d\alpha d\beta = \int_{B_1}^\varphi (1 - e^{2(\alpha-\varphi)/h})[-\frac{h}{2}a^3a''(1 + r)](\alpha) d\alpha,$$

where we simplified by changing the order of integration or integrating by parts. We then transform back to the x variables and get

$$r(\varphi(x)) = -\frac{h}{2} \int_{A_1}^x \left(1 - e^{-\frac{2}{h} \int_y^x \sqrt{V-E}}\right) a(y)a''(y)(1 + r(\varphi(y))) dy. \quad (1.2)$$

EXERCISE 1.3. Verify the steps leading up to (1.2).

We now solve this by iteration. Let $K(x, y) = -\frac{h}{2} \left(1 - e^{-\frac{2}{h} \int_y^x \sqrt{V-E}}\right) a(y) a''(y)$,

$$r_1(x) = \int_{A_1}^x K(x, y) dy, \quad r_{n+1}(x) = \int_{A_1}^x K(x, y) r_n(y) dy.$$

Adding the equations shows that

$$r(\varphi(x)) := \sum_{n=1}^{\infty} r_n(x) \quad (1.4)$$

solves (1.2), provided the infinite sum converges, and switching the order of sum and integral is correct. Using

$$0 \leq 1 - e^{-\frac{2}{h} \int_y^x \sqrt{V-E}} \leq 1 \quad (1.5)$$

and setting

$$\varepsilon(x) := \frac{h}{2} \int_{A_1}^x a(y) |a''(y)| dy,$$

yields

$$|r_1(x)| \leq \varepsilon(x), \quad |r_{n+1}(x)| \leq \varepsilon(x) \sup_{(A_1, A_2)} |r_n|.$$

Thus we have $|r_n(x)| \leq \varepsilon^n$ for all n and for all x in (A_1, A_2) , and the sum in (1.4) converges as least geometrically fast whenever $\varepsilon(x) < 1$, and switching the order of sum and integral is then justified by the dominated convergence theorem, provided $\sup_{x \in (A_1, A_2)} \varepsilon(x) < 1$.

Summing up, we have proved:

THEOREM 1.6. *Let E be a real number, $h > 0$, and V a twice continuously differentiable function on a (possibly infinite) interval (A_1, A_2) such that $V(x) > E$ for all x in (A_1, A_2) . Let*

$$a(x) = (V(x) - E)^{-1/4}, \quad \varphi(x) = \int_{x_0}^x \sqrt{V-E}, \quad \varepsilon(x) := \frac{h}{2} \int_{A_1}^x a |a''|,$$

where x_0 is any point in (A_1, A_2) . If

$$\sup_{x \in (A_1, A_2)} \varepsilon(x) < 1,$$

Then there is a solution ψ of

$$-h^2 \psi'' + V\psi = E\psi$$

on (A_1, A_2) such that

$$\psi(x) = a(x) e^{\varphi(x)/h} (1 + R(x)),$$

where

$$|R(x)| \leq \frac{\varepsilon(x)}{1 - \varepsilon(x)}$$

for all x in (A_1, A_2) .

Note that, as long as the integral defining $\varepsilon(x)$ converges, we have $\varepsilon(x) \rightarrow 0$ as $x \rightarrow A_1$, and so $R(x)$ is always a small remainder at least for x near A_1 , even if it becomes large as x grows.

EXERCISE 1.7. Let ψ be the solution given by Theorem 1.6, and let $\tilde{\psi}$ be the solution given by the same theorem, but where we replace x_0 by another point $\tilde{x}_0$ in (A_1, A_2) . How are ψ and $\tilde{\psi}$ related?

EXERCISE 1.8. Use a change of variables $x \mapsto -x$ (or redo the whole argument for practice) to get a similar result about a solution of the form

$$\psi(x) = a(x) e^{-\varphi(x)/h} (1 + r(\varphi(x))).$$

EXERCISE 1.9. Let $V \in C^2(\mathbb{R})$, $E < \inf V$, $a = (V - E)^{-1/4}$. Verify that $\int_{-\infty}^{\infty} a|a''|$ converges in one or more of the following cases:

- (1) V is a polynomial,
- (2) V is a rational function,
- (3) V is an *elliptic symbol*, in the sense that there are real constants m and C such that
 - $|V(x)| \leq C(1 + |x|^m)$, $|V'(x)| \leq C(1 + |x|^{m-1})$, $|V''(x)| \leq C(1 + |x|^{m-2})$, for all x ,
 - and $|V(x)| \geq |x|^m/C$ for $|x|$ sufficiently large.

(Note that each case includes the previous. You may also enjoy coming up with a still more general case that includes all of these.)

EXERCISE 1.10. What happens to (1.5) if alternate endpoints are used in the integration steps which go from (1.1) to (1.2)?

EXERCISE 1.11. Prove a similar but more complicated bound for $R'(x)$. Why is it superfluous to go on and prove such bounds for higher derivatives of R ?

EXERCISE 1.12. Prove an analogous theorem for the case where $V(x) < E$ for all x in (A_1, A_2) . The proof is very similar, although the exponents are now imaginary rather than real. Pay attention to how the issues of Exercise 1.10 play out in this case.