# WKB APPROXIMATION

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 8.1.

We now look at another approximation technique used in quantum mechanics. This is the WKB (named for the German physicist Gregor Wentzel (1898 - 1978), the Dutch physicist Hendrik Kramers (1894 - 1952) and the French physicist Léon Brillouin (1889 - 1969)) approximation, which is a mathematical technique applicable to one-dimensional differential equations.

We'll start with the usual one-dimensional time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V(x)\psi=E\psi \tag{1}$$

and rewrite it as

$$\frac{d^2\psi}{dx^2} = -\frac{2m[E-V(x)]}{\hbar^2}\psi \tag{2}$$

$$\equiv -\frac{p^2}{\hbar^2}\psi \tag{3}$$

where $p=\sqrt{2m[E-V(x)]}$ is the classical formula for the momentum of a particle with total energy $E$ moving in a one-dimensional potential $V(x)$, provided we assume $E\ge V(x)$ for all $x$.

In general, the wave function $\psi(x)$ is a complex function so we can write it in complex exponential form as

$$\psi(x)=A(x)e^{i\phi(x)} \tag{4}$$

where $A(x)$ is the amplitude and $\phi(x)$ is the phase, both of which are real functions. In this form, we have (using a prime to denote a derivative with respect to $x$):

$$\psi' = \left(A' + iA\phi'\right)e^{i\phi} \tag{5}$$

$$\psi'' = \left(A'' + iA'\phi' + iA\phi'' + iA'\phi' - A\left(\phi'\right)^2\right)e^{i\phi} \tag{6}$$

$$= \left(A'' + 2iA'\phi' + iA\phi'' - A\left(\phi'\right)^2\right)e^{i\phi} \tag{7}$$

Inserting this into 3 and cancelling off $e^{i\phi}$ we get

$$A'' + 2iA'\phi' + iA\phi'' - A\left(\phi'\right)^2 = -\frac{p^2}{\hbar^2}A \tag{8}$$

Everything in this equation is real apart from $i$ itself, so we can separate this equation into its real and imaginary parts to get two differential equations:

$$A'' - A\left(\phi'\right)^2 = -\frac{p^2}{\hbar^2}A \tag{9}$$

$$2A'\phi' + A\phi'' = 0 \tag{10}$$

The second of these equations can always be solved as

$$2A'\phi' + A\phi'' = \frac{1}{A}\left[A^2\phi'\right]' = 0 \tag{11}$$

$$\left[A^2\phi'\right]' = 0 \tag{12}$$

$$A^2\phi' = C^2 \tag{13}$$

where $C$ is a constant, which may be complex (since $\phi'$ could be negative). We can therefore write the amplitude as

$$A(x) = \frac{C}{\sqrt{\phi'}} \tag{14}$$

We've taken the positive square root, since any difference in sign can be accounted for by changing the integration constant $C$.

Equation 9 can't be solved in general since it depends on $V(x)$ which could in principle be anything. However, we can rewrite it as

$$\frac{A''}{A} = \left(\phi'\right)^2 - \frac{p^2}{\hbar^2} \tag{15}$$

This is where the approximation comes in. If $V(x)$ were constant then we can solve the Schrödinger equation exactly (as we did with the finite square well and finite square barrier). If $E > V$ we get a travelling wave with a constant amplitude $A$ and constant wavelength $\lambda = 2\pi\hbar/p$, while if $E < V$ we get an exponential decay with a characteristic decay length of $\ell = \hbar/\sqrt{2m[V(x)-E]}$. Now suppose that $V(x)$ is not constant, but that it varies slowly compared to either $\lambda$ or $\ell$. In this case, we'd expect that the wave function is close to $\psi$ for a constant potential, except that its amplitude and phase will vary slightly. The approximation comes by assuming that the variation in amplitude is small enough that the derivatives of $A(x)$ are negligible compared to $A(x)$ itself. That is, we can set the LHS of 15 to zero, which allows us to write down a solution of the RHS:

$$\phi' = \pm\frac{p}{\hbar} \tag{16}$$

$$\phi(x) = \pm\frac{1}{\hbar}\int p\,dx \tag{17}$$

This is written as an indefinite integral, since the constant of integration ($K$ say) can be absorbed into $C$:

$$\phi(x) = \pm\frac{1}{\hbar}\int p\,dx + K \tag{18}$$

$$\psi(x) = A(x)\,e^{i\phi(x)} \tag{19}$$

$$= \frac{C}{\sqrt{\phi'}}e^{iK}e^{\pm i\int p\,dx/\hbar} \tag{20}$$

$$= \frac{C\sqrt{\hbar}e^{iK}}{\sqrt{p(x)}}e^{\pm i\int p\,dx/\hbar} \tag{21}$$

$$= \frac{C_1}{\sqrt{p(x)}}e^{\pm i\int p\,dx/\hbar} \tag{22}$$

where

$$C_1 \equiv C\sqrt{\hbar}e^{iK} \tag{23}$$

The WKB approximation for the wave function is thus

$$\boxed{\psi(x) \approx \frac{C_1}{\sqrt{p(x)}}e^{\pm i\int p\,dx/\hbar}} \tag{24}$$

Provided we can do the integral in the exponent, we can find the wave function and, by imposing boundary conditions, we can often find the allowed energies as well.

**Example.** We have an infinite square well with a shelf in the well, with the potential given by

$$V(x)=\begin{cases}V_0 & 0<x<\frac{a}{2}\\ 0 & \frac{a}{2}<x<a\\ \infty & x<0 \text{ or } x>a\end{cases} \tag{25}$$

The classical momentum is

$$p(x)=\begin{cases}\sqrt{2m(E-V_0)} & 0<x<\frac{a}{2}\\ \sqrt{2mE} & \frac{a}{2}<x<a\end{cases} \tag{26}$$

so we have

$$\int_0^x p\,dx'=\begin{cases}x\sqrt{2m(E-V_0)} & 0<x<\frac{a}{2}\\ \frac{a}{2}\sqrt{2m(E-V_0)}+\left(x-\frac{a}{2}\right)\sqrt{2mE} & \frac{a}{2}<x<a\end{cases} \tag{27}$$

We've put limits on the integral with the understanding that any constant of integration is absorbed into the overall constant that multiplies the amplitude. This constant will be determined by normalization as usual.

We thus have

$$\phi(x)=\begin{cases}\pm\frac{x}{\hbar}\sqrt{2m(E-V_0)} & 0<x<\frac{a}{2}\\ \pm\frac{1}{\hbar}\left[\frac{a}{2}\sqrt{2m(E-V_0)}+\left(x-\frac{a}{2}\right)\sqrt{2mE}\right] & \frac{a}{2}<x<a\end{cases} \tag{28}$$

We can now write the wave function as

$$\psi(x)=\begin{cases}\frac{1}{[2m(E-V_0)]^{1/4}}\left(C_+e^{i\phi(x)}+C_-e^{-i\phi(x)}\right) & 0<x<\frac{a}{2}\\ \frac{1}{[2mE]^{1/4}}\left(C_+e^{i\phi(x)}+C_-e^{-i\phi(x)}\right) & \frac{a}{2}<x<a\end{cases} \tag{29}$$

where the constants $C_+$ and $C_-$ can be determined from boundary conditions and normalization as usual. (Actually, it's worth pointing out here that although $\phi(x)$ is continuous at $x=\frac{a}{2}$, the WKB wave function $\psi(x)$ is *not* continuous at this point. This violates one of the central conditions imposed on wave functions. The discontinuity arises from the discontinuity in the potential at this point, which violates one of the assumptions of WKB theory: that the potential varies slowly. Thus at the boundaries, the WKB assumptions don't hold, so it's a bit surprising that WKB gives a reasonable result for this problem since there are infinite discontinuities at $x = 0$ and $x = a$.)

To get the allowed energies, we can impose continuity at the end points of the well. That is

$$\psi(0) = \psi(a) = 0 \tag{30}$$

To use this condition, it's easier to write the wave function using trigonometric functions:

$$\psi(x) = \begin{cases} \frac{1}{[2m(E-V_0)]^{1/4}}\left(C_1 \sin\phi(x) + C_2\cos\phi(x)\right) & 0 < x < \frac{a}{2} \\ \frac{1}{[2mE]^{1/4}}\left(C_1 \sin\phi(x) + C_2\cos\phi(x)\right) & \frac{a}{2} < x < a \end{cases} \tag{31}$$

The condition $\psi(0) = 0$ gives us $C_2 = 0$ while the other condition $\psi(a) = 0$ tells us

$$\sin(\phi(a)) = 0 \tag{32}$$

$$\phi(a) = n\pi \tag{33}$$

$$\left[\sqrt{2m(E_n - V_0)} + \sqrt{2mE_n}\right]\frac{a}{2\hbar} = n\pi \tag{34}$$

Doing a bit of algebra we get

$$E - \frac{V_0}{2} + \sqrt{E(E-V_0)} = \frac{n^2\pi^2\hbar^2}{ma^2} \tag{35}$$

The quantity on the RHS is twice the allowed energies $E_n^0$ of the ordinary infinite square well. Solving this for $E$ we get

$$E = E_n^0 + \frac{V_0}{2} + \frac{V_0^2}{16E_n^0} \tag{36}$$

Griffiths shows in his Example 6.1 that first-order perturbation theory gives a result of

$$E = E_n^0 + \frac{V_0}{2} \tag{37}$$

This agrees with the WKB result when $V_0 \ll E_n^0$, which occurs either when the height of the shelf is very small, or when $E_n^0$ is very large; the latter case occurs when $n$ is large and we're approaching the classical zone.

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