WKB and Schrödinger's Equation for the Harmonic Oscillator

Consider the Sturm-Liouville type eigenvalue problem:

$$y'' + (\lambda - V(x))y = 0, \quad y \to 0 \text{ as } x \to \pm\infty, \tag{13.1}$$

where λ is an unknown eigenvalue and $V(x)$ is a specified function which goes to ∞ as $x \to \pm\infty$. For simplicity we'll assume $V(x)$ is smooth and has a single minimum. In general, (13.1) has a countably infinite set of eigenvalues $\lambda_v >> 1$ and corresponding eigenfunctions $y_n(x)$. This eigenvalue problem arises in numerous contexts, including in calculating eigenfunctions and energy states of the steady-state 1D Schrödinger equation, for which λ is proportional to the total energy, and $V(x)$ is proportional to a specified potential energy. For instance $V(x) = x^2$ is the potential energy of a harmonic oscillator such as a spring displaced a distance x from its rest position.

WKB theory can give excellent approximations to large eigenvalues $\lambda_v >> 1$ of (13.1) and their corresponding eigenfunctions $y_n(x)$. The approach is to pick an arbitrary λ and find a *quantization condition* on λ under which there is a WKB solution to (13.1) that obeys both BCs, which will then be the approximate eigenfunction

WKB asymptotics are accurate where $1 \gg \left|\dfrac{(\lambda - V(x))'}{(\lambda - V(x))^{3/2}}\right|$. If λ >> 1, this will hold for all x away from left and right turning points x_L and x_R where $V(x) = \lambda$. For $x < x_L$ and $x > x_R$, the solution is evanescent (exponentially growing/decaying). For $x_L < x < x_R$, the WKB solution is oscillatory. Defining the local wavenumber $m(z) = \left(\lambda - V(x)\right)^{1/2}$, it must be a linear combination of the two fundamental WKB solutions: (13.2)

$$y_{WKB}(x) = ay^+(x;x_L) + by^-(x;x_L) \quad \text{for } x_L < x < x_R$$

where $y^\pm(x;x_t) = |m(x)|^{-1/2} \exp\left\{\pm i\varepsilon^{-1}\int_{x_t}^{x} m(\zeta)d\zeta\right\}$. Note we have arbitrarily used the left turning point as the starting point for the phase integral.

We now implement the BCs using the WKB turning point formulas. We start at x_L, using (12.6):

$$y \text{ decaying for } x < x_L \quad \Rightarrow \quad y_{WKB}(x) = a\left\{y^+(x;x_L) + iy^-(x;x_L)\right\} \text{ for } x > x_L \quad \Rightarrow \quad b = ia \tag{13.3}$$

We've chosen the arbitrary constant in this formula to match the arbitrary constant in (13.2). The other turning point formula (12.5) is:

$$y \text{ decaying for } x > x_R \quad \Rightarrow \quad y_{WKB}(x) = c_R\left\{y^+(x;x_R) - iy^-(x;x_R)\right\} \text{ for } x < x_R \tag{13.4}$$

To use it, we note that

$$\int_{x_R}^{x} m(\zeta)d\zeta = \int_{x_L}^{x} m(\zeta)d\zeta - \alpha, \quad \text{where } \alpha = \int_{x_L}^{x_R} m(\zeta)d\zeta,$$

so

$$y^{\pm}(x;x_R) = |m(x)|^{-1/2}\exp\left\{\pm i\int_{x_R}^{x} m(\zeta)d\zeta\right\} = |m(x)|^{-1/2}\exp\left\{\pm i\left(\int_{x_L}^{x} m(\zeta)d\zeta - \alpha\right)\right\} = e^{\mp i\alpha}y^{\pm}(x;x_L)$$

so (13.4) is equivalent to

$$y_{WKB}(x) = c\left\{y^{+}(x;x_L)e^{-i\alpha} - iy^{-}(x;x_L)e^{i\alpha}\right\} \quad \Rightarrow \quad ce^{-i\alpha} = a, -ice^{i\alpha} = b \quad \Rightarrow \quad b = -ie^{2i\alpha}a \quad (13.5)$$

For both turning point conditions (13.3) and (13.5) to be consistent, $e^{2i\alpha} = -1 = e^{i\pi(2n+1)}$, which gives the *quantization condition*

$$\alpha = \int_{z_L}^{z_R}\left[\lambda - V(x)\right]^{1/2}d\zeta = (n+\frac{1}{2})\pi \quad (13.6)$$

whose solutions are the eigenvalues λ_n. Because it is derived from WKB, it is asymptotically accurate for large λ, i. e. for $n >> 1$. It is remarkable how elegantly WKB exposes the basic structure of this eigenvalue problem!

As a specific example, consider the harmonic oscillator potential $V(x) = x^2$. In this case, the turning points are $x_{L,R} = \pm\lambda^{1/2}$ and

$$\alpha = \int_{-\lambda^{1/2}}^{\lambda^{1/2}}\left[\lambda - \zeta^2\right]^{1/2}d\zeta$$

Using the substitution $\zeta = \lambda^{1/2}\cos\theta$,

$$\alpha = \lambda\int_{\pi}^{0}\sin\theta(-\sin\theta\, d\theta) = \lambda\pi/2 = (n+\frac{1}{2})\pi \quad \Rightarrow \quad \lambda_n = 2n+1 \quad (13.7)$$

Remarkably, for this problem, this approximation proves to be exactly correct for all $n = 0, 1, 2, \ldots$! The corresponding WKB eigenfunction in the oscillatory region is

$$y_{WKB}(x) = a\left\{y^{+}(x;x_L) + iy^{-}(x;x_L)\right\} = am^{-1/2}\left\{\exp(i\phi) + i\exp(-i\phi)\right\} \quad (13.8)$$

where, defining $\xi = \cos^{-1}(x/\lambda^{1/2})$,

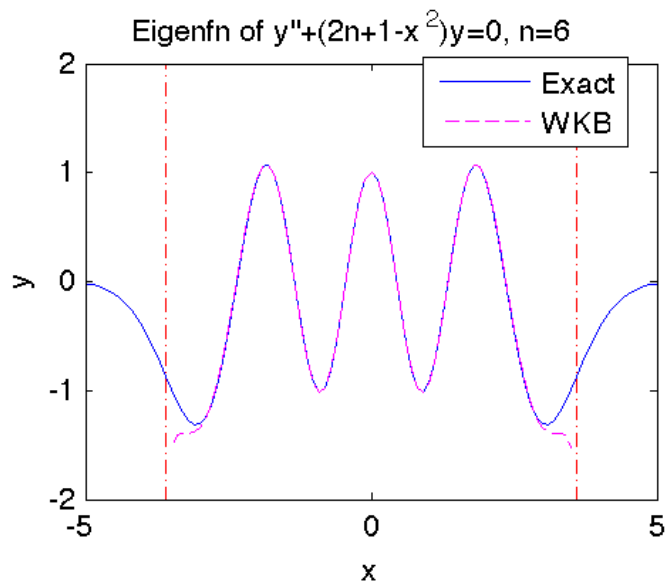
$$\phi(x) = \int_{-\lambda^{1/2}}^{x}\left[\lambda - \zeta^2\right]^{1/2}d\zeta = \lambda\int_{\pi}^{\xi}\sin\theta(-\sin\theta\, d\theta) = \lambda\left[-\frac{\theta}{2} + \frac{\sin 2\theta}{4}\right]_{\pi}^{\xi} = \lambda\left[\frac{\pi-\xi}{2} + \frac{\sin 2\xi}{4}\right]$$

To normalize $y_{WKB}(x)$ to be real, set $a = Ae^{-i\pi/4}/2$ in (13.8). Then

$$y_{WKB}(x) = \frac{A}{2} e^{-i\pi/4} m^{-1/2} \left\{ e^{i\phi} + ie^{-i\phi} \right\} = Am^{-1/2} \left\{ \frac{e^{i(\phi-\pi/4)} + e^{-i(\phi-\pi/4)}}{2} \right\} = Am^{-1/2} \cos(\phi - \frac{\pi}{4}) \quad (13.9)$$

The exact eigenfunctions are $y_n(x) = H_n(x)e^{-x^2/2}$; where $H_n(x)$ are the *Hermite polynomials* recursively defined as $H_0(x) = 1, H_1(x) = 2x, H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$.

In the plot below, these are compared with the WKB eigenfunctions (13.9) for $n = 6$. To facilitate the comparison, both eigenfunctions are scaled so that $y(0) = 1$. The WKB eigenfunctions are only plotted in the oscillatory region where they are valid. The agreement is extremely good except (as expected) near the turning points (red lines). Note that the solution oscillates the fastest near the origin where $m(x)$ is largest and the oscillation amplitude is largest near the turning points where $m(x)$ is smallest (it should go as $m^{-1/2}$ according to WKB).



A fairer comparison of the exact and asymptotic approaches would use a matching region and Airy functions near the turning points. Even for small n, this would give remarkably good approximations to the exact eigenfunctions for all x.