The WKB Method: Solved Problems

1. The WKB approximation for the transmission probability through a finite square barrier.

Since we know the exact result for the transmission probability through a square barrier, we can compare the WKB approximation with the exact result. The square barrier is also a good choice because it is fairly easy to calculate the integral required to obtain the WKB approximation. Of course, the most interesting cases for the WKB approximation are the cases where we cannot calculate the exact analytic transmission probability. By studying the square potential barrier, you should also obtain some valuable insight into the conditions that make the WKB approximation work well—*i.e.,* you should understand when the WKB method is a good approximation, and why!

(a) Calculate the WKB exponential transmission coefficient γ where

$$\gamma = (1/\hbar) \int_0^{2a} \mid p(x) \mid \ dx.$$

(b) Then calculate the WKB transmission probability $T_{wkb} = e^{-2\gamma}$.

(c) The WKB approximation works well when the transmission probability is small. This occurs when γ is large. Find the large γ expansion of the exact result.

$$T(E) = [\ 1 + [V_0{}^2 \ / \ 4\ E\ (V_0 - E)\ ]\ \sinh^2 \gamma\ ]^{-1}.$$

Show that for large γ the exact solution takes the form

$$T(E) \sim [16E(V_0 - E)/V_0{}^2]\ e^{-2\gamma}$$

and consequently show that the exact solution has the same functional form as the WKB approximation ($T_{wkb} \sim e^{-2\gamma}$) whenever the behavior is dominated by the exponential term.

1.(a) First calculate the WKB exponential transmission coefficient

$$\gamma = \frac{1}{\hbar} \int_0^{2a} |p(x)|\ dx = \frac{1}{\hbar} \int_0^{2a} \left| \sqrt{2m(E - V_0)} \right| dx\,.$$

Since $V(x) = V_0$ with $V_0 > E$, we have $p(x) = \sqrt{2m(E - V(x))}$. When $V_0 > E$ as it is in this problem, the momentum will be imaginary. But note that we need only the magnitude of the momentum which is given by $|p(x)| = \sqrt{2m(V_0 - E)}$. Doing the integral, we find

$$\gamma = \frac{1}{\hbar} \int_0^{2a} \sqrt{2m(V_0 - E)}\, dx = \frac{1}{\hbar} \sqrt{2m(V_0 - E)} \int_0^{2a} dx = \frac{1}{\hbar} \sqrt{2m(V_0 - E)}\, [\ x\ ]_0^{2a}$$

$$\boxed{\Rightarrow \quad \gamma = \frac{2a}{\hbar}\sqrt{2m(V_0 - E)}\,.}$$

1.(b) The WKB transmission probability is given by

$$T_{\rm WKB} = e^{-2\gamma} = \exp\left\{-2\left(\frac{2a}{\hbar}\sqrt{2m(V_0 - E)}\right)\right\}$$

$$\boxed{\Rightarrow \quad T_{\rm WKB} = \exp\left\{-\left(\frac{4a}{\hbar}\sqrt{2m(V_0 - E)}\right)\right\}.}$$

1.(c) Now let's compare this approximate WKB result with the exact result, which is given by

$$\frac{1}{T} = 1 + \frac{V_0^2}{4E(V_0 - E)}\sinh^2(\gamma),$$

where $\gamma = 2a\sqrt{2m(V_0 - E)}\,/\hbar$ as above. Expanding the hyperbolic sine function

$$\sinh^2(\gamma) = \left(\frac{e^{\gamma} - e^{-\gamma}}{2}\right)^2$$

for large γ, we find

$$\sinh^2(\gamma) \approx \left(\frac{e^{\gamma}}{2}\right)^2 = \frac{1}{4}\,e^{2\gamma}$$

$$\Rightarrow \quad \frac{1}{T} \approx 1 + \frac{V_0^2}{16E(V_0 - E)}\,e^{2\gamma}.$$

Since γ is large, we must have $V_0 >> E$, so we can neglect the 1 and write

$$\frac{1}{T} \approx \frac{V_0^2}{16E(V_0 - E)}\,e^{2\gamma} \quad \Rightarrow \quad T \approx \frac{16E(V_0 - E)}{V_0^2}\,e^{-2\gamma}.$$

Note that this has exactly the same functional form as our WKB result in part b, and that the addition, the coefficient

$$\frac{16E(V_0 - E)}{V_0^2}$$

is of order 1. Note further that the dependence on $(V_0 - E)$ is dominated by the exponential factor, and that the WKB method provides a good approximation for the finite square barrier when $V_0 >> E$.

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2. The WKB solution to the quantum mechanical bouncing ball problem.

(a) First write down the WKB quantization condition for a potential with one hard wall and one soft wall

$$\int_{x_1}^{x_2} p(x)\, dx = (n - \frac{1}{4})\, \pi\hbar.$$

Then find the classical turning points, which are the limits of integration. Since $p(x) = 0$ at the two turning points, and since $p(x) = \sqrt{2m(E - mgx)}$, we find immediately that the two turning points are given by $x_1 = 0$ and $x_2 = (E/mg)$.

(b) Do the integral to find the bound state energies. You should find

$$E_n = [\ \frac{9}{8}\pi^2 mg^2\hbar^2\ (n - \frac{1}{4})^2\ ]^{\frac{1}{3}}.$$

(c) Put in the numbers and compare your results with the exact results, you should find that E_1 agrees to one percent and that E_2, E_3, and E_4 agree to three significant figures!

(d) Find the principal quantum number n required to make the expectation value $< x >$ = one meter. Use the result:

$$< x > = \ (2E_n/3mg)$$

and your expression for E_n from part b.

2.(a) The potential energy above the surface of the earth is given by

$$\boxed{V(x) = mgx \quad \text{for} \quad x > 0.}$$

Since the ball cannot pass through the surface, we also have

$$\boxed{V(x) = \infty \quad \text{for} \quad x \leq 0.}$$

So our idealized potential for the quantum mechanical bouncing ball looks like this

2.(b) The time-independent Schrodinger equation is given by,

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\,\psi(x) + (mgx)\,\psi(x) = E\,\psi(x).$$

Change variables

$$y = x - \frac{E}{mg} \quad \Rightarrow \quad \frac{d}{dy} = \frac{d}{dx} \quad \Rightarrow \quad \frac{d^2}{dy^2} = \frac{d^2}{dx^2}\ .$$

Then our TISE becomes

$$\begin{aligned} & -\frac{\hbar^2}{2m}\frac{d^2}{dy^2}\,\psi(y) + mg\left(y + \frac{E}{mg}\right)\psi(y) - E\,\psi(y) = 0 \\ \Rightarrow \quad & -\frac{\hbar^2}{2m}\frac{d^2}{dy^2}\,\psi(y) + mgy\,\psi(y) + E\,\psi(y) - E\,\psi(y) = 0 \\ \Rightarrow \quad & \frac{d^2}{dy^2}\,\psi(y) - \left(\frac{2m^2 g}{\hbar^2}\right) y\,\psi(y) = 0. \end{aligned}$$

Let

$$\alpha = \left(\frac{2m^2 g}{\hbar^2}\right)^{1/3}$$

so that the above equation becomes

$$\boxed{\left(\frac{d^2}{dy^2} - \alpha^3 y\right)\,\psi(y) = 0.}$$

This is Airy's equation. To put this in the standard form, let

$$z = \alpha y = \alpha\left(x - \frac{E}{mg}\right) \quad \Rightarrow \quad \frac{d^2}{dy^2} = \left(\frac{d}{dz}\frac{dz}{dy}\right)\left(\frac{d}{dz}\frac{dz}{dy}\right) = \frac{d}{dz}(\alpha)\frac{d}{dz}(\alpha) = \alpha^2\frac{d^2}{dz^2}.$$

Then the boxed equation becomes

$$\alpha^2\frac{d^2}{dz^2}\,\psi(z) - (\alpha^2 z)\,\psi(z) = 0 \quad \Rightarrow \quad \left(\frac{d^2}{dz^2} - z\right)\psi(z) = 0,$$

The solutions to Airy's equation are the Airy functions. There are two linearly independent Airy functions called $Ai\,(z)$ and $Bi\,(z)$. The $Bi\,(z)$ are unbounded for large z, so they do not apply to our problem. We require finite solutions and these are given by $Ai\,(z)$.

2.(c) The first four values of the argument z_n for which $Ai(z_n) = 0$, are given by

n	z_n
1	-2.338
2	-4.088
3	-5.521
4	-6.787

To convert this information into the eigenenergies, first relate z_n to y_n and then relate y_n to x and E_n:

$$z_n = \alpha y_n = \alpha \left(x - \frac{E_n}{mg} \right).$$

Now use the boundary condition at $x = 0$, namely that $\psi(0) = 0$, to obtain

$$\psi(x = 0) = 0 \quad \Rightarrow \quad \psi(z_n) = 0 \;\text{ when }\; z_n = -\frac{\alpha E_n}{mg} = -\left(\frac{2m^2 g}{\hbar^2}\right)^{1/3} \frac{E_n}{mg}\,.$$

So, we obtain

$$z_n = -\frac{2^{1/3} m^{2/3} g^{1/3}}{\hbar^{2/3} mg} E_n = -\frac{2^{1/3}}{\hbar^{2/3} m^{1/3} g^{2/3}} E_n.$$

Solving for the eigenenergies, we find

$$E_n = -\frac{\hbar^{2/3} m^{1/3} g^{2/3}}{2^{1/3}} z_n.$$

Then using $g = 9.80\,\mathrm{m/s^2}$ and $m = 0.100\,\mathrm{kg}$, we obtain

$$\begin{aligned} E_n &= -\frac{(1.05 \times 10^{-34}\mathrm{J \cdot s})^{2/3} (0.100\,\mathrm{kg})^{1/3} (9.80\,\mathrm{m/s^2})^{2/3}}{2^{1/3}} z_n \\ &= -\frac{(2.226 \times 10^{-23})(0.464)(4.579)}{1.260} z_n \\ &= -3.755 \times 10^{-23} z_n \,\text{joules}. \end{aligned}$$

We conclude that eigenenergies are given by

n	z_n	E_n
1	-2.338	8.779×10^{-23} J
2	-4.088	1.535×10^{-22} J
3	-5.521	2.073×10^{-22} J
4	-6.787	2.548×10^{-22} J

2.(d) From the Virial theorem, we have

$$\langle T \rangle = \frac{1}{2}\langle V \rangle = \frac{1}{2}\langle mgx \rangle = \frac{1}{2}mg\langle x \rangle$$

So, the total energy is given by

$$\langle H \rangle = \langle T \rangle + \langle V \rangle = \frac{1}{2}\langle V \rangle + \langle V \rangle = \frac{3}{2}\langle V \rangle = \frac{3}{2}mg\langle x \rangle.$$

To calculate the size $\langle x \rangle$ versus the quantum number n, solve for $\langle x \rangle$ in terms of E_n

$$E_n = \frac{3}{2}mg\langle x \rangle \quad \Rightarrow \quad \langle x \rangle = \frac{2E_n}{3mg} \, .$$

So, for the ground state of the "point baseball" we find

$$\boxed{\langle x \rangle = \frac{2(8.779 \times 10^{-23}\,\mathrm{J})}{3(0.100\,\mathrm{kg})(9.80\,\mathrm{m/s^2})} = 5.97 \times 10^{-23}\,\mathrm{m}\,.}$$

To calculate the mean separation of an electron in its ground state, start with

$$E_n = -\frac{\hbar^{2/3} m^{1/3} g^{2/3}}{2^{1/3}} z_n$$

and use the mass of an electron 9.11×10^{-31} kg to obtain

$$\begin{aligned} E_1 &= -\frac{(1.05 \times 10^{-34}\mathrm{J \cdot s})^{2/3}(9.11 \times 10^{-31}\,\mathrm{kg})^{1/3}(9.80\,\mathrm{m/s^2})^{2/3}}{2^{1/3}}(-2.338) \\ &= -\frac{(2.226 \times 10^{-23})(9.69 \times 10^{-11})(4.579)}{1.260} z_n\,\mathrm{J} \\ &= 1.833 \times 10^{-32}\,\mathrm{J} \end{aligned}$$

$$\boxed{\langle x \rangle = \frac{2(1.833 \times 10^{-32}\,\mathrm{J})}{3(9.11 \times 10^{-31}\,\mathrm{kg})(9.80\,\mathrm{m/s^2})} = 1.369 \times 10^{-3}\,\mathrm{m} = 1.369\,\mathrm{mm}.}$$

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3. The WKB solution to the simple harmonic oscillator problem.

(a) First write down the WKB quantization condition for a potential with two soft walls

$$\int_{x_1}^{x_2} p(x)dx = (n - \frac{1}{2})\, \pi\hbar.$$

Then find the classical turning points, which are the limits of integration. Since $p(x) = 0$ at the two turning points, and since $p(x) = \sqrt{2m(E - \frac{1}{2}m\omega^2 x^2)}$, you should find immediately that the two turning points are given by $x_2 = -x_1 = \sqrt{(2E/m\omega^2)}$.

(b) Do the integral to find the bound state energies. You should find

$$E_n = (n - \frac{1}{2})\, \hbar\omega.$$

This turns into the standard form $E_n = (n + \frac{1}{2})\, \hbar\omega$ when we use the simple harmonic oscillator convention of starting from $n = 0$ instead of the WKB convention of starting from $n = 1$. Note that the WKB approximation yields the exact energies for the simple harmonic oscillator!

3.(a) For a potential well with two "soft" walls, the WKB quantization condition becomes

$$\int_{x_1}^{x_2} p(x)\, dx = \left(n - \frac{1}{2}\right) \pi\hbar \quad \text{with} \quad n = 1, 2, 3, \ldots$$

The classical turning points for the SHO are given by

$$\frac{1}{2}m\omega^2 x^2 = E_n \quad \Rightarrow \quad x^2 = \frac{2E_n}{m\omega^2}$$

$$\boxed{\Rightarrow \quad x = \pm \left(\frac{2E_n}{m\omega^2}\right)^{1/2}.}$$

3.(b) To evaluate the WKB quantization condition integral, we need the momentum which is given by

$$p(x) = \sqrt{2m(E - V(x))} = \left[2mE - 2m\left(\frac{1}{2}m\omega^2 x^2\right)\right]^{1/2} = \left[2mE - m^2\omega^2 x^2\right]^{1/2}.$$

Putting this in the integral and noting $E = \frac{1}{2}m\omega^2 x_2^2$, we obtain

$$\int_{x_1}^{x_2} p(x)\,dx = \int_{x_1}^{x_2} \left[2mE - 2m\left(\frac{1}{2}m\omega^2x^2\right)\right]^{1/2} dx = \int_{x_1}^{x_2} \left[2m\left(\frac{1}{2}m\omega^2x_2^2\right) - 2m\left(\frac{1}{2}m\omega^2x^2\right)\right]^{1/2} dx$$

$$= m\omega \int_{x_1}^{x_2} \left[x_2^2 - x^2\right]^{1/2} dx = 2m\omega \int_{0}^{x_2} \left[x_2^2 - x^2\right]^{1/2} dx.$$

Form 4.3.3.1.2 on page 158 of Jeffrey is the indefinite integral we need, namely

$$\int (a + cx^2)^{1/2}\,dx = \frac{1}{2}x(a+cx^2)^{1/2} + \frac{1}{2}\frac{a}{\sqrt{-c}}\sin^{-1}\left(x\sqrt{\frac{-c}{x_2^2}}\right), \quad a > 0, \quad c < 0.$$

For our integral, $a = x_2^2$ and $c = -1$, so both qualifying conditions are met, and our integral becomes

$$\begin{aligned}
2m\omega \int_{0}^{x_2} \left[x_2^2 - x^2\right]^{1/2} dx &= 2m\omega \left[\frac{1}{2}x(x_2^2 - x^2)^{1/2} + \frac{1}{2}\frac{x_2^2}{\sqrt{1}}\sin^{-1}\left(x\sqrt{\frac{1}{x_2^2}}\right)\right]_0^{x_2} \\
&= 2m\omega \left[\frac{1}{2}x(x_2^2 - x_2^2)^{1/2} - \frac{1}{2}(0)(x_2^2 - 0)^{1/2} + \frac{x_2^2}{2}\sin^{-1}\left(\frac{x}{x_2}\right)\Bigg|_0^{x_2}\right] \\
&= m\omega x_2^2 \left[0 - 0 + \sin^{-1}(1) - \sin^{-1}(0)\right] \\
&= m\omega x_2^2 \left[\frac{\pi}{2} - 0\right] = m\omega\frac{\pi}{2}x_2^2 \\
&= m\omega\frac{\pi}{2}\left(\frac{2E_n}{m\omega^2}\right) = \frac{\pi E}{\omega}.
\end{aligned}$$

So, the WKB quantization condition becomes

$$\frac{\pi E}{\omega} = \left(n - \frac{1}{2}\right)\pi\hbar \quad \Rightarrow \quad E = \left(n - \frac{1}{2}\right)\hbar\omega, \quad n = 1, 2, 3, \ldots.$$

Switching to the standard convention $n = 0, 1, 2, 3$, we find

$$\boxed{E_n = \left(n + \frac{1}{2}\right)\hbar\omega.}$$

Note that we have obtained the exact eigenenergies of the quantum mechanical SHO.
