Graduate QM (PHYS 517) Handout 11/23/10
WKB approximation and applications

Calculations in these notes are done with the Mathematica notebook `wkb.nb`, which is posted on the class web site.

1 Oscillator with a hard wall

The potential is

$$V(x) = \begin{cases} \frac{m\omega^2}{2}x^2 & -a < x < a \\ \infty & a \le |x| \end{cases} \tag{1}$$

As discussed in class, the WKB wavefunction is

$$u_{WKB}(x) \propto \frac{1}{\sqrt{k(x)}} \sin\left[\int_{-a}^{x} dx' k(x')\right], \qquad (|x| \le a), \tag{2}$$

where

$$k(x) = \frac{\sqrt{2m(E - V(x))}}{\hbar}. \tag{3}$$

In order for $u_{WKB}(a) = 0$, we need

$$\int_{-a}^{+a} k(x)dx = n\pi, \quad n = 1, 2, 3, \ldots \tag{4}$$

This result is valid as long as

$$E \ge V(a) = \frac{m\omega^2 a^2}{2}, \tag{5}$$

for otherwise the turning points occur for $|x| < a$, and the BC we have used are invalid. (In this case, one needs to do a standard WKB analysis, matching to exponentially falling solutions.)

It is convenient to measure energies relative to the ground state oscillator energy, $E_0 = \hbar\omega/2$ and distances relative to $\sqrt{2}$ times the ground-state oscillator spread,

$$x_0 = \sqrt{2\langle x^2\rangle_{g.s.}} = \sqrt{\frac{\hbar}{m\omega}}. \tag{6}$$

Thus we use

$$\epsilon = E/E_0, \quad \text{and} \quad \tilde{a} = a/x_0. \tag{7}$$

Doing the integral, one finds that the WKB condition becomes

$$n\pi = \epsilon\left(\theta_0 + \frac{\sin(2\theta_0)}{2}\right), \quad \sin\theta_0 = \frac{\tilde{a}}{\sqrt{\epsilon}}. \tag{8}$$

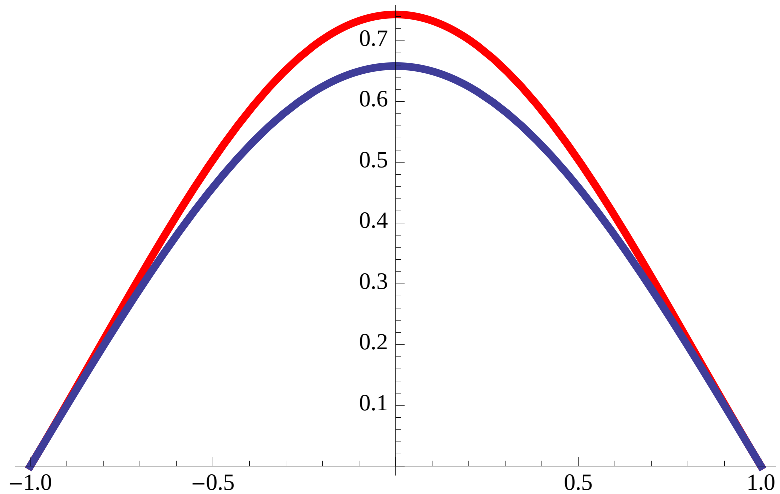

Figure 1: Comparison of exact wavefunction for ground state in cut-off SHO (red) with WKB wavefunction (blue). Horizontal scale is x/x_0; vertical scale is arbitrary. Both wavefunctions have the same slope at $x/x_0 = -1$.

This is a non-linear condition that can be solved numerically. The validity requirement (5) simplifies to $\epsilon > \tilde{a}^2$ in our new variables.

For $\tilde{a} = 1$ the energies are given in Table 1, and compared with the exact energies. The WKB approximation improves as n increases. The exact and WKB wavefuctions for $n = 1, 2$ are shown in Figs. 1 and 2.

n	E_{WKB}	E_{exact}
1	2.81	2.60
2	10.21	10.15
3	22.54	22.51
4	39.81	39.80

Table 1: Comparison of bound-state energies from WKB approximation and "exact" result (obtained numerically) for cut-off SHO potential with $\tilde{a} = 1$.

2 Airy functions

In the neighborhood of a turning point, and using in suitable variables, Schrödinger's equation becomes the equation

$$\frac{d^2u(z)}{dz^2} = zu(z)\,, \tag{9}$$

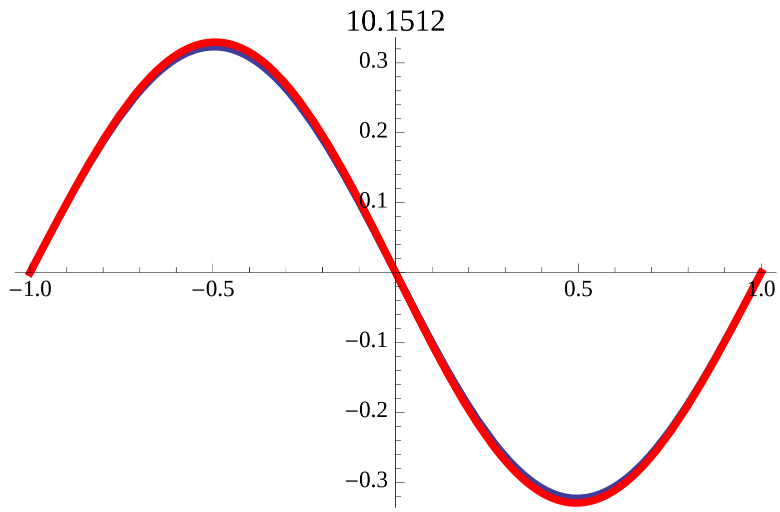

Figure 2: As for Fig. 1 but for first excited state. The difference between exact and approximate wavefunctions are only visible at the peak and trough.

whose solutions are Airy functions. (Here we have chosen to consider a turning point where the classically allowed region is $z < 0$.) The two standard solutions are labeled $Ai(z)$ and $Bi(z)$. The former falls to zero as $z \to \infty$, while the latter grows to infinity. Thus we are interested in $Ai(z)$ for normalizable solutions.

As discussed in class, it turns out that the WKB approximation applied to this equation leads to the leading term in the asymptotic expansion of the Airy functions as $|z| \to \infty$. For $Ai(z)$ the explicit forms are

$$Ai(z) \quad \overset{z\to+\infty}{\longrightarrow} \quad \frac{1}{2\sqrt{\pi}z^{1/4}} \exp\left(-2z^{3/2}/3\right)\left[1 + O(z^{-3/2})\right] , \tag{10}$$

$$\overset{z\to-\infty}{\longrightarrow} \quad \frac{1}{\sqrt{\pi}|z|^{1/4}} \cos\left(2|z|^{3/2}/3 - \pi/4\right)\left[1 + O(|z|^{-3/2})\right] . \tag{11}$$

Figure 3 compares $Ai(z)$ to the asymptotic forms, showing that they work well for $|z| > 1$.

For completeness, Fig. 4 compares $Ai(z)$ and $Bi(z)$.

3 Quartic potential in WKB approximation

Here we apply the WKB quantization condition,

$$\int_{x_1}^{x_2} dx \frac{\sqrt{2m(E - V(x))}}{\hbar} = (n + 1/2)\pi \tag{12}$$

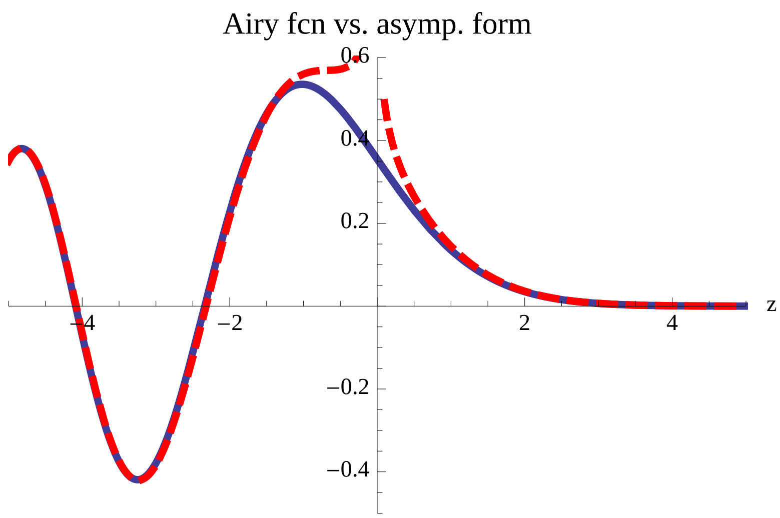

Figure 3: Airy function $Ai(z)$ (blue) compared to its asymptotic forms (dashed red).

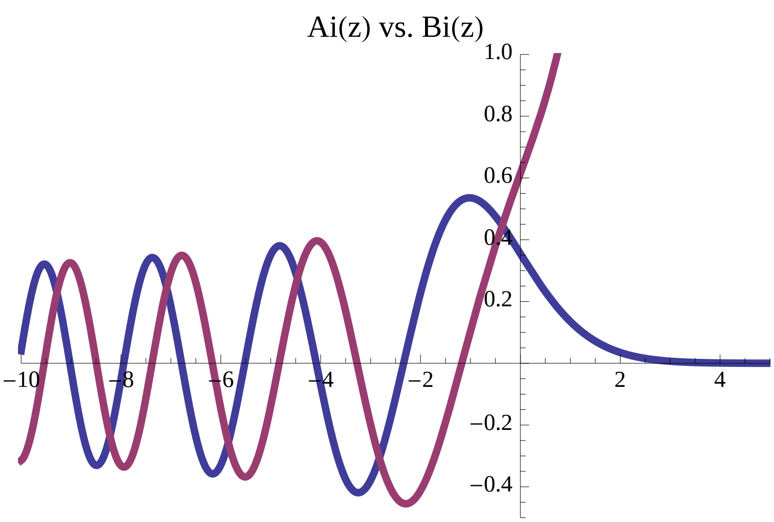

Figure 4: Comparison of $Ai(z)$ (blue) and $Bi(z)$ (red).

(where $x_{1,2}$ are the classical turning points) to the quartic potential

$$V(x) = V_0(x/x_0)^4 \,. \tag{13}$$

This parametrization is redundant (V_0 could be absorbed into x_0) but allows the units to be kept straight more easily.

Doing the integral, one finds

$$\begin{aligned} E_n &= E_0 \left(\frac{(n+1/2)\pi}{I} \right)^{4/3} , \qquad n = 0, 1, 2, \ldots \\ I &= \int_{-1}^{+1} dy \sqrt{1 - y^4} \approx 1.74804 \\ E_0 &= \left(\frac{\hbar^2 V_0^{1/2}}{2 m x_0^2} \right)^{2/3} . \end{aligned}$$

The first five energy levels are given in Table 3. The WKB approximation does increasingly well as n increases.

n	E_{WKB}/E_0	E_{exact}/E_0
0	0.87	1.06
1	3.75	3.80
2	7.41	7.46
3	11.61	11.64
4	16.23	16.26

Table 2: Comparison of bound-state energies from WKB approximation and “exact” result (obtained numerically) for quartic potential.

The “exact” (from numerical solution) and WKB wavefunctions are compared in Fig. 5. The horizontal axis is x/L, where

$$L = \left(\frac{\hbar^2 x_0^4}{2 m V_0} \right)^{1/6} \tag{14}$$

is the distance at which $V(L) = E_0$. Both solutions are normalized to equal unity for $x = 0$. (Normalizing the inside solution automatically normalizes the outside solution through the matching formula.) One sees that the WKB approximant captures only a small part of the inside wavefunction.

The figure also shows the Airy function which “does” the matching (normalized to match the exact wavefunction at the turning point). One sees that it actually matches quite poorly onto the WKB solutions. This is because keeping only the

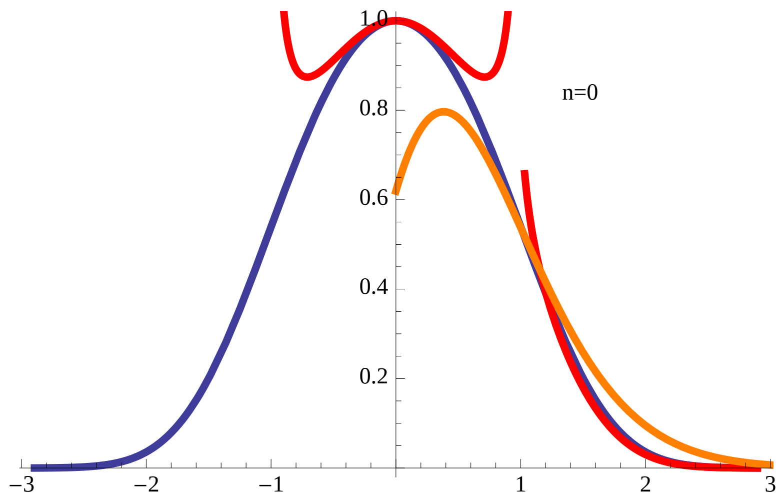

Figure 5: Comparison of exact ground-state ($n = 0$) wavefunction (blue) and WKB approximants (red). The orange curve shows the Airy function solution that is used to match across the turning point. For more details see text.

leading term in the Taylor expansion of the potential about the turning point is accurate only for a very small neighborhood of the turning point in this case. Similar plots for $n = 2, 4, 8$ are shown in Figs. 6, 7 and 8, respectively. The WKB wavefunction captures the exact behavior inside and outside increasingly well (there is hardly any blue curve visible!), but it is only at $n = 8$ that we can see the Airy function match onto the inside wavefunction. Note that it is *not* expected that the Airy function match the WKB curve away from the turning point—they are solutions to a different problem.

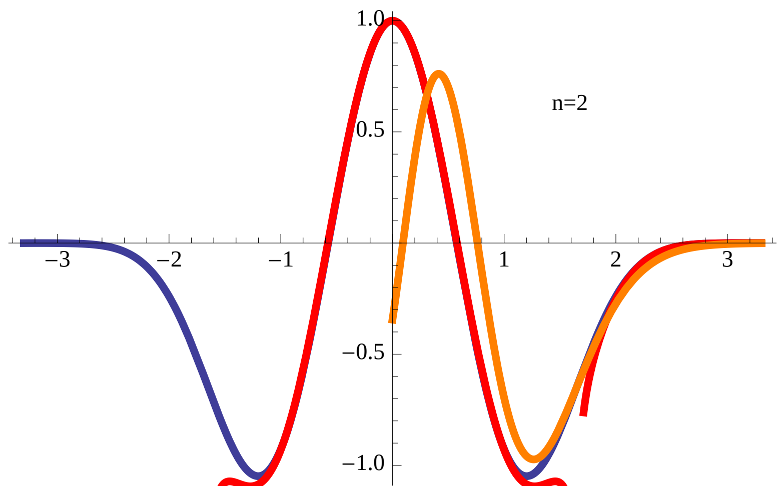

Figure 6: As for Fig. 5 except for the $n = 2$ state.

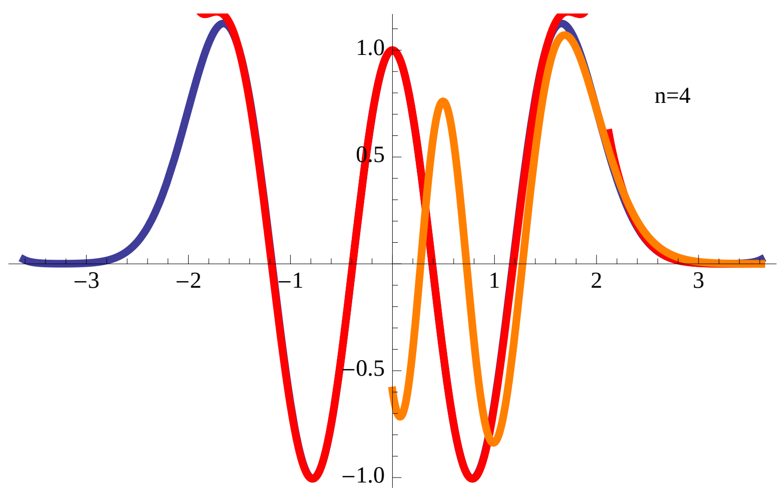

Figure 7: As for Fig. 5 except for the $n = 4$ state.

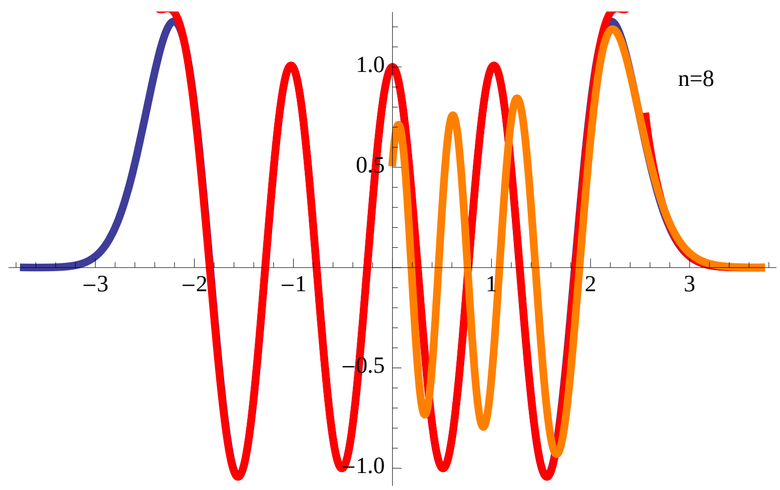

Figure 8: As for Fig. 5 except for the $n = 8$ state.