Phys 472 Assignment 10 Due Nov. 20, 2020, before 9:00 am Marsiglio, Fall 2020

1. Use the step potential in an infinite square well, with a step-up of size $\Delta V \equiv V_1 - V_0$ at $b = a/2$, where a is the width of the well. To be clear,

$$V(x) = \begin{cases} V_0 & \text{if} \quad 0 < x < b \\ V_1 & \text{if} \quad b < x < a \\ \infty & \text{elsewhere} \end{cases}$$

and determine the WKB approximation for *all* the energy levels (i.e. both below and above the step in potential energy). For the energy levels below (i.e. in the narrower portion of the well) the step, use the WKB formula for one vertical wall at $x = 0$,

$$\int_0^{x_2} p(x)\ dx = \left(n - \frac{1}{4}\right)\pi\hbar \tag{1}$$

as explained in Example 9.3 in Griffiths (Eq. 9.48). For the levels above the step, use the WKB formula for two vertical walls, as described by Eq. 9.17 in Griffiths,

$$\int_0^{a} p(x)\ dx = n\pi\hbar. \tag{2}$$

Plot the energies you obtain, along with the exact results, obtained either analytically (still have to solve a transcendental equation) or through your numerical program (this is probably easier!). For definiteness, plot $E/E_1^{(0)}$ vs. n for $n = 1, 2, 3, ...100$, and also provide another plot for $24 \leq n \leq 36$ with the appropriate scale for the energy to "zoom in" on the region where the step in the potential occurs. Are you impressed? (correct answer is yes! since the potential is anything but smoothly varying at the step). For your numerical results use $V_0 = 0$ and $V_1/E_1^{(0)} = 4000$, where $E_1^{(0)} \equiv \pi^2\hbar^2/(2m_0a^2)$.

2. (a) Assume a potential of the form,

$$V(x) = \lambda|x|^q,$$

where q is a real positive number. Use the WKB approximation to find the allowed energies as a function of n for arbitrary q. Use the WKB result for a potential without any vertical walls, i.e. Eq. (9.52) in Griffiths:

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

You will need the recognize the Beta function integral,

$$B(u, z) \equiv \int_0^1 dt\ t^{u-1}(1-t)^{z-1} = \frac{\Gamma(u)\Gamma(z)}{\Gamma(u+z)},$$

where $\Gamma(z)$ is the Gamma function. Write your answer for the energy in terms of the Gamma function [specifically, $\Gamma(1/q+3/2)$, and $\Gamma(1/q+1)$]. You need to use $\Gamma(z+1) = z\Gamma(z)$ and $\Gamma(1/2) = \sqrt{\pi}$.

(b) What do you get for the harmonic oscillator ($q = 2$), for the quartic potential ($q = 4$) and for the string potential ($q = 1$). For the ground state, your answers should be very impressive for the harmonic oscillator (indeed!) not so impressive for the quartic, and... you don't know how impressive for the string potential.

(c) [**Bonus!** 15% extra marks on this assignment] Since you have a program for the quartic, compare to your exact answers up to $n = 50$ (you will be amazed). Use $N_{\rm max}$ large enough so everything is well converged ($N_{\rm max} = 1000$ will definitely do it).

Do the same for the linear potential. In this case, you should find,

$$V_{nm} = \lambda a \begin{cases} \delta_{n,m}\frac{1}{4}\left[1 - \frac{4}{(\pi n)^2}\left(\frac{1-(-1)^n}{2}\right)\right] \\ (1-\delta_{nm})\frac{4}{\pi^2}\frac{1+(-1)^{n+m}}{2}\left[\frac{1-(-1)^{(n-m)/2}}{(n-m)^2} - \frac{1-(-1)^{(n+m)/2}}{(n+m)^2}\right]. \end{cases}$$

Use $\lambda a/E_1^{(0)} = 5000$ and do a comparison with the WKB results, like with the quartic potential, up to $n = 50$, i.e. plot both results on the same graph (two different kinds of points). For the potential you will have to divide your numerical results (assuming you are using units of $E_1^{(0)}$) by $(g/\pi)^{2/3}$.

Note added Nov. 17, 2020: The choice $\lambda a/E_1^{(0)} = 5000$ is not a sufficiently wide well, and you should use $\lambda a/E_1^{(0)} = 15000$.

And finally, plot the exact results for $q = 1$ and $q = 4$ all on the same figure, with E (in the suitable units for the given q)[1] vs. n up to $n = 50$. Now produce another plot of $a_q E^{[(q+2)/(2q)]}$ vs. n up to $n = 50$ (obviously inspired by the WKB). Choose $a_1 = 8\pi/3$ (I had 8/3 until today (9:30 am, Nov. 19) – thanks, Matt!) and $a_4 = \frac{\Gamma(1/4)}{\Gamma(3/4)}\frac{2}{3\sqrt{\pi}} \approx 1.113$ (again obtained from the WKB result, but we are plotting exact results!).

[1] This means units of $\lambda^{2/3}\left(\frac{\hbar^2}{2m_0}\right)^{1/3}$ for $q = 1$ and $\lambda^{1/3}\left(\frac{\hbar^2}{2m_0}\right)^{2/3}$ for $q = 4$.