Phys 472 Assignment 2 Due Sept. 18, 2020, before 9:00 am Marsiglio, Fall 2020

1. Consider the problem discussed in class — a harmonic oscillator potential, centred at $x = a/2$, and 'imbedded' in an infinite square well potential:

$$V(x) = \frac{1}{2} m_0 \omega^2 (x - a/2)^2 \theta(x) \theta(a - x),$$

where m_0 is the mass of the particle and ω is the frequency associated with the oscillator. Write everything with dimension length in units of a, and everything with units energy in units of $E_1^{(0)} \equiv \pi^2 \hbar^2 / (2 m_0 a^2)$. Set up this problem for solution using an eigenvalue formulation (as in class) and a computer, by following these steps (please submit a copy of all computer programs or scripts used):

(a) In class we derived the following equation for the matrix elements ($\rho \equiv \hbar\omega / E_1^{(0)}$):

$$\frac{H_{ij}}{E_1^{(0)}} = \delta_{ij} \left\{ j^2 + \frac{\pi^2 \rho^2}{48} \left(1 - \frac{6}{(\pi j)^2}\right) \right\} + [1 - \delta_{ij}] \left\{ \frac{\rho^2}{2} \frac{(-1)^{i+j} + 1}{2} \left(\frac{1}{(i-j)^2} - \frac{1}{(i+j)^2} \right) \right\}.$$

Use $\rho \equiv \hbar\omega / E_1^{(0)} = 50$, and plot the first 50 eigenvalues as a function of eigenvalue index, along with the corresponding expected (analytical) solutions for the infinite square well and the harmonic oscillator, i.e. reproduce Fig. 1 of the (2009 American Journal of Physics (AJP) paper. Beware the index numeration: here it begins with $n = 1$ whereas in the usual harmonic oscillator solution it begins with $n = 0$. Also plot the various expected analytical solutions for the various regimes: the answer for the infinite square well, the one for the infinite square well with account for a constant shift due to the harmonic oscillator potential, and the expected result for the harmonic oscillator potential (see Fig. 1). Comment on the degree to which your results agree or disagree with the expected analytical results. Check on the truncation error, i.e. try to solve a 50×50 matrix, and then a 100×100 one, and finally a 200×200 (my computer takes less than a second for this last one). Show a separate plot with 200 or so values, so you can better see the large values approaching the (corrected) infinite square well values.

(b) For $\rho \equiv \hbar\omega / E_1^{(0)} = 50$, now examine both the ground state and first excited state wave functions.

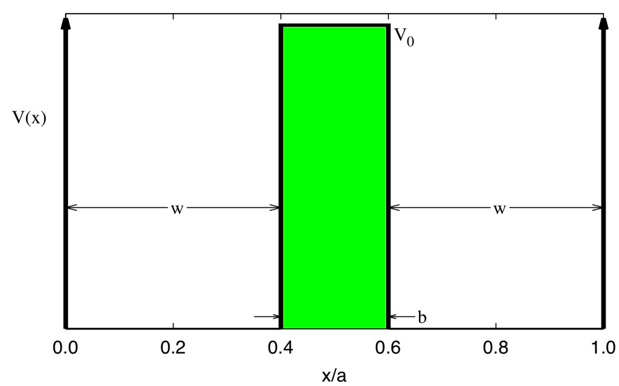
(i) Based on your eigenvector (obtained numerically), plot the wave function (not absolute value) for the ground state as a function of position, for $N_{\max} = 10, 20, 50$, and for the exact analytical result [see Eq. (14) in AJP 77, 253 (2009)], all on the same plot. This looks a little like Fig. 2 in the paper except that (erroneously) had the absolute value. To make the axes dimensionless you should be plotting $\sqrt{a}\psi_{n=1}(x)$ vs x/a.

(ii) Do the same thing with the first excited state.

For results based on a 50×50 matrix diagonalization, your results should agree to high accuracy with the analytical result.

2. We want to study the solutions for a double square well. There are many examples one can choose from; a particularly simple one is defined as follows: start with an infinite

square well between $x = 0$ and $x = a$, with a barrier inserted in the centre with height V_0 and width b. This means the barrier begins at $(a - b)/2$ and ends at $(a + b)/2$. With V_0 positive, this defines two square wells separated by a barrier of height V_0 and width b, and creates two wells, each of width $w \equiv (a - b)/2$. Assume the 'floor' of both wells has potential zero. See the figure.



(a) We can solve this analytically. Assume first an even solution (even around $a/2$) and then an odd (around $a/2$) solution; for each match the wave functions and their derivatives to derive the following two equations, first

$$\tan(z - \pi/2) = \left[\sqrt{\left(\frac{z_0}{z}\right)^2 - 1}\right] \tanh\left(\frac{b}{2w}\sqrt{z_0^2 - z^2}\right)$$

for the even solution, where $z \equiv kw$ and $z_0 \equiv \sqrt{\frac{2mV_0}{\hbar^2}}w$, with $k = \sqrt{\frac{2mE}{\hbar^2}}$, and then for the odd solution, derive

$$\tan(z - \pi/2) = \left[\sqrt{\left(\frac{z_0}{z}\right)^2 - 1}\right] \coth\left(\frac{b}{2w}\sqrt{z_0^2 - z^2}\right).$$

These equations could be solved iteratively for solutions for z (and therefore E), but we will instead proceed with a qualitative analysis.

(i) First consider V_0 infinite. A single particle can reside in either well. Enumerate the first 6 states and their energies, taking careful note of their degeneracies. *Hint: this part is easy.*

(ii) Now consider decreasing V_0. Physically, for large values of V_0 you expect even and odd (again defined with respect to $a/2$) solutions to have similar energy, since they essentially correspond to even and odd combinations of the single solutions corresponding to the ground state for each of the single wells to the left or to the right of the middle barrier. This is born out by the structure of these equations; they differ only in the presence of a *tanh* function in the first vs. a *coth* function in the second. The argument of these functions is quite large, so the function values are both very close to unity (one is slightly below and one is slightly above), and so the solutions to the two equations are very close to one another. Show a graph (a sketch will suffice) illustrating the left-hand-side and the right-hand-side (RHS) of these two equations (like Fig. 2.17 in G3 or Fig. 2.18 in G2), along with the RHS where the *tanh* (or *coth*) function is replaced by unity, and make this argument based on the graphical solutions.

(iii) Present an argument to determine whether or not a minimum barrier height V_0 is required to have a state with $E < V_0$. *Hint: think of* $V_0 \to 0$.

(b) Now solve this problem using matrix mechanics.

(i) Set up the matrix H for this problem, and then derive the following matrix elements (use units of energy as $E_1^{(0)} \equiv \frac{\hbar^2\pi^2}{2m_0a^2}$):

$$H_{nm} = \delta_{nm}\left(n^2E_1^{(0)} + V_0\frac{b}{a} + 2V_0\frac{w}{a}\ \mathrm{sinc}(2\pi n\frac{w}{a})\right)$$

$$-(1-\delta_{nm})\,2V_0\frac{w}{a}\left[\mathrm{sinc}(\pi(n-m)\frac{w}{a}) - \mathrm{sinc}(\pi(n+m)\frac{w}{a})\right]\left[\frac{(-1)^{n+m}+1}{2}\right],$$

where

$$\mathrm{sinc}(x) \equiv \frac{\sin(x)}{x}.$$

Use $b = a/5$ so that the individual wells have $w = 2a/5$. Again check your diagonalization routine both by setting $V_0 = 0$ and by setting V_0 to some very high value. What do you expect for the eigenvalues in these two cases? Compare your result, say for $V_0/E_1^0 = 2000000$, to what you said in part (a).

(ii) Finally, use $V_0/E_1^{(0)} = 500$; determine the two lowest eigenvalues and plot the two wave functions as a function of position. Are they even and odd, respectively, about the centre of the well? Also plot the probability, $|\psi(x)|^2$ corresponding to these two solutions on the same figure, and note how they are similar and how they are different.

3. Read the first 2 sections of American Journal of Physics 83, 861-865 (2015). Don't worry about the math so much. Write a few sentences (at most one paragraph) of what you learned from this paper. See Eclass or use the DOI link:
http://dx.doi.org/10.1119/1.4923249