PHYS 410: Homework 4
Numerical Solutions to the Schrödinger Equation

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All figures included in this report can be generated by running the MATLAB script hw4.m.

We first have to rearrange the Schrödinger equation to solve for $\frac{d^2\psi}{dx^2}$:

$$\frac{d^2\psi}{dx^2} = \frac{2m(V(x) - E)}{\hbar^2}\psi \tag{1}$$

Then, we can rewrite the second order ODE as a system of two first order ODEs by making the substitution $y_1 = \psi$ and $y_2 = \psi'$:

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} \psi \\ \psi' \end{bmatrix} \tag{2}$$

$$\begin{bmatrix} y_1' \\ y_2' \end{bmatrix} = \begin{bmatrix} \psi' \\ \psi'' \end{bmatrix} \tag{3}$$

$$= \begin{bmatrix} y_2 \\ \frac{2m(V(x)-E)}{\hbar^2} y_1 \end{bmatrix} \tag{4}$$

And now with $xspan = [-x_0, x_0]$ and $y0 = [0, \epsilon]$, we can solve the differential equation with RK4.m.

1 Question 1

Figure 1 does show that $\psi(x)$ blows up as x increases, just as noted in the assignment. This can be explained by the hint that in the classically forbidden regions, the Schrödinger equation admits two linearly independent solutions, one which increases, and the other which decreases. In particular, for a finite square potential, the solutions in the classically forbidden regions are:

$$\psi_1(x) = Ae^{-\alpha x} \tag{5}$$

$$\psi_2(x) = Be^{\alpha x} \tag{6}$$

where ψ_1 decreases exponentially and ψ_2 increases exponentially. Normally, when solving the equation analytically, we would throw out the exponentially growing solution as it is not square integrable. Assuming that the solutions for the anharmonic oscillator are similar, we would expect a similar set of exponentially growing and exponentially decaying solutions. But since we are solving the Schrödinger equation numerically instead of analytically, it is not possible to "throw out" one of the solutions and that would lead to the exponential growth behaviour we see in Figure 1.

2 Question 2

- For even solutions: $\psi'(0) = 0$
- For odd solutions: $\psi(0) = 0$

And for both even and odd solutions, the previous boundary conditions still apply:

- $\psi(-x_0) = 0$
- $\psi'(-x_0) = \epsilon$

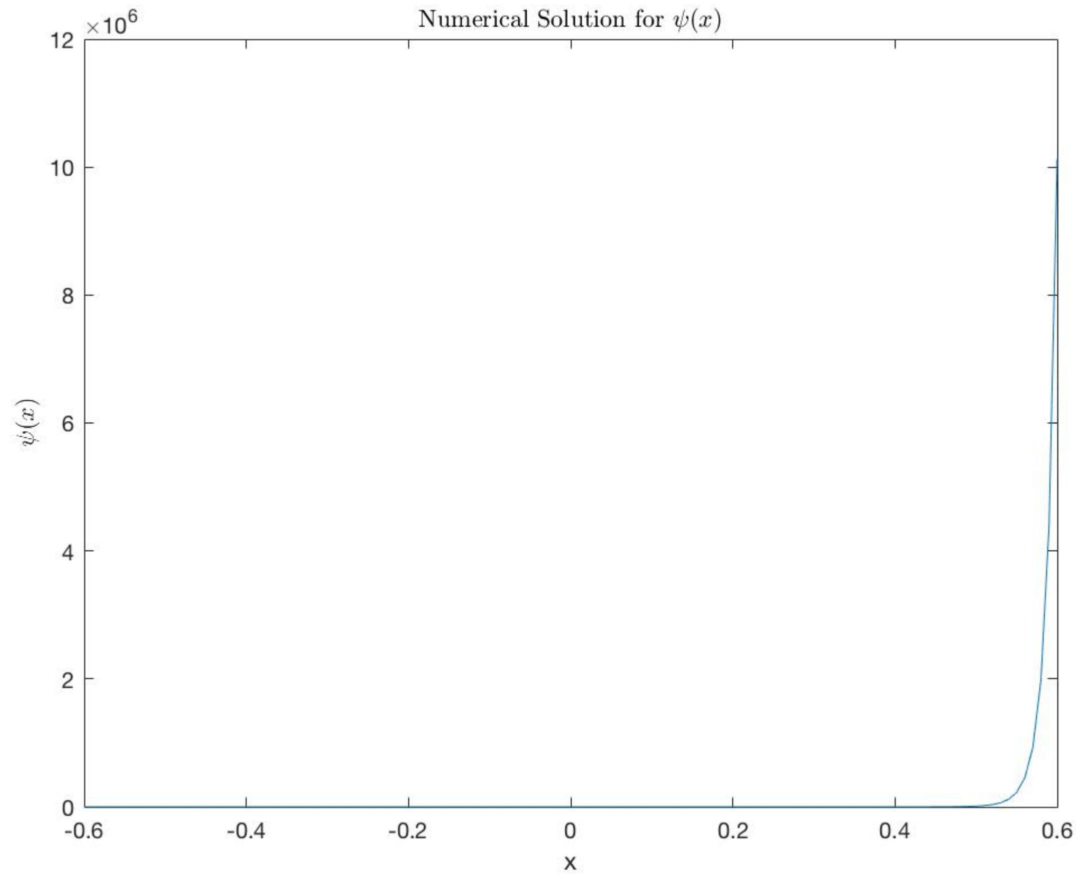

Figure 1: E=1. Initial conditions: $\psi(-x_0) = 0$, $\psi'(-x_0) = \epsilon$.

3 Question 3

Using the shooting method (details in the MATLAB files), I just manually guessed and checked from E=0 and increased the guess by 1 each time until fzero returned 3 different values for each of the odd and even functions. They are:

- $E_0 = 5.8533$ eV (even)
- $E_1 = 5.8896$ eV (odd)
- $E_2 = 15.3591$ eV (even)
- $E_3 = 16.6691$ eV (odd)
- $E_4 = 22.5864$ eV (even)
- $E_5 = 27.6577$ eV (odd)

4 Question 4

Figure 2 shows that the two lowest eigenstates are "trapped" in the two small potential oscillators. They also exhibit tunneling behaviour across the middle potential hump.

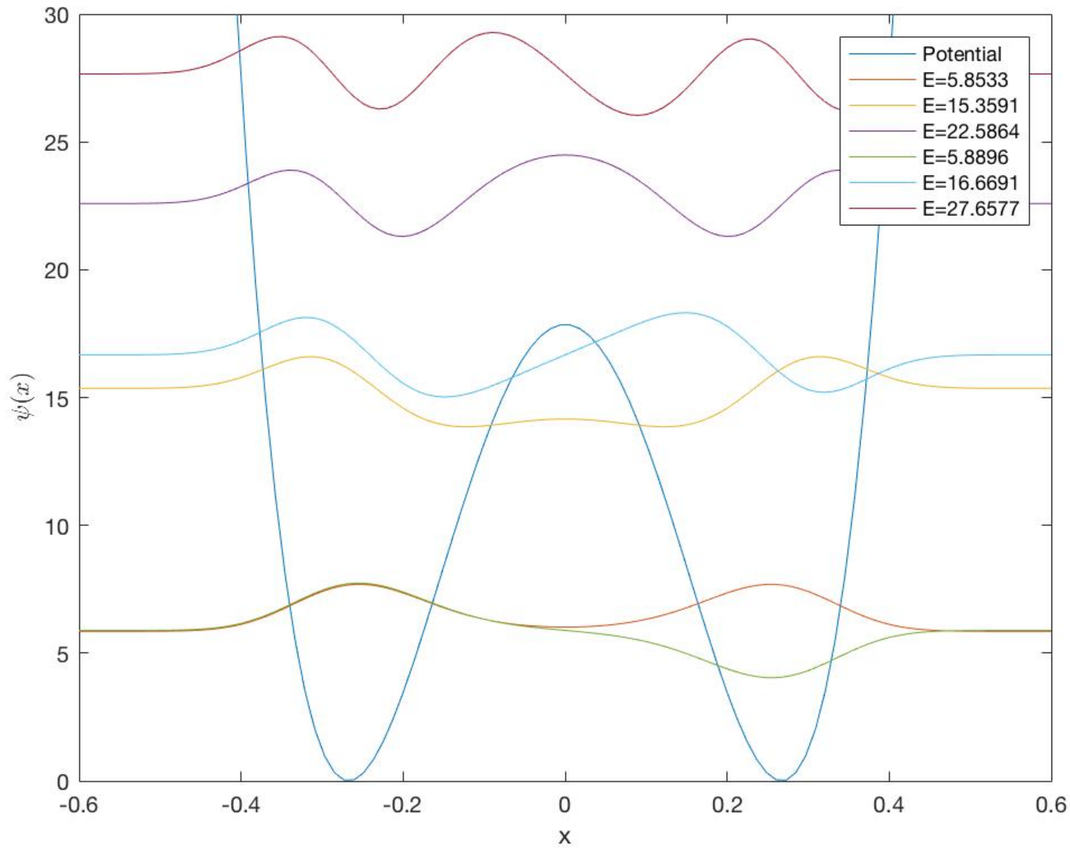

Figure 2: Six lowest energy bound states of the anharmonic oscillator.

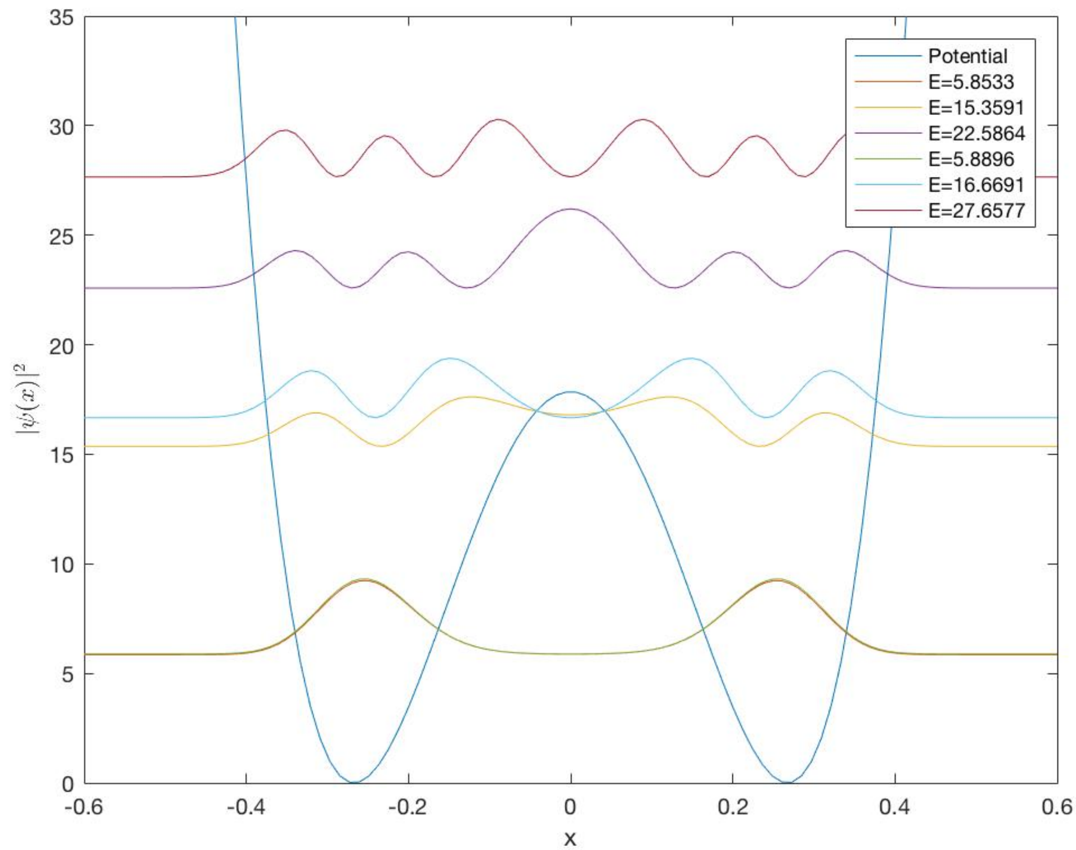

Figure 3: $|\psi|^2$ of the six lowest energy bound states of the anharmonic oscillator.