PHYS 410 - Homework 4

In this homework, we revisit the Schrödinger equation

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

We will be working in a system of units defined by electron masses, nanometers and eV's. In these units,

$$\hbar^2 = 0.076199682 \text{ eV } m_e \text{ nm}^2. \tag{2}$$

Our goal is to find the bound states of an electron that lies in an anharmonic oscillator potential of the form

$$V(x) = -\alpha x^2 + \beta x^4 + \frac{\alpha^2}{4\beta}, \tag{3}$$

where we take $\alpha = 500$ eV nm^{-2} and $\beta = 3500$ eV nm^{-4}.

1. (2 pts) Use the fourth-order explicit Runge-Kutta solver RK4 (found on the course website) to solve the Schrödinger equation on the domain $[-x_0, x_0]$, where we take $x_0 = 0.6$ nm and set $E = 1$ eV for now. Use the initial conditions $\psi(-x_0) = 0$ and $\psi'(-x_0) = \epsilon$, with $\epsilon = 10^{-5}$ so that $\psi(x) \neq 0$ on the entire domain. You should observe that the solution $\psi(x)$ blows up when x increases; explain why.

   Hint: In the classically forbidden regions, equation (1) admits two linearly independent solutions, one of which increases while the other decreases.

2. (2 pts) Notice the parity symmetry (symmetry under $x \to -x$) of equation (1), from which we deduce that the eigenstates $\psi(x)$ are either even or odd functions of x. This tells us that we only need to numerically integrate the equation on the interval $[-x_0, 0]$, with appropriate boundary conditions at $x = 0$. What boundary conditions should we impose for even solutions? What about odd solutions?

3. (6 pts) Write your own shooting method to find the six lowest energy eigenvalues for the anharmonic oscillator bound states. Write them down to 4 decimal places.

4. (5 pts) In a single figure, plot the six corresponding eigenstates, as well as the potential $V(x)$, on the domain $[-x_0, x_0]$. Align the zero baseline of each wavefunction with its energy eigenvalue, and use the MATLAB function *trapz* (trapezoidal integration) to normalize them appropriately, i.e. to ensure that

   $$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1. \tag{4}$$

   What can you say about the two lowest eigenstates?