Computational Quantum Physics
Exercise 2

Problem 2.1 Bound states in 1-D Schrödinger equation and eigenvalue problem

Find the bound state solutions of the 1D Schrödinger equation with $E < 0$ using the Numerov algorithm and a root solver. Note that the solution exists only for discrete energy eigenvalues.
Proceed as described in lecture notes in section 3.1.3.
Take the potential zero outside the interval [0,1] and inside the interval it can be taken as

$$v(x) = c(x^2 - x), 0 \leq x \leq 1, \tag{1}$$

where c is a constant. Please check the dependency of the number of bound states on the values of c.

Start with finding the ground state energy (which has zero nodes) and proceed further with 1, 2, 3... nodes.
Hint: Check the number of zeros (nodes) in the solution. For your guessed energy, if you find more nodes in your solution than the desired number of nodes, decrease the guess-energy and vice versa.

Problem 2.2 Anharmonic oscillator

In this exercise we will calculate properties of the anharmonic oscillator. The quantum mechanical description is based on an eigenvalue problem (the stationary Schrödinger equation),

$$H|\Psi\rangle = E|\Psi\rangle \tag{2}$$

where

- $|\Psi\rangle \in \mathcal{H}$ is a vector in some Hilbert space $\mathcal{H}$,
- H is the Hamilton operator which acts on vectors in $\mathcal{H}$,
- E are the energy eigenvalues.

To solve this problem, we will choose a basis set and truncate to a finite dimension, set up the eigenvalue problem and find the eigenvalues numerically.
The Hamiltonian of the anharmonic oscillator is given by

$$\begin{aligned} H &= H_{\text{harmonic}} + H_{\text{anharmonic}} && (3) \\ &= \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + Kx^4, && (4) \end{aligned}$$

where x and p are operators that generally do not commute, $xp - px \neq 0$.
The harmonic part of this Hamiltonian can be written as

$$H_{\text{harmonic}} = \hbar\omega(a^\dagger a + \frac{1}{2}) \tag{5}$$

with the operators a and $a^\dagger$ defined by

$$a = \sqrt{\frac{m\omega}{2\hbar}}x + \frac{ip}{\sqrt{2m\hbar\omega}} \tag{6}$$

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}x - \frac{ip}{\sqrt{2m\hbar\omega}}, \tag{7}$$

where $[a, a^\dagger] = 1$.
The eigenstates $|n\rangle$ of the count operator $N = a^\dagger a$ build a natural set of basis states for the harmonic oscillator. Their energy eigenvalues are given by $\langle n|H_{harm}|n\rangle = \hbar\omega(n + \frac{1}{2})$. We will use this as a basis set for the anharmonic oscillator, but truncate at a finite n.

1. Using the definitions of a and $a^\dagger$, express the anharmonic part of the oscillator in second-quantized form.

2. Calculate the non-vanishing matrix elements of $\mathcal{H}$ in the basis $|n\rangle$.

3. Set up the matrix and diagonalize it numerically for finite n and small K.