Exercise 5
Numerov's method

Solve computationally the Schrödinger equation for an anharmonic oscillator potential using Numerov method

$$-\frac{1}{2m}\nabla^2\psi(x) + V(x)\psi(x) = E\psi(x), \text{ where} \tag{1}$$

$$V(x) = \frac{C}{2}x^2 - \frac{D}{2}x^3 + \frac{E}{2}x^4, \tag{2}$$

where C, D and E are larger than zero. Note that the equation is written in atomic units. Obtain at least 5 eigenenergies and eigenstates, plot eigenstates as a function of x. There is no need to normalize eigenstates, but they must be continuous.

First make the calculation for the case of $D = 0$ and $E = 0$ and check that your eigenvalues agree with the analytical ones. Select some values D and E such that the anharmonic term is NOT the dominating one and such that the potential does not decay for any x. Study how eigenenergies and eigenfunctions change, if you change D and E.

Choice of parameters
Please select C of order ∼500 – 1500 N/m, which is a typical values for force constants of diatomic molecules. Please select the mass of order from 0.5 to 20 Dalton, which corresponds approximately the mass of 900 to 4000 Hartree atomic units. This is a typical reduced mass of light diatomic molecules.

Output of results
All parameters that can be varied must be defined and read from an input file. The output of results - a pdf file/presentation. The calculated energy must be presented in eV. Length must be presented in nm, Ångstrom or Bohr.

Tipp
Use double precision for Numerov's method to avoid rounding errors. Make small enough iteration step in energy or use a Cooley method to guess an energy for a new iteration.