Scientific Programming
(Wissenschaftliches Programmieren)

Exercise 5

1. Matplotlib quick start guide

- Read and try (type – do not copy paste! – and run) the Matplotlib quick start guide.
- Make sure you understand the examples.
- If you encounter any unknown functions, arguments, look it up in the Numpy/Matplotlib documentation.

2. *Plotting the results of simple QM-calculations

- Visualize the results of a QM-program which solves the 1D time-independent non-relativistic one-particle Schrödinger-equation for an electron in a given potential.
- The program produces following output files:
  - discrpot.dat: Potential on a grid.
  - energies.dat: Calculated eigenenergies.
  - wfuncs.dat: Calculated eigenfunctions on a grid.
- All data is given in atomic units (length unit 1 Bohr ≈ 0.529177 Å, energy unit 1 Hartree ≈ 27.2114 eV)
- The files have following formats:
  - energies.dat

    ```
    energy1
    energy2
    energy3
    :
    ```

  - discrpot.dat:

    ```
    x1  V(x1)
    x2  V(x2)
    x3  V(x3)
    :
    ```

  - wfuncs.dat:

    ```
    x1  Psi1(x1)  Psi2(x1)  Psi3(x1) …
    x2  Psi1(x2)  Psi2(x2)  Psi3(x2) …
    x3  Psi1(x3)  Psi2(x3)  Psi3(x3) …
    :
    ```

    - The x-values (grid) in the files discrpot.dat and wfuncs.dat are equidistant and identical.
- Write a function, which accepts a directory name as argument, reads the three files (energies.dat, discrpot.dat and wfuncs.dat) from that directory and returns the contained energies, x-coordinates, potential and wave functions as four numpy arrays.
- Write a function which visualizes the eigenfunctions by plotting them within the potential on a base line shifted by the energy of the corresponding eigenstate.
- With the help of those functions and the sample data provided with the exercise, reproduce the figures below.
- Write each figure into a PDF-file.