Scientific Programming
(Wissenschaftliches Programmieren)

Exercise 5

1. Matplotlib quick start guide

- Go through the Matplotlib quick start guide trying out the examples to see how they work.
- Ensure you have a good grasp of the examples provided.
- Should you come across any unfamiliar functions or arguments, consult the Numpy/Matplotlib documentation to understand their usage.

2. Plotting the results of simple QM-calculations

- Create a visualization for the output of a (hypothetical) quantum mechanics simulation program that calculates the one-dimensional, time-independent, non-relativistic Schrödinger equation for an electron within a specified potential.
- The program generates the following output files:
  - **discrpot.dat**: Contains the potential on a grid.
  - **energies.dat**: Contains the calculated eigenenergies.
  - **wfuncs.dat**: Contains the calculated eigenfunctions on a grid.

All data is presented in atomic units, where the unit of length is 1 Bohr (≈ 0.529177 Å) and the energy unit is 1 Hartree (≈ 27.2114 eV).

Tasks:

- Develop a function that takes a directory name as an argument, reads the three files (`energies.dat`, `discrpot.dat`, and `wfuncs.dat`) from that directory, and returns the energies, x-coordinates, potentials, and wave functions as four separate numpy arrays.
- Create a function which plots the eigenfunctions together with the potential, formers offset by the energy of the respective eigenstates (as shown in the example figures).
- Make sure, the function is generic enough to plot any eigenstate-like function, such as the spatial probability densities (the square of the wave functions), when the right data is passed.
- Recreate the example figures using these functions and the sample data included with the exercise,.
- Save each generated figure as a PDF file.

File formats:

energies.dat:	**discrpot.dat:**	**wfuncs.dat:**
`energy1`	`x1 V(x1)`	`x1 Psi1(x1) Psi2(x1) Psi3(x1) …`
`energy2`	`x2 V(x2)`	`x2 Psi1(x2) Psi2(x2) Psi3(x2) …`
`energy3`	`x3 V(x3)`	`x3 Psi1(x3) Psi2(x3) Psi3(x3) …`
`:`	`:`	`:`

(The x-values (grid point coordinates) in the files **discrpot.dat** and **wfuncs.dat** are equidistant and identical.)