

Scientific Programming (Wissenschaftliches Programmieren)

Exercise 5

1. Matplotlib finger exercise

- Try (type – do not copy paste! – and run) all examples in Sections 1.5.1, 1.5.2, and 1.5.3 in [Chapter 1.4. Matplotlib: plotting](#) of the [Scipy lecture notes](#)
- Make sure you understand the examples.
- If you encounter any unknown functions, arguments, look it up in the Numpy/Matplotlib documentation.
- Note: You may have to set `plt.rcParams["axes.axisbelow"] = False` in order to make the example with the overlaid bboxes working correctly.

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.

3. Matplotlib for advanced users*

- Reproduce the examples in Section 1.5.4. [Chapter 1.5. Matplotlib: plotting](#) of the [Scipy lecture notes](#).
- Make sure you understand the examples.
- If you encounter any unknown functions, arguments, look it up in the Numpy/Matplotlib documentation.

