Computational Physics: Introductory Course

Assignment 1:

Introduction to Python

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Installing software

Install Python

To follow the course you are expected to have a personal computer with Python installed. We recommend that you install the Spyder Integrated Development Environment (IDE) `https://www.spyder-ide.org/`, where you can do your exercises. The lecture notes describe how to use Spyder.

Install screen recording program

In addition, in some of the exercises, you are expected to perform screen recordings of various activities, and therefore you should also install a screen recording program suitable for the operating system on your personal computer. There are various non-commercial and commercial screen recording programs on the market. If you are using Windows or Mac we recommend `ScreenPal` which is free of charge. For information see the page:

`https://screenpal.com/`

If you are using Mac, you can also do screen recordings in the Quick time player.

For Linux distributions, `recordMyDesktop` is a popular screen recording application and more information can be found here:

`http://recordmydesktop.sourceforge.net/about.php`

Writing reports

Writing reports in LaTeX

For writing reports, we strongly encourage you to use LaTeX. LaTeX is a command based document preparation system, which is developed for scientific writing. It is extremely powerful, and once you master it, writing will be much faster than with other document preparation systems. Check this page for installation on different operating systems:

`https://latex-project.org/ftp.html`

In case you don't want to install LaTeX on your computer, we recommend that you try `Overleaf` which is an online tool for the generation of LaTeX-based articles:

`https://www.overleaf.com/`

At Canvas you can download zip-files with report templates. Just drag them to `Overleaf`, and they will automatically unzip and produce a pdf-file.

What the report should contain

A report should contain:

- The py-files, with carefully commented Python code, that were used to solve the exercises. Before the code a few sentences describing what the code is doing should always be included. Each py-file should be embedded in the LaTeX or Word document.

- When applicable, you should include the output or plots produced by your code as part of the exercise.
- When you, as part of an exercise, are asked to draw physical conclusions it is important that these conclusions are included in the report. If you are unable to draw any conclusion you should explicitly write 'I was not able to draw any conclusion'.

Important things to keep in mind for producing a good report that adheres to the general rules in scientific writing.

- All variables in the report should be in math font, e.g. the distance was $d = 1.5$ (do not write the distance was d = 1.5, wrong).
- All units in the report should be in correct font, e.g. the acceleration is $a = 1.5\ \mathrm{ms}^{-2}$ (do not write the acceleration is $a = 1.5\, ms^{-2}$, wrong).
- Write $a = 1.5 \cdot 10^{-3}$ instead of $a = 1.5 * 10^{-3}$ (wrong, never use * in equations or text)
- If you give computed values, round them to a reasonable number of decimals.
- The font size in plots should be large enough for the axis texts and legends to be read.

Reading instructions for assignment 1

Start to read chapters 1 - 6 in the lecture notes, which are available at Canvas, in a overview fashion. You will now be in a good position to do the exercises. For the plotting exercises have a detailed look at the relevant plotting examples in sections 6.3 - 6.6. For defining lambda functions, see section 2.6. Relevant information on how to determine roots and integrals can be found in examples 17.3 and 20.3 in the lecture notes.

Exercises

1. The title of this course is "Computational Physics: Introductory Course". But how is Computational Physics defined and what are the applications? Look around for information and summarize what you find in maximum half a page. At least two independent sources should be cited.
2. (a) Plot the functions $f(x) = e^{-x^2}$ and $g(x) = e^{-(x-2)^2}$ over the interval $[-2, 3]$. Both functions should be in the same plot. Choose colors red and blue. Add title, legends, axis labels and grid lines.

   Make a screen recording of the task above. Create a Youtube account on `www.youtube.com` and upload the recorded video.
   Provide the link to the video, for example `https://www.youtube.com/watch?v=tKGWFrWXuk0`

   (b) Plot the function

   $$f(x) = \frac{x^2 - x + 1}{(x-1)(x-2)}$$

   in the interval $[-2, 5]$. To handle the undefined points, plot the function in three pieces from -2 to 1, from 1 to 2 and from 2 to 5. Use the command `axis` to adjust your plot so that you get a good scale for the y-axis (compare example 6.7). The plot should be as informative as possible.

Be very careful so that you don't make any error with the parenthesis. Note that

```
(x**2 - x + 1)/(x - 1)*(x - 2)
```

is wrong (why?). It is probably better to write the numerator and the denominator separately and then put them together.

3. In an experiment, the radioactivity as a function of time $A(t)$ of a sample is recorded and the following data are obtained:

t [s]	0	1	2	3	4	5	6
$A(t)$ [kBq]	205	130	85	65	42	25	15

Plot the data above as discrete data points together with the model function

$$A(t) = 202e^{-0.42t} \text{ [kBq]}$$

in the same plot. Use a vector t with 100 points in the interval between 0 and 6 to plot $A(t)$. Estimate as accurately as possible the half-life of the sample, i.e. the instance in time when the radioactivity of the sample is 50 % of its original value.

Hint: If you have defined the model function as a lambda function, try different values of t until $A(t) \approx A(0)/2 = 101$ kBq. Alternatively define $f(t) = 202e^{-0.42t} - 101$ as a lambda function and use the command `brentq` to solve the equation $202e^{-0.42t} - 101 = 0$ for t .

4. The radial wave function of the $4p$ electron in hydrogen as a function of the distance r from the nucleus in atomic units [a.u.] is given by

$$P(r) = Ar^2e^{-r/4}\left(1 - \frac{1}{4}r + \frac{1}{80}r^2\right),$$

where A is a constant. Plot the radial wave function in some suitable interval from $r = 0$ extending out to a point where the wave function drops down to virtually zero. Use the information from the plot to find the roots of the wave function (define the function as a lambda function and use `brentq`).

The square of a radial wave function reflects the probability of finding the electron at a certain distance. Since the probability of finding the electron somewhere between $r = 0$ and $r = \infty$ must be identically equal to 1, we require the following normalization criterion to be fulfilled

$$\int_0^\infty |P(r)|^2\, dr = 1.$$

Find an approximate value of the constant A so that the normalization criterion is fulfilled. Please note that you are not only supposed to give a value of A, but also explain how you computed it.

Physics background

The course is in computational physics, and we provide the physics background for many of the exercises together with links, that make it possible to read more if you find it interesting.

Radioactivity
Some isotopes are unstable with a well defined probability λ per unit time for a decay. If we at a given time t have a sample of $N(t)$ nuclei then the change $N'(t)$ per unit time satisfies

$$N'(t) = -\lambda N(t),$$

where we have a negative sign since the change per unit time is negative. Integrating the differential equation we have

$$N(t) = N_0 e^{-\lambda t},$$

where N_0 is the number of nuclei at time $t = 0$ when we start to study the system. Thus the number of nuclei in the sample decreases exponentially. The half-life $t_{1/2}$ is defined as the time for which the original number of nuclei N_0 has gone down to half, that is the time for which

$$\frac{N_0}{2} = N_0 e^{-\lambda t}.$$

Solving this equation gives

$$t_{1/2} = \frac{\ln(2)}{\lambda}.$$

The activity $A(t)$ of a sample is defined as the number of decays per unit time and is given in units of becquerel (Bq) in honor of the discoverer of radioactivity

$$A(t) = \lambda N(t) = \frac{\ln(2)}{t_{1/2}} N(t).$$

Thus the activity and the number of nuclei in the sample are proportional.

You can read more about radioactivity at `https://www.radioactivity.eu.com/site/pages/Home_Page.htm`. The page covers nuclear physics very broadly, including radioactive decay, the theory for alpha and beta decay, applications in energy production and medicine etc. Much recommended reading!

Wave function
Light has wave properties as is demonstrated by Young's double-slit experiment `https://en.wikipedia.org/wiki/Double-slit_experiment`. Light also has particle properties, read for example about the photoelectric effect `https://en.wikipedia.org/wiki/Photoelectric_effect`, and can be viewed as a swarm of discrete energy packets, known as photons. Conversely, material particles have wave properties at the nanometer scale `https://en.wikipedia.org/wiki/Wave%E2%80%93particle_duality`, and the states of a particle system are described by wave functions that are solutions to a differential equation known as the Schrödinger equation (we will solve this equation later on during the course).

The hydrogen atom consists of an electron bound to a single proton (the nucleus). The electron can be in different states with well defined energies. The states of the electron are specified by three so called quantum numbers nlm_l. n is called the principal quantum number and can take on positive integer values

$$n = 1, 2, 3, \ldots$$

l is the angular quantum number for which

$$l = 0, 1, 2, \ldots, n-1,$$

where $l = 0, 1, 2, 3$ often are denoted s, p, d, f. m_l is the magnetic quantum number and can take on the vales

$$m_l = -l, -l+1, -l+2, \ldots, l.$$

The states are described by wave functions $\psi_{nlm_l}(x, y, z)$ in three dimensional space. The wave function $\psi_{nlm_l}(x, y, z)$ for a state has a probabilistic interpretation such that

$$\left|\psi_{nlm_l}(x, y, z)\right|^2 \Delta x \Delta y \Delta z$$

gives the probability to find the electron in a cube with edges Δx, Δy, Δz centered around (x, y, z). The probability distributions for some of the states are shown below. We see that states with $l = 0$ have spherically symmetric distributions whereas states with $l > 0$ have distributions that goes out in lobes, the orientation of which depends on m_l.

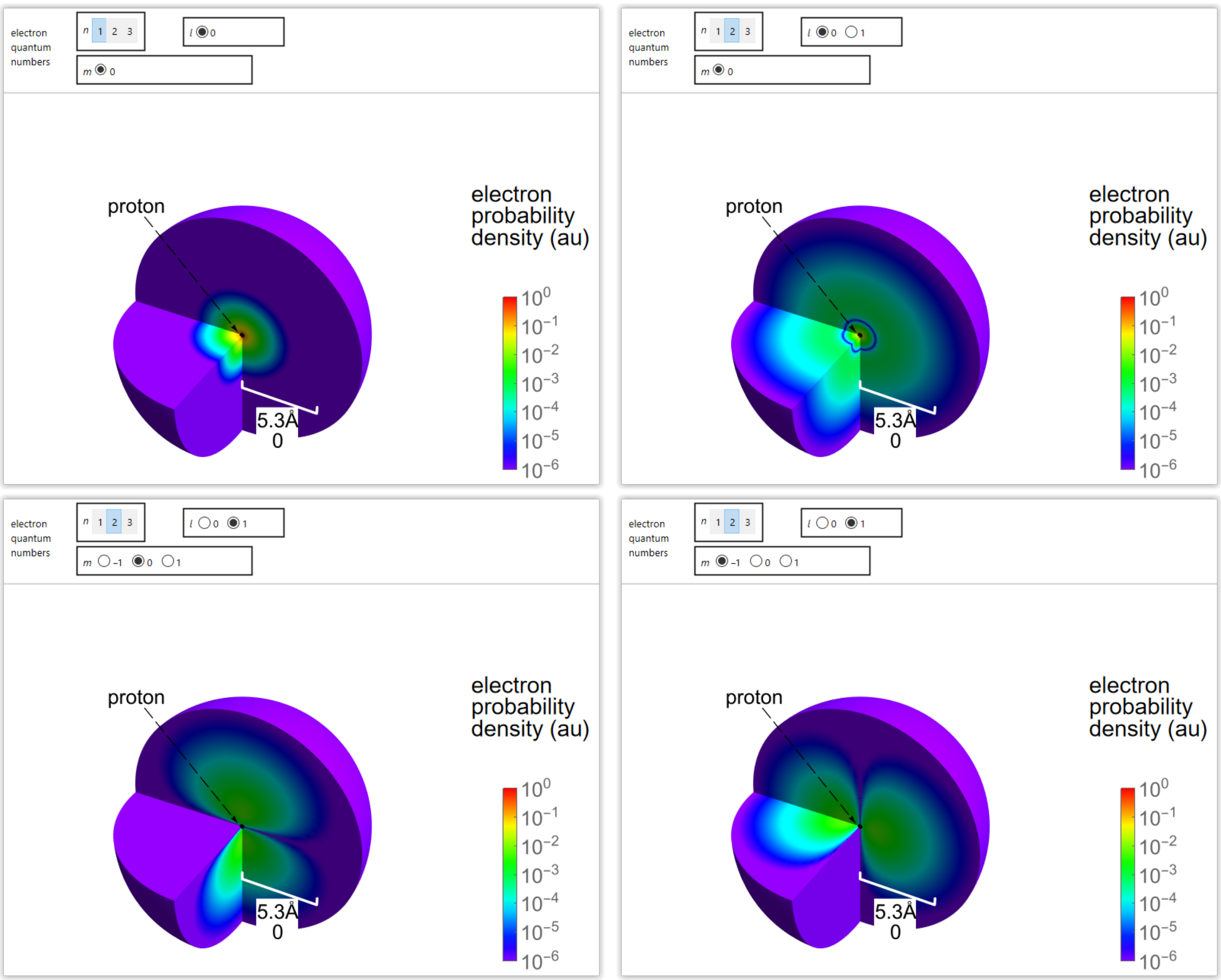
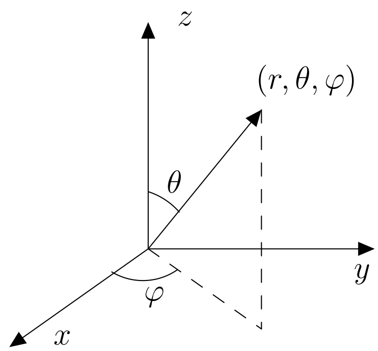


Figure 1: *Probability distributions for some electronic states in hydrogen.*

In spherical co-ordinates (r, θ, φ), as illustrated below



the wave function can be decomposed into a radial and an angular part

$$\psi_{nlm_l}(r, \theta, \varphi) = \frac{P_{nl}(r)}{r} Y_{lm_l}(\theta, \varphi),$$

where the angular part is given by so called spherical harmonics. The radial part $P_{nl}(r)$ extends from $r = 0$ to ∞. We can interpret

$$|P_{nl}(r)|^2 \, dr$$

as the probability to find the electron in a spherical shell with radius r and width dr centered at the nucleus. Points where $P_{nl}(r) = 0$ are called nodes, and at the nodes the probability to find the electron drops down to zero. For convenience r is measured in so called atomic units (a.u.), where the atomic unit for length is $a_0 = 5.29 \times 10^{-11}$ m. The probability interpretation leads to the condition

$$\int_0^\infty |P_{nl}(r)|^2 \, dr = 1,$$

which is the mathematical way to say that the total probability to find the electron somewhere in space must be one. Plots of the radial distributions for some states can be fond here, see `http://hyperphysics.phy-astr.gsu.edu/hbase/hydwf.html`. Note the nodal structure of the functions and the similarity with standing waves on a string. So, forget about the picture of the Hydrogen atom as an electron moving in an orbit around the nucleus in a similar way as the earth orbits the sun. Think about the electronic states in terms of probability distributions with similarities with standing waves on a string and with lobes extending in different angles. The atom is a wave!