Practice Work 3
Differential Equations

This practice work deals with numerically solving a differential equation with an eigenvalue. Since the calculations required here are presented in the lecture notes, you must carefully show that you understand what you are doing, i.e. give good comments among the calculations.

The Equation

The equation which you'll be studying is the same as in the lectures, the Schrödinger equation for the Hydrogen atom (with $l = 0$):

$$-\frac{d^2y(r)}{dr^2} - \frac{2}{r}y(r) = Ey(r), \tag{1}$$

which holds for energy values $E < 0$. Here $y(r) = rR(r)$, where R is the actual radial wave function. The function R satisfies the normalization condition

$$4\pi \int_0^\infty r^2 R(r)\, dr = 1, \tag{2}$$

from which follows a normalization condition for the function y (see lectures and excercises).

Assignment I

Before attacking the numerical solution of (1), here are a few warm-up excercises concerning differential equations of various types:

1. Solve the differential equation

$$\frac{d^2y}{dx^2} + cx\frac{dy}{dx} + xy = 0 \tag{3}$$

with the initial conditions $y(0) = 0$ and $y'(0) = 1$. Let the parameter c have the values $0.25, 0.5, 1.5, 4.0, 10.0$ and 40.0 and plot all the solutions, corresponding to different values of c, in the same picture.

2. Solve the eigenvalue equation

$$\frac{dy^2}{dx^2} + \frac{dy}{dx} = \lambda y \tag{4}$$

on the interval $0 \le x \le 5$, in *matrix form.* This means that you must search for the solution of (4) in discrete points $x_0, x_1, \ldots, x_n$, where in this case $x_0 = 0$ and $x_n = 5$. Suppose that the points are equally spaced, i.e. $x_i - x_{i-1} = h$, for all $i = 1, \ldots, n$. Then you can approximate the derivatives which appear in on the left hand side of the equation with finite differences,

$$y''(x_i) \approx \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} \quad \text{and} \quad y'(x_i) \approx \frac{y_{i+1} - y_{i-1}}{2h}. \tag{5}$$

Then the problem reduces to a set of linear equations for the variables $y_0, y_1, \ldots, y_n$, where $y_i = y(x_i)$. This can be presented in matrix form as

$$MY = \lambda Y, \tag{6}$$

where $Y = (y_0, \ldots, y_n)^\top$. As boundary conditions you can set $y_{-1} = y_{n+1} = 0$. Now the eigenvalues and -vectors of M are straightforward to calculate in *Mathematica*. As a result, plot a few of the eigenfunctions which correspond to the lowest (in terms of absolute value) eigenvalues.

3. In the file `ass1e3.txt`, located in the folder `pw3_datafiles`, values of a function $y(x)$ are tabulated, along with the corresponding values of x. Vefify, by means of interpolation, that the function y satisfies (to some precision) the differential equation

$$\frac{d^3y}{dx^3} + x\frac{d^2y}{dx^2} = 1. \tag{7}$$

Also, calculate the analytical solution of the equation (you must determine some appropriate boundary conditions) and plot it in the same figure with the interpolating function.

Assignment II

Your first Hydrogen-related task is to reproduce the solution of this equation which was presented in the lectures. First, you must determine the interval $[r_0, r_1]$ in which you search for the solution, in the way that $0 < r_0 < r_1 < \infty$. Then, to ensure numerical accuracy and stability, you must divide this interval into two, $[r_0, r_m]$ and $[r_m, r_1]$ and search the solution in these two parts separately. Denote y_0 the solution in $[r_0, r_m]$ and y_∞ in $[r_m, r_1]$. The asymptotic behavior of y,

$$y(r)|_{r\to 0} \sim r \quad \text{and} \quad y(r)|_{r\to\infty} \sim e^{-\sqrt{-E}r}, \tag{8}$$

determines the boundary conditions in these subintervals, i.e.

$$y_0(r_0) = r_0, \quad \text{and} \quad y_0'(r_0) = 1, \tag{9}$$

and

$$y_\infty(r_1) = e^{-\sqrt{-E}r_1} \quad \text{and} \quad y_\infty'(r_1) = -\sqrt{-E}e^{-\sqrt{-E}r_1}. \tag{10}$$

Now, corresponding to these boundary conditions, only some certain values of E yield an acceptable solution of (1). The condition for acceptability is that the solution and its derivative are continuous, i.e. $y_0(r_m) = y_\infty(r_m)$ and $y_0'(r_m) = y_\infty'(r_m)$. Dividing the latter by the former yields

$$\delta(E) := \frac{y_0'(r_m)}{y_0(r_m)} - \frac{y_\infty'(r_m)}{y_\infty(r_m)} = 0. \tag{11}$$

The task is, basically, to find the zeros of the function δ. There are two possible ways of achieving this. You can proceed as in the lectures, find two initial guessed values for E which give a different sign to δ and iterate your way to a more accurate eigenvalue. Or, you can proceed as in the excercises and implement δ as a *Mathematica* function using the `Module` command.

From the eigenvalues E, calculate the two longest wavelengths of the Lyman series. The Lyman series is the set of spectral emission lines from a Hydrogen atom, resulting from transitions to the ground state from some excited state. In this transition, the atom emits a photon with wavelength

$$\lambda = \frac{hc}{\Delta E}, \tag{12}$$

where h is Planck's constant, c is the speed of light in vacuum and ΔE is the energy difference of the states in question. To calculate these wavelengths, you need the energies of the three lowest states. Note that the units employed here are not SI-units. Instead, the eigenvalue of (1) comes out in *Rydbergs*. One Rydberg is $1\,\text{Ry}= 13.6\,\text{eV}$, and one electron volt is $1\,\text{eV}= 1.602 \cdot 10^{-19}\,\text{J}$.

Also, plot the third state (i.e. the second excited state). First, you must match the partial solutions and normalize the function as was done in the lectures and excercises.

Bonus Assignment

In the file `code.txt`, in the folder `pw3_datafiles`, there is a secret message. It has been encrypted using so-called Caesar's decryption method. This method consists of first assigning numbers to the different letters, i.e. $A = 1, B = 2, \ldots, Z = 26$, and then adding some number, which preferably is known only to the sender and the receiver, and then converting the resulting numbers back to letters.

For example, the word BONUS could be encrypted as follows: First, convert the original letters to numbers: $(B, O, N, U, S) \to (2, 15, 14, 21, 19)$. Then, add for example 13 to each number. Note that if the sum exceeds 26, the enumeration starts again from 1, i.e. $27 \to 1, 28 \to 2, \ldots$ This procedure results in $(15, 28, 27, 34, 32) \to (15, 2, 1, 8, 6)$. Then, convert the numbers back to letters and obtain the word OBAHF.

Your task is to discover the added number in the case of the text in `code.txt` and decrypt the message. You can of course do it manually, by trying all possible alternatives, but the most rewarding way to complete this task is to write a *Mathematica* function which does the aforedescribed encryption, which can then be used also to decryption.

This is a bonus assignment, so you don't have to do this, but I highly encourage it! You can use the `Module` command to wrap up a set of commands to a function. Also, the `Mod` command might turn out to be useful. *Hint*: First, make a function which assigns numbers to letters, then one which does the opposite.

Practical Issues

Carry out the above tasks and do *all* of your calculations with *Mathematica*. This time you must write the *Mathematica* commands in a separate file and execute the file using the commands `SetDirectory["path//to//file"]` and `<<"file.m"`. Note that you cannot refer to previous output using the `%n` command inside the file. Also, if you suppress output using the semicolon (`;`), that output is also inreferrable with `%`. This way you will learn to be more efficient using *Mathematica*, and other programming languages as well.

Write a work report, which includes the following:

- (on the first page) your name and e-mail address, practice work number and date of return
- the assignment, briefly in your own words
- a print-out of the files containing your *Mathematica* calculations, and the output generated by it
- a separate section for the results of the calculations

  First task 1. The plot of the set of solutions. 2. Plots of the eigenfunctions, and the corresponding eigenvalues. 3. Plot of the interpolating function and the analytical solution.

  Second task The two longest wavelengths, and a plot of the second excited state

  Bonus task The message decrypted!

Return the report into the IN-box in the theoretical physics lobby. If you experience problems, help is available Tuesdays until April 24th, at 8–11 in classroom KO130. Also, you can ask questions by e-mail. My address is `jmattas@mail.student.oulu.fi`. Furthermore, I am available at the physics tutor room FY1043 on Wednesdays from 2 p.m. to 4 p.m.

The exam of this class is on Friday, May 4th in the classroom KO150. Sign up for the exam at the theoretical physics lobby. Remember to return all your practice works before the exam!