

Cool Title

Project 2, FYS-3150

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All source codes can be found at: https://github.com/inakbk/Project_1.git in the folders `exercise_b` and `exercise_d`.

Contents

1	Motivation and purpose	2
2	Numerical method: Jacobis method	2
3	Physics 1: One electron in a three-dimentional harmonic oscillator potential.	2
3.1	Rewriting the Schrödinger's equation to a dimentionaless form	2
3.2	Discretizing the Schrödingers equation to solve numerically.	3

[illegible]

We are only interested in the solution of the radial part of the Schrödinger equation given by

$$-\frac{\hbar^2}{2m} \left(\frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} - \frac{l(l+1)}{r^2} \right) R(r) + V(r)R(r) = ER(r). \quad (1)$$

Then we use the substitution $R(r) = (1/r)u(r)$ and obtain

$$-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} u(r) + \left(V(r) + \frac{l(l+1)}{r^2} \frac{\hbar^2}{2m} \right) u(r) = Eu(r).$$

The boundary conditions are $u(0) = 0$ and $u(\infty) = 0$.

We will modify equation 1 further by introducing a dimensionless variable $\rho = (1/\alpha)r$ where α is a constant with dimension length and get

$$-\frac{\hbar^2}{2m\alpha^2} \frac{d^2}{d\rho^2} u(\rho) + \left(V(\rho) + \frac{l(l+1)}{\rho^2} \frac{\hbar^2}{2m\alpha^2} \right) u(\rho) = Eu(\rho).$$

Now inserting $l = 0$ and the rewritten potential $V(\rho) = (1/2)k\alpha^2\rho^2$ we obtain:

$$-\frac{\hbar^2}{2m\alpha^2} \frac{d^2}{d\rho^2} u(\rho) + \frac{k}{2}\alpha^2\rho^2 u(\rho) = Eu(\rho).$$

and then multiply by $2m\alpha^2/\hbar^2$ on both sides

$$-\frac{d^2}{d\rho^2} u(\rho) + \frac{mk}{\hbar^2} \alpha^4 \rho^2 u(\rho) = \frac{2m\alpha^2}{\hbar^2} Eu(\rho).$$

We fix the constant α so that

$$\frac{mk}{\hbar^2} \alpha^4 = 1 \Rightarrow \alpha = \left(\frac{\hbar^2}{mk} \right)^{1/4}.$$

and then define

$$\lambda = \frac{2m\alpha^2}{\hbar^2} E,$$

Finally equation 1 can be written as

$$-\frac{d^2}{d\rho^2} u(\rho) + \rho^2 u(\rho) = \lambda u(\rho). \quad (2)$$

which is the equation we want to solve numerically. We know¹ that this equation has the eigenvalues $\lambda_0 = 3, \lambda_1 = 7, \lambda_2 = 11, \dots$ for $l = 0$. These analytical values will be used to test the precision of the numerical method.

3.2 Discretizing the Schrödingers equation to solve numerically.

We will now rewrite the Schrödingers equation on a discretized form to be able to solve it as an matrix eigenvalue problem.

¹This is given in the assignment text for Project 2, FYS3150..

We use the expression for the second derivative of the function $u(\rho)$

$$u'' = \frac{u(\rho + h) - 2u(\rho) + u(\rho - h)}{h^2} + O(h^2), \quad (3)$$

where h is our step. We define the minimum and maximum values for the variable ρ , $\rho_{\min} = 0$ and ρ_{\max} so that:

$$h = \frac{\rho_{\max} - \rho_{\min}}{n_{\text{step}}}.$$

where n_{step} is a given number of steps. Since $\rho \propto r$ and $r \in [0, \infty)$ the maximum value of ρ should be $\rho_{\max} = \infty$. But we cannot set a infinite value when computing the solution numerically. We will therefore have to choose a significantly large enough ρ that give stable results for different n_{step} (test noe noe ??)

We can then define an arbitrary value of ρ as

$$\rho_i = \rho_{\min} + ih \quad i = 0, 1, 2, \dots, n_{\text{step}}$$

so that the Schrödinger equation for ρ_i reads

$$-\frac{u(\rho_i + h) - 2u(\rho_i) + u(\rho_i - h)}{h^2} + \rho_i^2 u(\rho_i) = \lambda u(\rho_i),$$

or in a more compact way with the harmonic oscillator potential $V_i = \rho_i^2$:

$$-\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + V_i u_i = \lambda u_i,$$

Then we can define first the diagonal matrix element

$$d_i = \frac{2}{h^2} + V_i,$$

and the non-diagonal matrix element:

$$e_i = -\frac{1}{h^2}.$$

We observe that in this case all the non-diagonal matrix element is given by a constant, so we can denote them all as $e = -\frac{1}{h^2}$ instead. (insert e og ikke ei hele veien??)

With these definitions the Schrödinger equation (2) takes the following form

$$d_i u_i + e_{i-1} u_{i-1} + e_{i+1} u_{i+1} = \lambda u_i,$$

where u_i is unknown. This can be written as a matrix eigenvalue problem

$$\begin{pmatrix} d_1 & e_1 & 0 & 0 & \dots & 0 & 0 \\ e_1 & d_2 & e_2 & 0 & \dots & 0 & 0 \\ 0 & e_2 & d_3 & e_3 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & \dots & d_{n_{\text{step}}-2} & e_{n_{\text{step}}-1} \\ 0 & \dots & \dots & \dots & \dots & e_{n_{\text{step}}-1} & d_{n_{\text{step}}-1} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \dots \\ \dots \\ \dots \\ u_{n_{\text{step}}-1} \end{pmatrix} = \lambda \begin{pmatrix} u_1 \\ u_2 \\ \dots \\ \dots \\ \dots \\ u_{n_{\text{step}}-1} \end{pmatrix} \quad (4)$$

Project 2, Schrödinger's equation for two electrons in a three-dimensional harmonic oscillator well

or if we wish to be more detailed, we can write the tridiagonal matrix as

$$\begin{pmatrix} \frac{2}{h^2} + V_1 & -\frac{1}{h^2} & 0 & 0 & \dots & 0 & 0 \\ -\frac{1}{h^2} & \frac{2}{h^2} + V_2 & -\frac{1}{h^2} & 0 & \dots & 0 & 0 \\ 0 & -\frac{1}{h^2} & \frac{2}{h^2} + V_3 & -\frac{1}{h^2} & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & \dots & \frac{2}{h^2} + V_{n_{\text{step}}-2} & -\frac{1}{h^2} \\ 0 & \dots & \dots & \dots & \dots & -\frac{1}{h^2} & \frac{2}{h^2} + V_{n_{\text{step}}-1} \end{pmatrix} \quad (5)$$

Recall that the solutions are known via the boundary conditions at $i = n_{\text{step}}$ and at the other end point, that is for ρ_0 . The solution is zero in both cases.

- a) Your task here is to write a function which implements Jacobi's rotation algorithm (see Lecture notes chapter 7) in order to solve Eq. (4).

We Define the quantities $\tan \theta = t = s/c$, with $s = \sin \theta$ and $c = \cos \theta$ and

$$\cot 2\theta = \tau = \frac{a_{ll} - a_{kk}}{2a_{kl}}.$$

We can then define the angle θ so that the non-diagonal matrix elements of the transformed matrix a_{kl} become non-zero and we obtain the quadratic equation (using $\cot 2\theta = 1/2(\cot \theta - \tan \theta)$)

$$t^2 + 2\tau t - 1 = 0,$$

resulting in

$$t = -\tau \pm \sqrt{1 + \tau^2},$$

and c and s are easily obtained via

$$c = \frac{1}{\sqrt{1 + t^2}},$$

and $s = tc$.

Explain why we should choose t to be the smaller of the roots. Convince yourself that this choice ensures that $|\theta| \leq \pi/4$ (and has the effect of minimizing the difference between the matrices \mathbf{B} and $\mathbf{A} \Rightarrow$ so that the iterations goes 'faster')

We need: $|\theta| \leq \pi/4 \Rightarrow \theta \leq \pi/4$ and $\theta \geq -\pi/4$. Start with the first:

$$\theta = \arctan t \leq \pi/4$$

$$t \leq \tan(\pi/4) = 1$$

and

$$\theta = \arctan t \geq -\pi/4$$

$$t \geq \tan(-\pi/4) = -1$$

so $|t| \leq 1 \Rightarrow -\tau \pm \sqrt{1 + \tau^2} \leq 1$. I then look at the case where $\tau > 0$ and try the positive root of t :

$$\begin{aligned} -\tau + \sqrt{1 + \tau^2} &\leq -|\tau| + 1 + |\tau| = 1 \\ \Rightarrow t &\leq 1 \Rightarrow \theta \leq \pi/4 \end{aligned}$$

Then try the case when $\tau < 0$ and try the negative root of t :

$$\begin{aligned} -\tau - \sqrt{1 + \tau^2} &= |\tau| - \sqrt{1 + \tau^2} \geq |\tau| - (1 + |\tau|) = -1 \\ \Rightarrow t &\geq -1 \Rightarrow \theta \geq -\pi/4 \end{aligned}$$

So we see then that when $\tau > 0$ we choose the positive root, and when $\tau < 0$ we choose the negative root to make shure that $|\theta| \leq \pi/4$. This is to make shure that the operations does not make bigger changes to the other elements while making another element zero \rightarrow also making shure that we get to the solution faster (or at all?).

- b) How many points n_{step} do you need in order to get the lowest three eigenvalues with four leading digits? Remember to check the eigenvalues for the dependency on the choice of ρ_{max} .

How many similarity transformations are needed before you reach a result where all non-diagonal matrix elements are essentially zero? Try to estimate the number of transformations and extract a behavior as function of the dimensionality of the matrix.

You can check your results against the code based on Householder's algorithm, *tqli* in the file `lib.cpp`. Alternatively, you can use the Armadillo function for solving eigenvalue problems.

Comment your results (here you could for example compute the time needed for both algorithms for a given dimensionality of the matrix).

- c) We will now study two electrons in a harmonic oscillator well which also interact via a repulsive Coulomb interaction. Let us start with the single-electron equation written as

$$-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} u(r) + \frac{1}{2} k r^2 u(r) = E^{(1)} u(r),$$

where $E^{(1)}$ stands for the energy with one electron only. For two electrons with no repulsive Coulomb interaction, we have the following Schrödinger equation

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dr_1^2} - \frac{\hbar^2}{2m} \frac{d^2}{dr_2^2} + \frac{1}{2} k r_1^2 + \frac{1}{2} k r_2^2 \right) u(r_1, r_2) = E^{(2)} u(r_1, r_2).$$

Note that we deal with a two-electron wave function $u(r_1, r_2)$ and two-electron energy $E^{(2)}$.

With no interaction this can be written out as the product of two single-electron wave functions, that is we have a solution on closed form.

We introduce the relative coordinate $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and the center-of-mass coordinate $\mathbf{R} = 1/2(\mathbf{r}_1 + \mathbf{r}_2)$. With these new coordinates, the radial Schrödinger equation reads

$$\left(-\frac{\hbar^2}{m} \frac{d^2}{dr^2} - \frac{\hbar^2}{4m} \frac{d^2}{dR^2} + \frac{1}{4}kr^2 + kR^2 \right) u(r, R) = E^{(2)} u(r, R).$$

The equations for r and R can be separated via the ansatz for the wave function $u(r, R) = \psi(r)\phi(R)$ and the energy is given by the sum of the relative energy E_r and the center-of-mass energy E_R , that is

$$E^{(2)} = E_r + E_R.$$

We add then the repulsive Coulomb interaction between two electrons, namely a term

$$V(r_1, r_2) = \frac{\beta e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} = \frac{\beta e^2}{r},$$

with $\beta e^2 = 1.44$ eVnm.

Adding this term, the r -dependent Schrödinger equation becomes

$$\left(-\frac{\hbar^2}{m} \frac{d^2}{dr^2} + \frac{1}{4}kr^2 + \frac{\beta e^2}{r} \right) \psi(r) = E_r \psi(r).$$

This equation is similar to the one we had previously in (a) and we introduce again a dimensionless variable $\rho = r/\alpha$. Repeating the same steps as in (a), we arrive at

$$-\frac{d^2}{d\rho^2} \psi(\rho) + \frac{1}{4} \frac{mk}{\hbar^2} \alpha^4 \rho^2 \psi(\rho) + \frac{m\alpha\beta e^2}{\rho\hbar^2} \psi(\rho) = \frac{m\alpha^2}{\hbar^2} E_r \psi(\rho).$$

We want to manipulate this equation further to make it as similar to that in (a) as possible. We define a 'frequency'

$$\omega_r^2 = \frac{1}{4} \frac{mk}{\hbar^2} \alpha^4,$$

and fix the constant α by requiring

$$\frac{m\alpha\beta e^2}{\hbar^2} = 1$$

or

$$\alpha = \frac{\hbar^2}{m\beta e^2}.$$

Defining

$$\lambda = \frac{m\alpha^2}{\hbar^2} E_r,$$

we can rewrite Schrödinger's equation as

$$-\frac{d^2}{d\rho^2} \psi(\rho) + \omega_r^2 \rho^2 \psi(\rho) + \frac{1}{\rho} = \lambda \psi(\rho).$$

We treat ω_r as a parameter which reflects the strength of the oscillator potential.

Here we will study the cases $\omega_r = 0.01$, $\omega_r = 0.5$, $\omega_r = 1$, and $\omega_r = 5$ for the ground state only, that is the lowest-lying state.

With no repulsive Coulomb interaction you should get a result which corresponds to the relative energy of a non-interacting system. Make sure your results are stable as functions of ρ_{\max} and the number of steps.

We are only interested in the ground state with $l = 0$. We omit the center-of-mass energy.

You can reuse the code you wrote for (a), but you need to change the potential from ρ^2 to $\omega_r^2 \rho^2 + 1/\rho$.

Comment the results for the lowest state (ground state) as function of varying strengths of ω_r .

For specific oscillator frequencies, the above equation has answers in an analytical form, see the article by M. Taut, Phys. Rev. A 48, 3561 - 3566 (1993). The article can be retrieved from the following web address http://prola.aps.org/abstract/PRA/v48/i5/p3561_1.

- d) In this exercise we want to plot the wave function for two electrons as functions of the relative coordinate r and different values of ω_r . With no Coulomb interaction you should have a result which corresponds to the non-interacting case. Plot either the function itself or the probability distribution (the function squared) with and without the repulsion between the two electrons. Varying ω_r , the shape of the wave function will change.

We are only interested in the wave function for the ground state with $l = 0$ and the two first excited states with the same symmetry and omit again the center-of-mass motion.

You can choose between three approaches; the first is to use the existing *tqli* function. Here the eigenvectors are obtained from the matrix $z[i][j]$, where the index j refers to eigenvalue j . The index i points to the value of the wave function in position ρ_j . That is, $u^{(\lambda_j)}(\rho_i) = z[i][j]$.

The eigenvectors are normalized. Plot then the normalized wave functions for different values of ω_r and comment the results.

Another alternative is to add a piece to your Jacobi routine which also returns the eigenvectors. This is the more difficult part. You will also need to normalize the eigenvectors.

Finally, the armadillo function *eig_sys* can be used to find eigenvalues and eigenvectors.

- e) Here you are asked to implement unit tests in either your C++ program or your Fortran program. For C++ users, please follow the guidelines on how to install unit tests with `c++` on the webpage. For Fortran user, the software package Fortran Unit Test Framework (FRUIT), sourceforge.net/projects/fortranxunit. These issues will be discussed in more detail at the lab and lectures during week 38.
- f) This exercise is optional and is meant more as a challenge. Implement the iterative Lanczos' algorithm discussed in the lecture notes and compute the lowest eigenvalues as done in exercise c) above. Compare your results and discuss faults and merits of the iterative method versus direct methods like Jacobi's method.