UNIVERSITY OF OSLO

COMPUTATIONAL PHYSICS

Project 2

Authors:

Birgitte Madsen

Magnus Isaksen

Soumya Chalakkal

Autumn 2015

UiO : University of Oslo

Department of Physics
University of Oslo
Sem Sælands vei 24
0371 Oslo, Norway
+47 22 85 64 28
http://www.mn.uio.no/fysikk/english/

Course:

Computational Physics

Project number:

2

Link to GitHub folder:

`https://??`

Hand-in deadline:

Monday, October 5, 2015

Project Members:

Birgitte Madsen
Magnus Isaksen
Soumya Chalakkal

Copies: 1
Page count: 15
Appendices: 0
Completed: ??

TABLE OF CONTENTS

CHAPTER

1 INTRODUCTION

Bla bla bla

The codes written in this project and the results gained from the codes, can be found by following the link: `https://?` to the GitHub repository. [1]

We can ref. to sections etc. using ”secref”-command like: Sec. 2

Vectors can be written using ”v”-command like: **v**

.... and a lot of other cool stuff!

[1] FiXme Note: correct the these lines

CHAPTER

2 METHOD

Intro to chapter

The source code itself can be found in the GitHub folder `https://??.` [1]

2.1 Nature of the problem

The aim of the first part of the project is to solve Schrödingers equations for one electron in a harmonic oscillator potential with angular momentum $l = 0$. The radial part of the Schrödingers equation is then given as

$$\left[-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}+V(r)\right]R(r) = ER(r). \tag{2.1}$$

In order to solve this equation numerically, it is rewritten after a series of transformation and substitution as

$$-\frac{d^2}{d\rho^2}u(\rho)+\rho^2u(\rho) = \lambda u(\rho) \tag{2.2}$$

Eq. (2.2) is discretized by rewriting the second derivative of u as

$$u'' = \frac{u(\rho+h)-2u(\rho)+u(\rho-h)}{h^2}+O(h^2) \tag{2.3}$$

In Eq. (2.3) h is the step length, ρ_{max} and ρ_{min} are the maximum and minimum values of the variable ρ, respectively. For a given number of steps n, the step length is calculated as

$$h = \frac{\rho_{max}-\rho_{min}}{n} \tag{2.4}$$

In order to solve (2.2), the differential equation is, by the use of Eq. (2.3), transformed into a matrix eigenvalue problem

$$\mathbf{Au} = \lambda\mathbf{u} \tag{2.5}$$

[1] FiXme Note: correct the above lines

in which **A** is a tridiagonal matrix of the form

$$\mathbf{A} = \begin{pmatrix} \frac{2}{h^2}+V_1 & -\frac{1}{h^2} & 0 & 0 & \dots & 0 & 0 \\ -\frac{1}{h^2} & \frac{2}{h^2}+V_2 & -\frac{1}{h^2} & 0 & \dots & 0 & 0 \\ 0 & -\frac{1}{h^2} & \frac{2}{h^2}+V_3 & -\frac{1}{h^2} & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & \dots & \frac{2}{h^2}+V_{n-2} & -\frac{1}{h^2} \\ 0 & \dots & \dots & \dots & \dots & -\frac{1}{h^2} & \frac{2}{h^2}+V_{n-1} \end{pmatrix} \tag{2.6}$$

A is obtained from Eq. (2.2) and (2.3) by discretizing ρ as

$$\rho_i = \rho_{min} + ih \qquad i = 0,1,2,\dots,n \tag{2.7}$$

This discretization yields the following Schrödinger equation:

$$-\frac{u(\rho_i+h)-2u(\rho_i)+u(\rho_i-h)}{h^2} + \rho_i^2 u(\rho_i) = \lambda u(\rho_i) \tag{2.8}$$

By introducing $u(\rho_i) = u_i$, this can be rewritten as

$$-\frac{u_{i+1}-2u_i+u_{i-1}}{h^2} + V_i u_i = \lambda u_i \tag{2.9}$$

in which $V_i = \rho_i^2$ is the harmonic oscillator potential. When comparing this problem to the general eigenvalue problem given in Eq. (2.5), it is evident that the diagonal elements of the matrix **A** is given as

$$d_i = \frac{2}{h^2} + V_i \tag{2.10}$$

whilst all off diagonal matrix elements are zero apart from those adjacent to the diagonal (that is, those multiplied by u_{i-1} and u_{i+1} when entering row i), which is given as a mere constant:

$$e_i = -\frac{1}{h^2} \tag{2.11}$$

which is exactly the matrix given in Eq. (2.6).

2.2 Description of the Algorithm

About the algorithm.....

This is how we write c++ code in the report:

```
// I am a comment

    double please define me;

    for (int i=1 ; i<n ; i++)
    {
        I do this for a lot of i's;
    }
```

2.2.1 Change in Matrix Elements after Iterations and Choice of θ

The algorithm for solving the eigenvalue problem given in [2] contains of multiply similarity transformations of the matrix **A**, in which we assume a_{kl} to be the largest off-diagonal element. The matrix **B** constructed by the similarity transformation is given by

$$\mathbf{B} = \mathbf{S}^T \mathbf{A} \mathbf{S} \tag{2.12}$$

in which **S** is an orthogonal transformation matrix with its non-zero matrix elements:

$$\begin{aligned}
&s_{kk} = s_{ll} = \cos\theta \\
&s_{kl} = -s_{lk} = -\sin\theta \\
&s_{ii} = 1, \qquad i \neq k, i \neq l
\end{aligned}$$

After matrix multiplication with the orthogonal transformation matrix **S** and its transverse (as in (2.12)) the entrances of **B** becomes

$$\begin{aligned}
&b_{ii} = a_{ii}, \qquad i \neq k, i \neq l \\
&b_{ik} = a_{ik}\cos\theta - a_{il}\sin\theta, \qquad i \neq k, i \neq l \\
&b_{il} = a_{il}\cos\theta + a_{ik}\sin\theta, \qquad i \neq k, i \neq l \\
&b_{kk} = a_{kk}\cos^2\theta - 2a_{kl}\cos\theta\sin\theta + a_{ll}\sin^2\theta \\
&b_{ll} = a_{ll}\cos^2\theta + 2a_{kl}\cos\theta\sin\theta + a_{kk}\sin^2\theta \\
&b_{kl} = (a_{kk} - a_{ll})\cos\theta\sin\theta + a_{kl}(\cos^2\theta - \sin^2\theta)
\end{aligned}$$

Due to the symmetry in (2.12) with **A** being a tridiagonal symmetric matrix, $b_{lk} = b_{kl}$, $b_{ki} = b_{ik}$, and $b_{li} = b_{il}$. [3] Since θ can be chosen arbitrarily, we choose θ to be the angle at which b_{kl}, and hence b_{lk}, becomes zero. In this way, the largest element of **A** is eliminated, and it can be shown that this choice of θ reduces the norm of the off-diagonal elements of **A**, which ensures that the algorithm terminates towards the eigenvalues. [4]

This yields the equation

$$0 = (a_{kk} - a_{ll})\cos\theta\sin\theta + a_{kl}(\cos^2\theta - \sin^2\theta) \tag{2.13}$$

By introducing $\tan\theta = \sin\theta/\cos\theta$ and the quantity

$$\tau = \frac{a_{ll} - a_{kk}}{2a_{kl}} \tag{2.14}$$

(2.13) can be rewritten as the quadratic equation in $\tan\theta$

$$\tan^2\theta + 2\tau\tan\theta - 1 = 0 \tag{2.15}$$

which has the solutions

$$\tan\theta = -\tau \pm \sqrt{1+\tau^2} \tag{2.16}$$

[2] FiXme Note: eqref

[3] FiXme Note: check that this is actually correct

[4] FiXme Note: this, I can write, right??

From the solutions for $\tan\theta$ given in (2.18), $\cos\theta$ and $\sin\theta$ can be found using the formulas

$$\cos\theta = \frac{1}{\sqrt{1+\tan^2\theta}} \qquad \text{and} \qquad \sin\theta = \tan\theta\cos\theta$$

If $\tau < 0$, $\tan\theta$ is chosen to be

$$\tan\theta = -\tau - \sqrt{1+\tau^2} \tag{2.17}$$

whilst if $\tau \geq 0$, $\tan\theta$ is calculated as

$$\tan\theta = -\tau + \sqrt{1+\tau^2} \tag{2.18}$$

This choice is made to always make $\tan\theta$ the smaller of the two roots given in (2.18). Furthermore, this choice ensures that $|\tan\theta| \leq 1$, yielding that $|\theta| \leq \pi/4$.

This is true since $|\tau| \leq 1$, because $|a_{kl}| \geq |a_{ij}|$ for all i, j, from which it follows that

$$|\tan\theta| = \left|-\tau - \sqrt{1+\tau^2}\right| \leq 1, \qquad \text{for } \tau < 0 \tag{2.19}$$

and

$$|\tan\theta| = \left|-\tau + \sqrt{1+\tau^2}\right| \leq 1, \qquad \text{for } \tau \geq 0 \tag{2.20}$$

since $\sqrt{1+\tau^2} \leq \sqrt{2}$.

The fact that $|\theta| \leq \pi/4$ ensures that $\cos\theta \geq 0$ which ultimately ensures that the difference between **A** and the new matrix **B** is minimized, since

$$||\mathbf{B}-\mathbf{A}||_F^2 = 4(1-c)\sum_{i=1,i\neq k,l}^{n}(a_{ik}^2 + a_{il}^2) + \frac{2a_{kl}^2}{c^2}. \tag{2.21}$$

[5]

[5] FiXme Note: and why is this minimization a good thing?? :-P

CHAPTER

3 RESULTS

When running the code presented in Chap. 2.... blah blah blah.... Let's have an intro to this chapter...

The results from running the code ... can be found in the GitHub folder `https://??`. [1]

3.1 Interpretation of Results

WOW, an awesome interpretation of the results :D

3.1.1 Dependence of ρ_{max} and n on Eigenvalue

[2] For a single electron moving in a three-dimensional harmonic oscillator potential, the analytical solution for first three eigenvalues to the rewritten Schrdinger's equation [3] is $\lambda_0 = 3$, $\lambda_1 = 7$, and $\lambda_2 = 11$, for $l = 0$. [4]

In the code given in ?? the two parameters ρ_{max} and n can be modified to give a more or less accurate numerical solution to the problem. If not considering the computational time, limit in memory, and round-off errors, the obvious [5] choice of ρ_{max} and n would be to make both numbers infinite. This is, however, not a realistic possibility, and this sections is therefore dedicated to find (discuss) on the optimal choices for ρ_{max} and n to obtain acceptable values for the eigenvalues of [6].

Changing ρ_{max} causes the interval $[\rho_{min}, \rho_{max}]$, in which the wave function is considered, to change. Since the wave function goes to zero as the distance goes to infinity, it is acceptable to neglect the contribution from some ρ_{max}. It is a [7] to decrease ρ_{max} and hence making the interval smaller, in the sense that a smaller n then is needed to create a sufficient step length and ultimately a good enough "resolution". However, if this ρ_{max} is too close to ρ_{min} the neglected part can actually not be neglected, if an acceptable result is wished for.

[1] FiXme Note: correct the above lines
[2] FiXme Note: include e.g. a section called "1 electron case" or smt similar
[3] FiXme Note: eq. ref to nature eq
[4] FiXme Note: ref. to project description
[5] FiXme Note: mest fordelagtige
[6] FiXme Note: eqref
[7] FiXme Note: fordel

In the figure below, the dependence of different integer valued ρ_{max} on the three first eigenvalues gained by the algorithm described in [8] is plotted for $n = 100$. [9]

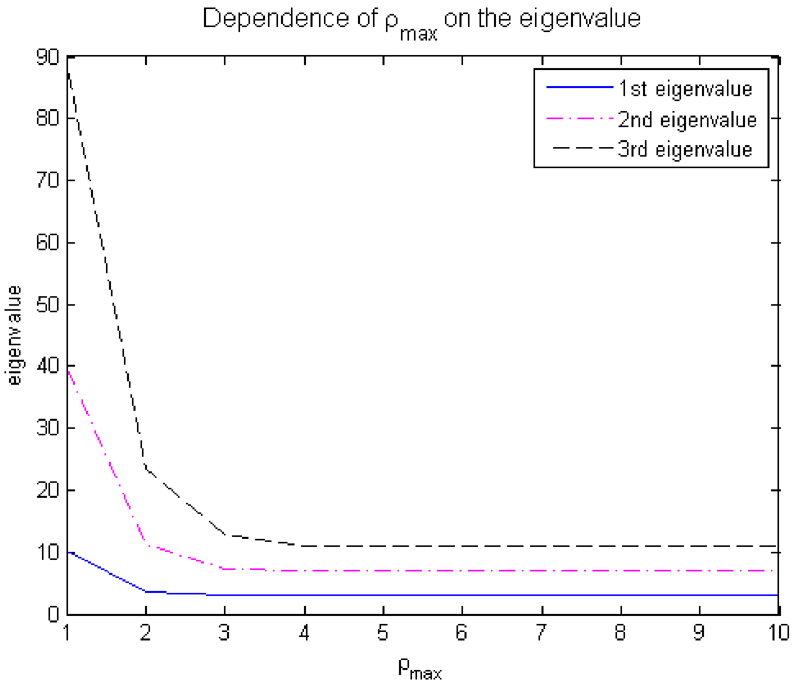

Figure 3.1. Awesome caption

From the figure that if $\rho_{max} < 3$ the eigenvalues are varying dramatically. This happens due to neglection ?? of strongly contributing parts of the eigenfunction. [10] [11] The ρ_{max} that, with $n = 100$, gives the most accurate result for all three of the first eigenvalues is $\rho_{max} = 5$. Since this ρ_{max} gives the most accurate result for a relatively small n, this is chosen as the optimal ρ_{max} in this and the following sections for this specific problem.

With this ρ_{max}, we wish to find the number of n that gives the first three eigenvalues with four leading digits. This optimal n is found by steady increment of n, as seen in [12].

[8] FiXme Note: sec ref

[9] FiXme Note: comment on, why we only have integer $\rho_m ax$

[10] FiXme Note: is this ok??

[11] FiXme Note: comment on the flat part!!

[12] FiXme Note: figref below

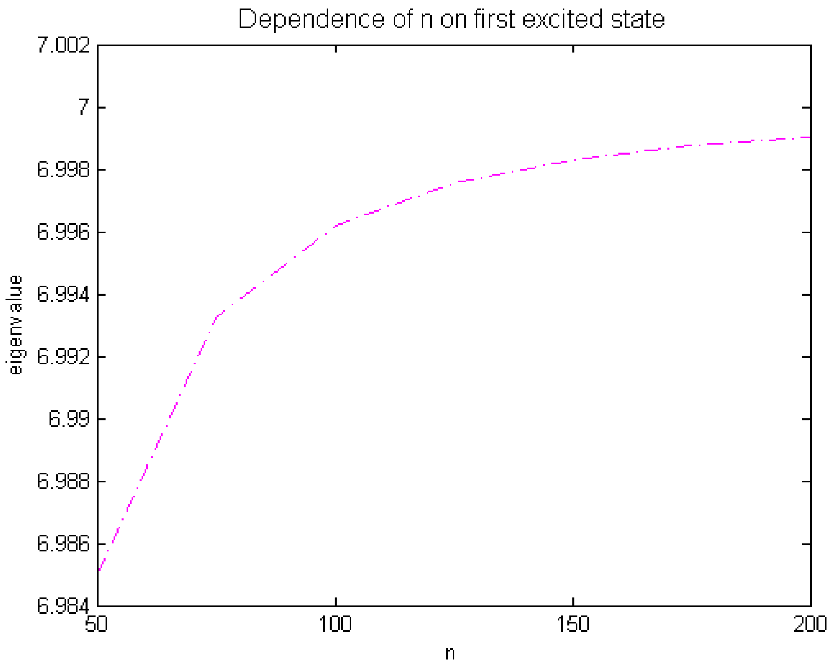

Figure 3.2. Awesome caption

The eigenvalue of the first exited is seen to be asymptotic to the analytical solution $\lambda_1 = 7$, and at a matrix size of $n = 200$, the eigenvalue of the first exited state has the numerical solution 6.99904. This yields an accuracy up to four leading digits, which is also found to be the case for the ground state and the third eigenstate. Hence, the optimal ρ_{max} and n is 5 and 200, respectively.

3.1.2 Dependence of n on Number of Iterations

In here I want to put the last two figures side by side, but I'm tired now :P

CHAPTER

4 CONCLUSION

Conclude.... conclude.... conclude....

BIBLIOGRAPHY

Appendix

A MatLab code for smt....

This is how, we write MatLab code in the report

```
close all
clear all
clc
%I am a comment

filename = ’Results.xlsx’;
sheet = 4;
xlRange = ’B3:C12’;

[v,T,vT] = xlsread(filename, sheet, xlRange);
x10=v(:,1);y10=v(:,2);

figure
plot(??)
legend(??)

xlim([??])
ylim([??])

title(??)
xlabel(’x’)
ylabel(’y’)
```