Project 2 FYS4150

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Abstract

In this report we used Jacobi's method to solve the eigenvalue problems of finding the energy of a single electron in a harmonic potential and two electrons in a harmonic potential that are interacting by a Coulomb potential. The results were the energies of the ground state of the single electron and the energies of the ground state for the two electrons for different oscillator frequencies. How the eigenvalues converge with Jacobi's method for increasing mesh points was investigated and the CPU time of Jacobi's method was compared to armadillo's solver for eigenvalues, to be able to analyse the method.

Contents

1 Introduction

Many problems in physics are eigenvalue problems [referanse. er dette sant egentlig? Ifølge wikipedia ja...]. Especially when we are at the quantum level. The Schrödinger equation with different potentials are an important example and that is the eigenvalue problem this report will attend to.

In this report we will use Jacobi's method to solve an eigenvalue problem. The eigenvalue problem is the Schrödinger equation for both a single electron in a harmonic potential and two electrons in a harmonic potential that are interacting by a Coulomb potential.

The report starts with some theory on how the equations are scaled and made dimensionless and how the problem ends up being a eigenvalue problem with a tridiagonal matrix. On this form, the problem can be solved numerically with Jacobi's method. After that, the algorithm with the unit tests are described in the method. Then, the results are presented in different tables. In the end a discussion of the results are made. At last the report is summarized in the conclusion.

2 Theory

2.1 Dimensionless and scaled Schrödinger Equation

In this report we are looking at how to solve an eigenvalue problem using Jacobi's method. The eigenvalue problem we will solve is the Schrödinger Equation for the ground state and the harmonic oscillator potential. We then start out with the one particle radial Schrödinger Equation (Equation 1 for the ground state which means that the quantum number $l = 0$. Here R is the radial part of the wave function, r is the distance from the origin to the electron, m is the mass of the particle, $\hbar$ is Planck's constant and E is the energy. The harmonic oscillator potential is shown in Equation 2. Here k is the wave number and ω is the oscillator frequency.

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

$$V(r) = \frac{1}{2}kr^2 \qquad \text{where } k = m\omega^2 \tag{2}$$

After substituting $R(r) = \frac{1}{r}u(r) = \frac{\alpha}{\rho}u(\rho)$ where $\rho = \frac{r}{\alpha}$, a dimensionless variable, and α is subsequently a constant with dimension length, the radial Schrödinger equation with the harmonic oscillator potential looks like Equation 3.

$$-\frac{\hbar^2}{2m\alpha^2}\frac{d^2}{d\rho^2}u(\rho) + \frac{1}{2}k\alpha^2\rho^2u(\rho) = Eu(\rho) \tag{3}$$

To make the equation a pure eigenvalue problem, we need to scale the equation properly, that we can to with the help of the inserted α. We start by multiplying Equation 3 with $\frac{2m\alpha^2}{\hbar^2}$:

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

If we set $\frac{m\alpha^4}{\hbar^2}k = 1$ then $\alpha = \left(\frac{\hbar^2}{mk}\right)^{\frac{1}{4}}$ and the equation is then written as Equation 4.

$$-\frac{d^2}{d\rho^2}u(\rho) + \rho^2u(\rho) = \lambda u(\rho) \qquad \text{where } \lambda = \frac{2m\alpha^2}{\hbar^2}E \tag{4}$$

This problem has an analytical solution and the three lowest eigenvalues for the ground state are $\lambda_1 = 3$, $\lambda_2 = 7$ and $\lambda_3 = 11$.

2.2 An eigenvalue problem

We have the scaled and dimensionless Schrödinger Equation (Equation 4) and the next move is to make it into a numerical eigenvalue problem. We start by making the continuous function $u(\rho)$ a discrete number of values $u_i = u(\rho_i)$. Here $\rho_i = \rho_0 + ih$ where h is the step length $h = \frac{\rho_{max}}{N}$, N is the number of mesh points and $\rho_0 = 0$. ρ_{max} should be infinitely big which is not possible, since $r \in [0, \infty)$, but we will come back to that in the method part of the report. Using the expression for the second derivative we get:

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

from Equation 4.

This equation can be rewritten into a matrix eigenvalue equation shown in Equation 5

$$\begin{bmatrix} d_1 & e_1 & 0 & \cdots & 0 & 0 \\ e_1 & d_2 & e_2 & \cdots & 0 & 0 \\ 0 & e_2 & d_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & d_{N-1} & e_{N-1} \\ 0 & 0 & 0 & \cdots & e_{N-1} & d_N \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{N-1} \\ u_N \end{bmatrix} = \lambda\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{N-1} \\ u_N \end{bmatrix} \tag{5}$$

where $d_i = \frac{2}{h^2} + \rho_i^2$ and $e_i = -\frac{1}{h^2}$.

2.3 Interacting case

In this report we will also study the eigenvalue problem that is the Schrödinger equation of two particles interacting with each other by a Coulomb potential. With relative and center-off-mass coordinates and discarding the center-off-mass energy, a new scaling and insertion of the Coulomb interaction the two particle Schrödinger Equation is shown in Equation 6.

$$-\frac{d^2}{d\rho^2}\psi(\rho) + \omega_r^2\rho^2\psi(\rho) + \frac{1}{\rho}\psi(\rho) = \lambda\psi(\rho) \tag{6}$$

Here $\rho = r/\alpha$ as before, $\omega = \frac{1}{4}\frac{mk}{\hbar^2}\alpha^4$ and reflects the strength of the oscillator, $\alpha = \frac{\hbar^2}{m\beta e^2}$ to get the right scaling, β is Coulomb's constant, $\lambda = \frac{m\alpha^2}{\hbar^2}E$ and E is the energy.

Because of good scaling, this case is almost the same eigenvalue problem as before. The only change is the potential, V_i, which is now $V_i = \omega_r^2\rho_i^2 + \frac{1}{\rho_i}$ instead of only $V_i = \rho_i$. That means that the diagonal of the matrix changes to $d_i = \frac{2}{h^2} + \omega_r^2\rho_i^2 + \frac{1}{\rho_i}$.

This equation has analytical solutions for some frequencies and the resulting energies are listed in 2.1.

Table 2.1: This table lists the eneries of the lowest states in the ground state for two electrons in the harmonic potential and Coulomb potential [?].

Frequency []	Energies $\left[\frac{\hbar^2}{m\alpha^2}\right]$
ω_r	λ_0
0.005	0.35
0.25	1.25

2.4 Jacobi's method

We are using Jacobi's method to solve the eigenvalue problem from Equation 5 in the previous section. We know that for a symmetric matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$ there exists a real orthogonal matrix $\mathbf{S}$ so that $\mathbf{S}^T A S = D$ where D is a diagonal matrix with the eigenvalues on the diagonal.

The idea of eigenvalue problem solving is to do a series of similarity transformations of the matrix $\mathbf{A}$ so that eventually the matrix A is reduced to the matrix D and we have the eigenvalues. $\mathbf{B}$ is a similarity transformation of $\mathbf{A}$ if $\mathbf{B} = \mathbf{S}^T\mathbf{A}\mathbf{S}$.

In Jacobi's method the matrix $\mathbf{S}$ used in the similarity transformations is the orthogonal transformation matrix on the form:

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \cos\theta & 0 & 0 & \sin\theta \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & -\sin\theta & 0 & 0 & \cos\theta \end{bmatrix}$$

Let s_{ij} be an element in the matrix $\mathbf{S}$ and then $s_{ii} = 1$, $s_{kk} = s_{ll} = \cos\theta$ and $s_{kl} = -s_{kl} = -\sin\theta$ where $i \neq k$ and $i \neq l$. Here k, l are the number of a row or a column and i is the index of the columns and row.

The similarity transformation of a matrix will then change the elements in the matrix. The clue of the method is to choose the angle, θ, so that the elements that are not on the diagonal become zero. Because of the nature of the similarity transformation the eigenvalues stay the same:

$$\begin{aligned} \mathbf{A}\mathbf{x} &= \lambda\mathbf{x} \\ \mathbf{S}^T\mathbf{A}\mathbf{x} &= \mathbf{S}^T\lambda\mathbf{x} \\ \mathbf{S}^T\mathbf{A}\mathbf{S}^T\mathbf{S}\mathbf{x} &= \lambda\mathbf{S}^T\mathbf{x} \\ (\mathbf{S}^T\mathbf{A}\mathbf{S})(\mathbf{S}^T\mathbf{x}) &= \lambda(\mathbf{S}^T\mathbf{x}) \\ \mathbf{B}(\mathbf{S}^T\mathbf{x}) &= \lambda(\mathbf{S}^T\mathbf{x}) \end{aligned}$$

The eigenfunctions change though, but their orthogonality remains because of $\mathbf{S}$ is an orthogonal matrix and then $\mathbf{S}^T\mathbf{x} = \mathbf{U}\mathbf{x}$, a unitary transformation. It can be shown like this:

$$\begin{aligned} \mathbf{w}_i &= \mathbf{U}\mathbf{v}_i \\ \mathbf{w}_i^T\mathbf{w}_j &= (\mathbf{U}\mathbf{v}_i)^T\mathbf{U}\mathbf{v}_j \\ &= \mathbf{v}_i^T\mathbf{U}^T\mathbf{U}\mathbf{v}_j \\ &= \mathbf{v}_i^T\mathbf{v}_j = \delta_{ij} \end{aligned}$$

After a similarity transformation on the matrix $\mathbf{A}$ the elements of the similarity transformation $\mathbf{B}$ becomes:

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

Jacobi's method is to reduce the norm of the non-diagonal elements of the matrix with similarity transformations. We change define $c = \cos\theta$ and $s = \sin\theta$. When we require the non-diagonal elements to be zero that implies that:

$$b_{kl} = (a_{kk} - a_{ll})cs + a_{kl}(s^2 - c^2) = 0$$

We can rearrange some variables and get:

$$(a_{ll} - a_{kk})cs = a_{kl}(s^2 - c^2) \implies \frac{(a_{ll} - a_{kk})}{2a_{kl}} = \frac{1}{2}\left(\frac{s^2}{sc} - \frac{c^2}{sc}\right)$$

We define $\tan\theta = t = s/c$ and $\cot 2\theta = \tau = \frac{a_{ll}-a_{kk}}{2a_{kl}}$ and insert that to the equation:

$$\frac{(a_{ll} - a_{kk})}{2a_{kl}} = \frac{1}{2}\left(\frac{s}{c} - \frac{c}{s}\right) \implies \cot 2\theta = \frac{1}{2}(\tan\theta - \cot\theta)$$

$$\cot\theta = \tan\theta - 2\cot 2\theta = (\tau - 2t)$$

$$\tau = \frac{1}{2}(t - (\tau - 2t)) \implies t^2 + 2\tau t - 1 = 0$$

Which then comes down to:

$$\begin{aligned} t &= \tau \pm \sqrt{1 + \tau^2} \\ c &= \cos\theta = \frac{1}{\sqrt{1 + \tan^2\theta}} = \frac{1}{\sqrt{1 + t^2}} \\ s &= \sin\theta = \tan\theta\cos\theta = tc \end{aligned}$$

3 Method

3.1 Jacobi's method

$$\begin{aligned} t &= \tau \pm \sqrt{1 + \tau^2} \\ c &= \cos\theta = \frac{1}{\sqrt{1 + \tan^2\theta}} = \frac{1}{\sqrt{1 + t^2}} \\ s &= \sin\theta = \tan\theta\cos\theta = tc \end{aligned}$$

3.2 The algorithm

Metode Algorigmer: Jacobi, rhomax valg av epsilon ("0")

Forelesning: Konvergens etter mellom 12n3 og 20n3, vi har mye kjappere!!!!! - fordi sym!!!

Our matrix $\mathbf{A}$ is symmetric, meaning that $\mathbf{A}^T = \mathbf{A}$. From this it follows that the product $\mathbf{S}^T AS$ also is symmetric, as is shown under:

$$\mathbf{S}^T\mathbf{AS} = \mathbf{S}^T\mathbf{A}^T(\mathbf{S}^T)^T \quad (7)$$

$$= \mathbf{S}^T\mathbf{AS} \quad (8)$$

Thus is it sufficient to search only the elements above the diagonal for the highest valued element in the matrix, instead of the entire matrix.

3.3 Unit tests

In this project we used two unit tests to ensure that the program performs as expected and delivers accurate enough results.

One way to be sure that our algorithm gives correct answers is to task it to find the eigenvalues of a matrix with known eigenvalues. These values had been pre calculated by Matlab.

The other unit test we utilized was to check that our algorithm to find the largest off-diagonal elements actually found the largest off-diagonal elements. This was done by setting up a known matrix and tasking our algorithm to find the largest off-diagonal element and checking it against the manually found largest element.

Other tests: Orthogonality, norm(A) = norm(B), symmetric

HVORFOR SØKER VI BARE ØVRE HALVDEL??????????????? We chose ?????? for all our calculations except when $\omega_r = 0.01$ then we changed it to be $\rho_{max} = 50$. The small frequency made the wave function smear out, and we needed a bigger interval to make sure we had the whole function in our calculations.

4 Result

Table 4.1: Convergence of eigenvalues for the non-interacting case using the Jacobi method. The energies corresponding to the eigenvalues λ_0, λ_1 and λ_2 are ?? eV, ?? eV and ?? eV respectively.

N	λ_1	λ_2	λ_3
10	2.9263	6.61967	10.0351
100	2.99928	6.99642	10.9919
200	2.99982	6.99911	10.9986
400	2.99996	6.99979	11.0003

Table 4.2: Comparisson of the time used between the Jacobi-algorithm and the Armadillo function *eig_sym* as a function of the mesh size N of matrix A. "Transforms" refers to the amount of similarity transforms the Jacobi method uses.

N	Transforms	time Jacobi (s)	time Armadillo (ms)
10	144	0.000	0.034
100	17681	0.241	1.789
200	71500	3.149	5.119
400	287490	57.175	23.045

Table 4.3: Eigenvalues for the interacting case. All the calculations are done with a mesh size of N=400. ρ_{max} was set to 7.9 for all ω_r, except for $\omega_r = 0.01$ ($\rho_{max} = 50$).

ω_r	λ_0	λ_1	λ_2
0.01	0.106	0.142	0.178
0.25	1.250	2.193	3.192
0.5	2.230	4.134	6.074
1	4.058	7.909	11.818
5	17.445	37.057	56.817

x

5 Discussion

5.1 The boundaries - ρ_{max}

Because we used the radial Schrödinger Equation our boundary conditions are given by $r \in [0, \infty)$ and since $\rho = r/\alpha$ the same boundary conditions are still relevant. That means that ρ_{max} should be ∞ that is not possible however on a computer.

Therefore an approximation of the boundary conditions had to be made. We chose ?????? for all our calculations except when $\omega_r = 0.01$ then we changed it to be $\rho_{max} = 50$. The small frequency made the wave function smear out, and we needed a bigger interval to make sure we had the whole function in our calculations.

5.2 Efficiency of method. Vilde

Discuss the CPU time and the convergence. Not a perfect method?

Discuss iterations (symmetric matrix + tridiagonal).

Choose of tolerance.

Specialize the algorithm to a tridiagonal matrix?

5.3 Unit test. Kjetil

Good unit test? Better/other unit tests?

6 Conclusion

We used Jacobi's method to solve the eigenvalue problems of finding the energy of a single electron in a harmonic potential and two electrons in a harmonic potential that are interacting by a Coulomb potential. First we scaled the different Schrödinger equations and made them dimensionless. We then rewrote the equation to a matrix equation. Then the problem ended up being an eigenvalue problem with a tridiagonal matrix. The scaling made it easy to adapt the algorithm for both cases with just changing the matrix involved, in this case the term for the potential. Two unit tests made sure the program was doing what it was supposed to do and the results were the energies of the ground state of the single electron and the energies of the ground state for the two electrons for different oscillator frequencies. The results were compared with the analytical values and the accuracy was down to the third decimal point with 400 mesh point and a step length of ??. The CPU time of Jacobi's method was compared to armadillo's solver for eigenvalues and our algorithm using Jacobi's method was very slow compared to armadillo's.

How could the program be better?

- Investigate where the program uses a lot of time.

How to better the method:

- Specialize for a tridiagonal matrix?

References