FYS3150 - Computational Physics

Project 2

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September 30, 2016

Abstract

This project aims to simulate so-called quantum dots, electrons trapped in harmonic oscillator potentials. By rewriting the Schroedinger equation to an eigenvalue problem which we solved with Jacobi's rotational method.

We found that our calculations of the eigenvalues and eigenvectors matched analytical expectations, but that Jacobi's method was much slower than Armadillo's inbuilt eigenvalue solver.

- Github repository containing programs and results are in: `https://github.com/richaraf/Comphys_projects/tree/master/Project_2`

1 Introduction

In this project, we study the theory behind quantum dots, a highly relevant subject in modern physics. A quantum dot is one or two electrons trapped in an quantum well. These are often referred to as artificial atoms, as they, like natural atoms, have discrete energy levels [2].

Our goal in this project is to simulate a quantum dot, modelled as one or two electrons bound in a three-dimensional harmonic oscillator well. Quantum Mechanics tells us that we find the behaviour of these electrons by solving the radial equation with the harmonic oscillator potential, $V(r) = \frac{1}{2}m\omega^2 r^2$:

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

We do so by rewriting equation (1) with dimensionless variables, and reduce the equation to a single eigenvalue problem, which we solve by implementing Jacobi's rotation method. Thereafter, we compare the obtained wave functions for one and two electrons with and without Coulomb interaction, and interpret the results physically. We also examine what effect the strength of the harmonic potential has on the wave function in the two-electron case.

2 Theory

2.1 One electron

To solve the Schroedinger's equation (SE) for one electron in a three-dimensional harmonic oscillator well, we first assume spherical symmetry, which means we only need to solve the radial part of SE

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

where $\hbar = 6.582 \cdot 10^{-16}$ eV·s, m is the electron mass, $r \in [0,\infty)$ the radial distance, $V(r)$ is the potential, E is the energy and l is the orbital quantum number. For our harmonic oscillator the potential is $V(r) = (1/2)kr^2$, with $k = m\omega^2$. If we look at the case where $l = 0$, we get the energies to be

$$E_n = \hbar\omega\left(2n+\frac{3}{2}\right). \tag{3}$$

If we also substitute $R(r) = (1/r)u(r)$ in equation (2), the SE we want to solve becomes

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}u(r)+V(r)u(r)=Eu(r). \tag{4}$$

We introduce the dimensionless variable $\rho = r/\alpha$, which means our potential becomes $V(\rho) = k\alpha^2\rho^2/2$. Inserting ρ and $V(\rho)$ into equation (4) we get

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

We can set $mk\alpha^4/\hbar^2 = 1$ and $2m\alpha^2E/\hbar^2 = \lambda$ which allows us to write the Schroedinger's equation as

$$-\frac{d^2}{d\rho^2}u(\rho)+\rho^2u(\rho)=\lambda u(\rho). \tag{5}$$

The second derivative can be expressed as

$$u'' \approx \frac{u(\rho+h) - 2u(\rho) + u(\rho-h)}{h^2},$$

where h is the step length. We use N mesh points with $\rho_{min} = \rho_0$ and $\rho_{max} = \rho_{N-1}$ which means the step length is $h = (\rho_{N-1} - \rho_0)/N$. ρ is discretized by

$$\rho_i = \rho_0 + ih \qquad\qquad \text{with } i = 1, 2, ..., N,$$

which means we can write our discretized SE as

$$-\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + V_i^2 u_i = \lambda u_i, \tag{6}$$

where $V_i = \rho_i^2$. The discretized case in eq (6) can be written as a linear set of equations

$$A\mathbf{u} = \lambda\mathbf{u}, \tag{7}$$

where A is the tridiagonal matrix

$$A = \begin{pmatrix} \frac{2}{h^2} + V_1 & -\frac{1}{h^2} & 0 & ... & 0 & 0 \\ -\frac{1}{h^2} & \frac{2}{h^2} + V_2 & -\frac{1}{h^2} & ... & 0 & 0 \\ 0 & -\frac{1}{h^2} & \frac{2}{h^2} + V_3 & ... & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & -\frac{1}{h^2} & \frac{2}{h^2} + V_{N-2} & -\frac{1}{h^2} \\ 0 & 0 & 0 & 0 & -\frac{1}{h^2} & \frac{2}{h^2} + V_{N-1}. \end{pmatrix} \tag{8}$$

For the potential $V_i = \rho_i^2$, we would expect the three lowest eigenvalues to be $3, 7$ and 11.

2.2 Two electrons

In the case of two electrons without repulsive Coulomb interaction our SE is

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr_1^2} - \frac{\hbar^2}{2m}\frac{d^2}{dr_2^2} + \frac{kr_1^2}{2} + \frac{kr_2^2}{2}\right) u(r_1, r_2) = E^{(2)} u(r_1, r_2),$$

where $E^{(2)}$ is the two-electron energy. Introducing a relative coordinate $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and the center-of-mass coordinate $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$, we can write SE as

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

The energy can be split into relative energy E_r and the center-of-mass energy E_R as well as $u(r, R) = \psi(r)\phi(R)$. We can then separate the SE into an r-dependent part and an R-dependent part. The repulsive Coulomb interaction potential between the two electrons is expressed

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

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

We are interested in solving the equation with E_r, because the R-dependent equation is very similar to the case of no repulsive Coulomb interaction. Adding the repulsive Coulomb potential the to r-dependent part of SE gives

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

We again use the dimensionless variable $\rho = r/\alpha$ which gives us

$$\left(-\frac{d^2}{d\rho^2} + \frac{mk\alpha^4\rho^2}{4\hbar^2} + \frac{m\alpha\beta e^2}{\rho\hbar^2}\right)\psi(\rho) = \frac{m\alpha^2}{\hbar^2}E_r\psi(\rho), \tag{9}$$

which we can simplify and make look like equation (5) by fixing α, defining a "frequency" ω_r and "energy" λ_r

$$\frac{m\alpha\beta e^2}{\hbar^2} = 1 \qquad \omega_r^2 = \frac{mk\alpha^4}{4\hbar^2} \qquad \lambda = \frac{m\alpha^2 E}{\hbar^2}.$$

The equation to solve then becomes

$$-\frac{d^2}{d\rho^2}\psi(\rho) + \omega_r^2\rho^2\psi(\rho) + \frac{1}{\rho}\psi(\rho) = \lambda\psi(\rho), \tag{10}$$

which means we can write the potential for the interacting case as

$$V_r(\rho) = \omega_r^2\rho^2 + \frac{1}{\rho}$$

and in discretized form

$$V_{ir} = \omega_r^2\rho_i^2 + \frac{1}{\rho_i}.$$

The potential for the case where there is no interaction between the two electrons, we simply set β to 0, which means the potential becomes

$$V_{nr}(\rho) = \omega_r^2\rho^2,$$

which for discrete points can be expressed

$$V_{inr} = \omega_r^2\rho_i^2.$$

The eigenvalue-problem in equation (10) can then be written as equation (7), a set of linear equations, where A is as defined in expression (8), with the potential V_{ir} for the interacting case and V_{inr} for the case without interaction.

2.3 Conservation of dot product

If we consider a set of vectors $\{\mathbf{v}_i\}$, an orthogonal matrix U and the transformation $\mathbf{w}_i = U\mathbf{v}_i$. The dot product for our set of vectors an be expressed as

$$\mathbf{v}_j^T \mathbf{v}_i,$$

which in the case of $\{\mathbf{v}_i\}$ being an orthonormal basis means that $\mathbf{v}_j^T \mathbf{v}_i = \delta_{ij}$, where δ_{ij} is the Kronecker delta. The dot product of an orthogonal transformation is preserved

$$\mathbf{w}_j^T \mathbf{w}_i = (U\mathbf{v}_j)^T U\mathbf{v}_i = \mathbf{v}_j^T U^T U\mathbf{v}_i = \mathbf{v}_j^T \mathbf{v}_i,$$

which also means that orthogonality is preserved in the case where $\{\mathbf{v}_i\}$ is an orthogonal basis.

3 Method

3.1 Jacobi's method

In this project we are using Jacobi's method, which transforms a matrix A into a diagonal matrix D with the eigenvalues of A on the diagonal. This is done by repeat setting the largest non-diagonal element equal to zero until all the non-diagonal elements are smaller than a tolerance ε. From linear algebra we know that a symmetric matrix always can be transformed into a diagonal matrix, so this should be valid for our specific symmetric matrix described in the theory. For doing this we need a transformation matrix S which sets the largest non-diagonal element to zero:

$$S^T A S = B \tag{11}$$

Where B is the transformed A matrix where the largest non-diagonal element is set to zero. S is given by

$$S = \begin{pmatrix} 1 & 0 & \dots & 0 & 0 & \dots & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & \cos\theta & 0 & \dots & 0 & \sin\theta \\ 0 & 0 & \dots & 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 0 & \dots & 1 & 0 \\ 0 & 0 & \dots & -\sin\theta & 0 & \dots & 0 & \cos\theta \end{pmatrix} \tag{12}$$

where the locations of $sin\theta$ and $-sin\theta$ are depending on the indexes of the largest element of A. Therefore we first need to find this, something we can easily do numerically:

```
max = 0;                                //Largest element
for(k = [0,size A])
    for(l = [0,size A])
        if(k != l)                      //Not on diagonal
            if(abs(A(k,l)) > max)
                kmax = k;               //Store indexes of
                lmax = l;               //largest element
                max = abs(A(k,l));
```

After the indexes of the largest element are found, we can start doing the Jacobi method (also called Jacobi rotation since the matrix S is a rotation matrix). By doing the multiplication $S^T AS = B$ for an arbitrary matrix A, we will see that B is constructed by

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

where i is an arbitrary column or row index, k is the index of the row with the largest non-diagonal number (in A) and l is the index of the column with the largest non-diagonal number. This makes it easy to find B numerically, and by doing Jacobi's method on B a multiple times, the largest non-diagonal element will constantly be smaller. In the theory these elements should be equal to zero when the diagonal elements are equal to the exact eigenvalues, but we can get a good approximation of the eigenvalues even if the largest element is a small number. We implement this by choosing a small tolerance ε and continue doing Jacobi's method until the largest element is smaller than this. The smaller ε is, the better approach we have.

The eigenvectors are found by

$$\mathbf{w}_i = S\mathbf{v}_i \tag{13}$$

where **v** is a basis of eigenvectors, S is the transformation matrix and **w** are the eigenvectors of A. Numerically we are going to do this by updating the matrix R which is the identity matrix in the beginning.

- $R_{il} = \cos\theta r_{il} + \sin\theta r_{ik}$
- $R_{ik} = -\sin\theta r_{il} + \cos\theta r_{ik}$

3.2 Solve the eigenproblem using Armadillo

We are also calculating the eigenvectors and eigenvalues with Armadillo, just to compare them with the eigenvalues and eigenvectors found by Jacobi's method. For a symmetric matrix, this is done by this script:

```
vec eigval;
mat eigvec;
eig_sym(eigval, eigvec, A);
```

where we assume that armadillo is included.

3.3 Tests

3.3.1 Largest element test

To ensure that the indexes of the largest non-diagonal element are found correctly, we have implemented a test for this. The test is a function which takes k and l as arguments (the indexes of the largest non-diagonal element) and placing the number 1 at this index while the remaining elements are zero. It will not allow us to place the element on the diagonal. Then we have a matrix where we know the exact location of the largest (non-diagonal) element. The next step is to send this matrix into the function which finds the largest element and returns the indexes of this. If this function returns the same indexes as where we placed the largest element, the largest element function passes the test.

The reason why we want the test function to take the indexes as arguments, is to be able to vary the test matrix to ensure that the solver is not giving the right result accidentally.

We are also testing if the matrix sent into the largest element finder is quadratic. This is simply done by comparing the number of rows and the number of columns. The test raises an error if the matrix is not quadratic.

3.3.2 Check of orthogonality

The eigenvectors should be orthogonal since they cannot be linear combination of each other. This means that the inner product between two different eigenvectors needs to be zero. The mathematical expression can be written as

$$\langle \mathbf{v}_i | \mathbf{v}_j \rangle = \begin{cases} c, & \text{if } i = j, \\ 0, & \text{if } i \neq j. \end{cases} \tag{14}$$

where c is a constant. We are not interested in c, but we want to check if the inner product between two *different* vectors are zero. The test loops over all the different combinations of eigenvectors (but not equal eigenvectors), and takes the inner product between them. Thereafter it compares the inner product with a given tolerance, and the test passes as long as the inner product is smaller than the tolerance.

4 Results

4.1 Run time

We ran our program for different numbers of grid points N, and noted the run times of our Jacobi rotation algorithm and the armadillo solver. The run times are presented in Table 1.

Table 1: Run time of our Jacobi-algorithm vs the Armadillo solver

N, number of grid points	**Jacobi runtime [s]**	**Armadillo runtime [s]**
5	4e-06	9.7e-05
100	0.301168	0.003286
350	63.5475	0.064743

4.2 One electron system

4.2.1 Plot of the wave functions

We found the ground states of the single electron system, and plotted the square of the wave functions. The resulting plot is shown in Figure 1.

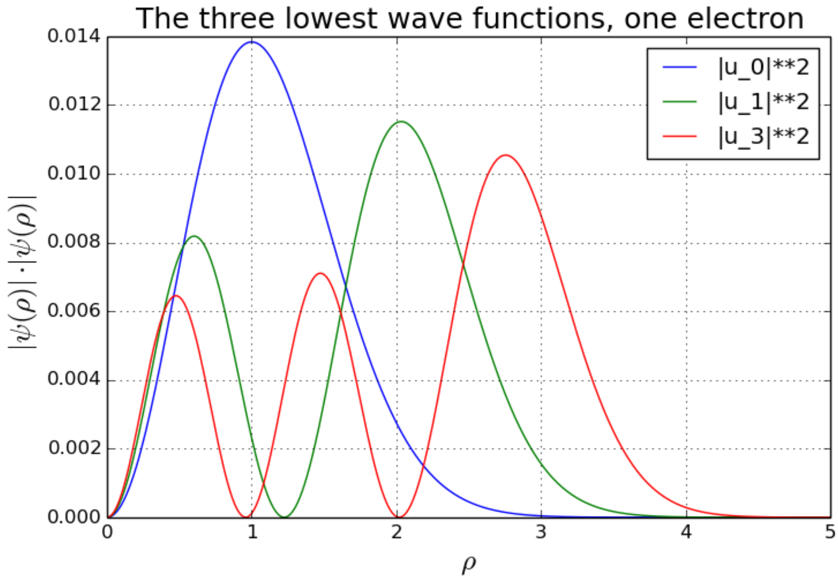

Figure 1: Plot of the wave functions of the three lowest states for the single electron system

4.2.2 Accuracy of the lowest eigenvalue vs N and ρ_{max}

We experimented with how the precision of the lowest eigenvalue λ_0 changed with number of grid point used and the chosen value og ρ_{max}. The results are presented in Table 2.

Table 2: Calculated value of the lowest eigenvalue λ_0, compared with number of grid points N and chosen value of ρ_{max}

N, number of grid points	**Calculated value of λ_0**	**Value of ρ_{max}**
5	9.82996	1
100	10.1504	1
350	10.1511	1
5	2.68672	5
100	2.99922	5
350	2.99994	5
5	4.49479	10
100	2.99687	10
350	2.99974	10

4.2.3 Number of similarity transforms needed

We experimented with how the number of iterations needed to transform the matrix A into a diagonal matrix D changed with the number of grid points we used. The results are presented in Table 3. We also found from both Tables 1 and 3, that for $N = 350$ there are approximately 3218 iterations per second and for $N = 100$ there are 53731 iterations per second.

Table 3: Number of iterations needed to transform A into a diagonal matrix D, our tolerance is $\epsilon = 10^{-8}$

N, number of grid points	**Number of iterations**
5	14
50	3862
100	16182
200	65920
350	204523
400	268235

4.3 Two electron system

4.3.1 Plot of the wave functions

We plotted the wave functions ground states for the two-electron system both with and without interaction, and varied the "frequency" ω of the potential. For $\omega = [0.01, 0.5, 1, 5]$, the resulting plots are shown in Figure 2-5.

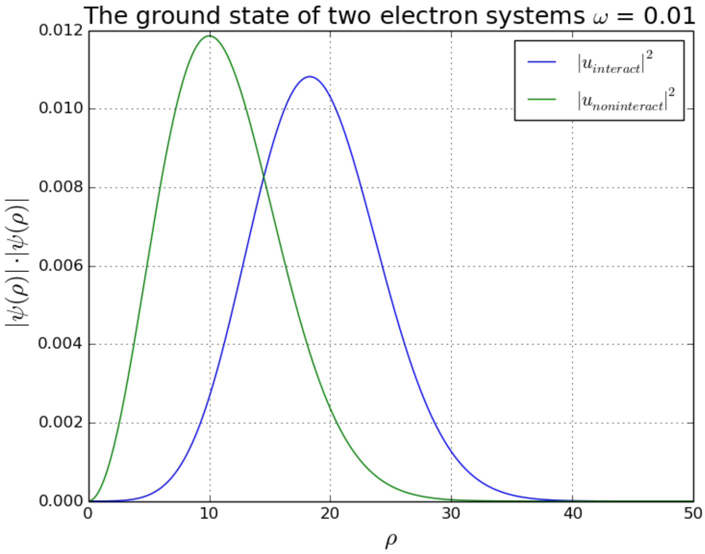

Figure 2: Plot of the ground state wave functions for two electron system with and without interaction, with the "frequency" $\omega = 0.01$

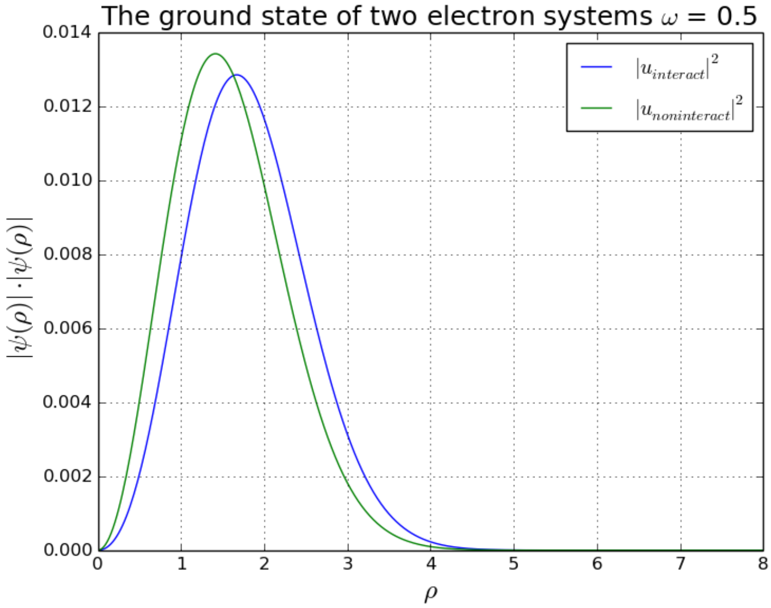

Figure 3: Plot of the ground state wave functionsfor the two electron system with and without interaction, with the "frequency" $\omega = 0.5$

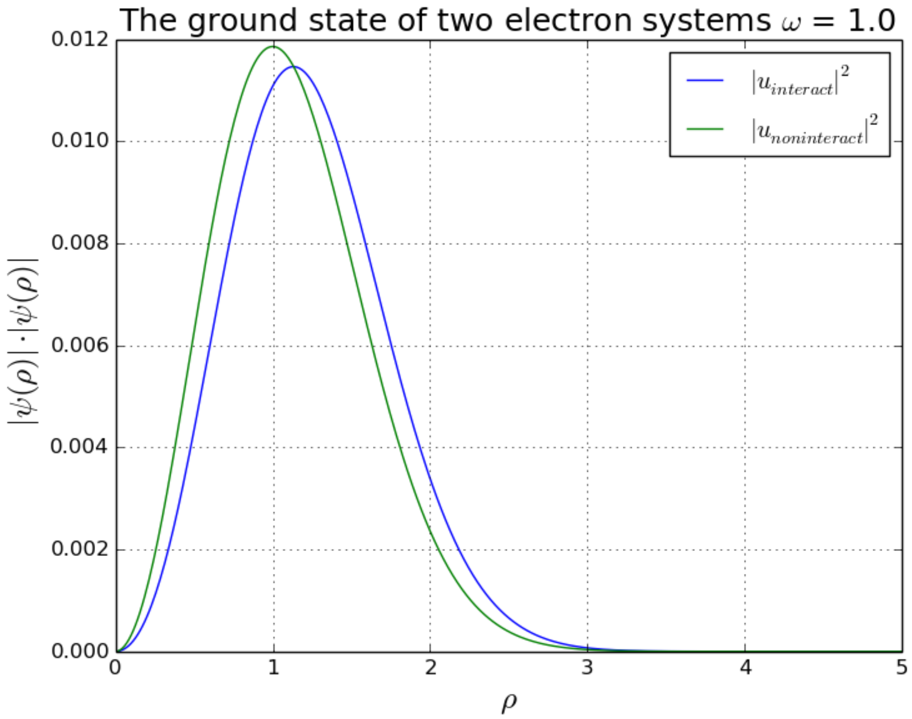

Figure 4: Plot of the ground state wave functions for the two electron system with and without interaction, with the ”frequency” $\omega = 1$

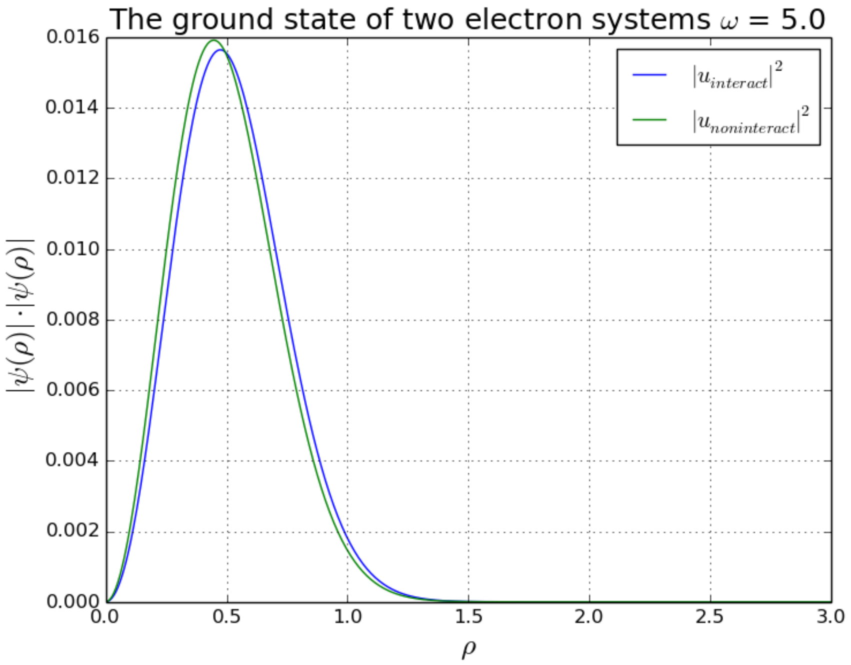

Figure 5: Plot of the ground state wave functions for the two electron system with and without interaction, with the "frequency" $\omega = 5$

4.4 Benchmarks

We have done some benchmarks for both the single electron case and case with two interacting electrons.

4.4.1 Single electron

In Table 4 we present the benchmark results for one electron.

Table 4: The exact analytical eigenvalues for the single electron case, compared with our numerical eigenvalue solution and the deviation. Included the three lowest eigenvalues. We are running the program for $N = 350$.

Eigenvalue	Analytical	Numerical	Deviation
0	3	2.99984	0.000163275
1	7	6.99918	0.000816424
2	11	10.998	0.0019922

As we can see, the numerical solutions are close to the analytical with deviation of order $\sim 10^{-4}$. The analytical solutions are gotten from the well-known energy formula for the harmonic oscillator, $E_n = \hbar\omega(2n + 3/2)$.(3) In our case, we are multiplying with $2/\hbar\omega$.

4.4.2 Two interacting electrons

Here we have compared the analytical solution of SE when we have two interacting electrons with our numerical solution. We are running the program with $N = 350$, and the analytical solution is gotten from [[3]], see Table 5.

Table 5: The exact analytical eigenvalue for the interacting electron case, compared with our numerical eigenvalue solution and the deviation for the lowest eigenvalue.

Eigenvalue	**Analytical**	**Numerical**	**Deviation**
0	1.2500	1.24996	3.54887e-05

The deviation in this case is small, in order $\sim 10^5$.

NB: In the analytical solution source they are working with a SE where all the terms are divided by two compared with the SE we are studying. Therefore we have to correct the analytical value given by multiplying with two.

5 Discussion

From Table 1, we saw that our Jacobi rotation method for finding the eigenvalues and eigenvectors was considerably slower than the armadillo method. In fact as the size of the matrix increases the Jacobi method slows down much faster than armadillo, which would suggest that the number of floating point operations in the Jacobi method is of a higher order than that of the armadillo method.

For the one electron case shown in Figure 1, we saw that higher energies meant that the expected value of the radius grew, which is what we would expect from equation (5). Additionally, for the second and third lowest energies, the probability distributions had several local maxima. These maxima can be interpreted as possible "orbits" around the center of the oscillator or if we wish we can think of the as "orbits" around a nucleus.

When calculating the eigenvalues λ, we found as shown in Table 2 that the eigenvalues both depend one the chosen number of grid points N and the boundary condition ρ_{max}. In the single electron case we found that

$N = 350$ and $\rho_{max} = 5$ gave sufficient accuracy. The method was actually quite sensitive to which value of ρ_{max} we chose. When choosing N and ρ_{max}, we have to make a compromise between the number of grid points resulting in computing time, and our approximation of infinity ρ_{max}. If we wanted to increase our accuracy further, and time or computer memory was of no concern, we could make a better approximation of infinity and use a much larger amount of grid points, which would result in very high accuracy in the eigenvalues and eigenvectors.

The number of iterations as a function of grid points shown in Table 3, appeared to follow the relation $\approx 1.6N^2$. Interestingly, the time required per iteration increases substantially for larger Ns. The only part of our algorithm which we would expect to take considerably longer time per iteration for different N values, is the function that searches through our matrix A to find the largest element. This time difference suggests that a large part of the CPU time is spent finding the largest element in our matrix. In Figure 2-5 we observe that for the two electron system the probability distribution comes wider when we lower the value of ω. This is what we would expect since lower ω corresponds to a weaker potential well, and thus the electrons can move more freely. The maxima of the probability distribution will therefore be found at higher values of ρ, which correspond to longer distances between the two electrons. When we choose larger values for ω, the potential well becomes steeper. The electrons are forced together, and the maxima of the probability density is found at lower values of ρ.

In Figure 2-5, we also compare the two electron system when we have included the Coulomb interaction between the electrons, and when we have neglected the interaction. The figures show that for lower "frequencies" ω the difference between the interacting and the non-interacting wave functions becomes larger. This is as expected. When the potential is weaker, the electrons have lower kinetic energy, and the Coulomb interaction is therefore more important than with higher kinetic energies.

Table 5 and 6 consist of different benchmarks, where the first contains analytical solutions compared with numerical solutions of the one electron case and the latter contains analytical solution compared with numerical solution of the two interacting electrons case. We saw that the deviations were small when we ran for $N = 350$, something which indicates that our implementations are correct.

6 Conclusion

In this project we have seen that the Armadillo algorithm was more efficient than our implemented Jacobi rotation algorithm. We have also seen that the "frequency" ω of the harmonic oscillator potential affects the probability distribution of the position of the electrons, and that it affects the non-interacting and the interacting electron system differently. Furthermore, we have seen that when calculating the wave functions, the choice of ρ_{max} is essential for obtaining the correct eigenvalues and -vectors.

7 References

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