

Schrödingers Equation for two Electrons in a 3D harmonic Oscillator Potential FYS 4150

Vegard SØRDAL

December 14, 2013

Instructor: Morten Hjort-Jensen

Abstract

In this second project of the semester we are interested in the properties of a two-electron system in an harmonic oscillator potential well. Specifically we want to use the Schrödinger equation to find the energy eigenvalues, and we want to solve this equation numerically. We will rewrite the equation into a tri-diagonal matrix-vector multiplication, using the same definition for the second derivative that we used in project 1. Following this we will use Jacobi's algorithm to diagonalize this matrix through a similarity transform, and the elements on the diagonal will be to the eigenvalues. The source-code for this project can be found at www.github.com/vegardbs/project2

1 Introduction

1.1 Quantum Dots

The two-electron problem we are looking at is a very relevant topic for research going on in academia today. Whenever you have a spatially confined electron the continuity of the possible energies which the electron can have is broken. The possible energy states of the electron is split into discrete levels. This separation of states in phase space is the essence of quantum mechanics. This *quantization*(quanta=) is not unique for the energy states and the same effect is observed for angular moment, spin, magnetic moment, and many other characteristic elementary properties.

Our space-confined electrons are not a thought experiment only interesting for its theoretical properties. It is a hot research topic in condensed matter physics today. Quantum dots, as they are called, is usually semiconductors which are so small that the excitons (hole-electron pair) have a bigger radius than the size of the semiconductor particle. This squeezes the excitons into a confined quantum state. The quantum states available depends on the physical size of

the semiconducting particle, in much the same way as the states of a particle trapped in a potential square well (a popular example for introduction to quantum mechanics) depends on the size of the well.

1.2 Schrödinger's equation for the single-electron system

First we will focus on a system of a single electron trapped in a harmonic oscillator potential. The radial Schrödinger equation for a single trapped in an harmonic oscillator potential is

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

The harmonic oscillator potential is well known, and given as $V(r) = (1/2)m(\omega r)^2$. We are also familiar with the energy-eigenfunction $E_{nl} = \hbar\omega(2n + l + \frac{3}{2})$. To simplify this equation we use the substitution $R(r) = u(r)/r$ while introducing the dimensionless $\rho = r/\alpha$ and obtain

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

with the boundary conditions $u(0) = u(\infty) = 0$

1.3 A numerical approach

We are only interested in the spherically symmetric case, so we set $l=0$, multiply both sides by $2m\alpha^2/\hbar^2$, and insert the harmonic potential $V(r)$ to get

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

Now we fix the constant α and define a new variable λ such that

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

and

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

We have the following form of the Schrödinger equation

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

This is a clean equation which we can solve numerically. Using the definition for the derivative which was discussed in the previous project

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

where h is the step length defined by

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

Then we quantize ρ as

$$\rho = \rho_{min} + ih \quad \text{for } i = 1, 2, 3, \dots, n_{step}$$

We can then write the Schrödinger equation in the following form

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

or in a more compact way

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

where $V_i = \rho_i^2$.

We are now in a position to rewrite the problem as a matrix eigenvalue problem.

Defining the diagonal elements as

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

and the non-diagonal elements as

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

we obtain a symmetric tri-diagonal matrix where elements on the diagonals next to the main diagonal are all equal ($1/h^2$) and all other matrix elements are zero.

The final form of the Schrödinger equation is

$$d_i u_i + e_{i-1} u_{i-1} + e_{i+1} u_{i+1} = \lambda u_i \quad (3)$$

which can be written in a matrix representation as

$$\begin{pmatrix} d_1 & e_2 & 0 & \dots & \dots & 0 \\ e_1 & d_2 & e_3 & 0 & \dots & \dots \\ 0 & e_2 & d_3 & e_4 & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & e_{n-1} \\ 0 & \dots & \dots & \dots & e_{n-2} & d_{n-1} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \dots \\ \dots \\ u_{n-2} \\ u_{n-1} \end{pmatrix} = \lambda \begin{pmatrix} u_1 \\ u_2 \\ \dots \\ \dots \\ u_{n-2} \\ u_{n-1} \end{pmatrix}$$

1.4 Two-Electron system

Next we want to investigate a system of two electrons simultaneously trapped in a harmonic oscillator potential. For a single electron in an harmonic oscillator well, we have

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

where $E^{(1)}$ denotes the single-electron energy. Adding another electron into the potential well, we get additional potential and kinetic terms in the Schrödinger, but we are still ignoring the interaction between the electrons.

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dr_1^2} - \frac{\hbar^2}{2m} \frac{d^2}{dr_2^2} + \frac{1}{2}kr_1^2 + \frac{1}{2}kr_2^2 \right) u(r_1, r_2) = E^{(2)}u(r_1, r_2).$$

Here $u(r_1, r_2)$ represents the two-electron wave function, and $E^{(2)}$ the two-electron energy. Now we want to write the equation in a form that includes the center-of-mass coordinate and the relative coordinate between the two particle, but not their absolute position in space. The relative coordinate is simply $r = r_1 - r_2$ and the center-of-mass coordinate is $R = 1/2(r_1 + r_2)$. Substituting these two definitions into Schrödinger's equation we obtain

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

We assume (with good reason) that the relative coordinate is independent of the centre-of-mass coordinate and vice versa, thus allowing us to separate the equation via $u(r, R) = \psi(r)\phi(R)$. This also implies that the energy of the whole system is the sum of the centre-of-mass energy, E_R , and relative energy, E_r .

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

Finally we include the repulsive Coulomb interaction between two electrons

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

Adding this term into the Schrödinger equation we obtain

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

Comparing this equation to Eq.1 we see the similarity. As previously done, we introduce the dimensionless variable $\rho = r/\alpha$ which gives us

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

We want to make this equation as similar to Eq.2 as possible. If we can do this we might be able to solve the problem including Coulomb interaction with a small modification of the solution without Coulomb interaction. We start by introducing the frequency ω_r .

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

Just like we did previously we fix the constant α

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

and introduce another constant λ

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

This leaves us with the final result

$$-\frac{d^2}{d\rho^2}\psi(\rho) + \left(\omega_r^2\rho^2 + \frac{1}{\rho}\right)\psi(\rho) = \lambda\psi(\rho). \quad (4)$$

Comparing this equation to Eq.2 we see that we have reached our goal, and that the problem with and without Coulomb interaction can be solved in a very similar way. The only difference is that we need to change the potential from ρ^2 to $\omega_r^2\rho^2 + 1/\rho$. We see that the potential is proportional to ω_r^2 , thus we treat it as a parameter which determine the strength of the harmonic oscillator potential.

2 Methods

To solve this eigenvalue equation we will use a technique called Jacobi's Eigenvalue Method (or Givens's rotations). It is an iterative method for calculating of the eigenvalues and eigenvectors of a real symmetric matrix.

2.1 Similarity Transforms

If a matrix A is real and symmetric it is also diagonalizable and there exist a diagonal matrix D where the eigenvalues of A is the elements of the diagonal.

$$D = \begin{pmatrix} \lambda_1 & 0 & 0 & \dots & \dots & 0 \\ 0 & \lambda_2 & 0 & 0 & \dots & \dots \\ 0 & 0 & \lambda_3 & 0 & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & 0 \\ 0 & \dots & \dots & \dots & 0 & \lambda_n \end{pmatrix}$$

To obtain this diagonalized matrix D we have to perform a series of similarity transform on the original matrix A . If S is a real and orthogonal matrix, the matrix D is a similarity transform of A if

$$D = S^T A S$$

where $S^T = S^{-1}$ and $S^T S = S^{-1} S = I$. Similarity transforms like this is very useful since the eigenvalues are conserved in the transformation and they can be read right out off the diagonal of D . To show this, assume

$$Ax = \lambda x \quad \text{and} \quad D = S^T A S$$

which can be rewritten as

$$(S^T A S)(S^T x) = \lambda S^T x$$

by multiplying with $S^T S = I$ on the left of both sides. Since $D = S^T A S$ we have

$$D(S^T x) = \lambda(S^T x)$$

and this is just another eigenvalue equation with the same eigenvalue λ and the diagonalized transform D . Notice however that the eigenvector $S^T x$ is not the same as in the original equation. Normally we need to perform more than one similarity transform in order to diagonalize A , thus a more general expression is

$$S_N^T \dots S_1^T A S_1 \dots S_N = D$$

2.2 Jacobi's Method

Jacobi's method is an useful similarity transform which we will use to solve our eigenvalue equation. The transformation matrix is called Given's rotation matrix and is defined as

$$S = \begin{pmatrix} 1 & 0 & \dots & \dots & \dots & 0 \\ 0 & 1 & \dots & \dots & \dots & 0 \\ \dots & \dots & \cos(\theta) & \dots & \dots & \sin(\theta) \\ \dots & \dots & \dots & \dots & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & -\sin(\theta) & 0 & \dots & \cos(\theta) \end{pmatrix}$$

we see that $S^T = S^1$ as required by definition. This transformation matrix performs a rotation of angle Θ in the n -dimensional space. All matrix elements are zero except

$$S_{kk} = S_{ll} = \cos(\theta)$$

$$S_{kl} = -S_{lk} = -\sin(\theta)$$

$$S_{ii} = 1, \text{ where } i \neq k \text{ or } l$$

If we perform the similarity transform $B = S^T A S$ the elements of B will be

$$B_{ii} = A_{ii}$$

$$B_{ik} = A_{ik} \cos(\theta) - A_{il} \sin(\theta)$$

$$B_{il} = A_{il} \cos(\theta) + A_{ik} \sin(\theta)$$

$$B_{kk} = A_{kk} \cos^2(\theta) - 2A_{kl} \cos(\theta) \sin(\theta) + A_{ll} \sin^2(\theta)$$

$$B_{ll} = A_{ll} \cos^2(\theta) + 2A_{kl} \cos(\theta) \sin(\theta) + A_{kk} \sin^2(\theta)$$

$$B_{kl} = (A_{kk} - A_{ll}) \cos(\theta) \sin(\theta) + A_{kl} (\cos^2(\theta) - \sin^2(\theta))$$

The trick is now to choose the angle θ in such a way that all the non-diagonal matrix elements A_{kl} becomes zero. We then perform the transformation again on the new matrix \tilde{B} for another off-diagonal element and choose the new angle to make those elements zero. We repeat this process until all off-diagonal elements are zero, and we will then be left with the diagonalized matrix D .

In reality we will not be able to make all the elements zero, since after we

perform the transformation a second time the values previously made zero will be made non-zero by the second transformation. Thus the main idea is to systematically reduce the norm of the off-diagonal elements until it is below the tolerated value.

$$off(A) = \sqrt{\sum_{i=1}^n \sum_{i \neq j}^n A_{ij}^2}$$

We define the shorthand notations $t = \tan(\theta)$, $c = \cos(\theta)$, $\sin(\theta)$ and

$$\cot(2\theta) = \tau = \frac{A_{ll} - A_{kk}}{2A_{kl}}$$

Using $\cot(2\theta) = 1/2(\cot(\theta) - \tan(\theta))$ we obtain the quadratic equation

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

which has the solution

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

and finally for c and s

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

$$s = tc$$

We want to choose t to be the smaller of the roots. This will minimize the difference between the original and transformed matrix since a smaller t results in a larger c . The difference between the two matrices is

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

and we see that a larger c will minimize this expression. Jacobi's method can now be summarized as follows

- a. Choose a tolerated minimum value for the non-diagonal matrix elements.
- b. Find the largest element of the matrix and check if it is larger than the tolerance.
- c. Compute the τ, t, s and c value corresponding to that element as described above.
- d. Perform the first similarity transform using the calculated angle θ .
- e. Repeat all steps until the size of the largest element is smaller than the tolerance.

3 Code Details

The Armadillo[1] library was again used in this project. We will later show comparisons between Armadillo and self-made functions and once again Armadillo will prove to be an efficient high performance library.

3.1 Single Electron System

For the first part of this project we were only interested in a single electron in an harmonic oscillator potential. The theory behind this is discussed in section 1.3. We began by initializing the matrix A as follows

```
for(int i=0;i<n;i++){
    for(int j=0;j<n;j++){
        if(i==j){ A(i,j) = (2/(h*h)) + pow((i+1)*h,2); }
        else if(j==i+1||j==i-1) { A(i,j) = -1/pow(h,2); }
        else { A(i,j) = 0; }}
```

This matrix corresponds to the matrix below Eq.3. First we wanted to find the largest off-diagonal element and we do this by searching through every element and updating the size and the (row,column) position each time an element larger than the previous is found.

```
max_off=0.0;
for(int i=0;i < n;i++){
    for(int j=i+1;j<n;j++){
        if(fabs(max_off) < fabs(A(i,j)))
            { max_off = fabs(A(i,j));
              l = i;
              k = j; }
    }
}
```

Since we are implementing Jacobi's method, we need to find the rotation angle which makes the largest element we just found zero. Using the equations we discussed in section 2.2 we write the following lines of code.

```
if(A(k,l)!= 0.0)
{
    T = (A(l,l)-A(k,k))/(2*A(k,l));
    if(T >= 0.0) {t = (-T + sqrt(1+pow(T,2)));}
    else {t = (-T - sqrt(1+pow(T,2)));}
    c = 1/sqrt(1+pow(t,2));
    s = t*c;
}
else { c = 1.0 ; s = 0.0; }
```

This gives us the desired values for $\sin(\theta)$, $\cos(\theta)$ and $\tan(\theta)$ which we need to perform the similarity transformation. If the symmetric opposite element (k,l) of the largest element (l,k) is zero we directly set $c = 1$ and $s = 0$. Next change all the matrix elements to create the new matrix B as discussed in 2.2

```

A_kk = A(k,k);
A_ll = A(l,l);
A(k,k) = pow(c,2)*A_kk - 2*c*s*A(k,l) + pow(s,2)*A_ll;
A(l,l) = pow(s,2)*A_kk + 2*c*s*A(k,l) + pow(c,2)*A_ll;
A(k,l) = 0;
A(l,k) = 0;

for(int i=0;i<n;i++){
    if(i!=k && i!=l){
        A_ik = A(i,k);
        A_il = A(i,l);
        A(i,k) = c*A_ik - s*A_il;
        A(k,i) = A(i,k);
        A(i,l) = c*A_il + s*A_ik;
        A(l,i) = A(i,l);
    }
}

```

All of the code is in a while-loop and will be reiterated until the largest off-diagonal element is smaller than a tolerance we set.

3.2 Two-Electron System

The only thing we need to change when we handle the two-electron system is the way we initialize the matrix A. In the diagonal elements need to include the Coulomb interaction between the two electrons and a constant ω_r to control the potential strength. Thus the new way we initialize the matrix is

```

for(int i=0;i<n;i++){
    for(int j=0;j<n;j++){
        if(i==j){ A(i,j) = (2/(h*h)) + pow((i+1)*h,2)*pow(w,2) + 1/((i+1)*h); }
        else if(j==i+1||j==i-1) { A(i,j) = -1/pow(h,2); }
        else { A(i,j) = 0; }}}

```

The code used to solve the problem with the Armadillo library is short and elegant. We first create a vector to store the eigenvalues and a matrix to store the eigenvectors.

```

vec eigenval;
mat eigenvec;
eig_sym(eigenval,eigenvec,A);

```

Then the function $\text{eig_sym}(\text{vec}, \text{mat}, A)$ solves the eigenvalue problem for us and store the values in the previously declared vector and matrix. The eigenvalues and their corresponding eigenvectors are stored in ascending order, i.e. the eigenvector $\text{eigenvec}(i,0)$ running over all i has its eigenvalue stored in $\text{eigenval}(0)$.

4 Results

The first three eigenvalues of the single electron problems are analytically given as $\lambda_0 = 3, \lambda_1 = 7$ and $\lambda_2 = 11$. The first part of the project was to find these values using our program. In Fig. 1 the normalized value of the calculated

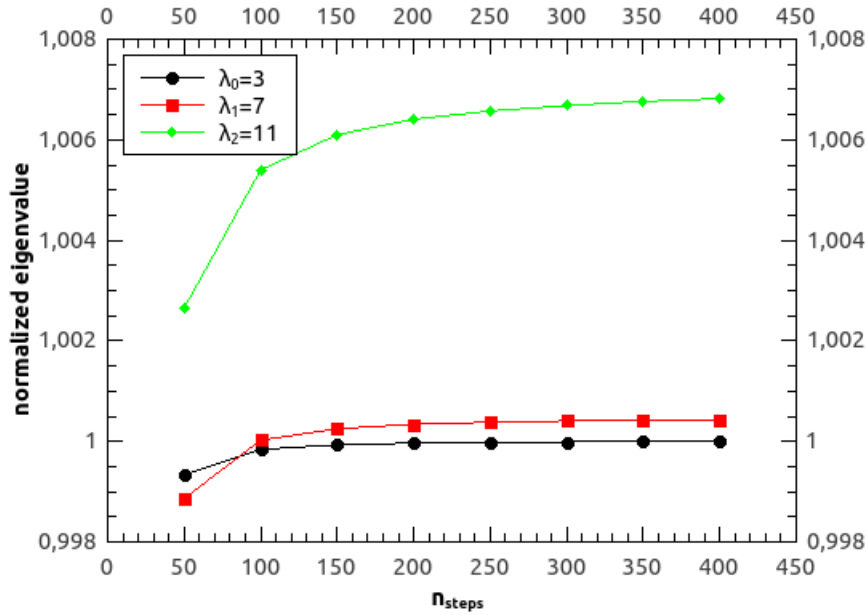


Figure 1: Each line is the calculated normalized eigenvalue as a function of the number of steps used. We see that all the values converges towards a final value as n increases.

eigenvalues are plotted with each coloured line corresponding to the eigenvalue as indicated in the legend. The lowest eigenvalue $\lambda_0 = 3$ converged fastest and at $n = 400$ the exact value of 3 was found. Further increasing n gave us a result that deviated from the exact answer, indicating higher n is not necessarily beneficial. The higher eigenvalues $\lambda_1 = 7$ (red line) and $\lambda_2 = 11$ (green line) did not converge to the exact answer but had a small deviation. The deviation increased with the value of the eigenvalue and this trend continued for even higher eigenvalues.

Next we wanted to see how many iterations of the while loop we needed to repeat until we got a satisfactory answer, and how the number of iterations depended on the number of steps. As seen in Fig.2 the number of iterations needed

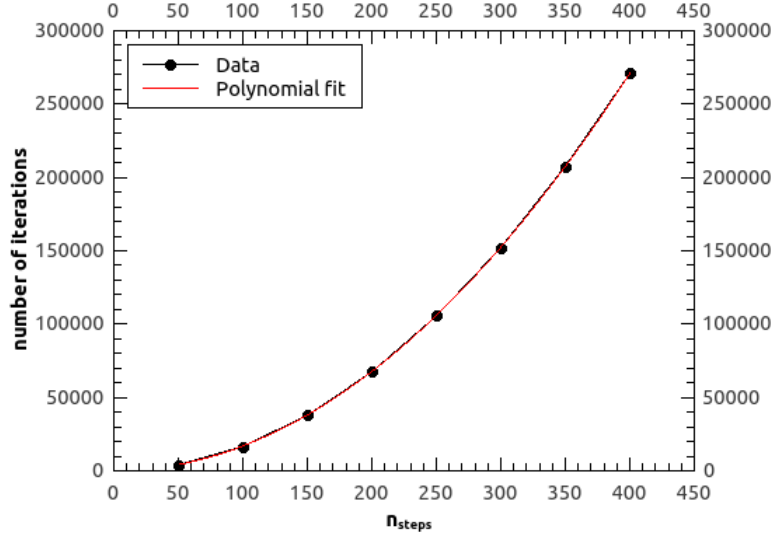


Figure 2: The number of iterations versus number of steps is plotted here. The data was fitted to the polynomial Ax^2 with the result $A = 1,69 \pm 1,05 \cdot 10^{-3}$

roughly increases as n_{steps}^2 . We fitted the data to a second order polynomial Ax^2 using a scaled Levenberg–Marquardt fit, with the result $A = 1,69 \pm 1,05 \cdot 10^{-3}$. This fits adequately with the predicted value of $3n^2 - 5n^2$ from the Computational Physics Lecture Notes[2].

Moving on to the two-electron system, we were interested in the wave functions of the electrons. In Figure 3 below we have plotted the wave functions for the ground state, with different values of ω_r which determines the strength of the oscillator potential. As expected when the oscillator potential increases in strength the two electrons is squeezed together more tightly.

Furthermore, the shape of the wave function is not the only thing that changes when varying ω_r , but as seen in Figure 4, the calculated value for the ground state eigenvalue is also deviating from the true value as a function of ω_r . The ground value eigenstates are analytically calculated (M.Taut,1993)[3] and given by

$$\lambda_0 = 2 \left[\frac{3}{2} \left(\frac{\omega_r}{2} \right)^{2/3} + \frac{\sqrt{3}}{2} \omega_r \right]$$

This expression is only valid for small ω_r so the deviation we observe is expected.

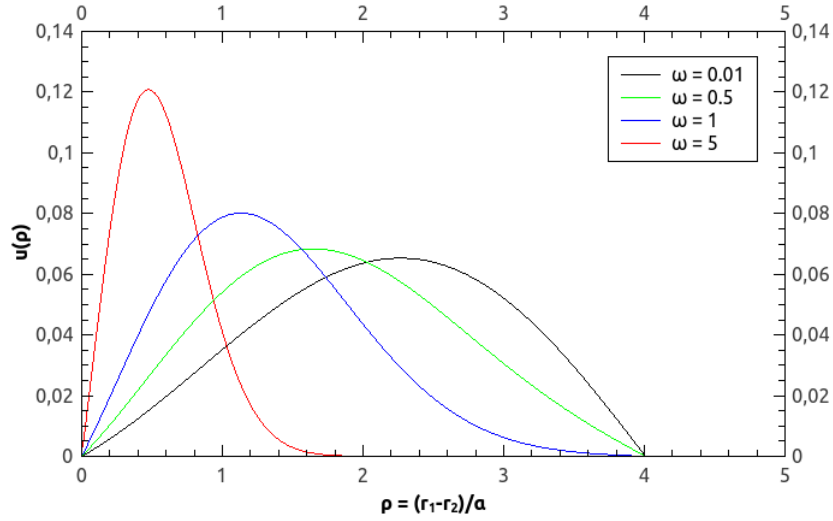


Figure 3: Here we have the ground state wave function as a function of the relative distance between the two electrons.

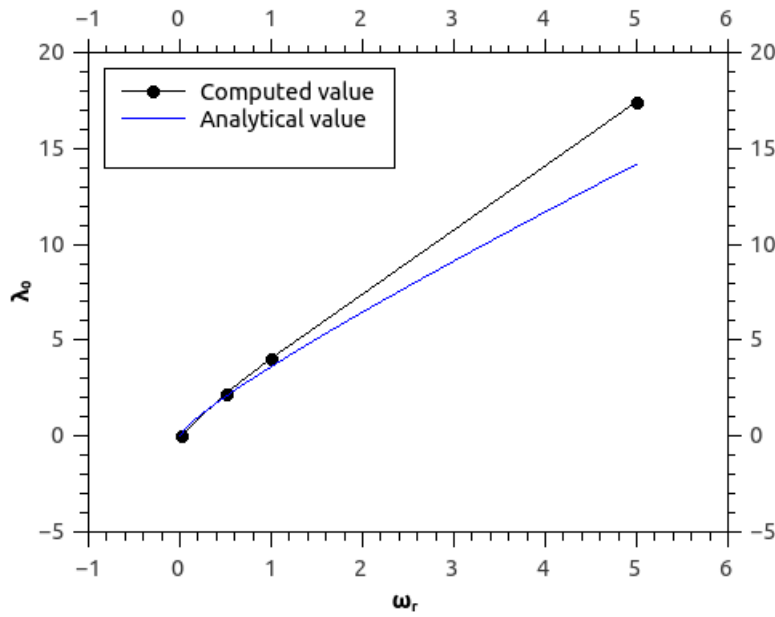


Figure 4: As we increase the strength of the potential, the computed values of the ground state eigenvalue deviates from the analytical value.

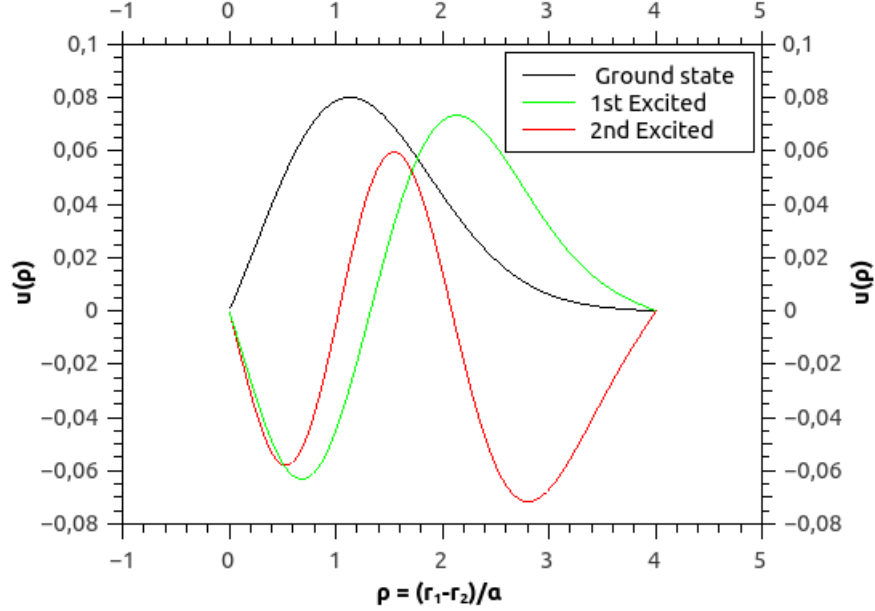


Figure 5: The wave function for the ground state, first excited state and the second excited state is plotted here. Here $\omega_r = 1$.

Next we wanted to plot the wave-function for the ground state and two higher excited states. We first plot the wave functions for the three first eigenstates with $\omega_r = 1$, as seen in Figure 5. The physical interpretation of the wave-function is somewhat obscure so it is in our interest to rather look at the probability distribution which is the square of the wave-function. In Figure 6 we plot the probability distributions for the same wave-functions we saw in Figure 5. In Figure 7 the probability distribution is again plotted, but this time without Coulomb interaction. Both Figure 6 and 7 have in common that the highest probability separation between the two electron increases for the excited states. In Figure 8 and 9 we have similar probability distributions, but this time with $\omega_r = 0.01$. This severely decreases the strength of the potential when compared to $\omega_r = 1$. This is obvious from the expression

$$V(\rho) = \rho^2 \omega_r^2 + 1/\rho$$

We also observe that with a low ω_r the Coulomb interaction term, $1/\rho$, becomes more dominant. This is also seen when comparing the difference between Figure 8 and 9 to the difference between Figure 6 and 8. There is not a big difference between the probability distribution with and without Coulomb interaction for $\omega_r = 1$, but the distortion is obvious for $\omega_r = 0.01$.

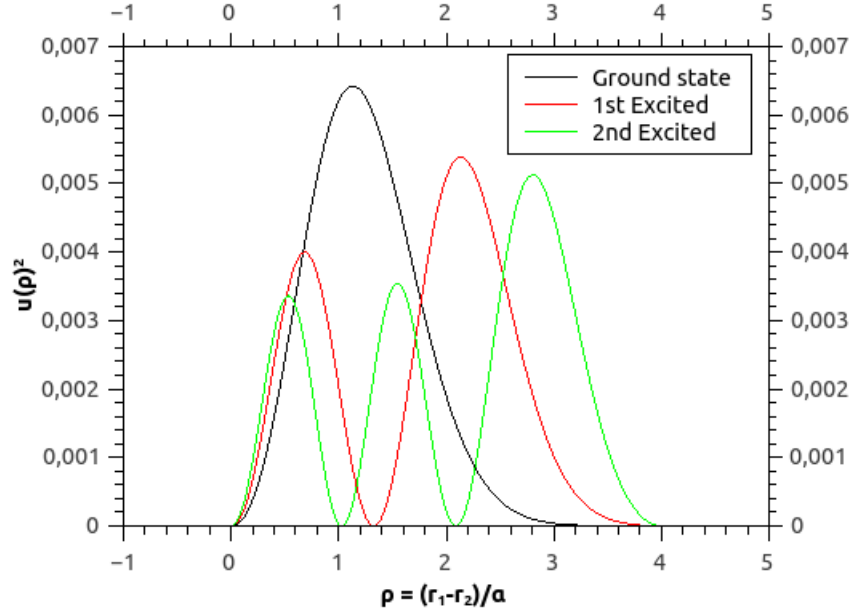


Figure 6: This is the wave function squared, in other words the probability distribution, plotted. Again we set $\omega_r = 1$. Coulomb interaction is included in these calculations.

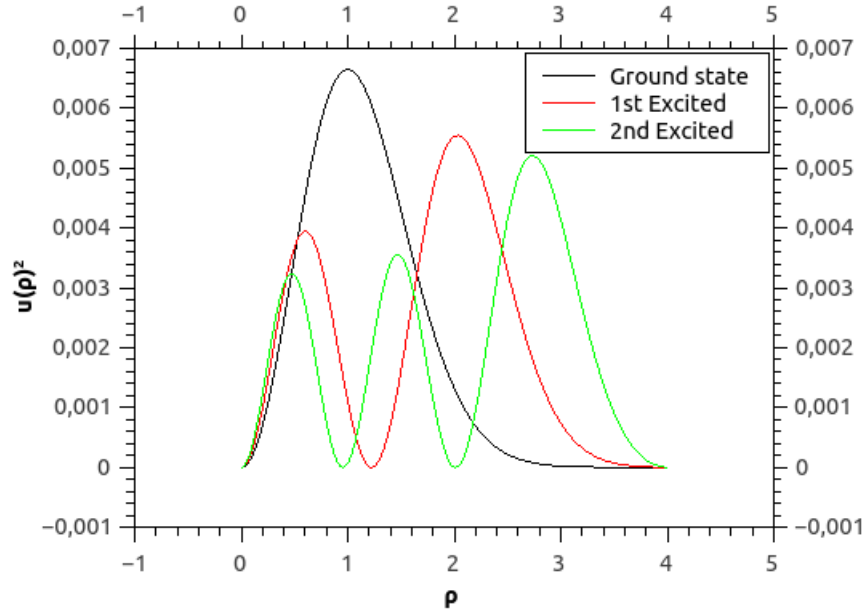


Figure 7: We plot the probability distribution again, but this time without Coulomb interaction. ω_r is still set to 1.

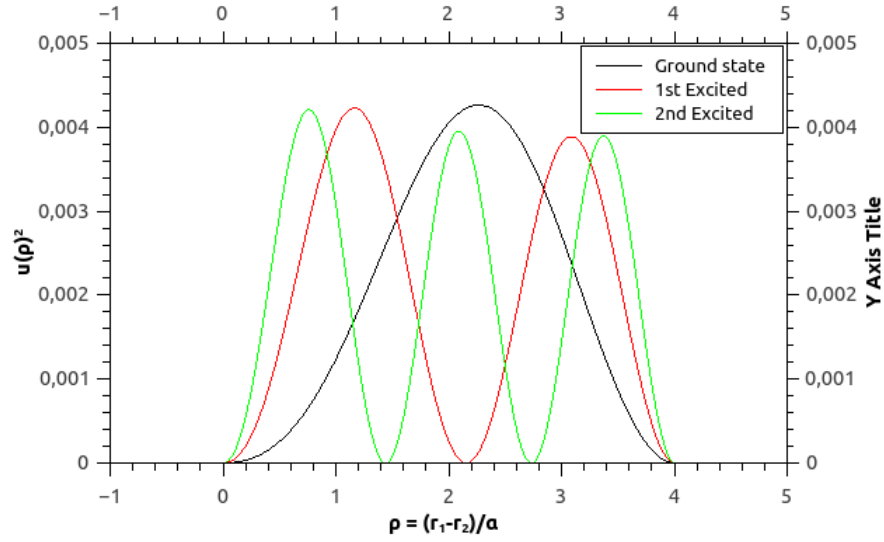


Figure 8: Here we plot the probability distribution for the three first eigenstates again, but this time with $\omega_r = 0.01$. Coulomb interaction is included.

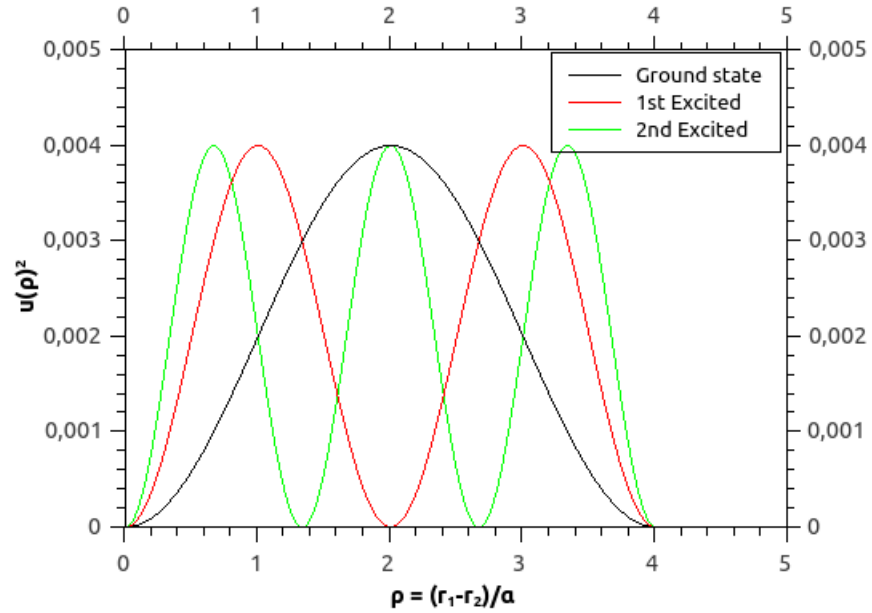


Figure 9: We plot the probability distribution again, but this time without Coulomb interaction. ω_r is still set to 0.01.

5 Discussion

In this project we have investigated the properties of quantum dots. Spatially confined electrons will obtain discreteness in the energy levels and we have calculated those energy levels. First we looked at a single electron in a oscillator potential, we set up the Schrödinger equation for the system and solved it using Jacobi's method. We found the three first eigenstates of the system and our result corresponded well with the known values. The trend was that the lower eigenvalues were more accurate than the higher. We also saw that the computational cost of Jacobi's method was proportional to the square of the number of steps used.

Next we added another electron in the potential and plotted the wave function of the two-electron system as a function of the relative distance between the two electrons. We found that in the excited states of the system the distance between the electrons was increased and that by increasing the strength of the potential the electrons were forced closer together.

References

- [1] Conrad Sanderson. Armadillo: An Open Source C++ Linear Algebra Library for Fast Prototyping and Computationally Intensive Experiments. Technical Report, NICTA, 2010.
- [2] Morten Hjorth-Jensen. Computational Physics Lecture Notes Fall 2012. October 12, 2012.
- [3] M. Taut, 1993, Two electrons in an external oscillator potential: Particular analytic solutions of a Coulomb correlation problem, Physical Review A, v. 48, p. 3561.