Quantum dots in three dimensions

FYS3150 – Project 2

github.com/henrikx2/FYS3150

Contents

Abstract

In this report, the eigenvalue problem of a system with electrons in a harmonic oscillator potential is explored. The well-known and stable Jacobi's rotation algorithm is used to diagonalize the Hamiltonian matrix into an eigenvalue matrix. The equilibrium between calculation speed and decimal precision of the eigenvalues are discussed as a function of step size, interval length and numbers of iterations. The impact of Coulomb interaction between the electrons is also an interesting aspect of the system to examine.

1. Introduction

The experiment aims to solve the general eigenvalue equation of the type

$$H\hat{v} = \lambda\hat{v}$$

Where H is going to be the Hamiltonian operator of the harmonic oscillator well potential and λ is the energy eigenvalue of the given state $\hat{v}$.

The equation is solved by firstly; constructing a tridiagonal Hamiltonian matrix. This matrix is derived by simplifying the Schroedinger's equation for one or two electrons in the HO potential and making it dimensionless. Then, the matrix is processed with orthogonal transformation through Jacobi's rotation algorithm. This reveals a diagonal matrix with the eigenvalues of the Hamiltonian at its diagonal. The eigenvalues are then compared to the analytic eigenvalues. Lastly, the ground state of the system's dependence on Coulomb interactions and varying HO potential will be explored.

2. Theory

2.1 One electron in the HO potential

The solution to the radial part of the Schroedinger's equation for one electron in the HO potential is given as

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

Where $V(r)$ is the HO potential $\frac{1}{2}kr^2$ with $k = m\omega^2$ and $r \in [0, \infty\rangle$, $R(r)$ is the wavefunction and E is the energy of the harmonic oscillator. The energies can be written as a function of the frequency ω as

$$E_{nl} = \hbar\omega\left(2n + l + \frac{3}{2}\right) \qquad (2)$$

Where $n = 0,1,2,\dots$ is the principal quantum number and $l = 0,1,2,\dots$ is the angular momentum quantum number of the electron. Substituting $R(r) = \frac{1}{r}u(r)$, Eq. 1 becomes

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}u(r) + \left(V(r) + \frac{l(l+1)}{r^2}\frac{\hbar^2}{2m}\right)u(r) = Eu(r) \qquad (3)$$

Where the Dirichlet boundary conditions give $u(0) = 0$ and $u(\infty) = 0$. To make the Eq. 3 dimensionless, it is rewritten as a function of the dimensionless variable $\rho = r/\alpha$ where α has dimensions length. The HO potential is then given $V(\rho) = \frac{1}{2}k\alpha^2\rho^2$. This project only focuses on a system where $l = 0$, which makes the expression of the centrifugal barrier go to zero and Eq. 3 simplifies to

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

To make Eq. 4 suitable for solving numerically, it is multiplied by $\frac{2m\alpha^2}{\hbar^2}$, so that

$$-\frac{d^2}{d\rho^2}u(\rho) + \frac{mk}{\hbar^2}\alpha^4\rho^2u(\rho) = \frac{2m\alpha^2}{\hbar^2}Eu(\rho) \qquad (5)$$

Which is further manipulated with the condition

$$\frac{mk}{\hbar^2}\alpha^4 = 1 \rightarrow \alpha = \left(\frac{\hbar^2}{mk}\right)^{\frac{1}{4}} \qquad (6)$$

So that defining

$$\lambda = \frac{2m\alpha^2}{\hbar^2}E \qquad (7)$$

Gives the simplified Schroedinger's equation which is to be solved as

$$-\frac{d^2}{d\rho^2}u(\rho) + \rho^2u(\rho) = \lambda u(\rho) \qquad (8)$$

The analytical eigenvalues of this equation are $\lambda = 3,7,11, \dots$

Since the maximum value ρ_{max} cannot be set to ∞, this will be varying as to get the most correct energies. The values of ρ_{min} is defined $\rho_{min} = 0$. The number of mesh points are given as N and the step length reads

$$h = \frac{\rho_N - \rho_0}{N} \qquad (9)$$

Which in turn gives the expression for the value of ρ at a given iteration i as

$$p_i = p_0 + ih, \quad i = 1,2, \dots, N \qquad (10)$$

An approximation to the 2ⁿᵈ derivative can be expressed

$$\frac{d^2}{df^2} = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + O(h^2) \tag{11}$$

Using Eq. 11 and the HO potential $V_i = \rho_i^2$ to describe the discrete case of the Schroedinger's equation as

$$-\frac{1}{h^2} u_{i-1} + \left(\frac{2}{h^2} + \rho_i^2\right) u_i - \frac{1}{h^2} u_{i+1} = \lambda u_i \tag{12}$$

It is easy to notice the tridiagonal matrix equation $\hat{A}\hat{u} = \lambda\hat{u}$ where the matrix $\hat{A}$ is defined as follows

$$\hat{A} = \begin{bmatrix}
\frac{2}{h^2} + \rho_i^2 & -\frac{1}{h^2} & 0 & 0 & 0 & \cdots & 0 \\
-\frac{1}{h^2} & \frac{2}{h^2} + \rho_i^2 & -\frac{1}{h^2} & 0 & 0 & \cdots & 0 \\
0 & -\frac{1}{h^2} & \frac{2}{h^2} + \rho_i^2 & -\frac{1}{h^2} & 0 & \cdots & 0 \\
0 & 0 & \ddots & \ddots & \ddots & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & -\frac{1}{h^2} & \frac{2}{h^2} + \rho_i^2 & -\frac{1}{h^2} \\
0 & 0 & 0 & 0 & \cdots & -\frac{1}{h^2} & \frac{2}{h^2} + \rho_i^2
\end{bmatrix}$$

In other words, the diagonal elements and the non-diagonal elements are denoted as

$$d_i = \frac{2}{h^2} + V_i \tag{13}$$

$$e_i = -\frac{1}{h^2} \tag{14}$$

2.2 Two electrons in the HO potential

Now, the two-electron system is a bit more exciting, because it opens the door to study the coulomb interactions between electrons. The general Schroedinger's equation for one electron in a HO potential well is as before

$$-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} u(r) + \frac{1}{2} kr^2 u(r) = E^1 u(r) \tag{15}$$

Where E^1 is the energy of the system with only one electron. Now, adding the other electron (but no Coulomb interactions) the equation reads

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr_1^2} - \frac{\hbar^2}{2m}\frac{d^2}{dr_2^2} + \frac{1}{2}kr_1^2 + \frac{1}{2}kr_2^2\right)u(r_1, r_2) = E^2 u(r_1, r_2) \qquad (16)$$

Now, using relative coordinate $r = r_1 + r_2$ and center-of-mass coordinate $R = \frac{1}{2}(r_1 + r_2)$, the Shroedinger equation becomes

$$\left(-\frac{\hbar^2}{m}\frac{d^2}{dr^2} - \frac{\hbar^2}{4m}\frac{d^2}{dR^2} + \frac{1}{4}kr^2 + kR^2\right)u(r, R) = E^2 u(r, R) \qquad (17)$$

Separating r and R can be done using the ansatz for the separation of the wave function $u(r, R) = \psi(r)\phi(R)$, where det energy is a sum of the relative and the center-of-mass energy given by $E^2 = E_r + E_R$.

The Coulomb interactions between the electrons is given by the expression

$$V(r_1, r_2) = \frac{\beta e^2}{|r_1 - r_2|} = \frac{\beta e^2}{r} \qquad (18)$$

In which the constant $\beta e^2 = 1.44 \ eVnm$. This can be added to the $\psi(r)$ part of the equation

$$\left(-\frac{\hbar^2}{m}\frac{d^2}{dr^2} + \frac{1}{4}kr^2 + \frac{\beta e^2}{r}\right)\psi(r) = E_r\psi(r) \qquad (19)$$

By making Eq. 19 dimensionless by using the same steps as in 2.1, the equation reads

$$-\frac{d^2}{d\rho^2}\psi(\rho) + \frac{1}{4}\frac{mk}{\hbar^2}\alpha^4\rho^2\psi(\rho) + \frac{m\alpha\beta e^2}{\rho\hbar^2}\psi(\rho) = \frac{m\alpha^2}{\hbar^2}E_r\psi(\rho) \qquad (20)$$

To make Eq. 20 "identical" to Eq. 8, a new "frequency" is defined as

$$\omega_r^2 = \frac{1}{4}\frac{mk}{\hbar^2}\alpha^4 \qquad (21)$$

Where the parameter ω_r mirrors the strength of the HO potential. Furthermore

$$\frac{m\alpha\beta e^2}{\hbar^2} = 1 \qquad (22)$$

Such that

$$\alpha = \frac{\hbar^2}{m\beta e^2} \qquad (23)$$

And the eigenvalue λ

$$\lambda = \frac{m\alpha^2}{\hbar^2} E_r \tag{24}$$

So that the final Schroedinger's equation reads

$$-\frac{d^2}{d\rho^2}\psi(\rho) + \omega_r^2\rho^2\psi(\rho) + \frac{1}{\rho}\psi(\rho) = \lambda\psi(\rho) \tag{25}$$

This equation has the analytical eigenvalues given by Eq. 26[1] underneath:

$$\epsilon = 2\epsilon'_m = 2 \cdot \left(V_0 + \omega_e\left[m + \frac{1}{2}\right]\right) \quad , \quad m = 0,1,2, \dots \tag{26}$$

Where:

$$V_0 = \frac{3}{2}\left(\frac{\omega_r}{2}\right)^{\frac{2}{3}}$$

$$\omega_e = \sqrt{3}\omega_r$$

The expression for the analytical eigenvalues with no electron-electron interaction, is given as:

$$\epsilon = 2\epsilon'_m = 2 \cdot \omega_r\left[2m + \frac{3}{2}\right] \quad , \quad m = 0,1,2, \dots \tag{27}$$

These expressions will be used to evaluate the experimental results from the program later.

The diagonal in the tridiagonal matrix is now defined (the off diagonals stay the same as in the single electron system):

$$d_i = \frac{2}{h^2} + \omega_r^2\rho_i^2 + \frac{1}{\rho_i} \tag{28}$$

If there where not to be a Coulomb interaction between the two particles, the d_i would be just like the one in the singe electron system, but with $\omega_r^2 = 1$ and hence α would be defined as:

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

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[1] *Eq. 26 and 27 are originating from equation (16a) and (16b) in the article: M. Taut, Phys. Rev. A 48, 3561 (1993).*

2.3 Preservation of orthogonality

For the method described in section 3 to work, it is essential to prove that a unitary transformation preserves the dot product and the orthogonality of vectors in a basis. Consider the orthogonal basis

$$\hat{v_i} = \begin{bmatrix} v_{i1} \\ v_{i2} \\ \vdots \\ v_{in} \end{bmatrix} \quad , \quad \hat{v}_j^T \hat{v}_i = \delta_{ij}$$

For a matrix U to be unitary it must have the property $U^T = U^{-1}$. Consider the transformation $\hat{w}_i = U\hat{v}_i$. The dot product is then

$$\hat{w}_j^T \hat{w}_i = \left(U\hat{v}_j\right)^T U\hat{v}_i = \hat{v}_j^T (U^T U)\hat{v}_i$$

$$= \hat{v}_j^T (U^{-1} U)\hat{v}_i$$

$$= \hat{v}_j^T \hat{v}_i = \delta_{ij}$$

Hence, the orthogonal/unitary transformation preserves the orthogonality ∎

3. Methods

3.1 Jacobi's rotation algorithm

Jacobi's rotation algorithm evolves around performing an orthogonal transformation with a rotation matrix of the type

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

Which has the property $S^T = S^{-1}$ and performs a rotation of angle θ in the Euclidean space. The elements of S that are not zero are given as

$$s_{kk} = s_{ll} = cos\theta, \quad s_{kl} = -s_{lk} = -sin\theta, \quad s_{ii} = 1 \quad i \neq k \, i \neq l$$

The algorithm is used to transform a symmetric matrix A into a diagonal matrix where the diagonal consists of the eigenvalues. This diagonalization is performed by doing the orthogonal transformation several times, so that the off-diagonal elements converge to zero.

Defining $c = cos\theta$ and $s = sin\theta$, a 2x2 system would look like this

$$\begin{bmatrix} b_{kk} & 0 \\ 0 & b_{ll} \end{bmatrix} = \begin{bmatrix} c & -s \\ s & c \end{bmatrix}\begin{bmatrix} a_{kk} & a_{kl} \\ a_{lk} & a_{ll} \end{bmatrix}\begin{bmatrix} c & s \\ s & c \end{bmatrix}$$

The requirement that $b_{kl} = b_{lk} = 0$ implies that

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

Where it's easy to see that if the off-diagonal element $a_{kl} = 0$, then $cs = 0$, which implies that $cos\theta = 1$ and $sin\theta = 0$, or in other words; no rotation needed as off-diagonals is close to zero. Next, defining

$$t = tan\theta = s/t$$

$$cot2\theta = \tau = \frac{a_{ll} - a_{kk}}{2a_{kl}}$$

A quadratic equation can be derived from the relation $cot2\theta = \frac{1}{2}(cot\theta - tan\theta)$ so that

$$t^2 + 2\tau t - 1 = 0 \qquad\qquad (29)$$

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

From the relation $cos\theta = \frac{1}{\sqrt{1+tan\theta^2}}$, c and s are defined as

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

$$s = tc$$

The equations for the new matrix elements when iterating are:

$$\begin{aligned} b_{ii} &= a_{ii}, i \neq k, i \neq l \\ b_{ik} &= a_{ik}c - a_{il}s, i \neq k, i \neq l \\ b_{il} &= a_{il}c + a_{ik}s, i \neq k, i \neq l \\ b_{kk} &= a_{kk}c^2 - 2a_{kl}cs + a_{ll}s^2 \\ b_{ll} &= a_{ll}c^2 + 2a_{kl}cs + a_{kk}s^2 \\ b_{kl} = b_{lk} &= (a_{kk} - a_{ll})cs + a_{kl}(c^2 - s^2) = 0 \end{aligned}$$

This gives a new matrix B, on which the same procedure is done until it's off-diagonal elements are under a certain tolerance

The rate of which the Jacobi's method converges to the diagonal matrix with the eigenvalues is horribly slow. It takes somewhat $3n^2 - 5n^2$ rotations to make the off-diagonals zero, and each rotation uses approximately $4n$ FLOPS. This makes the algorithm use at least somewhere around $12n^3 - 20n^3$ FLOPS.

3.2 Code structure

1. Build the matrix A by implementing the diagonal elements from the corresponding problem in section 2.
2. Find the off-diagonal element with the largest absolute value and assign its matrix index to l and k.
3. Calculate t, c and s.
4. Calculate the 6 equations with the obtained l and k and update the matrix A.
5. Repeat until off-diagonal elements are lower than the specified tolerance.

3.3 Running the calculations

To run the calculations using the provided source code in the git repository, it is required to have Python 3 with the `NumPy`, `SciPy`, `matplotlib` and `numba` packages installed. Run the calculations by executing `main.py`, this will start a UI. Choose to either; calculate all necessary data and make plots, just plot data which is already calculated or do individual calculation with your own variables.

4. Results and discussion

4.1 Single electron

The single electron system has the analytical eigenvalues $\lambda = 3,7,11,15,\dots$. To achieve these eigenvalues, it was necessary to run the algorithm several times trying different values of ρ_{max} and n. It was also found that it was not possible to achieve 4 decimal precision of the eigenvalues of the third lowest states at the same time. This resulted in Table 6.2.1, which shows which conditions on ρ_{max} and n that gave the eigenvalues with 4 decimal precision.

Figure 4.1.1a-c shows how the probability distribution, $|u(\rho)|^2$, of the three lowest states look like with the conditions from Table 6.2.1. From these figures, it is easy to notice how the higher excited states have a larger spatial distribution than that of the lower energetic states.

The limitations on how many eigenvalues that can be calculated at the same time evolves from the fact that infinity has to be assigned to something smaller than infinity. This makes it possible to get one eigenvalue correct (using a satisfying value of ρ_{max} and number of integration points), but the other values will likely be far off. To achieve several correct eigenvalues in the same matrix, the matrix would have to be very large (high n) and with a large value of ρ_{max}.

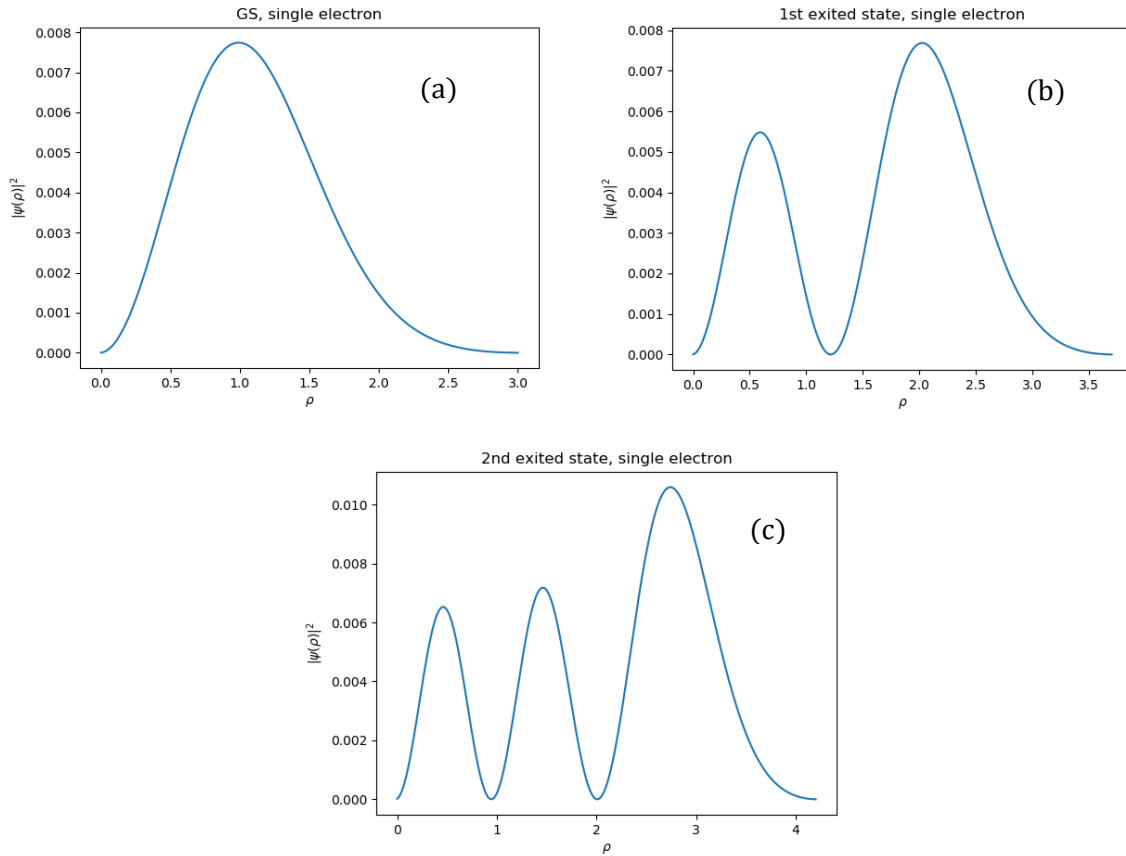*Figure 4.1.1: The probability density of the wave function in ground state (a), 1ˢᵗ exited state (b) and 2ⁿᵈ exited state (c). Calculated using the experimental eigenvalues with 4 decimal precision.*

4.2 Two electrons

In the two-electron system it is exciting to study how the Coulomb interactions and different values of ω_r impact the wavefunction and the energies of the ground state. So, first off is plotting the two different systems for values $\omega_r = 0.01$, $\omega_r = 0.5$, $\omega_r = 1$ and $\omega_r = 5$. One should be able to predict that the larger value of ω_r; the smaller the distribution of the wavefunction. This is shown in Figure 4.2.1 and Figure 4.2.2.

In these figures, it is clear how the HO frequency affects the wavefunction of the system to either broaden or shrink in ρ-space. This is intuitive, because a smaller potential would give the electrons more possibility of existing in a larger area.
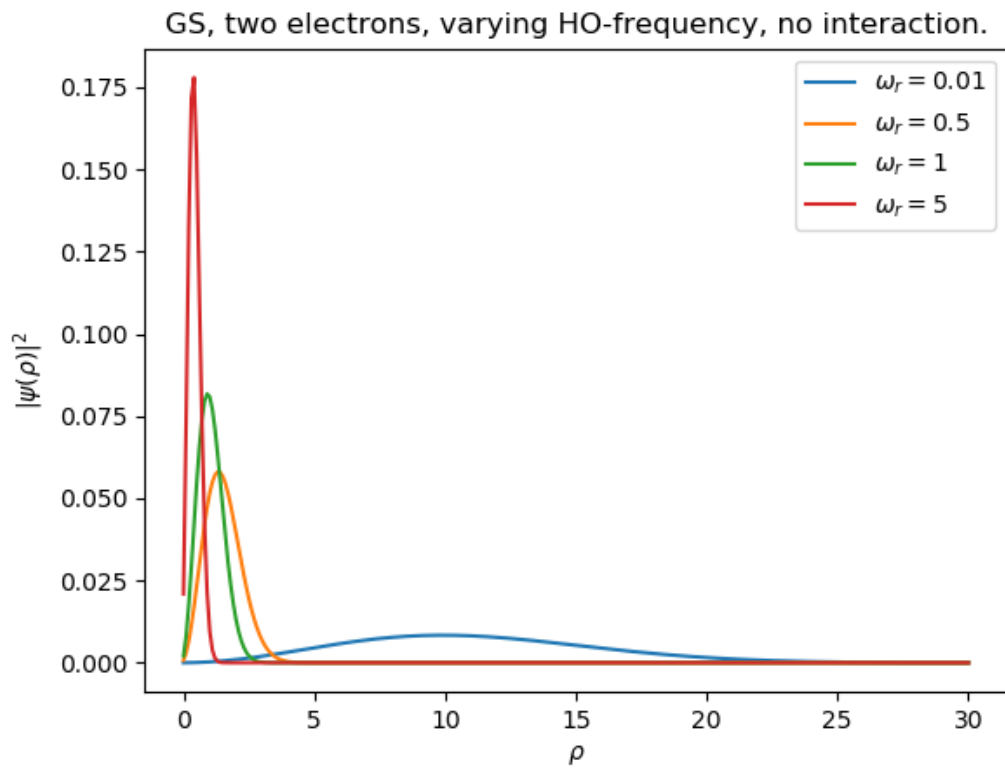
Figure 4.2.1: The probability density of the GS wavefunction without the electron-electron interaction for different values of the HO-potential strength ω_r. See how the distribution broadens for smaller potentials.
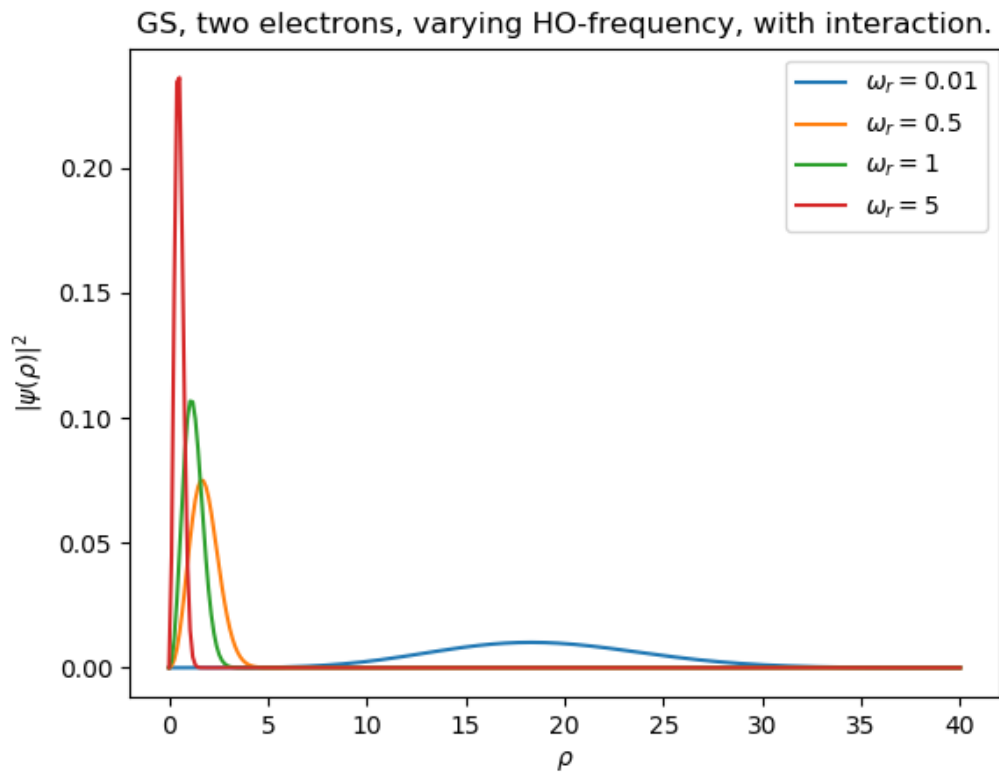

Figure 4.2.2: The probability density of the GS wavefunction with the electron-electron interaction for different values of the HO-potential strength ω_r. See how the distribution broadens for smaller potentials.

To figure out how the Coulomb interactions affect the systems energy, one may look at how the peaks in Figure 4.2.1 and Figure 4.2.2 are shifted. But this is hard to see with the naked eye, especially for the most energetic states. To see the difference between the two systems, let's look at the experimental eigenvalues. In Table 4.2.1, the eigenvalues in the two cases are compared as function of ω_r. The value of ρ_{max} and n are manipulated so that the wavefunction with $\omega_r = 0.01$ has the most correct eigenvalue (such that the error in the eigenvalues increases as ω_r increases). Table 6.1.1 in Appendix lists the analytical eigenvalues of the two-electron system with and without the Coulombs interactions.

Table 4.2.1: Comparison of eigenvalues in the Coulomb interacting systems and the non-Coulomb interacting systems.

HO frequency, ω_r	Two electrons, no interaction Experimental eigenvalues, λ:	Two electrons, with interaction Experimental eigenvalues, λ:	Increase in energy from interaction:
0.01	0.029990	0.105876	0.075886
0.5	1.426043	2.232772	0.806729
1	2.788140	4.060586	1.272446
5	12.642609	17.346902	4.704293

So, the energy of the system with Coulomb interaction has of course an increase in energy because of the repulsion forces between the electrons. By looking at how much the increase in energy is due to the Coulomb interaction as function of the HO-potential strength ω_r, one can see that the relation is at least not linear. This is likely since the higher the ω_r is, the narrower the peak of the probability density is (Figure 4.2.1 and Figure 4.2.2 shows this), and therefore the closer the electrons must be. Which again of course gives a large repulsion potential. As mentioned earlier, from Figure 4.2.1 and 4.2.2, one can also see how the Coulomb interactions actually makes the probability density function broader.

4.3 Jacobi's method

As much as this is a report solving the Schroedinger's equation for 1-2 electrons in a harmonic oscillator potential and analysing the aspects of this, there is also a numerical algorithm to discuss. One interesting aspect to investigate is how many similarity transformations are needed as function of the dimension of the matrix n. Figure 4.3.1 shows a plot of exactly this.
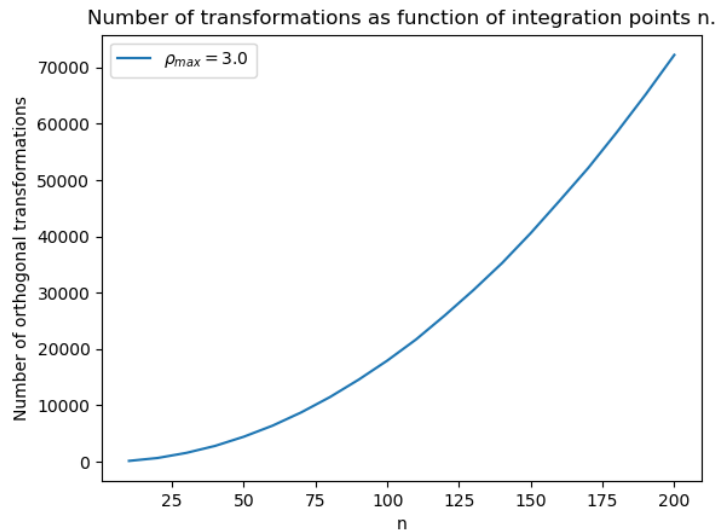
Figure 4.3.1: Number of similarity transformations as function of number of integration points in the Jacobi's algorithm. This should in theory be a 2ⁿᵈ degree curve.

Using the `SciPy` function `curve_fit` to interpret the points in this curve as a 2nd degree polynomial gives the equation:

$$y = 1.81n^2 - 79.42$$

This estimation of the number of similarity transformations falls somewhat short of the theoretic number ($3n^2 - 5n^2$) of rotations, but perhaps a larger interval of n could make the function more like the theoretic assumptions. When it comes to speed, Jacobi's method is a slow, but stable algorithm. One of the limiting factors when it comes to time usage are the integration points, n. As n increases, the double for-loop that finds the maximum off-diagonal element is rapidly getting more time consuming.

Though the algorithm itself is rather time consuming, it has no problems computing the eigenvalues of symmetric matrices of sizes up to $n = 500$ (with a tolerance where $0 \approx 10^{-10}$), if one has the time to wait a few minutes. The actual computation is in fact very precise, of course depending on the toleration limit for the zeros on the diagonal of the transformed matrix. This is also what gives the error of the method.

5. Conclusion

So, it has been shown that it is possible to calculate the analytic eigenvalues of the symmetric Hamiltonian with use of the Jacobi's algorithm. Also, the wavefunctions and the probability density of the different energy states of the systems is given by the algorithm. The algorithm is proved to be both stable and give exact eigenvalues.

One eye opener in this experiment is the realization of how slow Jacobi's method is compared to other known methods to solve eigenvalue problems. The next step would probably be to explore how much faster other algorithms (i.e. the House holders' algorithm or the Lanczos algorithm) can be. Though, this report has achieved to give a thorough explanation and presentation of the aspects of Jacobi's algorithm.

6. Appendix

6.1 Analytical eigenvalues

Using Eq. 26 and 27 with the fact that $l = m = 0$, the eigenvalues in Table 6.1.1 may be calculated.

Table 6.1.1: The analytical eigenvalues of the two-electron system with different frequencies.

	Two electrons, no interaction	Two electrons, with interaction
HO frequency, ω_r	Analytical eigenvalues, ϵ:	Analytical eigenvalues, ϵ:
0.01	0.03	0.1050
0.5	1.50	2.0566
1	3.00	3.6220
5	15.00	14.1864

6.2 Optimal values of n and ρ_{max}

Table 6.2.1 shows the optimal values of n and ρ_{max} to achieve 4 decimal precision of the three lowest energy eigenvalues of the single electron system.

Table 6.2.1: Optimal values of ρ_{max} and n to achieve 4 decimal precision of eigenvalues in the one-electron system.

Analytical eigenvalues	ρ_{max}	n	Experimental eigenvalues
3	3	325	2.999987
7	3.7	337	7.000073
11	4.2	254	10.999960

References

1. **Hjorth-Jensen, M. (2019)**, *Computational Physics, Project 2 Fall 2019*, Department of Physics, University of Oslo.
   https://github.com/CompPhysics/ComputationalPhysics/blob/master/doc/Projects/2019/Project2/pdf/Project2.pdf

2. **Hjorth-Jensen, M. (2019)**, *Computational Physics, Eigenvalue Problems,* Department of Physics, University of Oslo.
   http://compphysics.github.io/ComputationalPhysics/doc/pub/eigvalues/html/eigvalues.html

3. Analytical eigenvalues:
   https://journals.aps.org/pra/pdf/10.1103/PhysRevA.48.3561