Project 2
Computational Physics I
FYS3150/FYS4150

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October 1, 2018

Abstract

In this project we study how to solve eigenvalue problems using Jacobi's method of iterative diagonalization, and develop an eigenvalue solver based on the aforementioned method. The solver is tested on the equations of a buckling beam and Schrödinger's equation for two electrons in a three-dimensional harmonic oscillator well, recasted as eigenvalue problems by discretization and scaling of equations.

Our implementation reproduce the three first analytical eigenvalues of the buckling beam to at least 5 decimals. For single electron in harmonic oscillator, we easily reproduce eigenvalues to at least 4 decimals precision, but only for appropriate spacial intervals reflection the width of the wave function in question. Solving the two-electron interacting case produce ground state energies stable as functions of spacial interval and number of grid-points. The ground state eigenvalues tend to increase with increasing oscillator frequency ω. For $\omega = 0.25$ and $\omega = 0.05$, we produced ground state eigenvalues 1.24991 and 0.349995, in close correspondence to the known analytical values 1.25 and 0.35. When visualizing the eigenvectors of the interacting and non-interacting electrons case, we find that the relative coordinate wave function, that is, the relative spacing between the electrons, for the interacting case tend to be more "smeared out" than the non-interacting case. This effect was further amplified by lowering the frequency.

Studying the complexity of Jacobi's method, we find that the number of iterations needed to diagonalize a $(N \times N)$-matrix was proportional with N^2. The CPU-time need to fully diagonalize a matrix was approximately proportional to $N^{3.8}$, while Armadillo's built-in eigenvalue solver eig_sym solve it in time proportional to $N^{1.9}$.

GitHub repository: https://github.com/nicolossus/FYS3150/tree/master/Project2

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1 Introduction

In this project we study how to solve eigenvalue problems using Jacobi's method of iterative diagonalization, with the aim to develop an eigenvalue solver based on the aforementioned method. In order to test the solver, we apply it to solve the equations of a buckling beam and Schrödinger's equation for two electrons in a three-dimensional harmonic oscillator well, recasted as eigenvalue problems by discretization and scaling of equations.

We use Jacobi's method to solve the first three eigenvalues of the buckling beam and compare these to known analytical values. We also solve the eigenvalues of single electron in a harmonic oscillator and explore how the numerical precision behaves as function of the parameters number of mesh points N and interval $[\rho_0, \rho_N]$. We go onto finding the ground state eigenvalue and eigenvector for two interacting electrons in a harmonic oscillator and explore how they behave for different frequencies.

We benchmark our implementation of Jacobi's method and try to determine how the number of needed iterations and CPU-time depends on the dimmensionality of the matrix being diagonalized. In the case of CPU-time we also compare it to Armadillo's built-in eigenvalue solver *eig_sym*.

2 Theory

2.1 Eigenvalue Problems

Given a generic $n \times n$ matrix $\boldsymbol{A}$, an eigenvalue of that matrix is a number λ satisfying the equation

$$\boldsymbol{A}\boldsymbol{x} = \lambda \boldsymbol{x} \tag{2.1}$$

where the non-zero $\boldsymbol{x}$ are the eigenvectors [1, p. 213]. This matrix equation can be rewritten on the form

$$(\boldsymbol{A} - \lambda \boldsymbol{I})\, \boldsymbol{x} = 0$$

The solution to this equation is found by taking the determinant and setting it equal to zero, which means that

$$\det(\boldsymbol{A} - \lambda \boldsymbol{I}) = 0$$

This determinant gives the characteristic polynomial of degree n, and from the fundamental theorem of algebra there are n solutions. In other words are the eigenvalues of a matrix $\boldsymbol{A} \in \mathbb{C}^{n \times n}$ given by the n roots of it's characteristic polynomial. [1, p. 214] The polynomial can then be written as

$$P_n(\lambda) = det(\boldsymbol{A} - \lambda \boldsymbol{I}) = \prod_{i=1}^{n} (\lambda_i - \lambda), \tag{2.2}$$

and if the set $\{\lambda_1\lambda_2...\lambda_n\}$ is the eigenvalues of $\boldsymbol{A}$, the determinant is

$$\det(\boldsymbol{A}) = \prod_{i=1}^{n} \lambda_i$$

In order to solve Eq. (2.1) numerically a different approach is much more efficient. The general approach is to do a sequence of similarity transformations that either diagonalize the matrix or transform it to tridiagonal form.

2.2 Similarity Transformations

For a real symmetric matrix $\boldsymbol{A}$ which satisfies Eq. (2.1), and thus has n eigenvalues, there exist a real orthogonal matrix $\boldsymbol{S}$ which transform $\boldsymbol{A}$ into a diagonal matrix, $\boldsymbol{D}$, with the eigenvalues as its entries. The ideal case is if we have [1, p. 215]

$$\boldsymbol{S^T A S} = \boldsymbol{D}$$

In general, this transformation has to be implemented several times in order to fully diagonalize the matrix.

Using the eigenvalue equation,

$$\boldsymbol{Ax} = \lambda \boldsymbol{x},$$

as our point of depature, performing the transformation

$$\boldsymbol{S^T Ax} = \lambda \boldsymbol{S^T x}$$

and applying the orthogonality condition $\boldsymbol{SS^T} = \boldsymbol{1}$, gives

$$\boldsymbol{S^T ASS^T x} = \boldsymbol{BS^T x} = \lambda \boldsymbol{S^T x}$$

Here, the new matrix $\boldsymbol{B} = \boldsymbol{S^T AS}$ is the similar transform of $\boldsymbol{A}$, and thus their eigenvalues are the same, but it is important to note that the eigenvectors in general change. A sequence of similarity transformations can then give

$$\boldsymbol{S_N^T}....\boldsymbol{S_1^T A S_1}....\boldsymbol{S_N} = \boldsymbol{D}$$

where now $\boldsymbol{D}$ is the fully diagonalized matrix with the eigenvalues along the diagonal. This sequental transformation is known as Jacobi's method. Another method is to bring the matrix on tridiagonal form, which is known as Householder's method.

2.3 Orthogonal Transformation of Basis Vectors

A set of basis vectors $\boldsymbol{v_i}$ is orthogonal, which means that

$$\boldsymbol{v_i^T v_j} = \delta_{ij}$$

a transformation of a basis vector is given by

$$\boldsymbol{w}_i = \boldsymbol{U}\boldsymbol{v}_i$$

By demanding that the transformation is orthogonal, $\boldsymbol{U}^{\boldsymbol{T}}\boldsymbol{U} = \boldsymbol{I}$, the inner product of the transformed vectors is

$$\boldsymbol{w}_i^{\boldsymbol{T}}\boldsymbol{w}_j = \boldsymbol{v}_i^{\boldsymbol{T}}\underbrace{\boldsymbol{U}^{\boldsymbol{T}}\boldsymbol{U}}_{\boldsymbol{I}}\boldsymbol{v}_j = \boldsymbol{v}_i^{\boldsymbol{T}}\boldsymbol{v}_j = \delta_{ij},$$

which means that an orthogonal transformation preserves the inner product and orthogonality.

2.4 Jacobi's Method

The Jacobi (rotational) method is a method for solving eigenvalue problems using similarity transformations. Each transformation is a plane rotation around an angle θ in the Euclidian n-dimensional space. In order to construct a similarity transformation, we first define the real $(n \times n)$ orthogonal transformation matrix as

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

with the property $\boldsymbol{S}^{\boldsymbol{T}} = \boldsymbol{S}^{-\boldsymbol{1}}$ and matrix elements that differ from zero given by

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

where i is an index other than k or l, that is $i \neq k$ and $i \neq l$. Next, we define the matrix $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ as

$$\boldsymbol{A} = \begin{pmatrix} * & & & \dots & & & * \\ & \ddots & & & & & \\ & & a_{kk} & \dots & a_{kl} & & \\ \vdots & & \vdots & \ddots & \vdots & & \vdots \\ & & a_{lk} & \dots & a_{ll} & & \\ & & & & & \ddots & \\ * & & & \dots & & & * \end{pmatrix}$$

A transformation $\boldsymbol{S}$ on $\boldsymbol{A}$

$$\boldsymbol{B} = \boldsymbol{S}^{\boldsymbol{T}}\boldsymbol{A}\boldsymbol{S},$$

where $\boldsymbol{B}$ is the similarity transform of $\boldsymbol{A}$, then results in

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

The recipe is to choose θ so that all non-diagonal matrix elements b_{kl} become zero. That is, we need to solve

$$b_{kl} = (a_{kl} - a_{ll})\cos\theta\sin\theta + a_{kl}\left(\cos^2\theta - \sin^2\theta\right) = 0,$$

which gives

$$\cot 2\theta = \tau = \frac{a_{ll} - a_{kk}}{2a_{kl}} \tag{2.3}$$

Next, we define the quantities

$$\begin{aligned}
\sin\theta &= s, \\
\cos\theta &= c, \\
\tan\theta &= t = \frac{s}{c}
\end{aligned}$$

By using that $\cot 2\theta = 1/2(\cot\theta - \tan\theta)$ with Eq. (2.3), we obtain the quadratic equation

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

resulting in

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

From this, c and s are easily obtained with the relations

$$\begin{aligned}
c &= \frac{1}{\sqrt{1 + t^2}}, \\
s &= tc
\end{aligned}$$

Choosing t to be the smaller of the roots ensures numerical stability by performing the plane rotation around a small angle θ, rather than a large θ, at each iteration. This also has the effect of minimizing the difference

$$||\boldsymbol{B} - \boldsymbol{A}||$$

The algorithm is then quite simple. We perform a number of iterations until the sum over the absolute values of the non-diagonal matrix elements are less than a prefixed tolerance test (ideally equal zero). [1, p. 215-217]

2.5 Scaling of Equations

In the International System of Units (SI) there are seven base units with corresponding fundamental physical quantities that all other units derive from. In similar fashion, can the dimension of a physical quantity be expressed as a product of the dimensions of the fundamental physical quantities. In Table 2.1 are some of the fundamental physical quantities tabulated with the corresponding base units and dimensions (those omitted are not used in this project). [2, p. 1-2]

Table 2.1: *Some of the fundamental physical quantities and the corresponding base units and dimensions.*

Quantity	Unit	Dimension
Length	m	$[L]$
Mass	kg	$[M]$
Time	s	$[T]$

Scaling an equation means bringing it to a dimensionless form. The corresponding dimensionless variable $\bar{q}$ of a dimensional variable q, can be introduced as

$$\bar{q} = \frac{q - q_0}{q_c}, \tag{2.4}$$

where q_0 is a reference value of q (typically chosen as $q_0 = 0$) and q_c is a characteristic size of q. If q_c is the maximum value of $|q - q_0|$, then $\bar{q} \in [0, 1]$. [2, p. 17]

There are several reasons as to why scaling of equations may serve as an advantage:

- Scaled equations is less prone to machine error, especially if the nature of the problem deals with values that are very large (i.e. astronomy) or small (i.e. quantum physics).
- Having scaled equations means the problem only have to be solved once. By rescaling the solution back to dimensional form, a whole family of solutions may be obtained depending on how the rescaling is performed.

2.6 The Buckling Beam Problem

In this project we will apply Jacobi's method in order to solve the two point boundary problem of a buckling beam fastened at both ends, by recasting the differential equation as an dimensionless eigenvalue problem. The differential equation that describes the buckling beam problem with a beam of length L reads

$$\gamma \frac{d^2u(x)}{dx^2} = -Fu(x), \tag{2.5}$$

where $u(x)$ is the vertical displacement of the beam in the y-direction with $x \in [0, L]$, F is a force applied at $(L, 0)$ in the direction towards the origin and γ is a constant, with base units

Nm^2, defined by properties like the rigidity of the beam. In this project we apply Dirichlet boundary conditions, so that

$$u(0) = u(L) = 0$$

In order to scale the equation to a dimensionless form, we define the dimensionless variable

$$\rho = \frac{x}{L},$$

where L is the characteristic size and the maximum value of x, which implies that $\rho \in [0, 1]$ as explained in Section 2.5. We define the minimum and maximum values of ρ as $\rho_{\text{min}} = 0$ and $\rho_{\text{max}} = 1$, respectively.

By reordering the differential equation as

$$\frac{d^2u(\rho)}{d\rho^2} = -\frac{FL^2}{\gamma}u(\rho) = -\lambda u(\rho), \tag{2.6}$$

where $\lambda = FL^2/\gamma$, we have an equation that becomes an eigenvalue problem when discretized. Here, λ is also a dimensionless variable, which becomes evident by performing a dimensional analysis:

$$\dim \lambda = \frac{(\text{force}) \cdot (\text{length})^2}{\text{rigidity}} = \frac{(\text{force}) \cdot (\text{length})^2}{(\text{force}) \cdot (\text{length})^2} = \frac{[MLT^{-2}] \cdot [L^2]}{[MLT^{-2}] \cdot [L^2]} = 1$$

The discretization of the differential equation can be done by approximating the second derivative by the the three-point formula, that is

$$u'' = \frac{u(\rho + h) - 2u(\rho) + u(\rho - h)}{h^2} + \mathrm{O}\Big(h^2\Big), \tag{2.7}$$

where h is the step size and $\mathrm{O}\Big(h^2\Big)$ is the truncation error. With a given number of mesh points, N, we define the step size as

$$h = \frac{\rho_N - \rho_0}{N},$$

where $\rho_0 = \rho_{\text{min}}$ and $\rho_N = \rho_{\text{max}}$. The value of ρ at point i is then

$$\rho_i = \rho_0 + ih, \quad i = 1, 2, ..., N$$

We can thus rewrite the differential equation for a value ρ_i as

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

which, by adopting the notation $u(\rho_i) \to u_i$ and $u(\rho_i \pm h) \to u_{i\pm1}$, can be written more compactly as

$$-\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = \lambda_i u_i \tag{2.8}$$

with boundary conditions $u_0 = u_N = 0$. By writing out the explicit terms of the discretized differential equation,

$$\begin{aligned}
-\frac{1}{h^2}u_2 + \frac{2}{h^2}u_1 &= \lambda_1 u_1 \\
-\frac{1}{h^2}u_3 + \frac{2}{h^2}u_2 - \frac{1}{h^2}u_1 &= \lambda_2 u_2 \\
-\frac{1}{h^2}u_4 + \frac{2}{h^2}u_3 - \frac{1}{h^2}u_2 &= \lambda_3 u_3 \\
&\vdots \\
-\frac{1}{h^2}u_{N-1} + \frac{2}{h^2}u_{N-2} - \frac{1}{h^2}u_{N-3} &= \lambda_{N-2} u_{N-2} \\
\frac{2}{h^2}u_{N-1} - \frac{1}{h^2}u_{N-2} &= \lambda_{N-1} u_{N-1},
\end{aligned}$$

it becomes clear that the equation may be written in a more general form;

$$\begin{bmatrix} d & a & 0 & 0 & \dots & 0 & 0 \\ a & d & a & 0 & \dots & 0 & 0 \\ 0 & a & d & a & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & a & d & a \\ 0 & \dots & \dots & \dots & \dots & a & d \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \dots \\ u_{N-2} \\ u_{N-1} \end{bmatrix} = \lambda_i \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \dots \\ u_{N-2} \\ u_{N-1} \end{bmatrix}, \quad i = 1, 2, ..., N-1 \tag{2.9}$$

where the diagonal elements $d = 2/h^2$ and the non-diagonal elements $a = -1/h^2$.

We have thus recasted the buckling beam differential equation, Eq. (2.5), as an eigenvalue problem with a tridiagonal matrix equation, Eq. (2.9).

This eigenvalue problem has analytical eigenpairs, with eigenvalues given as

$$\lambda_j = d + 2a\cos\left(\frac{j\pi}{N+1}\right), \quad j = 1, 2, ..., N-1 \tag{2.10}$$

2.7 The Quantum Mechanical Harmonic Oscillator

The quantum harmonic oscillator holds a unique importance in quantum mechanics, as it is one of few problems that can be solved in closed form, and since many of the more complicated systems can be calculated as perturbations of these exact solutions.

2.7.1 The One Electron Equation

The Schrödinger equation for one electron moving in a harmonic oscillator potential is given by

$$-i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + \frac{1}{2}m^2\omega^2 r^2\psi$$

and since the potential is central symmetric it is possible to write the solution using separation of variables

$$\psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi)$$

Inserting this ansatz into the Schrödinger equation will give two uncoupled equations, one angular equation and one radial equation. The angular equation does frequently show up in physics and it's solutions is widely studied, and these are known as the spherical harmonics. Concentrating on the radial equation, which after insertion gives

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} - \frac{l(l+1)}{r^2}\right)R(r) + V(r)R(r) = ER(r). \tag{2.11}$$

Written for a general central symmetric potential $V(r)$. Note that l is defined since it will actually correspond to the angular momentum quantum number. Since the absolute value squared of the wavefunction represents the probability amplitude, a condition is that it has to be square integrable, and thus it has to vanish at infinity. Another condition is that it must vanish at $r = 0$. So by defining that $R(r) = u(r)/r$ we obtain the boundary conditions $u(0) = 0$ and $u(\infty) = 0$. By inserting this new definiton into Eq. (2.11) one obtains

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

Defining a dimensionless variable $\rho = r/\alpha$, where α is a constant with dimension length, the equation transforms to

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

By only looking at solutions where $l = 0$, and writing out the harmonic oscillator potential, the equation is given by

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

which can also be written as

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

The constant α can be fixed such that the term $\frac{mk}{\hbar^2}\alpha^4 = 1$, then defining

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

The final equation to solve is

$$-\frac{d^2}{d\rho^2}u(\rho) + \rho^2u(\rho) = \lambda u(\rho) \tag{2.12}$$

This equation has a closed form solution, which will be derived in detail in the next section.

When solving Eq. (2.12) numerically, there is a limit when representing infinity, i.e. there is a truncation that has to be done on ρ. We start by doing the exact same definition as in Section 2.6 for the step length and for the values of ρ at each point i. As in Eq. (2.7) we use the three-point formula on the differential Eq. (2.12), and rewrite it as

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

By adopting the notation $u(\rho_i)\rightarrow u_i$ and $u(\rho_i\pm h)\rightarrow u_{i\pm1}$, it can be written more compactly as

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

where $V_i=\rho_i^2$ is the harmonic oscillator potential, and the boundary conditions $u_0=u_N=0$. Writing out the explicit terms of the discretized equation yields

$$\begin{aligned}
-\frac{1}{h^2}u_2+\frac{2}{h^2}u_1+V_1&=\lambda_1u_1\\
-\frac{1}{h^2}u_3+\frac{2}{h^2}u_2-\frac{1}{h^2}u_1+V_2&=\lambda_2u_2\\
-\frac{1}{h^2}u_4+\frac{2}{h^2}u_3-\frac{1}{h^2}u_2+V_3&=\lambda_3u_3\\
&\vdots\\
-\frac{1}{h^2}u_{N-1}+\frac{2}{h^2}u_{N-2}-\frac{1}{h^2}u_{N-3}+V_{N-2}&=\lambda_{N-2}u_{N-2}\\
\frac{2}{h^2}u_{N-1}-\frac{1}{h^2}u_{N-2}+V_{N-1}&=\lambda_{N-1}u_{N-1},
\end{aligned}\tag{2.13}$$

where the only difference from Eq. (2.9) is that the potential is added along the diagonal. The diagonal and off-diagonal terms is thus given by

$$\begin{aligned}
d_i&=\frac{2}{h^2}+V_i,\\
a&=\frac{1}{h^2},
\end{aligned}$$

which gives us the tridiagonal matrix equation

$$\begin{bmatrix}
d_0 & a & 0 & 0 & \dots & 0 & 0\\
a & d_1 & a & 0 & \dots & 0 & 0\\
0 & a & d_2 & a & 0 & \dots & 0\\
\dots & \dots & \dots & \dots & \dots & \dots & \dots\\
0 & \dots & \dots & \dots & a & d_{N-2} & a\\
0 & \dots & \dots & \dots & \dots & a & d_{N-1}
\end{bmatrix}
\begin{bmatrix}u_1\\u_2\\u_3\\\dots\\u_{N-2}\\u_{N-1}\end{bmatrix}
=\lambda_i
\begin{bmatrix}u_1\\u_2\\u_3\\\dots\\u_{N-2}\\u_{N-1}\end{bmatrix},\quad i=1,2,...,N-1 \tag{2.14}$$

2.7.2 Analytical Solution to the One Electron Equation

The differential equation to solve is the scaled radial part of the Schrödinger equation for one electron in a harmonic oscillator potential. The equation was derived in Section 2.7.1, and is on the form

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

When solving differential equations of this type an important aspect is looking at the asymptotic behaviour. The approach is then to let ρ go to infinity and look for terms that dominate, so

$$\lim_{\rho\to\infty}\frac{d^2u(\rho)}{d\rho^2} = \lim_{\rho\to\infty}(\rho^2 - \lambda)u(\rho) \approx \rho^2 u(\rho) \tag{2.15}$$

An ansatz has to be made here, but since the function differentiated twice gives back the argument squared times the function, it is reasonable to think that an exponential will give that result. With that in mind try with

$$u(\rho) = e^{\beta\rho^2}$$

where β is a parameter to be decided in order to fit to the equation. Differentiating this ansatz will give

$$\frac{du(\rho)}{d\rho} = 2\beta\rho e^{\beta\rho^2}$$

and

$$\frac{d^2u(\rho)}{d\rho^2} = (2\beta + 4\beta^2\rho^2)e^{\beta\rho^2}$$

In the same limit, this is equal to

$$\lim_{\rho\to\infty}\frac{d^2u(\rho)}{d\rho^2} \approx 4\beta^2\rho^2 e^{\beta\rho^2}$$

In order to fit to Eq. (2.15), observe that $\beta^2 = \frac{1}{4}$. The most general solution is then

$$u(\rho) = f(\rho)e^{-\frac{\rho^2}{2}} + g(\rho)e^{\frac{\rho^2}{2}}$$

But since the wavefunction has to be normalizable, the last term has to be dropped. Then the solution to look for is on the form

$$u(\rho) = f(\rho)e^{-\frac{\rho^2}{2}} \tag{2.16}$$

The way to proceed further is by inserting this back into Eq. (2.12), which will give

$$\frac{d^2f}{d\rho^2} - 2\rho\frac{df}{d\rho} + (\lambda - 1)f = 0 \tag{2.17}$$

This differential equation is on known form, and can be solved by using Frobenius method. So expand $f(\rho)$ in the following way

$$f(\rho) = \sum_{n=0}^{\infty} a_n\rho^{n+s}$$

Again insert back into the differential equation and compare exponents

$$\sum_{n=0}^{\infty} a_n(n+s)(n+s-1)\rho^{n+s-2} - \sum_{n=0}^{\infty}(2(n+s)+1-\lambda)a_n\rho^{n+s} = 0$$

Now set $n = 0$ and look at the term with lowest power of s, which will give the indicial equation

$$s(s-1) = 0$$

Thus $s = 0$ or $s = 1$, but the lowest s will almost always give the full solution. Then set $s = 0$, and by manipulating the first term the equation is now reduced to

$$\sum_{n=0}^{\infty}((n+2)(n+1)a_{n+2} - (2n+1-\lambda)a_n)\rho^n = 0$$

This is to hold for all ρ, which will give the recursion relation

$$a_{n+2} = \frac{2n+1-\lambda}{(n+2)(n+1)}a_n \tag{2.18}$$

Look at the behaviour of the coefficients for large n

$$\lim_{n\to\infty} a_{n+2} \approx \frac{2n}{n^2}a_n = \frac{2}{n}a_n$$

With these coefficients the wave function will not be normalizable, so the series has to truncate. Then the recursion relation has to be equal to zero, which mean that

$$\lambda = 2n+1,$$

where n is an integer, but which values it takes is not decided. The definition of λ was set to be

$$\lambda = \frac{2E}{\hbar\omega}$$

Thus the energy eigenvalues are

$$E = \hbar\omega(n+\frac{1}{2})$$

Now Eq. (2.12) is a second order differential equation, and thus there are two coefficients that has to be determined. Then by determining a_0, one constructs all the even series solutions, and by determining a_1 one constructs all the odd series solutions.

The main interest is to look for the ground state eigenfunctions, so for $n = 0$ and $\lambda = 1$,

$$a_2 = \frac{2*0+1-1}{(0+2)(0+1)}a_0 = 0$$

Then the eigenfunction is given by

$$u(\rho) = a_0 e^{-\frac{\rho^2}{2}}$$

One boundary condition is that $u(0) = 0$, but then $a_0 = 0$, and there is no state. But this means that all the even terms are zero, which gives that n can only take odd values, $n = 1, 3, 5, 7, ..$

For $n = 1$ and $\lambda = 3$,

$$a_3 = \frac{2 * 1 + 1 - 3}{(1 + 2)(1 + 1)} a_1 = 0$$

Then the solution is

$$u(\rho) = a_1 \rho e^{-\frac{\rho^2}{2}} \tag{2.19}$$

This solution satisfies the boundary conditions, then this is the ground state eigenfunction. Instead of demanding that n only can take odd values, define that $n = 2n' + 1$, then the energy eigenvalues is equal to

$$E_{n'} = \hbar\omega(2n' + \frac{3}{2}) \quad n' = 0, 1, 2, 3... \tag{2.20}$$

The values for λ is then given by

$$\lambda = 4n' + 3 \quad n' = 0, 1, 2, 3 \tag{2.21}$$

and the lowest lying values are $\lambda_0 = 3, \lambda_1 = 7, \lambda_2 = 11, \lambda_3 = 15, ...$

2.7.3 The Two Electron Equation

The Schrödinger equation for two non interracting electrons in a harmonic oscillator potential is given by

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

where $\psi(r_1, r_2)$ is now a two electron wavefunction with two electron energy $E^{(2)}$. With no interactions this equation can be separated into two one particle equations, and thus has a closed form solution. Introducing the relative coordinates $\vec{r_1} - \vec{r_2}$ and the centre of mass coordinates $R = 1/2(\vec{r_1} + \vec{r_2})$. With these coordinates the radial equation can be written as

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

This equation is now on the form such that it can be separated into two equations, one for the relative coordinates r and one for the centre of mass R. So the anzats $\psi(r, R) = \psi(r)\phi(R)$ is made, which mean that the energy can be written as a sum of the two contributions.

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

in order to have an interaction the repulsive coulomb potential must be added to the equation, namely add

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

with $\beta e^2 = 1.44$ eVnm. By adding this term the r dependent schrödinger equation becomes

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

The general procedure is as before, where the dimensionless variable $\rho = \frac{r}{\alpha}$ is introduced. Insert into the Schrödinger equation and manipulate, which will give

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

By defining a frequency

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

the constant α can now be determined such that

$$\frac{m\alpha\beta e^2}{\hbar^2} = 1$$

which means that α is equal to

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

then the eigenvalue can be defined to be equal to

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

Thus the equation to solve is given by

$$-\frac{d^2}{d\rho^2}\psi(\rho) + \omega_r^2\rho^2\psi(\rho) + \frac{1}{\rho}\psi(\rho) = \lambda\psi(\rho). \tag{2.22}$$

The defined frequency ω_r is a parameter which decides the strength of the oscillator potential.

3 Method

3.1 Implementing Jacobi's Method

Algorithm 1 below shows a possible implementation of Jacobi's method described in Section 2.4.

Algorithm 1 Jacobi's Method

function MAXOFFDIAG(A, N) ▷ Find Max Value of Offdiag
  $\max(a_{ij}) := 0.0$
  for $i = 0$ **to** N **do**
    for $j = i + 1$ **to** N **do**
      if $|a_{ij}| < \max(a_{ij})$ **then**
        $\max(a_{ij}) := |a_{ij}|$
        $k := i$
        $l := j$
      end if
    end for
  end for
  return $\max(a_{ij}), k, l$
end function

function ROTATE(A, k, l, N) ▷ Perform Similarity Transformation
  $a'_{kk} := a_{kk}$
  $a'_{ll} := a_{ll}$
  $a'_{kl} := a_{kl}$
  $\tau := (a'_{ll} - a'_{kk})/2a'_{kl}$
  $t := -\tau \pm \sqrt{1 + \tau^2}$ ▷ $t \equiv \tan\theta$
  $c := 1/\left(\sqrt{1 + t^2}\right)$ ▷ $c \equiv \cos\theta$
  $s := tc$ ▷ $s \equiv \sin\theta$
  for $i = 1$ **to** N **do**
    $a'_{ik} := a_{ik}$
    $a'_{il} := a_{il}$
    $a_{ki} := ca'_{ik} - sa'_{il}$
    $a_{ik} := ca'_{ik} - sa'_{il}$
    $a_{li} := ca'_{il} - sa'_{ik}$
    $a_{il} := ca'_{il} - sa'_{ik}$
  end for
  $a_{kk} := c^2 a'_{kk} - 2sca'_{kl} + s^2 a'_{ll}$
  $a_{ll} := s^2 a'_{kk} + 2sca'_{kl} + c^2 a'_{ll}$
  $a_{kl} := 0$
  $a_{lk} := 0$
end function

```
function JACOBI(A, N)
    while max(a_ij) > ε do                          ▷ Tolerance ε ≤ 10^−8
        max(a_ij), k, l := MAXOFFDIAG(A, N)
        ROTATE(A, k, l, N)
    end while
end function
```

3.2 The Buckling Beam Problem

In order to solve the buckling beam eigenvalue problem, Eq. (2.9), Jacobi's method is implemented as described by Algorithm 1. The numerical eigenvalues will then be compared to the analytical eigenvalues given by Eq. (2.10). These results will be tabulated along with the the number n of similarity transformations needed before all non-diagonal matrix elements are essentially zero and the computational time T of the Jacobi method.

3.3 Benchmarking and Efficiency

In order to find the complexity of Jacobi's method, we extract the behavior as a function of the dimensionality of the matrix. The characteristics of particular interest is the number n of similarity transformations needed before all non-diagonal elements are essentially zero and the computational time T. The procedure is to benchmark the performance for an increasing number of mesh points N, and present the results in log-log plots. For obtaining a reference, the computational time of Armadillo's built eigenvalue solver *eig_sym* will be plotted with the computational time T of Jacobi's method .

3.4 Single Electron in the Harmonic Oscillator Well

The Hamiltonian solved here describes one electron trapped in a Harmonic Oscillator potential. This equation is solved analytically in Section 2.7.2, which will be vital in order to verify the precision of the numerical implementation. In order to solve the Schrödinger equation for one electron Eq. (2.12) numerically, Jacobis method is implemented as described by Algorithm 1. The numerical eigenvalues will then be tabulated several number of mesh points and for different values of ρ_N.

3.5 Two Interacting Electrons in the Harmonic Oscillator Well

The Hamiltonian solved here describes two electrons in a Harmonic Oscillator potential where the electrons also feel a repulsive coulomb potential. In order to solve the Schrödinger equation for two electrons Eq. (2.22) numerically, Jacobis method is implemented as described by Algorithm 1. The numerical eigenvalues will then be tabulated for several number of

mesh points and different values of ρ_N. The two electron wavefunction squared will also be plotted as a function of the separation between them.

3.6 Comparison of Numerical and Analytical HO Solutions

In [3] the analytical solution to the two electron in a Harmonic Oscillator potential with a repulsive coulomb potential between them is given. The numerical and analytical solution to the eigenvalues will tabulated and compared for different values of ω.

3.7 Comparison of Wave Functions

The absolute square of the two electron wavefunction will be plotted where there is a comparison between the wavefunctions with interaction and without interaction. This will be plotted as a function of the separation between the electrons, for several values of ω.

4 Results

4.1 Implementing Jacobi's Method

The program containing the implementation of Jacobi's method and accompanying programs that produces all the results presented in this project, can be found at the GitHub repository https://github.com/nicolossus/FYS3150/tree/master/Project2

4.2 The Buckling Beam Problem

In Table 4.1 are the results from implementing Jacobi's method in order to solve the buckling beam problem as described in Section 3.2.

Table 4.1: *Results from the implementation of Jacobi's method for solving the buckling beam eigenvalue problem. The parameters tabulated are; the number of mesh points N, the analytical eigenvalues λ_i, given by Eq. (2.10), with $i = 1, 2, 3$ for each N, the numerical eigenvalues $\hat{\lambda}_i$ with $i = 1, 2, 3$ for each N, the number n of similarity transformations needed before all non-diagonal elements are essentially zero, and the CPU time T needed to compute Jacobi's method in seconds*

N	i	λ_i	$\hat{\lambda}_i$	n	T [s]
50	1	9.86648	9.86648	4 666	0.0124487
	2	39.4285	39.4285		
	3	88.5739	88.5739		
100	1	9.86881	9.86881	18 731	0.176546
	2	39.4657	39.4657		
	3	88.762	88.762		
200	1	9.8694	9.8694	74 949	2.78244
	2	39.4752	39.4752		
	3	88.8102	88.8102		
400	1	9.86955	9.86955	303 084	55.3531
	2	39.4776	39.4776		
	3	88.8224	88.8224		

4.3 Benchmarking and Efficiency

In Figure 4.1 a comparison of the CPU-time of Jacobi's method vs Armadillo's eigenvalue solver is done. The plot is generated by making a log-log plot of the CPU-time as a function of the dimension N. The data have been linearly-fitted.

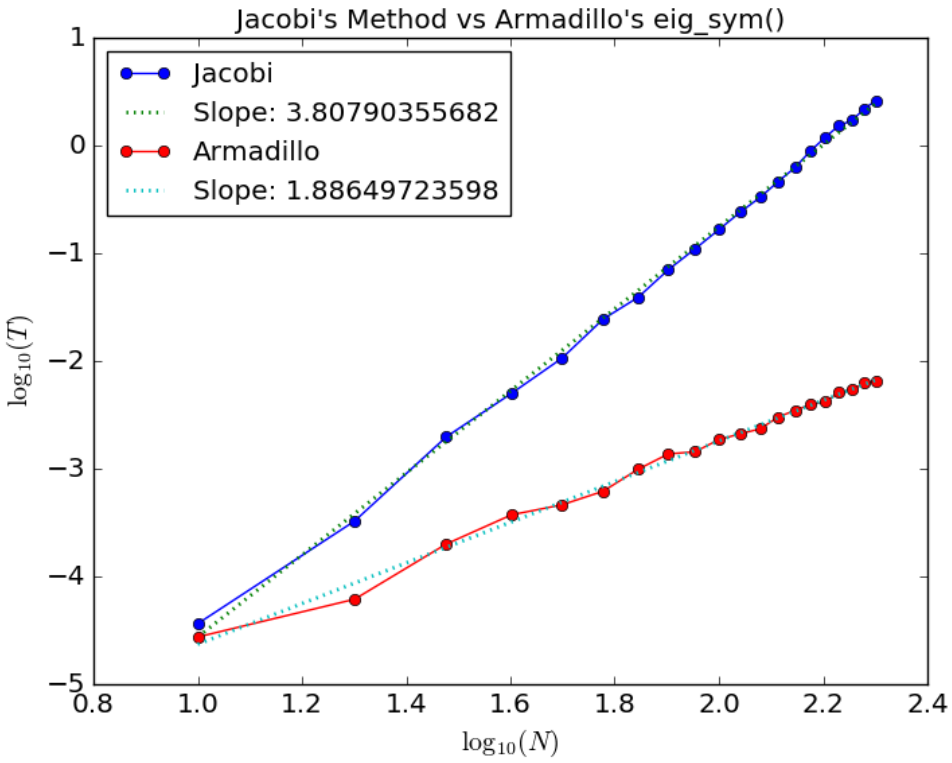

Figure 4.1: *Comparison of CPU-time of Jacobi's method vs Armadillo's eig_sym. This is a log-log plot of the CPU-time as a function of the dimension N. The data have been linearly fitted with expressions stated in the legend*

In Figure 4.2 shows a log-log plot of the number of iterations using Jacobi's method in order to diagonalize the matrix, as a function of the dimension of the matrix. The data have been linearly fitted.

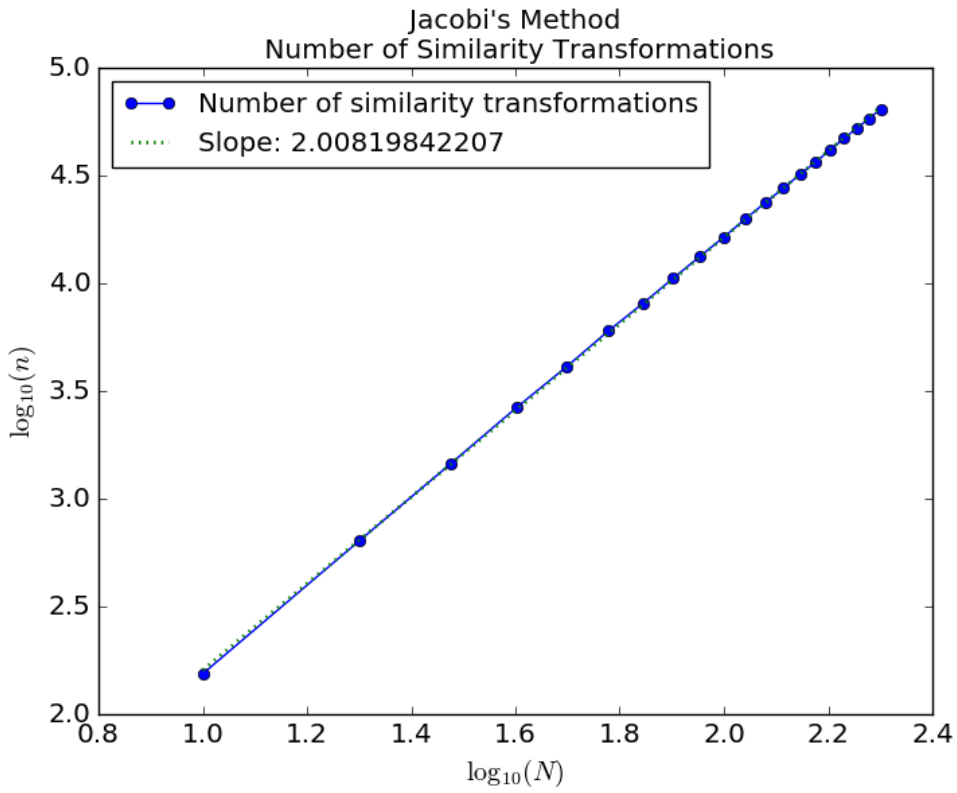

Figure 4.2: *This is a log-log plot of the number of iterations using Jacobi's method to sufficiently diagonalize the matrix, as a function of the dimension of the matrix N. The data have been linearly fitted*

4.4 Single Electron in the Harmonic Oscillator Well

In Table 4.2 are the first eigenvalues λ_0, λ_1, λ_2, and λ_3 of the single electron in the harmonic oscillator problem for a different number of mesh points N with $\rho_0 = 0$ and $\rho_N = 2.5$ tabulated.

Table 4.2: *The first eigenvalues λ_0, λ_1, λ_2, and λ_3 of the single electron in the harmonic oscillator problem for a different number of mesh points N with $\rho_0 = 0$ and $\rho_N = 2.5$*

N	λ_0	λ_1	λ_2	λ_3
50	3.102009	8.360085	16.26608	27.23212
100	3.102631	8.366371	16.29647	27.32740
200	3.10279	8.367979	16.30425	27.35182
400	3.10283	8.368386	16.30621	27.35800

In Table 4.3 are the first eigenvalues λ_0, λ_1, λ_2, and λ_3 of the single electron in the harmonic oscillator problem for a different number of mesh points N with $\rho_0 = 0$ and $\rho_N = 4$ tabulated.

Table 4.3: *The first eigenvalues λ_0, λ_1, λ_2, and λ_3 of the single electron in the harmonic oscillator problem for a different number of mesh points N with $\rho_0 = 0$ and $\rho_N = 4$*

N	λ_0	λ_1	λ_2	λ_3
50	2.998106	6.993741	11.05396	15.52967
100	2.999539	7.000927	11.07251	15.57266
200	2.999905	7.002763	11.07724	15.58365
400	2.999998	7.003227	11.07844	15.58643

In Table 4.4 are the first eigenvalues λ_0, λ_1, λ_2, and λ_3 of the single electron in the harmonic oscillator problem for a different number of mesh points N with $\rho_0 = 0$ and $\rho_N = 7$ tabulated.

Table 4.4: *The first eigenvalues λ_0, λ_1, λ_2, and λ_3 of the single electron in the harmonic oscillator problem for a different number of mesh points N with $\rho_0 = 0$ and $\rho_N = 7$*

N	λ_0	λ_1	λ_2	λ_3
50	2.994100	6.970437	10.92770	14.86574
100	2.998498	6.992486	10.98166	14.96600
200	2.999621	6.998104	10.99537	14.99143
400	2.999905	6.999524	10.99884	14.99785

In Table 4.5 are the first eigenvalues λ_0, λ_1, λ_2, and λ_3 of the single electron in the harmonic oscillator problem for a different number of mesh points N with $\rho_0 = 0$ and $\rho_N = 14$ tabulated.

Table 4.5: *The first eigenvalues λ_0, λ_1, λ_2, and λ_3 of the single electron in the harmonic oscillator problem for a different number of mesh points N with $\rho_0 = 0$ and $\rho_N = 14$*

N	λ_0	λ_1	λ_2	λ_3
50	2.976247	6.880143	10.70459	14.4469
100	2.993983	6.969846	10.92625	14.86304
200	2.998483	6.992411	10.98147	14.96566
400	2.999619	6.998095	10.99535	14.99139

4.5 Two Interacting Electrons in the Harmonic Oscillator Well

In Table 4.6 are the ground state eigenvalues λ_0 of two interacting electrons in a harmonic oscillator potential with oscillator frequency $\omega = 0.01$ for different maximum values ρ_N of the interval and number of mesh points N tabulated.

Table 4.6: *Ground state eigenvalues λ_0 of two interacting electrons in a harmonic oscillator potential with oscillator frequency $\omega = 0.01$ for different maximum values ρ_N of the interval and number of mesh points N*

N	λ_0 with $\rho_N = 40$	λ_0 with $\rho_N = 50$	λ_0 with $\rho_N = 60$
100	0.1058118	0.1057694	0.105767
200	0.1058144	0.1057735	0.1057729
400	0.1058151	0.1057745	0.1057743

In Table 4.7 are the ground state eigenvalues λ_0 of two interacting electrons in a harmonic oscillator potential with oscillator frequency $\omega = 0.5$ for different maximum values ρ_N of the interval and number of mesh points N tabulated.

Table 4.7: *Ground state eigenvalues λ_0 of two interacting electrons in a harmonic oscillator potential with oscillator frequency $\omega = 0.5$ for different maximum values ρ_N of the interval and number of mesh points N*

N	λ_0 with $\rho_N = 20$	λ_0 with $\rho_N = 30$	λ_0 with $\rho_N = 40$
100	2.226960	2.222982	2.217359
200	2.229325	2.228328	2.226929
400	2.229921	2.229671	2.229321

In Table 4.8 are the ground state eigenvalues λ_0 of two interacting electrons in a harmonic oscillator potential with oscillator frequency $\omega = 1.0$ for different maximum values ρ_N of the interval and number of mesh points N tabulated.

Table 4.8: *Ground state eigenvalues λ_0 of two interacting electrons in a harmonic oscillator potential with oscillator frequency $\omega = 1.0$ for different maximum values ρ_N of the interval and number of mesh points N*

N	λ_0 with $\rho_N = 4$	λ_0 with $\rho_N = 6$	λ_0 with $\rho_N = 8$
100	4.057433	4.056721	4.055821
200	4.057817	4.057585	4.057358
400	4.057914	4.057804	4.057747

In Table 4.9 are the ground state eigenvalues λ_0 of two interacting electrons in a harmonic oscillator potential with oscillator frequency $\omega = 5.0$ for different maximum values ρ_N of the interval and number of mesh points N tabulated.

Table 4.9: *Ground state eigenvalues λ_0 of two interacting electrons in a harmonic oscillator potential with oscillator frequency $\omega = 5.0$ for different maximum values ρ_N of the interval and number of mesh points N*

N	λ_0 with $\rho_N = 2$	λ_0 with $\rho_N = 3$	λ_0 with $\rho_N = 4$
100	17.44549	17.44147	17.43585
200	17.44788	17.44686	17.44545
400	17.44849	17.44823	17.44787

4.6 Comparison of Numerical and Analytical HO Solutions

In Table 4.10 are the numerical ground state eigenvalues of two interacting electrons in a harmonic oscillator potential for chosen oscillator frequencies ω tabulated with corresponding analytical solutions retrieved from [3].

Table 4.10: *Ground state eigenvalues λ_0 of two interacting electrons in a harmonic oscillator potential for chosen oscillator frequencies ω yielding analytical solutions. The energies have been calculated with $N = 400$ mesh points, and $\rho_N = 9$ and $\rho_N = 20$, respectively. The analytical values are retrieved from [3]*

ω	Numerical λ_0	Analytical λ_0
0.25	1.249991	1.2500
0.05	0.3499995	0.3500

4.7 Comparison of Wave Functions

In Figure 4.3 is a visual comparison between the wave functions with and without coulomb interaction. They are plotted as a function of the separation between the electrons. The wave function is generated by using Jacobi's method with oscillator frequency $\omega = 1$, number of mesh points $N = 400$, and maximum value of the interval $\rho_N = 20$.

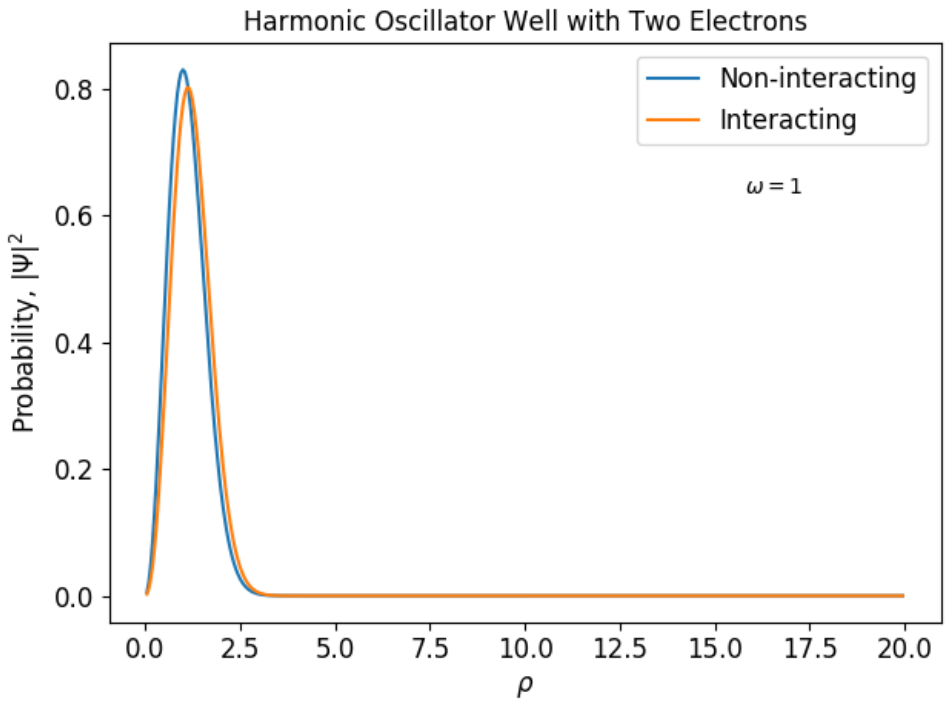

Figure 4.3: *Comparison of wave functions of two electrons in a harmonic oscillator potential, with and without interaction. The wave function is numerically calculated using Jacobi's method with* $\omega = 1$, $N = 400$ *and* $\rho_N = 20$

In Figure 4.4 is a visual comparison between the wave functions with and without coulomb interaction. They are plotted as a function of the separation between the electrons. The wave function is generated by using Jacobi's method with oscillator frequency $\omega = 0.3$, number of mesh points $N = 400$, and maximum value of the interval $\rho_N = 20$

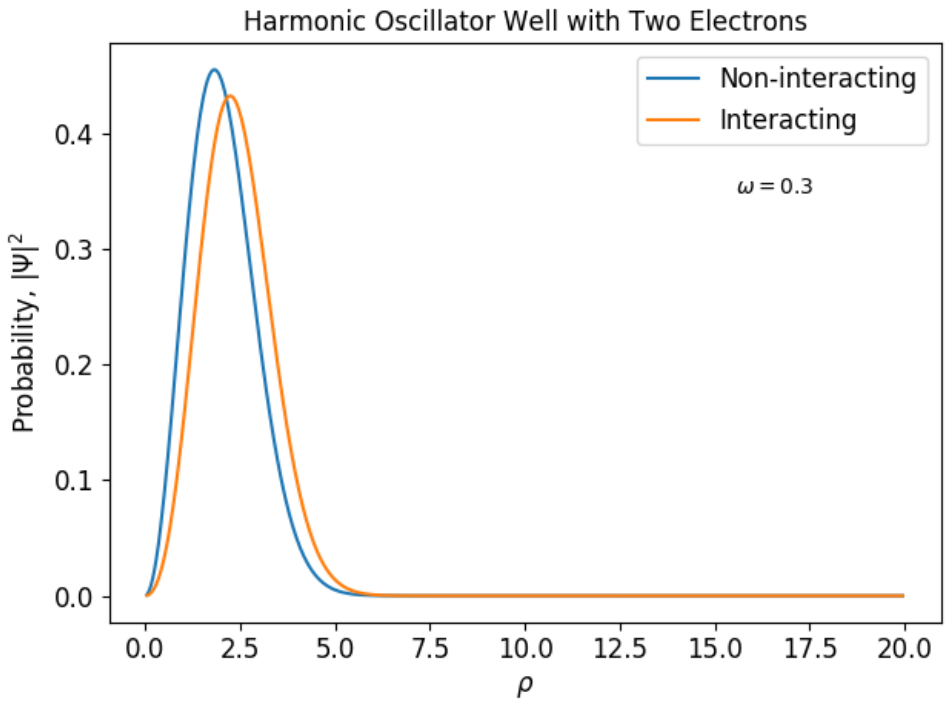

Figure 4.4: *Comparison of wave functions of two electrons in a harmonic oscillator potential, with and without interaction. The wave function is numerically calculated using Jacobi's method with* $\omega = 0.3$, $N = 400$ *and* $\rho_N = 20$

In Figure 4.5 is a visual comparison between the wave functions with and without coulomb interaction. They are plotted as a function of the separation between the electrons. The wave function is generated by using Jacobi's method with oscillator frequency $\omega = 0.06$, number of mesh points $N = 400$, and maximum value of the interval $\rho_N = 20$

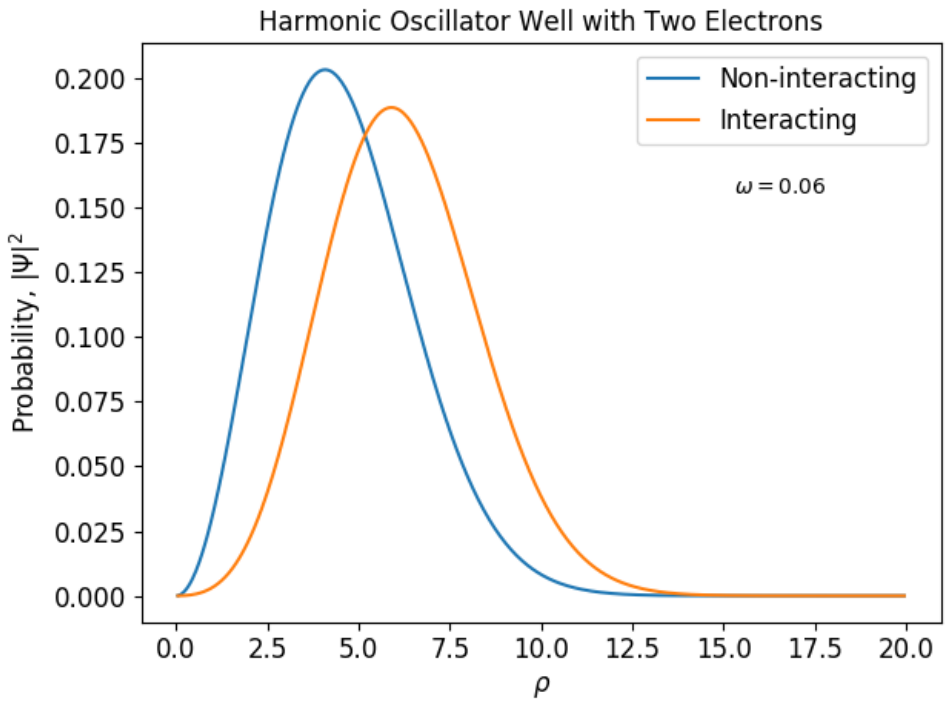

Figure 4.5: *Comparison of wave functions of two electrons in a harmonic oscillator potential, with and without interaction. The wave function is numerically calculated using Jacobi's method with* $\omega = 0.06$, $N = 400$ *and* $\rho_N = 20$

5 Discussion

5.1 The Buckling Beam Problem

Comparing the analytical and numerical eigenvalue solutions of the buckling beam problem tabulated in Table 4.1, shows that the numerical approximation to the eigenvalues are very accurate, to more than five decimals, for all the tested number of mesh points. The relative error could have been calculated to get a better sense of the exact accuracy, but the main purpose of solving the buckling beam problem was to verify that the implementation of the Jacobi method was correct. The accuracy of the method is looked closer upon in the problems regarding the quantum harmonic oscillator. Furthermore, the table shows the number of similarity transformations needed before all non-diagonal matrix elements are essentially zero and the computational time of the Jacobi method. The results of the former are discussed in detail in the next section. The computational time increases considerably with the dimension of the matrix. This is to some extent expected, but the true time of only the Jacobi rotation method is not shown in the table. In the code implementation there is also a procedure for sorting the eigenvalues and eigenvectors generated by the Jacobi method. This obviously slows down the computational time as the dimension increases. However, one may consider it necessary to sort the eigenpairs in the method from an end-user perspective, so all-in-all we may regard the times tabulated as the "true" times of the method. The computational time is also discussed in detail in the next section.

5.2 Benchmarking and Efficiency

In Figure 4.1 we can interpret the slope of the log-log plots as the complexity of the respective methods. For our implementation of Jacobi's method, the complexity goes approximately as $N^{3.8}$. The reason the complexity surpasses N^3 is likely because the complexity of max_element function inside the while loop goes as N^2. As seen in Figure 4.2, the number of iterations goes as N^2, meaning the method as a whole goes as approximately N^4 for large N.

Armadillo's eig_sym function for finding eigenvalues and eigenvectors of a matrix was much more efficient and had a complexity close to $N^{1.9}$. Though it is not documented, it is reasonable to assume that Armadillo uses an algorithm that exploits the fact that our matrix is sparse. Jacobi's method on the other hand has no way of doing this. Rather, it has the habit of setting zero-elements to small non-zero values after each iteration. Because of this it is needed to do additional iterations to correct these newly introduces values. One ends up diagonalizing the matrix as if it were a dense matrix. Although this is a reasonable way of solving matrices already dense, it is terribly inefficient for sparse matrices like our tridiagonal matrix.

5.3 Single Electron in the Harmonic Oscillator Well

As stated earlier, the first analytical eigenvalues of Eq. (2.21) are $\lambda = 3, 7, 11, 15$. The numerical approximations presented in Table 4.2 are off by $\sim 3\%$ for the ground state, with drastically worse precision for the excited states. The result also got worse with higher number of mesh points N. As stated in Eq. (2.19) the ground state wave function goes as $exp(-\rho^2/2)$, it still has an amplitude proportional to 0.04 at $\rho = 2.5$. Physical intuition tells this is not a big enough interval to represent infinity, as the wave function has not yet diminished to large degree. This is even more true for the exited states, as they tend to "live" longer for higher ρ's. The numerical errors introduced by using a too small ρ_N is amplified by introducing more mesh points.

In Table 4.3 we see that the numerical precision improves across the board by increasing $\rho_N = 4$. While the ground state and first excited energies have become very accurate(6 leading digits for $N = 400$!), the second and third are still a bit off, $\sim 0.7\%$ and $\sim 3.9\%$, respectively. This indicates we are sufficiently approximating infinity for the first two states, but not the higher excitations.

In Table 4.4 we see that for $\rho_N = 7$ also the higher states have good numerical precision, however the precision of the ground state have actually slightly worsened. A reasonable explanation is that infinity is already sufficiently approximated by $\rho_N = 5$. Increasing ρ_N yields nothing more than making the mesh points more sparse, hence decreasing the precision.

In Table 4.5 for $\rho_N = 14$, the numerical precision is worse across the board, of the same reasons stated in the previous paragraph.

5.4 Two Interacting Electrons in the Harmonic Oscillator Well

From Table 4.6, 4.7 and 4.8, it can be seen that the ground state energies are very constant both as function of number of mesh points and interval. However, this stability occurs for very different orders of intervals dependent of the frequency ω. Table 4.6 shows stable values for ρ_N in the interval 40 to 60 for $\omega = 0.01$. Further, the next tables shows that the stable values occur for smaller ρ_N for increasing ω. Going back to physical intuition, this can be explained by the interaction of the electrons. If ω has a high value, it means the harmonic potential is strong, causing the electrons to be strongly confined even though they also repeal each other. This results in a more narrow wave function, which we know from earlier is best approximated with a small ρ_N. However, when ω decrease, the electrons are not as strongly confined and their repulsion becomes much more relevant. Thinking in a classical way, this allows the electrons to drift more apart. This causes the wave function to be more smeared out, calling for a higher ρ_N to be used to preserve numerical accuracy.

We see from the same tables that the ground state energies increase rapidly as ω increases. This makes sense, since forcing the electrons closer together increases the potential energy because of the repelling term. Much the same way as loading a spring.

5.5 Comparison of Numerical and Analytical HO Solutions

The numerical estimates of the ground state energies discussed in the previous section are nice and stable for the given interval of ρ_N, and this dependency is expected because of the argument of the smearing of the wave function due to the repelling term. However, how can we be sure these values are correct? We are fortunate enough that the ground state energy is analytically solvable for given frequencies. As seen in Table 4.9, the accuracy is excellent. This gives confidence that the other estimates of the interacting case are good as well.

5.6 Comparison of Wave Functions

Figure 4.3, 4.4 and 4.5 shows how the wave function of the two electrons differ in the interacting and non-interacting case for different frequencies ω. For a strong potential with $\omega = 1$, both cases produces fairly narrow wave functions, meaning the electrons are very localized. For smaller ω, the wave functions tends to smear out, and even more so for repelling electrons as discussed earlier. This supports our suspicion of the behaviour discussed in Section 5.4.

6 Conclusion

To summarize, our implementation of Jacobi's method was able to reproduce the first three eigenvalues of the buckling beam to more than five decimals. When solving the eigenvalues for an electron in a harmonic oscillator, it was found that choosing a interval appropriate to the size of the wave function was important for producing eigenvalues accurate to 4 decimals. Intervals that failed to capture the significant parts of the wave function yielded values too large, and intervals that were too large caused loss of resolution.

For two electrons in a harmonic oscillator potential, the wave function tended to be less localized for lower oscillator frequencies ω. This was even more true in the interacting case, as the electrons repulsion allowed them to drift far apart when the harmonic potential decreased. For oscillator frequencies $\omega = 0.25$ and $\omega = 0.05$, Jacobi's method approximated the analytical ground state eigenvalues 1.25 and 0.35 to 1.24991 and 0.34995, respectively.

Our implementations of Jacobi's method for solving eigenvalue problems is inferior to Armadillo's eig_sym. The CPU-time went approximately as $N^{3.8}$ and $N^{1.9}$, respectively. This confirmed the already known fact that using Jacobi's method on a sparse matrix, like we did, is very inefficient.

References

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[2] H. P. Langtangen and G. K. Pedersen. *Scaling of Differential Equations*. Springer International Publishing AG, Switzerland, 2016 (cit. on p. 5).

[3] M. Taut. "Two electrons in an external oscillator potential: Particular analytic solutions of a Coulomb correlation problem". In: *Phys. Rev. A* 48 (5 Nov. 1993), pp. 3561–3566. DOI: 10.1103/PhysRevA.48.3561. URL: https://link.aps.org/doi/10.1103/PhysRevA.48.3561 (cit. on pp. 16, 22).