FYS3150 Report
Project 2 - Solving Eigenvalue Problems

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something abstract

ABOUT PROJECT 2

This is a report for Project 2 in FYS3150 Computational Physics at UiO, due October 1st, 2018. [3] The project description was accessed September22nd, 2018 with the following web address:
https://github.com/CompPhysics/ComputationalPhysics/blob/master/doc/Projects/2018/Project2/pdf/Project2.pdf
All material written for this report can be found in this GitHub repository:
https://github.com/njmikkelsen/comphys2018/tree/master/Project2

I. INTRODUCTION

Project 2 in FYS3150 Computational Physics is concerned with the problem of solving eigenvalue problems, in particular matrix eigenvalue problems. However, instead of solving arbitrary eigenvalue problems, this report will investigate some important examples from physics: the buckling beam and the radial harmonic oscillator. Most of the equations are already on the eigenvalue-problem format. However, further treatment will bring the equations to dimensionsless form in order to highlight their underlying similarities, especially in the context of solving them by numerical means. In the following sections, all the continuous problems will be introduced before the discretisation process.

The matrix eigenvalue equations will be solved using the famous Jacobi eigenpair/diagonalisation algorithm, which is an essential algorithm in the field of numerical Linear Algebra. More modern methods (such as Householder's algorithm, etc.) have been proven to be much more effective than the Jacobi algorithm with respect accuracy, stability and computation-time. Nonetheless, the Jacobi algorithm is historically important and serves as a stepping stone for future study of more complex methods.

Having applied the algorithm to the simpler cases, the project will expand its horizon and study a Coulomb-interaction pair of electrons, situated in a harmonic oscillator potential.

II. THEORY

All eigenvalue problems may be written as

$$\hat{\Lambda} f = \lambda f \tag{1}$$

where f and λ is an eigenvector-eigenvalue eigenpair of the operator $\hat{\Lambda}$. Other than requiring the existence of at least one eigenvector, the operator $\hat{\Lambda}$ does not need to be restricted in any particular way.

A. Eigenvalue Problems in Physics: The Buckling Beam

A straight non-rigid beam of length L is fastened at $x = 0$ and $x = L$. A constant uniform force $\mathbf{F} = -F\hat{\mathbf{e}}_x$ is applied to the beam at $x = L$ such that the beam is bended in the $\hat{\mathbf{e}}_y$ direction with displacement $y(x)$. Using infinitesimal analysis, one can show that the beam's bending behaves according to

$$\gamma \partial_x^2 y(x) = -F y(x), \quad x \in [0, L] \tag{2}$$

where γ is a rigidity parameter and $y(x)$ is restricted by Dirichlet boundary conditions $y(0) = y(L) = 0$.

The next step is to introduce the dimensionless variables $\xi = x/L$ and $v(\xi) = y(L\xi)$, which by definition implies that $\xi \in [0, 1]$. The new Dirichlet boundaries become $v(0) = v(1) = 0$ and the eigenvalue equation may be written as

$$\partial_\xi^2 v(\xi) = -\lambda v(\xi) \tag{3}$$

Here, $v(\xi)$ are eigenvectors with corresponding eigenvalues $-\lambda = FL^2/\gamma$.

B. Eigenvalue Problems in Physics: The Radial Schrödinger Equation

Provided the spherical coordinates basis $\{|r, \theta, \varphi\rangle\}$, the Hamiltonian for a particle of mass m in a spherically symmetric potential $V(r)$ may be written as

$$\hat{\mathcal{H}} = \frac{-\hbar^2}{2m}\nabla^2 + V(\hat{r}) \tag{4}$$

where the laplacian is given by

$$\nabla^2 = r^{-1}\partial_r^2 r + r^{-2}\Big(\csc\theta\partial_\theta[\sin\theta\partial_\theta] + \csc^2\theta\partial_\varphi^2\Big) \tag{5}$$

Using the canonical operatores $\hat{x} = x$ and $\hat{p} = -i\hbar\nabla$, one can show that the angular momentum operator $\hat{\mathbf{L}}^2 = \hat{\mathbf{L}}_x^2 + \hat{\mathbf{L}}_y^2 + \hat{\mathbf{L}}_z^2$ is given by

$$\hat{\mathbf{L}}^2 = -\hbar^2\Big(\csc\theta\partial_\theta[\sin\theta\partial_\theta] + \csc^2\theta\partial_\varphi^2\Big)$$

which implies that the hamiltonian may be rewritten in terms of $\hat{\mathbf{L}}^2$:

$$\hat{\mathcal{H}} = \frac{-\hbar^2}{2mr}\partial_r^2 r + \frac{\hat{\mathbf{L}}^2}{2mr^2} + V(\hat{r}) \tag{6}$$

All components of $\hat{\mathcal{H}}$ commutes, thus $[\hat{\mathcal{H}}, \hat{\mathbf{L}}^2] = 0$. Therefore, $\hat{\mathcal{H}}$ and $\hat{\mathbf{L}}^2$ must share eigenstates $\psi(r,\theta,\varphi)$. However, the eigenstates of $\hat{\mathbf{L}}^2$ are already known to be the spherical harmonics $Y_\ell^m(\theta,\varphi)$, meaning that the r-dependency of ψ must be independent of (θ,φ). Or in other words:

$$\psi(r,\theta,\varphi) = \mathcal{R}(r)Y_\ell^m(\theta,\varphi) \tag{7}$$

The eigenvalues of $\hat{\mathbf{L}}^2$ are $\hat{\mathbf{L}}^2 Y_\ell^m(\theta,\varphi) = \hbar^2\ell(\ell+1)Y_\ell^m$. Thus, the eigenvalues of $\hat{\mathcal{H}}$ are determined by

$$\begin{aligned}\hat{\mathcal{H}}\psi &= E\psi\\ \frac{-\hbar^2}{2mr}\partial_r^2 r\psi + \frac{\hbar^2\ell(\ell+1)}{2mr^2}\psi + V(r)\psi &= E\psi\\ \frac{-\hbar^2}{2mr}\partial_r^2 r\mathcal{R}(r) + \frac{\hbar^2\ell(\ell+1)}{2mr^2}\mathcal{R}(r) + V(r)\mathcal{R}(r) &= E\mathcal{R}(r)\end{aligned}$$

i.e. the so-called Radial Schrödinger equation. The equation may be further simplified by introducing the transformation $u(r) = r\mathcal{R}(r)$:

$$\frac{-\hbar^2}{2m}\partial_r^2 u(r) + \Big[V(r) + \frac{\hbar^2\ell(\ell+1)}{2mr^2}\Big]u(r) = Eu(r) \tag{8}$$

The Dirichlet boundary conditions for this equation are $u(0) = \lim_{b\to\infty} u(b) = 0$.

Finally, one may introduce the dimensionless variables $\xi = r/\alpha$ and $v(\xi) = u(\alpha\xi)$, where α is the system's so-called natural length scale. Note that $\xi \in [0,\infty)$ and that the Dirichlet boundary conditions for $v(\xi)$ are completely equivalent to those of $u(r)$. Equation (8) may thus, via a little algebra, be rewritten as the dimensionless eigenvalue equation:

$$\Big[\partial_\xi^2 - \frac{2m\alpha^2}{\hbar^2}V(\alpha\xi) - \frac{\ell(\ell+1)}{\xi^2}\Big]v(\xi) = -\lambda v(\xi) \tag{9}$$

Here, $v(\xi)$ are eigenvectors with corresponding eigenvalues $-\lambda = 2m\alpha^2 E/\hbar^2$.

It is now impossible to continue the analysis without specifying the potential energy function $V(r)$.

1. The harmonic oscillator potential

The harmonic oscillator potential is given by $V(r) = \frac{1}{2}m\omega^2 r^2$. This implies that

$$\frac{2m\alpha^2}{\hbar^2}V(\alpha\xi) = \frac{m^2\omega^2}{\hbar^2}\alpha^4\xi^2$$

Now if $\alpha = i\sqrt{\hbar/m\omega}$, then equation (9) simplifies to

$$\Big[\partial_\xi^2 - \xi^2 - \ell(\ell+1)\xi^{-2}\Big]v(\xi) = -\lambda v(\xi) \tag{10}$$

where $-\lambda = 2E/\hbar\omega$.

While it is possible to solve equation (10) analytically, this will not be done here. However, the resulting energy eigenvalues are given by:

$$E_{nl} = \hbar\omega\Big(2n + \ell + \frac{3}{2}\Big) \tag{11}$$

where $n = 0, 1, \ldots$ and $\ell = 0, 1, \ldots, n-1$. This implies that the analytic values for λ are

$$\lambda_{nl} = 4n + 2l + 3 \tag{12}$$

2. Two Coulomb-interacting electrons in a harmonic oscillator potential

To extend the case of a single particle to the case of two interacting particles, the Hamiltonian must change accordingly:

$$\hat{\mathcal{H}} = \frac{|\hat{\mathbf{p}}_1|^2}{2m_1} + \frac{|\hat{\mathbf{p}}_2|^2}{2m_2} + V(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2) \tag{13}$$

where in the case of two electrons: $m_1 = m_2 = m$. If placed in a harmonic oscillator potential, and allowed to interact via a Coulomb interaction, the potential for the electron-electron system is given by

$$V(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2) = V_H(\hat{\mathbf{r}}_1) + V_H(\hat{\mathbf{r}}_2) + V_C(\hat{\mathbf{r}}_1 - \hat{\mathbf{r}}_2) \tag{14}$$

where

$$V_H(\mathbf{r}) = \frac{1}{2}m\omega^2|\mathbf{r}|^2 \quad \text{and} \quad V_C = \frac{k}{|\mathbf{r}|}$$

with $k = e^2/4\pi\varepsilon_0$. In order to simplify the calculations, the following coordinate transformation is introduced:

$$\mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2) \quad \text{and} \quad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2 \tag{15}$$

Here, $\mathbf{R}$ represents the center of mass while $\mathbf{r}$ represents the electrons' relative frame of reference. Following standard definitions, the momenta $\mathbf{P}$ and $\mathbf{p}$ corresponding to $\mathbf{R}$ and $\mathbf{r}$ are defined as follows:

$$\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2 \quad \text{and} \quad \mathbf{p} = \mathbf{p}_1 - \mathbf{p}_2 \tag{16}$$

Hence, by definition:

$$\begin{aligned}4|\mathbf{R}|^2 + |\mathbf{r}|^2 &= 2\Big(|\mathbf{r}_1|^2 + |\mathbf{r}_2|^2\Big)\\ |\mathbf{P}|^2 + |\mathbf{p}|^2 &= 2\Big(|\mathbf{p}_1|^2 + |\mathbf{p}_2|^2\Big)\end{aligned}$$

Using $\mathbf{R}$, $\mathbf{r}$, $\mathbf{P}$ and $\mathbf{p}$, one may rewrite the Hamiltonian:

$$\hat{\mathcal{H}} = \frac{|\hat{\mathbf{P}}|^2}{4m} + \frac{|\hat{\mathbf{p}}|^2}{4m} + m\omega^2|\hat{\mathbf{R}}|^2 + \frac{1}{4}m\omega^2|\hat{\mathbf{r}}|^2 + \frac{k}{|\hat{\mathbf{r}}|} \tag{17}$$

This may be further seperated into two components $\hat{\mathcal{H}}_R$ and $\hat{\mathcal{H}}_r$, which are dependent on $\hat{\mathbf{R}}$ and $\hat{\mathbf{r}}$ respectively. All components of $\hat{\mathcal{H}}$ commute, thus $\hat{\mathcal{H}}_R$ and $\hat{\mathcal{H}}_r$ must share eigenstates ψ. Provided the spherical coordinate bases $\{|R, \theta_R, \varphi_R\rangle\}$ and $\{|r, \theta_r, \varphi_r\rangle\}$, the eigenstates may be written in terms of two separate components:

$$\psi(\mathbf{R}, \mathbf{r}) = \phi(\mathbf{R})\chi(\mathbf{r}) \tag{18}$$

Moreover, the eigenvalue equation $\hat{\mathcal{H}}\psi = E\psi$ may be simplified via the separation of variables technique (the details have been omitted):

$$E_R + E_r = E \tag{19a}$$

$$\left[\frac{-\hbar^2}{4m}\nabla_R^2 + m\omega^2 R^2\right]\phi = \hat{\mathcal{H}}_R\phi = E_R\phi \tag{19b}$$

$$\left[\frac{-\hbar^2}{4m}\nabla_r^2 + \frac{1}{4}m\omega^2 r^2 + \frac{k}{r}\right]\chi = \hat{\mathcal{H}}_r\chi = E_r\chi \tag{19c}$$

By following the exact same approach as the one laid out earlier in this section, the operators ∇_R^2 and ∇_r^2 may be rewritten in terms of $\hat{\mathbf{L}}_R^2$ and $\hat{\mathbf{L}}_r^2$ respectively. It follows that $\hat{\mathcal{H}}_R$ and $\hat{\mathcal{H}}_r$ commute with $\hat{\mathbf{L}}_R^2$ and $\hat{\mathbf{L}}_r^2$ such that ϕ and χ may be written as products of a radial component and spherical harmonics respectively:

$$\phi(R, \theta_R, \varphi_R) = \mathcal{R}_R(R)Y(\ell_R, m_R; \theta_R, \varphi_R) \tag{20a}$$

$$\chi(r, \theta_r, \varphi_r) = \mathcal{R}_r(r)Y(\ell_r, m_r; \theta_r, \varphi_r) \tag{20b}$$

As a result, equations (19b) and (19c) yield:

$$\left(\frac{-\hbar^2}{4mR}\partial_R^2 R + m\omega^2 R^2 + \frac{\hbar^2\ell_R(\ell_R+1)}{4mR^2}\right)\mathcal{R}_R = E_R\mathcal{R}_R$$

$$\left(\frac{-\hbar^2}{4mr}\partial_r^2 r + \frac{1}{4}m\omega^2 r^2 + \frac{\hbar^2\ell_r(\ell_r+1)}{4mr^2} + \frac{k}{r}\right)\mathcal{R}_r = E_r\mathcal{R}_r$$

Again, introduce transformations $u_R(R) = R\mathcal{R}_R(R)$ and $u_r(r) = r\mathcal{R}_r(r)$ such that

$$\left(\frac{-\hbar^2}{4m}\partial_R^2 + m\omega^2 R^2 + \frac{\hbar^2\ell_R(\ell_R+1)}{4mR^2}\right)u_R = E_R u_R$$

$$\left(\frac{-\hbar^2}{4m}\partial_r^2 + \frac{1}{4}m\omega^2 r^2 + \frac{\hbar^2\ell_r(\ell_r+1)}{4mr^2} + \frac{k}{r}\right)u_r = E_r u_r$$

The R-equation is actually the same as the harmonic oscillator studied above. To realise this, one must introduce the dimensionless variables $\xi = R/\alpha$ and $v_R(\xi) = u_R(\alpha\xi)$, now with $\alpha = i\sqrt{\hbar/2m\omega}$. In doing so the R-equation reduces to equation (10) with $E_R = E$ and $\lambda_R = 2E/\hbar\omega$. This implies E_R is given by equation (11) and λ_R is given by equation (12).

To continue with the r-equation, dimensionless variables $\rho = r/\beta$ and $v_r(\rho) = u_r(\beta\rho)$ are introduced:

$$\left(\partial_\rho^2 - \frac{m^2\omega^2}{\hbar^2}\beta^4\rho^2 - \frac{\ell_r(\ell_r+1)}{\rho^2} - \frac{4mk\beta}{\hbar^2\rho}\right)v_r = -\frac{4m\beta^2}{\hbar^2}E_r v_r$$

At this point, β may be chosen in order to scale the equation either according to the harmonic oscillator potential or the Coulomb interaction. In an experimental setting, a harmonic oscillator potential could be adjustable whereas the Coulomb interaction is fixed. This implies that the Coulomb interaction serves best as the system's natural scale: $\beta = \hbar^2/4mk$. Now let $\omega_r^2 = m^2\omega^2\beta^4/\hbar^2$ denote an adjustable dimensionless oscillatory parameter such that the final eigenvalue equation becomes

$$\left(\partial_\rho^2 - \omega_r^2\rho^2 - \ell_r(\ell_r+1)\rho^{-2} - \rho^{-1}\right)v_r = -\lambda_r v_r \tag{21}$$

Here, $v_r(\rho)$ are eigenvectors with corresponding eigenvalues $-\lambda_r = \hbar^2 E_r/4mk^2$.

In conclusion, the total energy of the electron-electron system is given by

$$E = E_R + E_r = \hbar\omega\left(2n_R + \ell_R + \frac{3}{2}\right) - \frac{4mk^2}{\hbar^2}\lambda_r \tag{22}$$

C. Eigenvalues Of Tridiagonal Matrices

The following theorem will not be proven here, but is included due to its comparative applications in this project.

Provided the following tridiagonal matrix equation:

$$\hat{A}\hat{\mathbf{x}} = \lambda\hat{\mathbf{x}} \tag{23}$$

where $\lambda \in \mathbb{R}$, $\hat{\mathbf{x}}^T = \begin{bmatrix} x_1 & \cdots & x_n \end{bmatrix}$ and $\hat{A}$ is composed by a central, upper and lower diagonal diagonal. All elements along the central diagonal are equal to b, while all elements along the upper and lower diagonals are equal to a. The eigenvalues are given by

$$\lambda_i = b + 2a\cos\left[\frac{i\pi}{n+1}\right] \quad \text{for} \quad i = 1, 2, \ldots, n \tag{24}$$

D. Discretisation

Let $\xi \in [a, b]$ denote an independent variable and $v(\xi) \in \mathbb{R}$ denote a dependent variable that satisfies some eigenvalue equation $\hat{\Lambda}v(\xi) = \lambda v(\xi)$, where the variables and the operator are continuous objects. The operator may be a linear combination of several operators $\hat{\Lambda} = \hat{\Lambda}_1 + \hat{\Lambda}_2 + \cdots$. The following section is concerned with the discretisation of these variables and operators.

1. The variables

The first step is to discretise the ξ-interval $[a, b]$ into $n+1$ slices such that ξ is replaced by a grid with $n+2$ ξ_i values:

$$\xi_i = a + ih \quad \text{for} \quad i = 0, 1, \ldots, n+1 \tag{25}$$

where

$$h = \frac{b-a}{n+1} \tag{26}$$

(Note that $\xi_0 = a$ and $\xi_{n+1} = b$.) Following the discretisation of ξ, $v(\xi)$ is now naturally discretised as follows:

$$v_i = v(\xi_i) \quad \text{for} \quad i = 0, 1, \ldots, n+1 \tag{27}$$

Any Dirichlet boundary conditions $v(a) = v_a$ and $v(b) = v_b$ are then imposed by setting $v_0 = v_a$ and $v_{n+1} = v_b$. As opposed to the continuous variable $v(\xi)$, the simplest way to represent the discrete variable-set $\{v_i\}_{i=0}^{i=n+1}$ is as a column vector:

$$\mathbf{v} = \begin{pmatrix} v_0 & v_1 & \cdots & v_{n+1} \end{pmatrix}^T \tag{28}$$

2. Operator: The second derivative

As $\mathbf{v}$ is not a continous object, it is incompatible with the continous second derivative operator $\hat{\Lambda} = \partial_\xi^2$. To work around this problem, the derivative must be approximated via some discretisation process. One such approach is the finite difference approximation, in particular the central finite difference approximation method for second order derivatives:

Consider the Taylor expansion of any single-variable function $f(y)$, centered about $y = x$:

$$f(y) = f(x) + f'(x)(y-x) + \frac{f''(x)}{2}(y-x)^2 + \frac{f'''(x)}{6}(y-x)^3 + \frac{f^{(4)}(x)}{24}(y-x)^4 + \cdots \tag{29}$$

Now consider $f(x \pm h)$:

$$f(x \pm h) = f(x) \pm f'(x)h + \frac{f''(x)}{2}h^2 \pm \frac{f'''(x)}{6}h^3 + \frac{f^{(4)}(x)}{24}h^4 + \cdots \tag{30}$$

It follows that

$$f(x+h) + f(x-h) = 2f(x) + f''(x)h^2 + \mathcal{O}\big(h^4\big)$$

where it assumed that $h \leq 1$. The central finite difference approximation for second order derivatives is now found by solving for $f''(x) = \partial_y^2 f(x) = \partial_x^2 f(x)$:

$$\partial_x^2 f(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + \mathcal{O}\big(h^2\big) \tag{31}$$

(Note that the *approximation* does not include the order-of term.) It is worth noting that equation (31) is exact in the limit $h \to 0$:

$$\lim_{h\to 0} \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + \mathcal{O}\big(h^2\big) = \lim_{h\to 0} \frac{\frac{f(x+h)-f(x)}{h} - \frac{f(x)-f(x-h)}{h}}{h} + \mathcal{O}\big(h^2\big) = \lim_{h\to 0} \frac{f'(x+h) - f'(x)}{h} + \mathcal{O}\big(h^2\big) = f''(x)$$

The idea of equation (31) is to approximate $v''(\xi_i)$ for each $i = 1, \ldots, n$:

$$\begin{aligned} v''(\xi_1) &\approx h^{-2}\big(v_0 - 2v_1 + v_2\big) \\ v''(\xi_2) &\approx h^{-2}\big(v_1 - 2v_2 + v_3\big) \\ &\vdots \quad \vdots \\ v''(\xi_n) &\approx h^{-2}\big(v_{n-1} - 2v_n + v_{n+1}\big) \end{aligned}$$

Note that $v''(\xi_0)$ and $v''(\xi_{n+1})$ cannot be approximated as v_{-1} and v_{n+2} are unknown. The above equations may be written as a matrix equation if the second derivatives are denoted as the column vector $\mathbf{v}'' = \big(v''(\xi_1) \ \cdots \ v''(\xi_n)\big)^T$:

$$\begin{pmatrix} v''(\xi_1) \\ \vdots \\ v''(\xi_n) \end{pmatrix} = h^{-2} \begin{pmatrix} 1 & -2 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & \cdots & \vdots & \vdots & \vdots \\ 0 & 0 & 1 & \ddots & \ddots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \ddots & 1 & 0 & 0 \\ \vdots & \vdots & \vdots & \cdots & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 & -2 & 1 \end{pmatrix} \begin{pmatrix} v_0 \\ v_1 \\ \vdots \\ v_n \\ v_{n+1} \end{pmatrix}$$

Or simply

$$\mathbf{v}'' = \hat{\Lambda}_D \mathbf{v} \tag{32}$$

where $\hat{\Lambda}$ is the giant matrix, including the factor h^{-2}. Note that while $\mathbf{v}$ contains $n+2$ points, $\mathbf{v}''$ only contains n points; this is also evident from the fact that $\hat{\Lambda}_D$ is an $n \times (n+2)$ matrix. [4] Furthermore, equation (32) is the discrete equivalent to the continous equation:

$$\partial_\xi^2 v(\xi) = v''(\xi)$$

As the local truncation error in each finite difference approximation is of order h^2, and there are n approximations, the global truncation error goes as $n\mathcal{O}\big(h^2\big) \cong \mathcal{O}(h)$. Hence, $\hat{\Lambda}_D$ makes a truncation error of order h when it is used to approximate the continuous second derivative operator.

3. Operator: Multiplication with another function

A "multiplication-with-another-function operator" may be written as $\hat{\Lambda} = g(\xi)$. Compared to the second derivative operator, these operators are much more simple to account for as they do not act on the eigenvector itself. The discretisation of these operators is simply given by $\hat{\Lambda}_g = \text{diag}\big(g(\xi_0)\cdots g(\xi_{n+1})\big)$, which yields:

$$\hat{\Lambda}_g \mathbf{v} = \begin{bmatrix} g(\xi_0)v_0 & \cdots & g(\xi_{n+1})v_{n+1} \end{bmatrix}^T \tag{33}$$

A common example of these kind of operators are polynomials: $g(\xi) = \xi^2$, $g(\xi) = \xi^{-2}$, etc.

E. Solving Matrix Eigenvalue Equations Via The Jacobi Algorithm

The following section presents the Jacobi eigenpair/-diagonalisation algorithm for solving matrix eigenvalue equations on the form:

$$\hat{A}\mathbf{v} = \lambda \mathbf{v} \tag{34}$$

where $\hat{A}$ is a symmetric matrix. The algorithm is based on the properties of similarity (orthogonal) transformations, and will therefore be dealt with first.

1. Similarity transformations

A symmetric matrix $\hat{A} \in \mathbb{R}^{n\times n}$ is said to be similar to another symmetric matrix $\hat{B} \in \mathbb{R}^{n\times n}$ if there exist a unitary matrix $\hat{S} \in \mathbb{R}^{n\times n}$ that is such that

$$\hat{B} = \hat{S}^T \hat{A} \hat{S} \tag{35}$$

Let $\{\mathbf{u}_i\}_{i=1}^{i=n}$ denote an orthonormal basis for the column space of $\hat{A}$: $\mathbf{u}_i^T \mathbf{u}_j = \delta_{ij}$. The similarity transformation $\mathbf{w}_i = \hat{S}^T \mathbf{u}_i$ preserves the orthonormality of the basis:

$$\mathbf{w}_i^T \mathbf{w}_j = \big(\hat{S}^T \mathbf{u}_i\big)^T \big(\hat{S}^T \mathbf{u}_j\big) = \mathbf{u}_i^T \hat{S}\hat{S}^T \mathbf{u}_j = \mathbf{u}_i^T \mathbf{u}_j = \delta_{ij}$$

The idea is to perform m number of transformations such that $\hat{A}$ is diagonalised to $\hat{D}$:

$$\hat{D} = \hat{S}_m^T \hat{S}_{m-1}^T \cdots \hat{S}_1^T \hat{A} \hat{S}_1 \cdots \hat{S}_{m-1}\hat{S}_m \tag{36}$$

where

$$\hat{D} = \text{diag}\big(\lambda_1 \;\; \lambda_2 \;\; \cdots \;\; \lambda_n\big) \tag{37}$$

Matrices $\hat{S}_1, \ldots, \hat{S}_m$ are guaranteeed to exist as $\hat{A}$ is a real symmetric matrix (the proof is not included here). Using (35), equation (34) yields:

$$\hat{S}^T \hat{A}\hat{I}\mathbf{v} = \hat{S}^T \lambda \mathbf{v} \implies \hat{S}^T A \hat{S}\hat{S}^T \mathbf{v} = \lambda \hat{S}^T \mathbf{v} \implies$$

$$\hat{B}\big(\hat{S}^T \mathbf{v}\big) = \lambda \big(\hat{S}^T \mathbf{v}\big) \tag{38}$$

As $\hat{A}$ is a real symmetric matrix, its eigenvectors $\mathbf{v}_1, \ldots, \mathbf{v}_n$ form an orthogonal basis for its column space. And as the transformation $\hat{S}^T\mathbf{v}$ conserves orthogonality, the final eigenvectors $\hat{S}_1 \cdots \hat{S}_m \mathbf{v}$ must also form an orthogonal basis for the column space of $\hat{A}$. Furthermore, equation (38) reveals that the eigenvalue λ of $\hat{A}$ is unaffected by each transformation.

Now let

$$\hat{V} = \begin{bmatrix} \hat{\mathbf{v}}_1 & \cdots & \hat{\mathbf{v}}_n \end{bmatrix} = \hat{S}_1 \cdots \hat{S}_m \hat{I} \tag{39}$$

so that $\hat{V}^T \hat{A} \hat{V} = \hat{D}$. This implies

$$\hat{A}\hat{V} = \begin{bmatrix} \hat{A}\hat{\mathbf{v}}_1 \cdots \hat{A}\hat{\mathbf{v}}_n \end{bmatrix} \tag{40a}$$

$$\hat{A}\hat{V} = \hat{V}\hat{D} = \begin{bmatrix} \lambda_1 \hat{\mathbf{v}}_1 & \cdots & \lambda_n \hat{\mathbf{v}}_n \end{bmatrix} \tag{40b}$$

which proves that the eigenvectors of $\hat{A}$ are the vectors $\hat{\mathbf{v}}_1, \ldots, \hat{\mathbf{v}}_n$. As orthogonal transformations preserves normalisation, the set $\{\hat{\mathbf{v}}_i\}_{i=1}^{i=n}$ must also form an orthonormal basis for the column space of $\hat{A}$.

2. The algorithm

The unitary matrix used in the Jacobi algorithm is the so-called Givens rotation matrix $\hat{G}(k, l, \theta)$, which is a generalisation of the rotation-matrix for planar (2-dimensional) coordinate systems. The elements in $\hat{G}(k, l, \theta)$ are given by

$$g_{ij} = \begin{cases} 1, & i = j \notin \{k, l\} \\ \cos\theta, & i = j \in \{k, l\} \\ \sin\theta, & i = k,\ j = l \\ -\sin\theta, & i = l,\ j = k \\ 0, & otherwise \end{cases} \tag{41}$$

Before continuing to the actual algorithm, consider first the transformation $\hat{B} = \hat{G}^T \hat{A} \hat{G}$, where the elements of the symmetric matrices $\hat{A}$ and $\hat{B}$ are denoted by a_{ij} and b_{ij}. The simplest case, i.e. with $n = 2$, is the following

$$\begin{pmatrix} b_{11} & b_{12} \\ b_{12} & b_{22} \end{pmatrix} = \begin{pmatrix} c & s \\ -s & c \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{pmatrix} \begin{pmatrix} c & -s \\ s & c \end{pmatrix}$$

That is:

$$\begin{aligned} b_{11} &= c^2\, a_{11} - 2sc\, a_{12} + s^2\, a_{22} \\ b_{12} &= (c^2 - s^2) a_{12} + sc(a_{22} - a_{11}) \\ b_{22} &= s^2\, a_{11} + 2sc\, a_{12} + c^2\, a_{22} \end{aligned}$$

So far, no criteria has been placed on the parameter θ. However, the Jacobi algorith designs the matrix $\hat{G}$, and thereby θ, such that $b_{12} = 0$:

$$a_{11} - a_{22} = \frac{\cos^2\theta - \sin^2\theta}{\sin\theta\cos\theta} a_{12} = (\cot\theta - \tan\theta) a_{12}$$

Using the identity $2\cot(2\theta) = \cot\theta - \tan\theta$ one finds:

$$\cot(2\theta) = \frac{a_{11} - a_{22}}{2a_{12}}$$

Let $t = \tan\theta$ and $\tau = \cot(2\theta)$ so that

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

Which further implies

$$t = -\tau \pm \sqrt{1 + \tau^2} \tag{42}$$

Having found t, finding s and c is simple:

$$c = \frac{1}{\sec\theta} = \frac{1}{\sqrt{1 + \tan^2\theta}} = \frac{1}{\sqrt{1 + t^2}} \tag{43a}$$

$$s = \cos\theta \frac{\sin\theta}{\cos\theta} = ct \tag{43b}$$

A special case of the transformation is when $a_{12} = 0$: it follows that $\theta = \pi/4$ and thus $c = 1$, $s = 0$.

By increasing the dimensionality of the transformation from $n = 2$ to any arbitrary n, only two extra cases arise: whether the element a_{ij} is affected or not depends on its location in the matrix.

The key detail is to realise how the structure of $\hat{G}$ is related to the identiy matrix: other than the k^{th} and l^{th} columns and rows, $\hat{G}$ is essentially an identity matrix. It follows that all elements a_{ij} where $i, j \notin \{k, l\}$ seemingly interact with the identity matrix; leaving them unchanged after the transformation: $b_{ij} = a_{ij}$.

Furthermore, the elements b_{kk}, b_{ll} and b_{kl} are the same elements as in the $n = 2$ case. The generalised τ is:

$$\tau = \frac{a_{kk} - a_{ll}}{2a_{kl}} \tag{44}$$

The remaining elements $b_{ik} = b_{ki}$ and $b_{il} = b_{li}$, where $i \notin \{k, l\}$, can be derived from the observation that the matrix product $\hat{G}^T\hat{A}$ only acts on the rows of $\hat{A}$, while the matrix product $\hat{A}\hat{G}$ only acts on the columns of $\hat{A}$. By computing $\hat{A}\hat{G}$ (details omitted here), one finds:

$$b_{ik} = ca_{ik} - sa_{il} \quad \text{and} \quad b_{il} = sa_{ik} + ca_{il}$$

In summary, the elements of $\hat{B}$ are given by:

$$b_{ij} = a_{ij}, \qquad i, j \notin \{k, l\} \tag{45a}$$

$$b_{ik} = ca_{ik} - sa_{il}, \qquad i \notin \{k, l\} \tag{45b}$$

$$b_{il} = sa_{il} + ca_{il}, \qquad i \notin \{k, l\} \tag{45c}$$

$$b_{kk} = c^2 a_{kk} - 2sca_{kl} + s^2 a_{ll} \tag{45d}$$

$$b_{ll} = c^2 a_{kk} + 2sca_{kl} + s^2 a_{ll} \tag{45e}$$

$$b_{kl} = 0 \tag{45f}$$

After performing the transformation, the eigenvectors (i.e. $\hat{V} = \begin{bmatrix}\hat{\mathbf{v}}_1 & \cdots & \hat{\mathbf{v}}_n\end{bmatrix}$) must also be updated in order to remain eigenvectors for the transformed matrix:

$$\hat{V}_{new} = \hat{V}_{old}\hat{G} \tag{46}$$

This operation exactly mirrors $\hat{A}\hat{G}$, hence:

$$v_{ik}^{\text{new}} = cv_{ik}^{\text{old}} - sv_{il}^{\text{old}}, \quad i \notin \{k, l\} \tag{47a}$$

$$v_{il}^{\text{new}} = sv_{il}^{\text{old}} + cv_{il}^{\text{old}}, \quad i \notin \{k, l\} \tag{47b}$$

The Jacobi algorithm is essentially comprised of performing orthogonal transformations $\hat{A}_{p+1} = \hat{G}^T\hat{A}_p\hat{G}$ until $\hat{A}$ is "successfully diagonalised". As this process is iterative, true diagonalisation is only guaranteed in the limit $p \to \infty$. In order to terminate the process, the quality of the diagonalisation must be measured by some criterion at the end of each iteration. A commonly used measure is whether the off-diagonal elements of $\hat{A}_p$ are sufficiently small:

$$\text{off}(\hat{A}) = \sqrt{\sum_{i=1}^{n}\sum_{j\neq i}^{n} a_{ij}^2} \leq \epsilon \tag{48}$$

for some error tolerance ϵ. However, it is computationally very ineffective to require the computation of off$(\hat{A})$ at each iteration. Instead, consider the following:

$$\text{off}(\hat{A}) \leq \sqrt{\sum_{i=1}^{n}\sum_{j\neq i}^{n} \max\{a_{ij}^2\}} = n\max\{|a_{ij}|\} \tag{49}$$

Finding $n\max\{|a_{ij}|\}$ is much more computation-friendly and is thus better suited for the algorithm. As n simply scales the tolerance, the essential measure is:

$$\max\{|a_{ij}|\} \leq \varepsilon \tag{50}$$

The number of iterations required to satisfy (50) is difficult to quantify. In order to avoid unpredictably long computation time, a maximum number of iterations $N_{\max}$ is also enforced in the algorithm.

Due to the miniscule effects of the transformation (it only affects the k^{th} and l^{th} columns and rows), the choice of coefficients k and l becomes very important. Seeing that the transformation defines $b_{kl} = 0$, a clever approach would be to choose k and l using $\max\{|a_{ij}|\}$. This approach is also the most effective with respect to equation (50) in that each step reduces the current $\max\{|a_{ij}|\}$ to zero.

The full Jacobi-diagonalisation algorithm can be summaried as follows:

1. Set $p = 0$, load $\hat{A}_0$ and define $\hat{V} = \hat{I}$.
2. Compute $a_{kl} = a_{max} = \max\{|a_{ij}|\}$.
3. `while` $\max\{|a_{ij}|\} > \varepsilon$ `and` $p \leq N_{\max}$:

   Compute τ, t, c and s using equations (44), (42) and (43) respectively.

   Use equations (45) to adjust $\hat{A}_{p+1}$.

   Use equations (47) to adjust $\hat{V}_{p+1}$.

   Find $a_{kl} = a_{max} = \max\{|a_{ij}|\}$.

   $p = p + 1$.
4. Extract

$$\begin{bmatrix}\lambda_1 & \cdots & \lambda_n\end{bmatrix} = \text{diag}(\hat{A}_p) \quad \text{and} \quad \begin{bmatrix}\hat{\mathbf{v}}_1 & \cdots & \hat{\mathbf{v}}_n\end{bmatrix} = \hat{V}$$

III. METHOD

A. Testing The Machinery On The Buckling Beam

This first problem serves mainly as a test for both the Jacobi algorithm and the mathematical formalism developed in the theory section. The existence of simple analytic eigenvalues makes the problem an excellent starting point.

Equation (3), which governs the system, contains the second derivative operator ∂_ξ^2. Employing the discretisation formalism yields the equation

$$\hat{\Lambda}_D \mathbf{v} = -\lambda \mathbf{v} \tag{51}$$

However, by imposing the Dirichlet boundary conditions $v_0 = v_{n+1} = 0$ it is apparent that the first and last columns of $\hat{\Lambda}_D$ serves no purpose. Ignoring these columns results in the symmetric tridiagonal matrix eigenvalue equation:

$$D\tilde{\mathbf{v}} = -\lambda \tilde{\mathbf{v}} \tag{52}$$

where D is the symmetric tridiagonal matrix (without the h^2 term), $\tilde{\mathbf{v}} = h^2 \begin{pmatrix} v_1 & \cdots & v_n \end{pmatrix}^T$ and the analytic eigenvalues $-\lambda$ are given by equation (24).

Equation (52) is solved using the Jacobi algorithm for all combinations of $\varepsilon \in \{10^{-2}, 10^{-6}, 10^{-10}\}$ and $n \in \{10, 100, 300\}$, where $N_{\max}$ is increased beyond the necessary amount of iterations. Our interest lies in the accuracy of the Jacobi algorithm. The simplest criteria to tell whether the algorithm is successful is to compare the eigenvalues to the analytic eigenvalues.

In order to add an additional layer of confidence to the accuracy of the algorithm, the same system will be analysed using the `eig_sym` function from the `Armadillo C++` library.

B. Evaluating The Discrete Formalism Via The Quantum Harmonic Oscillator Potential

Having succesfully completed a preliminary test of the algorithm, the machinery is now put to work on the quantum harmonic oscillator system, i.e. equation (10). Whereas the buckling beam system featured definite variable boundaries $0 \leq \xi \leq 1$, the harmoni oscillator system does not: $0 \leq \xi < \infty$. Seeing that this is impossible to represent using a grid, infinity must be approximated by some upper boundary ξ_∞. The goal is to study how the discrete mathematics behaves with respect to the parameters ξ_∞ and n.

To simplify the interpretations, the azimuthal quantum number is set to zero: $\ell = 0$. The remaining operators in (10) are thus the second derivative operator ∂_ξ^2 and a multiplication-operator $-\xi^2$. Employing the discretisation formalism yields:

$$\left[\hat{\Lambda}_D + \hat{\Lambda}_g\right]\mathbf{v} = -\lambda \mathbf{v} \tag{53}$$

where $g(\xi) = -\xi^2$. By imposing the boundary conditions $v(0) = v(\xi_{\text{upper}}) = 0$, the first and final columns of $\hat{\Lambda}_D$ is again found to be unecessary. The resulting tridiagonal matix may therefore be combined with $\hat{\Lambda}_g$ (which is diagonal) to produce the tridiagonal matrix equation:

$$E\tilde{\mathbf{v}} = -\lambda \tilde{\mathbf{v}} \tag{54}$$

where $\tilde{\mathbf{v}} = h^2 \begin{bmatrix} v_1 & \cdots & v_n \end{bmatrix}$ and E is a tridiagonal matrix whose coefficents are $-2 - h^2\xi_i^2$ along the central diagonal and 1 along both the upper and lower diagonals.

The problem will be studied for all combinations of $\xi_\infty \in \{0.5, 1, 1.5, 2, 4\}$ and $n \in \{10, 100, 500\}$, where $\varepsilon = 10^{-8}$ and $N_{\max}$ is increased beyond the necessary amount of iterations.

C. Applying The Machinery To The Electron-Electron System

As a final challenge, the machinery will now be put to use on the Coulomb-interacting electrons that are located in a harmonic oscillator potential. Seeing that the center-of-mass frame is essentially just the one-dimensional harmonic oscillator, the focus in this report will lie on the relative frame (i.e. equation (21)).

Again the simplification $\ell = 0$ is assumed, meaning the remaining operators are: ∂_ρ^2, $-\omega^2\rho^2$ and $-\rho^{-1}$, where ω is a parameter. Once more infinity is approximated by some large value ρ_∞ such that the mathematical formalism yields:

$$\left[\hat{\Lambda}_D + \hat{\Lambda}_{\tilde{g}} + \hat{\Lambda}_f\right]\mathbf{v} = -\lambda \mathbf{v} \tag{55}$$

where $\tilde{g}(\rho) = -\omega_r^2\rho^2$ and $f(\xi) = -\rho^{-1}$. Again $\hat{\Lambda}_D$ may be simplified by imposing the boundary conditions $v(0) = v(\rho_{\text{upper}}) = 0$, leading to the tridiagonal matrix

$$G\tilde{\mathbf{v}} = -\lambda \tilde{\mathbf{v}} \tag{56}$$

where $\tilde{\mathbf{v}} = h^2 \begin{bmatrix} v_1 & \cdots & v_n \end{bmatrix}$ and G is a tridiagonal matrix whose coefficients are $-2 - h^2(\omega^2\rho^2 + \rho^{-1})$ along the central diagonal and 1 along both the upper and lower diagonals.

The end-goal is to study the balance between the Coulomb-interaction and the harmonic oscillator potential: while the Coulomb potential repels the electrons, the harmonic oscillator potential centers the electrons about the origin, thereby forcing them closer together. This balance will be studied via the parameter $\omega \in \{0.1, 1, 2.5, 5\}$. Other parameters used in the program include $n = 200$, $\varepsilon = 10^{-8}$, sufficient $N_{\max}$ and a sufficient ρ_∞. [5] In order to gain some insight from the results, the resulting probability distributions $p(\rho) = |v(\rho)|^2$ will be compared. However, to avoid unecessary energy-considerations, only the ground state will be analysed.

IV. RESULTS

Only a handful of the prepared figures are featured, all figures are available at the GitHub address:
https://github.com/njmikkelsen/comphys2018/tree/master/Project2

A. The Buckling Beam

A clear trend revealed itself whilst studying this system: the Jacobi algorithm is slow, however accurate. Moreover, it's accuracy is dependent on a sufficient user-defined tolerance ε. Figure 1 shows an example with $n = 100$ and an error tolerence of only $\varepsilon = 10^{-2}$: the resulting eigenvector becomes terribly off. As long as the user is aware of this potential pitfall, this is not necessarily a big problem. Figure 2 shows another example with $n = 100$, however now with $\varepsilon = 10^{-10}$: the eigenvector comes out as expected.

While some of the eigenvectors in computations with large ε turned out completely wrong, the eigenvalues matched the analytic eigenvalues very well in almost every computation. Table I shows a Mean Square Error (MSE) score for every computation: most notably there are no immediately critical errors. `armadillo` performs especially impressive with zero error within the specified precision, Jacobi performs also quite well.

B. The Harmonic Oscillator

The importance of an appropriate approximation of infinity is summarised by figures 3 and 4: While figure 3 features greatly distorted wave functions, figure 4, which is much more generous in its approximation of infinity, yields therefore much more accurate results. One detail that is particulary noticeable between the two is the maximum height of the wave functions. Whereas all wave functions are more or less equally tall in figure 3, there is a clear difference between the different concentrations in figure 4.

C. The Coulomb-Interacting Electron-Electron Harmonic Oscillator

The effect of adjusting the harmonic oscillator frequency is immediately obvious from figures 5, 6 and 7: Increasing the frequency, which leads to a relative decrease in the repulsive Coulomb interaction, yields a concentration of the electrons. This is not surprising as there are only potentials working against each other: the Coulomb-interaction trying to pull the electrons a part, and the harmonic oscillator trying to concentrate the electrons about a common center. The relative increase in the strength of the harmonic oscillator is therefore expected to lead to a greater probability concentration closer to the origin.

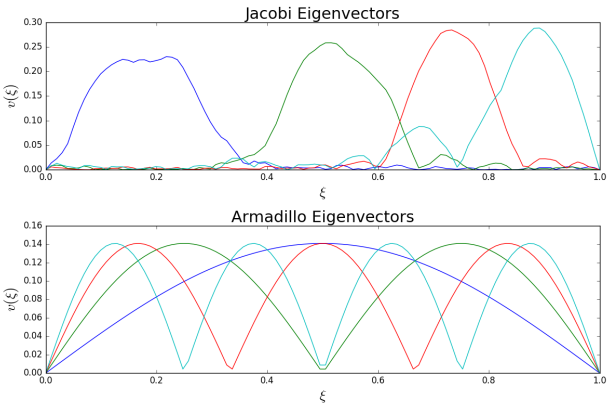

Figure 1. Some eigenvectors of the Buckling Beam system. The numerical calculation defined $n = 100$ and $\varepsilon = 10^{-2}$.

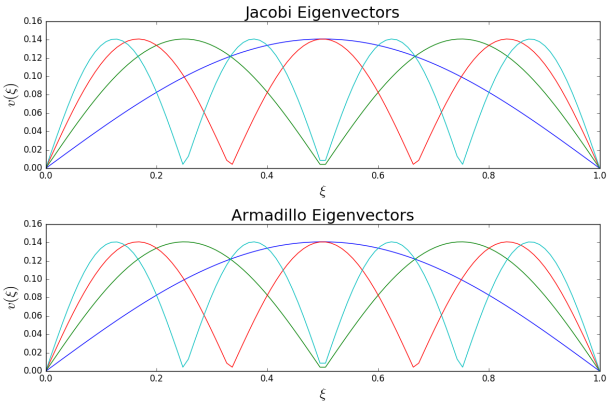

Figure 2. Some eigenvectors of the Buckling Beam system. The numerical calculation defined $n = 100$ and $\varepsilon = 10^{-10}$.

Table I. Mean Square Error score for both the Jacobi-calculated eigenvalues and the `armadillo`-calculated eigenvalues for every computation of the Buckling Beam system. The figures have been truncated due to uneccesary precision.

n	ε	Jacobi MSE	`armadillo` MSE
10	10^{-2}	$1.34 \cdot 10^{-7}$	0
10	10^{-6}	0	0
10	10^{-10}	0	0
100	10^{-2}	$9.17 \cdot 10^{-4}$	0
100	10^{-6}	$1.00 \cdot 10^{-20}$	0
100	10^{-10}	0	0
300	10^{-2}	$6.82 \cdot 10^{-3}$	0
300	10^{-6}	$1.02 \cdot 10^{-16}$	0
300	10^{-10}	0	0

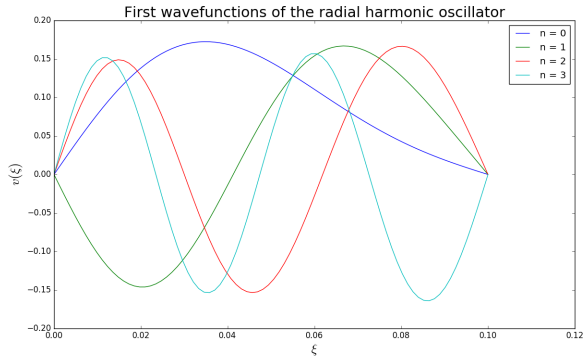

Figure 3. The first wavefunctions of the radial quantum harmonic oscillator. Here, infinity is approximated by $\xi_\infty = 0.1$.

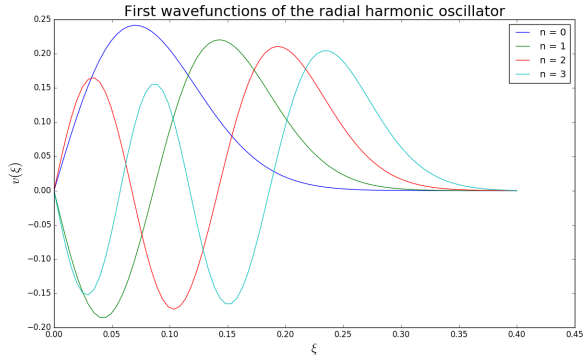

Figure 4. The first wavefunctions of the radial quantum harmonic oscillator. Here, infinity is approximated by $\xi_\infty = 0.4$.

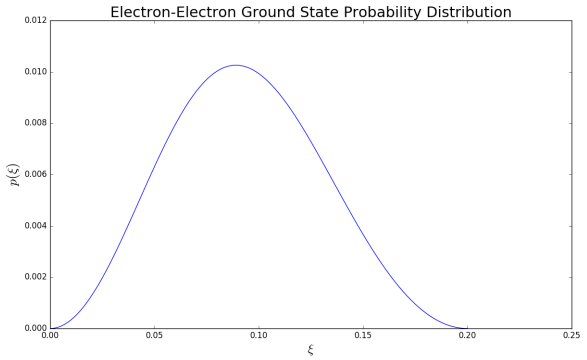

Figure 5. The radial ground state of the Coulomb-interacting electron-electron quantum harmonic oscillator. Here, infinity is approximated by $\xi_\infty = 0.2$ and the harmonic oscillator frequency is $\omega = 0.1$.

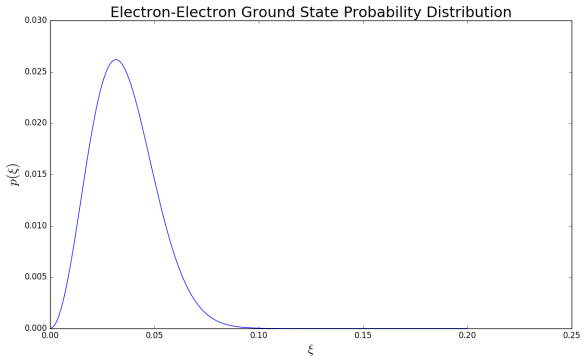

Figure 6. The radial ground state of the Coulomb-interacting electron-electron quantum harmonic oscillator. Here, infinity is approximated by $\xi_\infty = 0.2$ and the harmonic oscillator frequency is $\omega = 1.0$.

V. DISCUSSION

The goal of this project was to study eigenvalue problems using discrete mathematics and the Jacobi algorithm. Overall the project was a success: the systems in question were satisfactorily modelled, provided an appropriate set of parameters.

The discrete formalism was a little tedius to setup, especially due to its generality. Once introduced however, applying it to specific systems was increadibly easy. The mathematics is obviously dependent on the chosen number of grid points, in particular the complexity of the resulting matrix equation is directly affected. While increasing the number of grid points leads to more accurate results, the neccessary amount of operations required to solve the system grows exponentially.

The Jacobi algorithm proved well-equipped to handle low-dimensional equations: as the dimensionality increased, the efficiency dropped significantly. Furthermore, the accuracy of algorithm was very suceptible to the tolerance, and its efficiency did not scale well with improved tolerance. Nonetheless, provided an adequate set of parameters, the algorithm did reproduce the expected results. This is especially visible in figures 1 and 2 in which the tolerances are $\varepsilon = 10^{-2}$ and $\varepsilon = 10^{-10}$ (all other parameters kept constant). It's tempting to assign the errors of the Jacobi algorithm to a mixture of the algorithm and the chosen dimensionality of the problem, this is however proven wrong by the accuracy of the `armadillo` results. In particular, table I proves that the numerical errors produced by the Jacobi algorithm is entirely attributable to the algorithm tolerance.

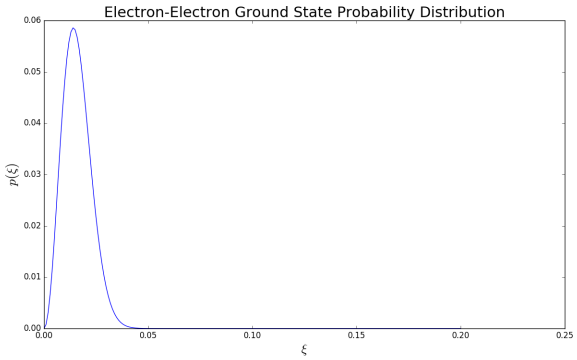

Figure 7. The radial ground state of the Coulomb-interacting electron-electron quantum harmonic oscillator. Here, infinity is approximated by $\xi_\infty = 0.2$ and the harmonic oscillator frequency is $\omega = 2.5$.

VI. CONCLUSION

In conclusion, project 2 has been an overall success. The major goals of project 2 was to study eigenvalue problems using discrete mathematics and the Jacobi algorithm. Three physical systems were studied: the buckling beam, the quantum harmonic oscillator and two Coulomb-interacting electrons in a harmonic oscillator potential. All the governing equations of these systems were derived using continuous mathematics. A discretisation process transformed the equations to matrix eigenvalue equations by introducing a fixed grid.

The buckling beam served as a test for the algorithm. The results indicated that the algorithm provided sufficiently accurate results as long as an appropriate tolerance was used. The results from the harmonic oscillator showed that for grids that approximate infinity, the choice of upper boundary has distinct effect on the shape of the eigenvectors if set to low. The final example, namely the electron-electron system, effectively showed the balance between the harmonic oscillator and the Coulomb-interaction: By increasing the oscillation frequency, the harmonic oscillator began dominating the Coulomb-interaction. This forced the repelling electrons closer to the origin, increasing the probability density of finding the electrons about the origin.

[1] Morten Hjorth-Jensen. Computational physics lectures: Ordinary differential equations, 2017. http://compphysics.github.io/ComputationalPhysics/doc/pub/ode/pdf/ode-print.pdf.

[2] Morten Hjorth-Jensen. Computational physics lectures: Linear algebra methods, 2018. http://compphysics.github.io/ComputationalPhysics/doc/pub/linalg/pdf/linalg-print.pdf.

[3] Morten Hjorth-Jensen. Fys3150 computational physics - project 2, 2018. https://github.com/CompPhysics/ComputationalPhysics/blob/master/doc/Projects/2018/Project2/pdf/Project2.pdf.

[4] The fact that $\hat{\Lambda}_D$ is an $n \times (n+2)$ matrix implies that it accepts an $(n+2)$-dimensional column vector and returns an n-dimensional column vector.

[5] The use of "sufficient" here implies that the parameter is determined such that it has no affect on the results.