# Numerical Solution of Eigenvalue Problem for Classical and Quantum Systems

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We consider the differential equations of the buckling beam and the three dimensional quantum oscillator for one and two electrons. Through discretization we obtain an eigenvalue problem that is solved by diagonalization using Jacobi's method. Our calculations result in numerous errors, making any physical interpretation impossible. Despite the problems with calculations, we found the number of iterations in Jacobi's method is proportional to $n^2$, with $n$ being the matrix dimension, as expected.

## I. INTRODUCTION

A large class of problems in physics fall under the category of eigenvalue problems. These show up in various settings, so having the knowledge of how to solve them is of great importance. What all of these problems have in common is that they can be written as a matrix equation

$$A\mathbf{x} = \lambda\mathbf{x}, \tag{1}$$

where we are interested in finding the eigenvectors $\mathbf{x}$ and eigenvalues $\lambda$ of the matrix $A$.

Examples of eigenvalue problems are calculating the motion of coupled oscillators[1] and finding the principal axes of rotation given an inertia tensor[2]. In this paper, we are going to study two other eigenvalue problems in detail.

The first problem is a classical case, where we look at the displacement of a buckling beam fastened at both ends. The other one is something that at first may seem unrelated, the quantum mechanical problem of a 3D harmonic oscillator. Both of these cases are going to be solved with the method known as Jacobi's eigenvalue algorithm. Since both cases are eigenvalue problems, only small changes are needed in how the algorithm is implemented.

We will begin by considering Newton's second law for the displacement of the buckling beam and the Schrödinger equation for the quantum oscillator. Both equations will be rewritten in terms of dimensionless parameters. Then we will discretize both of them and express them as an eigenvalue equation on the form (1). Finally, we will implement Jacobi's method to diagonalize and thereby solve the eigenvalue equation.

* Code repository: https://github.com/williameivikolsen/FYS4150

## II. THEORY

### A. Buckling beam

#### 1. Description of system

First of all, we start by setting up the system. We are looking at a one-dimensional beam along the $x$-axis with length $L$, so that the beam is located at $x \in [0, L]$. There is a force $F$ applied at $x = L$ directed towards the origin, which is what makes the beam buckle. We denote $u(x)$ to be the vertical displacement of the beam in the $y$-direction. Since we assume the endpoints to be fixed (Dirichlet boundary conditions), we let $u(0) = u(L) = 0$.

A possible way of modelling of the displacement $u(x)$ is by treating the beam as a line of connected springs. The displacement is then given as

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

where the parameter $\gamma$ is material-specific constant that encompasses properties such as the rigidity of the beam.

#### 2. Discretization and scaling

In order to make the solution of a differential equation as general as possible, the equation can be scaled so that it's dimensionless. We can introduce the dimensional variable

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

where $\rho \in [0, 1]$ and insert this this into Eq (2). Then

$$\frac{\gamma}{L^2}\frac{\mathrm{d}^2u(\rho)}{\mathrm{d}\rho^2} = -Fu(\rho),$$

such that the scaled equation becomes

$$\frac{\mathrm{d}^2u(\rho)}{\mathrm{d}\rho^2} = -\frac{FL^2}{\gamma}u(\rho) = -\lambda u(\rho), \tag{3}$$

where we have defined $\lambda = FL^2/\gamma$ in the last step.

We go on by discretizing the interval $[0,1]$ in $n+1$ points, with endpoints $\rho_0 = 0$ and $\rho_n = 1$. This gives a step length

$$h = \frac{\rho_n - \rho_0}{n},$$

and the values of $\rho$ and $u(\rho)$ become

$$\rho \to \rho_i = \rho_0 + ih \quad \text{for} \quad i = 1, 2, \ldots, n \tag{4}$$

and

$$u(\rho) \to u(\rho_i) = u_i. \tag{5}$$

The next step is to discretize the second derivative of $u(\rho)$. An expression for this is given by

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

which is derived by Hjort-Jensen in Ref.[3]. Using the notation in Eq. (4) and (5), this can be more compactly written as

$$u'' = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2}.$$

The final discretized version of the differential equation is then

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

Since Eq. (6) is in reality a set of linear equations, and it is shown in Ref.[4] that finding all $u_i$ is the same as solving the matrix equation

$$\begin{bmatrix} d & a & 0 & 0 & \ldots & 0 & 0 \\ a & d & a & 0 & \ldots & 0 & 0 \\ 0 & a & d & a & 0 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & \ldots & \ldots & \ldots & a & d & a \\ 0 & \ldots & \ldots & \ldots & \ldots & a & d \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \ldots \\ u_{n-1} \\ u_n \end{bmatrix} = \lambda \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \ldots \\ u_{n-1} \\ u_n \end{bmatrix}, \tag{7}$$

setting the diagonal elements $d = 2/h^2$ and the off-diagonal elements $a = -1/h^2$. The endpoints $u_0$ and $u_n$ do not appear in the matrix equation, as they're defined by the boundary conditions.

#### 3. Analytical solution

From the original differential equation Eq. (2), we see that we would expect solutions in terms of sines or cosines. Lyche shows (p.49 in Ref.[5]) that this eigenvalue problem has analytical eigenvalues given as

$$\lambda_j = d + 2a\cos\left(\frac{j\pi}{n+1}\right), \quad j = 1, 2, \ldots, n$$

with corresponding eigenvectors

$$\mathbf{u}_j = \left[\sin\left(\frac{j\pi}{n+1}\right), \sin\left(\frac{2j\pi}{n+1}\right), \ldots, \sin\left(\frac{nj\pi}{n+1}\right)\right]^T.$$

### B. Three-dimensional quantum oscillator

#### 1. One electron

It can be shown (Ref.[6]) that for a central potential $V(r)$, the solution $\psi_{n\ell m}(r,\theta,\phi)$ of the three-dimensional Schrödinger equation can be separated into a product of a radial and angular function:

$$\psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)Y_\ell^m(\theta,\phi), \tag{8}$$

where the radial function is the solution of the radial equation

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} - \frac{\ell(\ell+1)}{r^2}\right)R_{n\ell}(r) + V(r)R_{n\ell}(r) = E_{n\ell}R(r). \tag{9}$$

Here $m$ and $\ell$ is the mass and angular momentum of the particle, respectively. $E_{n\ell}$ is the energy eigenvalue of the state.

Changing variables to $u(r) = rR_{n\ell}(r)$, equation (9) simplifies to

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[V + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right]u = E_{n\ell}u. \tag{10}$$

For the three-dimensional harmonic oscillator, the potential $V(r)$ is given by

$$V(r) = \frac{1}{2}kr^2, \tag{11}$$

where $k = m\omega^2$ and $\omega$ is the oscillator frequency. The energies $E_{n\ell}$ are

$$E_{n\ell} = \hbar\omega\left(2n + \ell + \frac{3}{2}\right), \quad \text{for} \quad n, \ell = 0, 1, 2, \ldots \tag{12}$$

The boundary conditions of the system are $u(0) = u(\infty) = 0$.

We introduce the dimensionless variable $\rho = r/\alpha$ where $\alpha$ is a constant with dimension length and get

$$-\frac{\hbar^2}{2m\alpha^2}\frac{d^2}{d\rho^2}u(\rho) + \left(V(\rho) + \frac{l(l+1)}{\rho^2}\frac{\hbar^2}{2m\alpha^2}\right)u(\rho) = E_{n\ell}u(\rho) \tag{13}$$

For our calculations we will only consider the states with no angular momentum, $\ell = 0$. The potential (11) in terms of $\rho$ becomes

$$V(\rho) = \frac{1}{2}k\alpha^2\rho^2. \tag{14}$$

Inserting (14) into (13) for $\ell = 0$, we obtain

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

Multiplied with $2m\alpha^2/\hbar^2$, the equation becomes

$$-\frac{d^2}{d\rho^2}u(\rho) + \frac{mk}{\hbar^2}\alpha^4\rho^2u(\rho) = \frac{2m\alpha^2}{\hbar^2}E_nu(\rho). \tag{15}$$

Now we define the constant $\alpha$ to be

$$\alpha = \left(\frac{\hbar^2}{mk}\right)^{1/4}, \tag{16}$$

such that $(mk/\hbar^2)\alpha^4 = 1$. Finally, we define a dimensionless parameter $\lambda_n$ to be

$$\lambda_n = \frac{2m\alpha^2}{\hbar^2}E_n. \tag{17}$$

Inserting these parameters into equation (15), we obtain the dimensionless radial equation for zero angular momentum states:

$$-\frac{d^2}{d\rho^2}u(\rho) + \rho^2 u(\rho) = \lambda_n u(\rho), \tag{18}$$

where the eigenvalues $\lambda_n$ are given by

$$\lambda_n = 4n + 3 \text{ for } n = 0, 1, 2, ... \tag{19}$$

Now we discretize equation (18) in the same manner as for the buckling beam to obtain

$$-\frac{u(\rho_i+h)-2u(\rho_i)+u(\rho_i-h)}{h^2} + \rho_i^2 u(\rho_i) = \lambda u(\rho_i). \tag{20}$$

Notice the extra term $\rho_i^2 u(\rho_i)$ compared to the discretized equation for the buckling beam (6). Except from this difference, the equations are equivalent. Following the same derivation as before, we end up with the matrix equation

$$\begin{bmatrix} \tilde{d} & a & 0 & 0 & \dots & 0 & 0 \\ a & \tilde{d} & a & 0 & \dots & 0 & 0 \\ 0 & a & \tilde{d} & a & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & a & \tilde{d} & a \\ 0 & \dots & \dots & \dots & \dots & a & \tilde{d} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \dots \\ u_{n-2} \\ u_{n-1} \end{bmatrix} = \lambda \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \dots \\ u_{n-2} \\ u_{n-1} \end{bmatrix}, \tag{21}$$

where

$$\tilde{d}_i = \frac{2}{h^2} + \rho_i^2.. \tag{22}$$

### 2. *Two electrons*

If we add another electron to the quantum oscillator, the Hamiltionian will contain an additional interaction term. Consider first the Schrödinger equation for the non interactive case:

$$\left(-\frac{\hbar^2}{m}\frac{d^2}{dr^2} - \frac{\hbar^2}{4m}\frac{d^2}{dR^2} + \frac{1}{4}kr^2 + kR^2\right)u(r, R) = E^{(2)}u(r, R) \tag{23}$$

where the (2) denotes that $E^{(2)}$ is the energy eigenvalue for the two-particle system and $\mathbf{r}$ and $\mathbf{R}$ is the relative coordinate and the center-of-mass coordinate, respectively, defined as:

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2, \tag{24}$$

$$\mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2). \tag{25}$$

We assume the wave function $u(r, R)$ to be separable into independent functions of $r$ and $R$:

$$u(r, R) = \psi(r)\phi(R). \tag{26}$$

Defining the energy to be the sum of the relative energy $E_r$ and the center-of-mass energy $E_R$, we can now separate equation (23) into independent equations of $r$ and $R$. The $r$-dependent equation reads

$$\left(-\frac{\hbar^2}{m}\frac{d^2}{dr^2} + \frac{1}{4}kr^2\right)\psi(r) = E_r\psi(r). \tag{27}$$

Now we want to add the interaction between the electrons. They interact via the Coulomb potential, given by

$$V(r_1, r_2) = \frac{\beta e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} = \frac{\beta e^2}{r}, \tag{28}$$

with $\beta e^2 = 1.44$ eVnm. Adding this term to the Hamiltonian, the $r$-dependent equation ends up as

$$\left(-\frac{\hbar^2}{m}\frac{d^2}{dr^2} + \frac{1}{4}kr^2 + \frac{\beta e^2}{r}\right)\psi(r) = E_r\psi(r). \tag{29}$$

We now introduce another dimensionless variable $\rho = r/\alpha$. Going through the same steps as in the one electron-case, we arrive at

$$-\frac{d^2}{d\rho^2}\psi(\rho) + \frac{1}{4}\frac{mk}{\hbar^2}\alpha^4\rho^2\psi(\rho) + \frac{m\alpha\beta e^2}{\rho\hbar^2}\psi(\rho) = \frac{m\alpha^2}{\hbar^2}E_r\psi(\rho). \tag{30}$$

To simplify even further, we define a frequency $w_r$ by

$$\omega_r^2 = \frac{1}{4}\frac{mk}{\hbar^2}\alpha^4, \tag{31}$$

and fix the constant $\alpha$ by requiring

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

or

$$\alpha = \frac{\hbar^2}{m\beta e^2}. \tag{32}$$

Defining

$$\lambda = \frac{m\alpha^2}{\hbar^2}E, \tag{33}$$

we can rewrite Schrödinger's equation as

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

Following the previous derivation, this leads to a matrix equation equivalent to (21), but with diagonal elements

$$\tilde{d}_i = \frac{2}{h^2} + \rho_i^2 + \frac{1}{\rho_i}. \tag{34}$$

### C. Jacobi's method

#### 1. Similarity transformations

A well-known result from linear algebra is that if the matrix $A$ is real ($A \in \mathbb{R}^{n\times n}$) and symmetric, there exists a real orthogonal matrix $S$ such that

$$S^T AS = D = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n), \tag{35}$$

where $D$ is a diagonal matrix that contains the eigenvalues from $A$. In general, a matrix $B$ is a similarity transformation of $A$ if

$$B = S^T AS, \tag{36}$$

and orthogonal matrix $S$ has the properties that

$$S^T S = S^{-1} S = SS^T = \mathbb{1}.$$

It can be proved (not shown here) that the matrix $B$ is symmetric.

Our motivation is to show that we can transform $A$ into a diagonal matrix $D$ by a series of similarity transformations, so that

$$S_n^T \ldots S_1^T AS_1 \ldots S_n = D. \tag{37}$$

For this to be true, the eigenvalues have to be preserved after similarity transformations (even though this preservation generally doesn't apply for the eigenvectors). We will prove this by using the eigenvalue equation Eq.(1) and Eq.(39):

$$\begin{aligned} A\mathbf{x} &= \lambda\mathbf{x} \\ S^T A\mathbf{x} &= \lambda S^T\mathbf{x} \\ S^T A\underbrace{SS^T}_{\mathbb{1}}\mathbf{x} &= \lambda S^T\mathbf{x} \\ (S^T AS)S^T\mathbf{x} &= \lambda S^T\mathbf{x} \\ B(S^T\mathbf{x}) &= \lambda(S^T\mathbf{x}) \end{aligned}$$

The matrix $B$ thus have the same eigenvectors as $A$, but with eigenvectors $S^T\mathbf{x}$. Since the diagonal matrix $D$ has standard basis vectors $\mathbf{u}_i$ as eigenvectors, the eigenvectors $\mathbf{x}_i$ of matrix $A$ are related by

$$D\mathbf{u}_i = \lambda_i\mathbf{u}_i = \lambda_i(S^T\mathbf{x}_i).$$

Then

$$\mathbf{u}_i = S^T\mathbf{x}_i = S^{-1}\mathbf{x}_i,$$

and we find the eigenvectors $\mathbf{x}_i$ by

$$\mathbf{x}_i = S\mathbf{u}_i = S_n \ldots S_1\mathbf{u}_i. \tag{38}$$

We can also show that $S$ gives rise to unitary transformations that preserve the dot product and orthogonality. Given a basis of vectors $\mathbf{v}_i$ that is orthogonal, the inner product between the basis vectors is

$$\langle\mathbf{v}_i, \mathbf{v}_j\rangle = \mathbf{v}_i^T\mathbf{v}_j = \delta_{ij}.$$

Now, if we have the transformation

$$\mathbf{w}_i = S\mathbf{v}_i,$$

then

$$\langle\mathbf{w}_i, \mathbf{w}_j\rangle = \langle S\mathbf{v}_i, S\mathbf{v}_j\rangle = \mathbf{v}_i^T\underbrace{S^T S}_{\mathbb{1}}\mathbf{v}_j = \mathbf{v}_i^T\mathbf{v}_j = \delta_{ij},$$

so the dot product and orthogonality are preserved.

#### 2. Description of algorithm

In order to diagonalize the real and symmetric $n \times n$ matrix $A$, we can apply a series of similarity transformations as shown in Eq.(37). In Jacobi's method, these matrices represent a plane rotation about an angle $\theta$ in $n$-dimensional Euclidean space, with the form

$$S = \begin{bmatrix} 1 & 0 & \ldots & 0 & 0 & \ldots & 0 & 0 \\ 0 & 1 & \ldots & 0 & 0 & \ldots & 0 & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & 0 & \ldots \\ 0 & 0 & \ldots & \cos\theta & 0 & \ldots & 0 & \sin\theta \\ 0 & 0 & \ldots & 0 & 1 & \ldots & 0 & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & 1 & \ldots \\ 0 & 0 & \ldots & -\sin\theta & 0 & \ldots & 0 & \cos\theta \end{bmatrix}. \tag{39}$$

The most efficient way of diagonalizing the matrix is to choose $S$ so that it sets the pair of largest (in absolute size) non-diagonal elements of $A$ to zero. If these matrix elements are $a_{kl} = a_{lk}$, the matrix $B = S^T AS$ would have the property that $b_{kl} = b_{lk} = 0$. Finding the elements $a_{kl} = \max|a_{ij}|$ where $i \neq j$ is thus part of the algorithm.

Knowing which elements we want to eliminate, we can write out matrix elements in the transformed matrix $B$:

$$b_{ik} = a_{ik}\cos\theta - a_{il}\sin\theta, \quad i \neq k, l \tag{40a}$$

$$b_{il} = a_{il}\cos\theta + a_{ik}\sin\theta, \quad i \neq k, l \tag{40b}$$

$$\begin{aligned} b_{kk} &= a_{kk}\cos^2\theta - 2a_{kl}\cos\theta\sin\theta + a_{ll}\sin^2\theta \\ b_{ll} &= a_{ll}\cos^2\theta + 2a_{kl}\cos\theta\sin\theta + a_{kk}\sin^2\theta \\ b_{kl} &= (a_{kk} - a_{ll})\cos\theta\sin\theta + a_{kl}(\cos^2\theta - \sin^2\theta). \end{aligned} \tag{40c}$$

We now choose the value of $\theta$ such that $b_{kl} = 0$. In order to make notation easier, we introduce the abbreviations

$$c = \cos\theta, \quad s = \sin\theta \quad \text{and} \quad t = \tan\theta = \frac{s}{c}.$$

From Eq.(40c), we then have

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

Dividing by $c^2 = \cos^2\theta$, this becomes

$$a_{kl}(1 - t^2) + (a_{kk} - a_{ll})t = 0.$$

Then, by defining the value

$$\tau = (a_{ll} - a_{kk})/2a_{kl}, \tag{41}$$

we recognize the quadratic equation

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

which has solutions

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

Looking at Eq. (39), it's apparent that we only need the values of $c = \cos\theta$ and $s = \sin\theta$, and never the value of $\theta$ itself. Having found $t = \tan\theta$, we can relate $t$ to $c$ and $s$ by

$$c = \frac{1}{\sqrt{1+t^2}}. \tag{43}$$

and

$$s = tc, \tag{44}$$

and we are finally able to construct $S$.

By repeatedly doing these kinds of similarity transformations, we would expect $A$ to gradually be transformed in to a diagonal matrix $D$. However, a possible pitfall is shown in Eq.(40a) and (40b). After setting a pair of non-diagonal elements to zero, a subsequent transformation might reinstate a non-zero value to the same pair. This will slow down the diagonalization, but it can be shown that Jacobi's method leads to convergence (albeit extraneously slowly)[3].

#### 3. *Practical implementation of algorithm*

As we keep on doing similarity transformations on the matrix $A$, we would like to minimize the norm of the off-diagonal matrix elements of the computed matrix $B$

$$\text{off}(B) = \sqrt{\sum_{i=1}^{n}\sum_{j=1,j\neq i}^{n} a_{ij}^2} \tag{45}$$

so that it's less than a set tolerance $\epsilon$. Instead of computing the double sum in the above equation, we can stop the calculations when the largest non-diagonal elements $|b_{kl}|$ squared is smaller than some other tolerance $\epsilon$, i.e. when

$$\max(b_{kl}^2) \leq \epsilon.$$

Another detail is that Eq.(42) allows us to choose between two roots. We will choose the sign so that $|t|$ is minimized, as this will give the fastest convergence[3]. Thus, the sign chosen is

$$\begin{aligned} &+ \quad \text{if} \quad \tau > 0 \\ &- \quad \text{if} \quad \tau < 0. \end{aligned}$$

Another thing to be beware of is that if $|\tau|$ is large, we Eq.(42) becomes

$$t \simeq -\tau \pm |\tau| \simeq 0,$$

using the above sign convention in the last step. We are effectively subtracting two numbers that are very close in size, which is bad for numerical stability. We therefore rewrite Eq.(42) such that

$$t = \frac{(\tau \pm \sqrt{1+\tau^2})(-\tau \mp \sqrt{1+\tau^2})}{-\tau \mp \sqrt{1+\tau^2}},$$

and thus

$$t = \frac{1}{\tau \mp \sqrt{1+\tau^2}.} \tag{46}$$

We can now set up the algorithm that diagonalizes matrix $A$.

**while** $\max(a_{kl}^2) \leq \epsilon$ **do**
Find element $a_{kl}$ such that $|a_{kl}| = \max_{i\neq j}|a_{ij}|$
Find corresponding indexes $(k,l)$
Compute $\tau, t, s, c$
Compute elements in $B = S(k,l,\theta)^T A S(k,l,\theta)$
Set B $\rightarrow$ A
**end while**

## III. METHOD

We have written a program that does the following:

#### 1. *Buckling beam*

- Diagonalize the $(n \times n)$ matrix $A$ with Jacobi's method up to a tolerance $\epsilon = 10^{-8}$ for $n \in \{10, 100, 1000\}$.

#### 2. *One electron quantum oscillator*

- Repeat the step performed for the buckling beam. The parameter $\rho_{max}$ is set to $\rho_{max} = 100$.

#### 3. *Two electron quantum oscillator*

- Repeat the step performed for the one electron quantum oscillator for $\omega_r \in \{0.01, 0.5, 1, 5\}$.

The program also contains a unit test that compares the eigenvalues with the analytical eigenvalues.

## IV. RESULTS

Resulting data from calculations can be found in the linked code repository.

None of the calculated eigenvalues - for the three physical systems - managed to pass the eigenvalue unit test.

Figure 1 shows the eigenvector $u$ with the lowest eigenvalue as a function of $\rho$ for the case $n = 100$.

Figure 2 shows the number of iterations for values of $n$ on a logarithmically scaled interval $[10, 251]$ with a linear regression. The best fit value for the slope is found to be 2.039 with a standard error of 0.009.

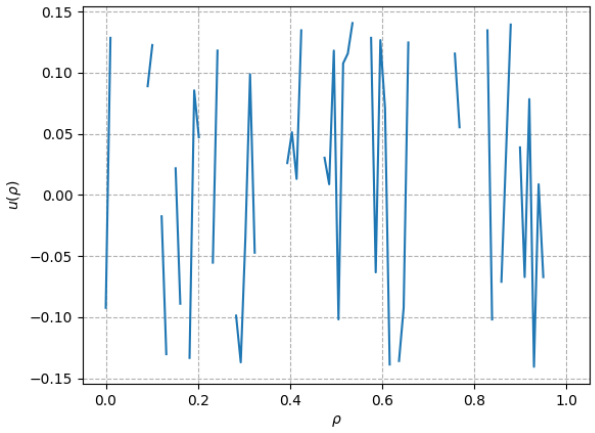


Figure 1. Eigenvector $u$ with lowest eigenvalue for the buckling beam with $n = 100$ as a function of $\rho$.

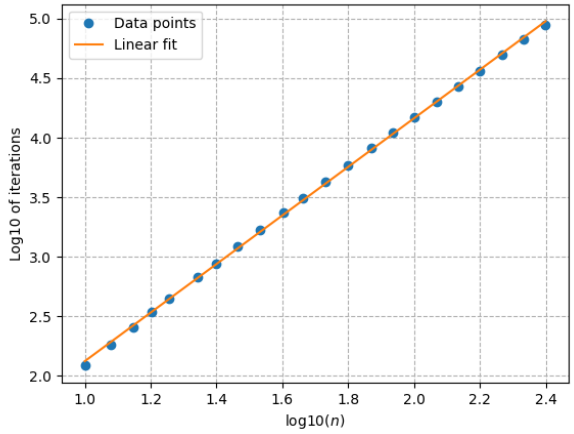


Figure 2. Logarithm of iterations for values of $n$ on a logarithmically scaled interval $[10, 251]$ with a linear regression. The best fit value for the slope is found to be 2.039 with a standard error of 0.009. Here, the tolerance is set to $\epsilon = 10^{-8}$.

## V. DISCUSSION

Figure 1 reveals that our calculations have been filled with errors. The data files reveal that many of the calculations have resulted in invalid numbers, which causes the discontinuities in the plot. When we in addition consider that none of the calculated eigenvalues pass the eigenvalue unit test, it should be safe to conclude that our implementation of the Jacobi algorithm has been unsuccessful.

Even though the quality of the generated data is poor, we can still compare how the amount of similarity transformations scales with the matrix dimension $n$. The linear regression shown in Figure 2 shows that the number of iterations is of order $\mathcal{O}(n^2)$. Theoretically [3], we expect the number of iterations to be $3n^2 \sim 5n^2$, which matches our findings. When each rotation requires $4n$ floating point operations (FLOPs), Jacobi's eigenvalue method requires $12n^3 \sim 20n^3$ FLOPs in total. This is very inefficient compared with more sophisticated methods. For example, Householder's method requires only $n - 2$ iterations[3].

## VI. CONCLUSION

In this paper, we have explored how to solve discretized eigenvalue problems by diagonalization. Even though we are confident in our understanding of the algorithm used, Jacobi's eigenvalue algortihm, the data generated by our numerical calculations neither looks correct, nor pass checks against analytical values. Constricted by time, we have not been able to find out where the implementation of the algorithm has gone wrong. We have however found that despite of its simplicity, Jacobi's method converges slowly (requires $\mathcal{O}(n^2)$ iterations), and that it's not a suitable method when the matrices become large.

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