Second Order Differential Equation as an Eigenvalue Problem

Solving the equations of a buckling spring to Schrödinger's equation for two electrons in a three dimensional harmonic oscillator well

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Abstract

We study eigenvalue problems using Jacobi's method. Dimensionless variables and scaling of equations are taken use of in order to to generalize three physical problems. This allows us to avoid changing large part of the code. The three problems investigated are a buckling spring, one and two electrons in three dimensions, trapped in an harmonic oscillator; also referred to as quantum dots. We find that the resulting eigenvectors act like the probability distribution which results from Schrodingers equation. The plotted eigenvectors for all three problems display very similar behavior. Also, the measured time needed for our self-made solve class is long. Compared to Armadillo's eigenvalue solver, the Jacobi method is very inefficient. Its iterations are proportional to n^2 and for a matrix dimension between $50 - 200$, the run time is also proportional to n^2. In general, matrix size and the determined interval have a great impact on accuracy. The code can be found at Github repository.

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1 Introduction

Ordinary differential equations appear in all types of physical problems. By discretizing the continuous equation, we can solve them numerically. Several of these can be solved as eigenvalue problems. An important necessity is scaling of equations. Creating a general program to solve such an issue, which then can be used for many physical problem, we make use of a Toeplitz matrix and the Jacobi rotation method. As long as the initial differential equation can be manipulated to match the basic one, we can simply add values to the diagonal elements.

Firstly, the ordinary differential equation is presented as an eigenpair problem. Then three different physical problems more in detail; buckling spring problem, one electron and two electrons in 3 dimensions, trapped in an harmonic oscillator potential. For the two electrons, the Coulomb interaction must be accounted for. Further, the Jacobi method for solving the eigenpair problems is explained. The results for the different problems are presented, which includes the time needed to solve and plotting the eigenpairs. Finally, the results are discussed, comparing the vectors for the different problems and verifying results with the analytical eigenvalues.

2 Methods

2.1 Discretization of the second derivative

Given an ordinary second order differential equation

$$\frac{d^2u(\rho)}{d\rho^2} + V(\rho)u(\rho) = -\lambda u(\rho) \tag{1}$$

and appliying Dirichlet boundary conditions, that is $\rho \in (0,1)$ and $u(0) = u(1) = 0$, u'' can be written as

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

Neglecting the error term $O(h^2)$, u'' can be approximated with

$$u'' \approx -\frac{u_{i+1} + u_{i-1} - 2u_i}{h^2}, \qquad for\ i = 1, ..., N-1 \tag{3}$$

where h stands for the stepsize given by the number of integration points N. Thus, eq. 1 can be rewritten as

$$-\frac{u(\rho_{i+1}) + u(\rho_{i-1}) - 2u(\rho_i)}{h^2} + V(\rho_i)u(\rho_i) = \lambda u(\rho_i). \tag{4}$$

Further, to modify the differential equation the equation can also be written as an eigenvalue problem (see 6.1 for deviation)

$$\begin{bmatrix} d & a & 0 & 0 & \dots & 0 & 0 \\ a & d & a & 0 & \dots & 0 & 0 \\ 0 & a & d & a & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & a & d & a \\ 0 & \dots & \dots & \dots & \dots & a & d \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \dots \\ u_{N-2} \\ u_{N-1} \end{bmatrix} = \lambda \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \dots \\ u_{N-2} \\ u_{N-1} \end{bmatrix}. \tag{5}$$

The diagonal elements are defined as $d = 2/h^2 + V(\rho_i)$ and the non-diagonal ones as $a = -1/h^2$. Note that the enpoints, u_0 and u_N, are not included and that the matrix is symmetric.
Chapter 1.2 and 1.3 in Tom Lyche's lecture notes (ref. [3]) present a detailed discussion of tridiagonal matrices and two-point boundary value problems.

2.2 Buckling spring problem

The starting point for modelling the spring is Newtons second law given as a differential equation

$$\gamma \frac{d^2u(x)}{dx^2} = -Fu(x). \tag{6}$$

The above equation can also be interpreted as a classical wave function in one dimension. The spring(length L) $x \in [0, L]$ experiences a force F at $(L, 0)$ in the direction towards the origin. The following vertical displacement of the beam in the y direction is given by $u(x)$. The material constant γ describes the specific properties of the material such as rigidity. Further, Dirichlet boundary conditions are applied, which set $u(0) = u(L) = 0$.
In our case, the parameters F and L are known. Thus, we are left with an eigenvalue problem in order to find γ.
To simplify the calculations, we introduce a dimensionless variable ρ

$$\rho = \frac{x}{L} \qquad \rho \in [0, 1]. \tag{7}$$

Rewriting eq. 6 we get

$$\frac{d^2u(\rho)}{d\rho^2} = -\frac{FL^2}{\gamma}u(\rho) = -\lambda u(\rho), \tag{8}$$

where $\lambda = FL^2/\gamma$.
Discretization of u'' leads to the described eigenvalue problem in 2.1 with $V(\rho) = 0$ for all ρ. This potential shall be referred to as $V0$.
Given matrix (5) and $V(\rho) = 0$ for all ρ, this eigenvalue problem has analytical eigenpairs:

$$\lambda_j = d + 2a\cos(\frac{j\pi}{N}), \quad j = 1, 2, \dots N-1 \tag{9}$$

$$\mathbf{u}_j = [\sin(\frac{j\pi}{N}), \sin(\frac{2j\pi}{N}), ..., \sin(\frac{(N-1)j\pi}{N})]^T, \quad j = 1, 2, \dots N-1. \tag{10}$$

Additionally, an excellent description of this matrix is provided by Tom Lyche lecture notes (ref. [3]).

2.3 Quantum dots in three dimensions - one electron

We shall look at the solution of the radial part of Schrödinger's equation for one electron. Assuming the potential is spherical symmetric, the radial part of Schrödinger's differential equation reads

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}-\frac{l(l+1)}{r^2}\right)R(r)+V(r)R(r)=ER(r). \tag{11}$$

In our case $V(r)$ is the harmonic oscillator potential $(1/2)kr^2$ with $k=m\omega^2$, E is the energy of the harmonic oscillator in three dimensions and ω is the oscillator frequency (see 6.2 for the different energy states).
In spherical coordinates, the radius of the electron, r, has theoretically a range from $[0,\infty]$. Looking solely at the ground state, the orbital momentum, l, is set to zero. Substituting $R(r)=u(r)/r$, the boundary conditions change to $u(0)=u(\infty)=0$. Additionally, by introducing a dimensionless variable $\rho=(1/\alpha)r$ (α is a constant with dimension length) the potential can be written as:

$$V(\rho)=\frac{1}{2}k\alpha^2\rho^2. \tag{12}$$

Inserting the newly defined variables into eq. 11 and multiplying with $2m\alpha^2/\hbar^2$ on both sides gives

$$-\frac{d^2}{d\rho^2}u(\rho)+\frac{mk}{\hbar^2}\alpha^4\rho^2u(\rho)=\frac{2m\alpha^2}{\hbar^2}Eu(\rho). \tag{13}$$

To simplify, we set

$$\frac{mk}{\hbar^2}\alpha^4=1, \tag{14}$$

that is

$$\alpha=\left(\frac{\hbar^2}{mk}\right)^{1/4}. \tag{15}$$

Schrödinger's equation can now be written as

$$-\frac{d^2u(\rho)}{d\rho^2}+\rho^2u(\rho)=\lambda u(\rho), \tag{16}$$

where $\lambda=\frac{2m\alpha^2}{\hbar^2}E$.
Discretization of u'' leads to the described eigenvalue problem in 2.1 with $V(\rho)=\rho^2$. This potential shall be referred to as $V1$. Note that the step size h is defined as

$$h=\frac{\rho_N-\rho_0}{N}, \tag{17}$$

where $\rho_0=0$ and $\rho_N=\infty$. However, since we can not set $\rho_N=\infty$, ρ_N must be replaced by ρ_{max}, which will be determined during computations.

2.4 Quantum dots in three dimensions - two electrons

For this part, we shall look at two electrons confined in a harmonic oscillator. Compared to the problem in 2.3, the repulsive Coulomb interaction between the two electrons must now be considered as well.
The radial Schrödinger equation for two electrons reads

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr_1^2} - \frac{\hbar^2}{2m}\frac{d^2}{dr_2^2} + \frac{1}{2}kr_1^2 + \frac{1}{2}kr_2^2\right) u(r_1, r_2) = E^{(2)}u(r_1, r_2), \tag{18}$$

where $u(r_1, r_2)$ represents the two-electron wave function and $E^{(2)}$ for the two-electron energy.
To simplify, we introduce the relative coordinate $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and the center-of-mass coordinate $\mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$. Inserting the newly defined variables into eq. 18 yields

$$\left(-\frac{\hbar^2}{m}\frac{d^2}{dr^2} - \frac{\hbar^2}{4m}\frac{d^2}{dR^2} + \frac{1}{4}kr^2 + kR^2\right) u(r, R) = E^{(2)}u(r, R). \tag{19}$$

The ansatz for the wave function, $u(r, R) = \psi(r)\phi(R)$, is used to separate the equations for r and R. Thus, the energy $E^{(2)}$ is given by the sum of the relative energy E_r and the center-of-mass energy E_R

$$E^{(2)} = E_r + E_R. \tag{20}$$

The Coulomb interaction can be modeled by

$$V(r_1, r_2) = \frac{\beta e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} = \frac{\beta e^2}{r}, \tag{21}$$

with $\beta e^2 = 1.44$ eVnm.
Setting this term into the r-dependent Schrödinger equation, we get

$$\left(-\frac{\hbar^2}{m}\frac{d^2}{dr^2} + \frac{1}{4}kr^2 + \frac{\beta e^2}{r}\right)\psi(r) = E_r\psi(r). \tag{22}$$

Note that eq. 22 has the same form as eq. 11. We proceed as above. Introducing a dimensionless variable $\rho = r/\alpha$ and rearrangement leads to

$$-\frac{d^2}{d\rho^2}\psi(\rho) + \frac{1}{4}\frac{mk}{\hbar^2}\alpha^4\rho^2\psi(\rho) + \frac{m\alpha\beta e^2}{\rho\hbar^2}\psi(\rho) = \frac{m\alpha^2}{\hbar^2}E_r\psi(\rho). \tag{23}$$

To simplify further, we introduce a new "frequency", ω_r, reflecting the strength for the oscillator potential

$$\omega_r^2 = \frac{1}{4}\frac{mk}{\hbar^2}\alpha^4. \tag{24}$$

Again, we fixate the constant α by demanding

$$\frac{m\alpha\beta e^2}{\hbar^2} = 1, \tag{25}$$

that is

$$\alpha = \frac{\hbar^2}{m\beta e^2}. \tag{26}$$

The Schrödinger equation can now be written as

$$-\frac{d^2\psi(\rho)}{d\rho^2} + \omega_r^2\rho^2\psi(\rho) + \frac{1}{\rho}\psi(\rho) = \lambda\psi(\rho), \tag{27}$$

where

$$\lambda = \frac{m\alpha^2}{\hbar^2}E. \tag{28}$$

As we are only interested in the ground state (l=0) and omitting the center-of-mass energy, discretization of ψ'' leads to the described eigenvalue problem in 2.1 with $V(\rho) = \omega_r^2\rho^2 + 1/\rho$. This potential shall be referred to as $V2$.
M. Taut's article (ref. [4]) lists analytic solutions for specific oscillator frequencies, which we shall take use of.

2.5 Mathematical properties of unitary transformations

Eigenvalue problems can be solved by applying a series of unitary transformation on a given matrix. Before looking at the actual method to solve the eigenvalue problem (here Jacobi's method), first some properties of an unitary transformations.

Preservation of orthonormality A unitary transformation preserves the orthogonality of the obtained eigenvectors. Given a symmetric matrix $\mathbf{A}$ with a set of eigenvectors $\mathbf{u_i}$,

$$\mathbf{u}_i = \begin{bmatrix} u_1 \\ \cdots \\ \cdots \\ u_n \end{bmatrix}$$

that are orthonormal

$$\mathbf{u}_j^T\mathbf{u}_i = \delta_{ij}, \tag{29}$$

let the unitary transformation be defined by $\mathbf{S}$ such that $\mathbf{S^T S} = I$.
Then, their inner product also preservers orthonormality

$$(\mathbf{Su_i})^\mathbf{T}(\mathbf{Sv_j}) = \mathbf{u_i^T S^T S u_j} = \mathbf{u_i^T I u_j} = \mathbf{u_i^T u_j} = \delta_{ij}, \tag{30}$$

where δ is the Kronecker delta.

Preservation of eigenvalues Given the matrices $\mathbf{A}$ (with eigenvalues $\{\lambda_i\}$ and eigenvectors $\{\mathbf{u_i}\}$) and $\mathbf{S}$ as defined above a similar matrix $\mathbf{B}$ is defined as:

$$\mathbf{B} = \mathbf{S}^T\mathbf{AS} \tag{31}$$

has the same eigenvalues as $\mathbf{A}$. Multiplying

$$\mathbf{A}\mathbf{u_i} = \lambda \mathbf{u_i} \tag{32}$$

with $\mathbf{S^T}$ on the left side and inserting $\mathbf{S^T S} = I$ between $\mathbf{A}$ and $\mathbf{u_i}$ results in

$$(\mathbf{S^T A S})(\mathbf{S^T u_i}) = \lambda(\mathbf{S^T u_i}) \tag{33}$$

which is the same as

$$\mathbf{B}(\mathbf{S^T u_i}) = \lambda(\mathbf{S^T u_i}). \tag{34}$$

In other words, $\mathbf{B}$ has eigenvectors of the form $\mathbf{S^T u_i}$ with eigenvalues λ_i.

Similar transform eigenvectors er orthonormal If a matrix $\mathbf{A}$ has orthonormal eigenvectors, then a similar matrix $\mathbf{B}$ has orthonormal eigenvectors as well. Making use of the results above, that is using that $\mathbf{B}$ has eigenvectors of the form $\mathbf{S^T u_i}$, their dot product is given by

$$(\mathbf{S^T u_i})^T(\mathbf{S^T u_j}) = (\mathbf{u_i^T S})(\mathbf{S^T u_j}) = \mathbf{u_i^T u_j} = \delta_{ij}. \tag{35}$$

2.6 Jacobi Method

The Jacobi method guarantees a solution for a given eigenvalue problem for all real symmetric matrices. The method rotates the initial matrix in a series of similarity transformations. By eliminating the off-diagonal elements, the eigenvalues appears along the diagonal. The corresponding eigenvectors, however, do change. For a real and symmetric $n \times n$ matrix $\mathbf{A}$ we get

$$\mathbf{S}^T\mathbf{A}\mathbf{S} = diag(\lambda_1\lambda_2 \dots \lambda_n). \tag{36}$$

where $\mathbf{S}$ is the transformation matrix and λ are the eigenvalues.
In order to understand this transformation, we first look at the transformation matrix $\mathbf{S}$, also called a unitary matrix. The transformation matrix is orthogonal since its inverse is equal to its transpose

$$\mathbf{S}^T = \mathbf{S}^{-1}.$$

In $\mathbb{R}^2$, the transformation matrix is given by

$$\mathbf{S} = \begin{bmatrix} cos(\theta) & sin(\theta) \\ -sin(\theta) & cos(\theta) \end{bmatrix}$$

and θ denotes the degree for the plane rotation in the Euclidean two dimensional space.
In $\mathbb{R}^3$, the rotation along the x, y and z axis respectively are

$$R_x = \begin{bmatrix} 1 & 0 & 0 \\ 0 & cos(\theta) & sin(\theta) \\ 0 & -sin(\theta) & cos(\theta) \end{bmatrix} \quad R_y = \begin{bmatrix} cos(\theta) & 0 & sin(\theta) \\ 0 & 1 & 0 \\ -sin(\theta) & 0 & cos(\theta) \end{bmatrix} \quad R_z = \begin{bmatrix} cos(\theta) & sin(\theta) & \\ -sin(\theta) & cos(\theta) & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Generally, a rotation in $\mathbb{R}^n$ is given by

$$S(k,l,\theta) = \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \begin{array}{ccccccc} & & l & & k & & \end{array} \\ \begin{bmatrix} 1 & \dots & 0 & \dots & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & & \vdots & & \vdots \\ 0 & \dots & cos(\theta) & \dots & sin(\theta) & \dots & 0 \\ \vdots & & \vdots & \ddots & \vdots & & \vdots \\ 0 & \dots & -sin(\theta) & \dots & cos(\theta) & \dots & 0 \\ \vdots & & \vdots & & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & \dots & 0 & \dots & 1 \end{bmatrix} \end{array} \begin{array}{c} \\ \\ l \\ \\ k \\ \\ \\ \end{array}$$

$cos(\theta)$ and $sin(\theta)$ are now placed in the l$^{\text{th}}$ row and l$^{\text{th}}$ column and k$^{\text{th}}$ row and k$^{\text{th}}$ column (ref. [2]).
The similarity transformation

$$\mathbf{A}' = \mathbf{S}^T(k,l,\theta) \cdot \mathbf{A} \cdot \mathbf{S}(k,l,\theta) \tag{37}$$

rotates row and column k and l of $\mathbf{A}$ an angle θ such as the entries $\mathbf{A}'(k,l)$ and $\mathbf{A}'(l,k)$ become zero. The new entries for $\mathbf{A}'$ are given with

$$a'_{ii} = a_{ii} \quad i \neq k, i \neq l \tag{38}$$
$$a'_{ik} = a_{ik}cos(\theta) - a_{il}sin(\theta) \quad i \neq k, i \neq l \tag{39}$$
$$a'_{il} = a_{il}cos(\theta) + a_{ik}sin(\theta) \quad i \neq k, i \neq l \tag{40}$$
$$a'_{kk} = a_{kk}cos^2(\theta) - 2a_{kl}cos(\theta)sin(\theta) + a_{ll}sin^2(\theta) \tag{41}$$
$$a'_{ll} = a_{ll}cos^2(\theta) + 2a_{kl}cos(\theta)sin(\theta) + a_{kk}sin^2(\theta) \tag{42}$$
$$a'_{kl} = (a_{kk} - a_{ll})cos(\theta)sin(\theta) + a_{kl}(cos^2(\theta) - sin^2(\theta)) \tag{43}$$

The goal is to end up with zero on all the non-diagonal elements a'_{kl}. Which is done by forcing them to be 0 and solving the following equation:

$$a'_{kl} = (a_{kk} - a_{ll})cos(\theta)sin(\theta) + a_{kl}(cos^2(\theta) - sin^2(\theta)) = 0. \tag{44}$$

For each iteration, θ must be chosen accordingly. Given the quantity $tan(\theta) = sin(\theta)/cos(\theta)$, abbreviated with $t = s/c$, and defining

$$\tau = \frac{a_{ll} - a_{kk}}{2a_{kl}}, \tag{45}$$

we get

$$t^2 + 2\tau t - 1 = 0. \tag{46}$$

The solutions for t are

$$t = -\tau \pm \sqrt{1 + \tau^2}. \tag{47}$$

In order to ensure maximal numerical stability the smallest root is chosen, which corresponds to the smaller rotation. Additionally, eq. 47 is rewritten as

$$1/(\tau \pm \sqrt{1+\tau^2}). \tag{48}$$

Consequently, c and s can be expressed as

$$c = \frac{1}{\sqrt{1+t^2}} \tag{49}$$

and $s = t/c$.
In the case of $a_{kl} = 0$, we have $cos(\theta) = 1$ and $sin(\theta) = 0$.
The Jacobi Method is an iterative method, thus this procedure is repeated until the sum over the squared non-diagonal matrix elements, $off(\mathbf{A})$, are less than a prefixed test, ϵ, (ideally equal zero). That is

$$off(\mathbf{A}) = \sqrt{\sum_{i=1}^{n} \sum_{j=1, j\neq i}^{n} = |a_{ij}|^2} < \epsilon \tag{50}$$

Since this is quite a time-consuming test, it can be replaced by finding the largest (absolute) value of the off-diagonal elements.

$$max|a_{ij}| < \epsilon \quad i \neq j. \tag{51}$$

Meaning i and j become the new indices equivalent to k and l. Even though $\mathbf{A}'(k,l)$ and $\mathbf{A}'(l,k)$ are set to zero for one iteration, these entries may become different from zero in the next iteration, which slows down the algorithm. The convergence rate can be approximated with $3n^2 - 5n^2$ rotations, where each rotation requires $4n$ operations. In other words, in order to zero out the non-diagonal matrix elements, it takes about $12n^3 - 20n^3$ operations. The mathematical problem is further described here ref. [1].

2.6.1 Code Implementation

We define n as $n = N - 1$.

Algorithm 1 Jacobi's method

while $max_{i \neq j} |a_{ij}| < \epsilon$ **do**
  $a_{kl} = max_{i \neq j} |a_{ij}$
  if $a_{lk} \neq 0$ **then**
    $\tau = (a_{ll} - a_{kk})/(2.0 a_{kl})$
    if $\tau \geq 0$ **then**
      $t = 1.0/(\tau + \sqrt{1.0 + \tau^2})$
    else
      $t = -1.0/(-\tau + \sqrt{1.0 + \tau^2})$
    end if
    $c = 1.0/\sqrt{1.0 + t^2}$
    $s = c \cdot t$
  else
    $c = 1.0$
    $s = 0.0$
  end if
  for $i = 0, 1, ..., n - 1$ **do**
    $a'_{kk} = a_{kk} c^2 - 2 a_{kl} c \cdot s + a_{ll} s^2$
    $a'_{ll} = a_{ll} c^2 + 2 a_{kl} c \cdot s + a_{kk} s^2$
    $a'_{kl} = 0$
    $a'_{l,k} = 0$
    if $i \neq k$ & $i \neq l$ **then**
      $a'_{ik} = a_{ik} c - a_{il} s$
      $a_{ki} = a_{ik}$
      $a'_{il} = a_{il} c + a_{ik} s$
      $a'_{li} = a_{il}$
    end if
  end for
end while

The code was tested with several unit test, described on the Github repository.

3 Results

3.1 Convergence Rate

In order to study the convergence rate of the Jacobi method for the buckling spring problem, figure 1 shows how many similarity transformations are needed to get all non-diagonal matrix elements essentially zero, for different matrix dimensionalities. The function has been approximated with a second order polynomial, $\sim 1.8n^2$, also displayed in the label. The stepsize Δn for the datapoints is 10.

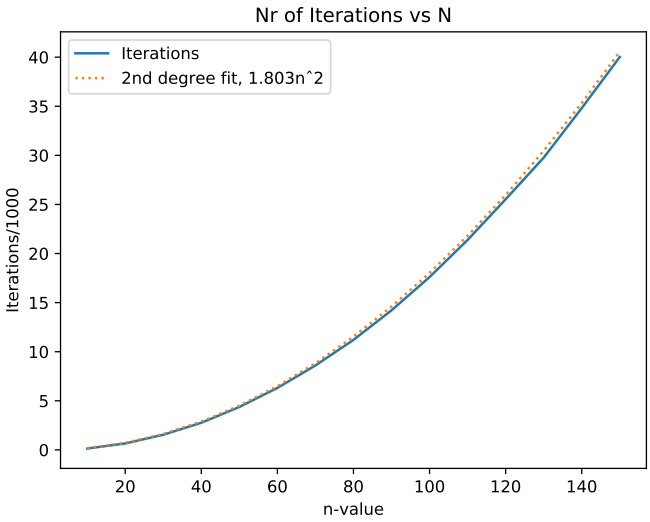

Figure 1: Number of iterations as a function of matrix dimension, n, (stepsize $\Delta n = 10$) needed for solving the buckling spring problem; label shows fitted approximated polynomial

3.2 CPU time

In section 2.6 we mentioned that the Jacobi method is relatively slow. Figure 2 shows the time needed to solve the eigenpair problem for the buckling spring with the Jacobi method and Armadillo, given different matrix dimensionalities, n. In other words, we measured the time needed for the initial matrix to be diagonalized and computing its eigenvectors. The figure also shows a second degree polynomial that is fit to the data points for the Jacobi method run time for $n > 50$.

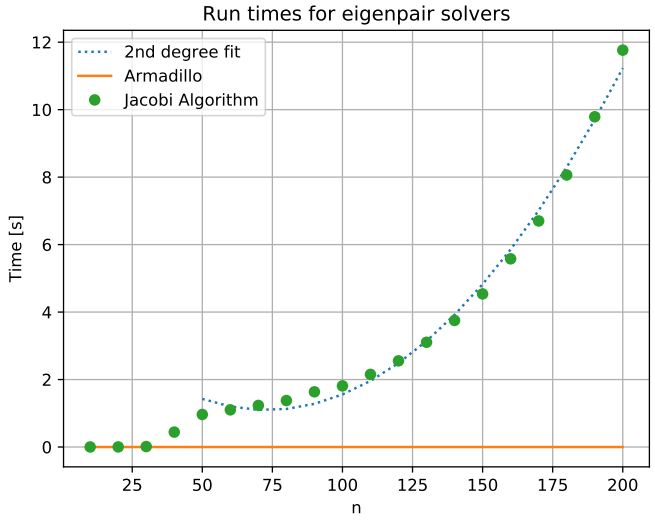

Figure 2: Jacobi and Armadillo run time for solving buckling spring eigenpair problem as a function of matrix dimension, n. A second degree fit for the Jacobi algorithm is also shown for $n > 50$.

3.3 Buckling Spring

For the buckling spring problem, we plotted the three eigenvectors for the lowest eigenvalues in figure 3 with $n = 300$. The eigenvectors computed with Armadillo's function for solving eigenvalue problems. The eigenvectors computed with Armadillo's function served as comparison for solving the eigenvalue problems. The solution of eigenvalues with both methods are approximately equally. "Num" stands for the numerical solution obtained with the Jacobi algorithm and "Arma" for Armadillo. The vertical displacement of the spring, $u(\rho)$ is given as a function of position, ρ. Note that Jacobi's and Armadillo's eigenvectors for $\lambda = 9.8695$ and $\lambda = 88.8190$ are alike. For $\lambda = 39.4770$ only the plus minus sign is changed.

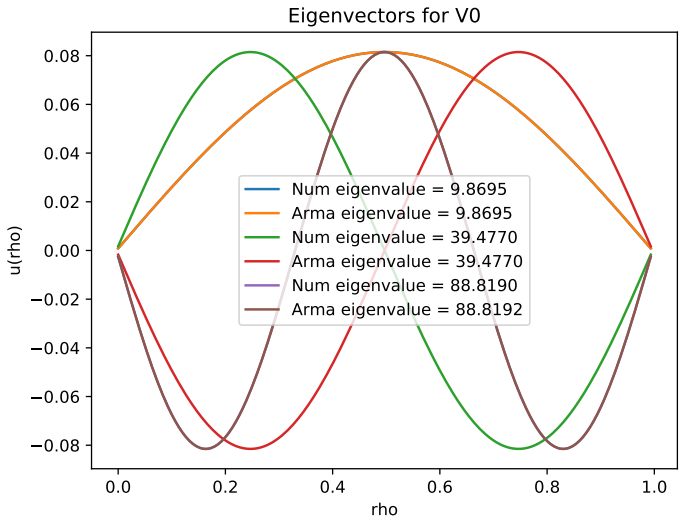

Figure 3: The plots shows the eigenvectors, $u(\rho)$, for the three first eigenvalues found with both the Jacobi Algorithm, "Num", and Armadillo, "Arma", for the buckling spring, as function of position ρ ($n = 300$).

3.4 Quantum Dots in three dimensions - one electron

Adding the harmonic oscillator potential to the tridiagonal matrix (see 2.3), the three eigenvectors for the lowest eigenvalues are displayed in figure 4. Note that the boundary interval has changed from $[0, 1]$ to $[0, \rho_{max}]$. The computational analysis states that, in order to reproduce the analytical results with four leading digits after the decimal point, $\rho_{max} \approx 4.6$ and $n \approx 400$. These values were determined by trial and error, slightly adjusting each time. ρ represents the absolute position of the electron. In addition, we plotted $u(\rho)^2$ (figure 5) which is proportional to the probability density, $\psi(\rho)$.

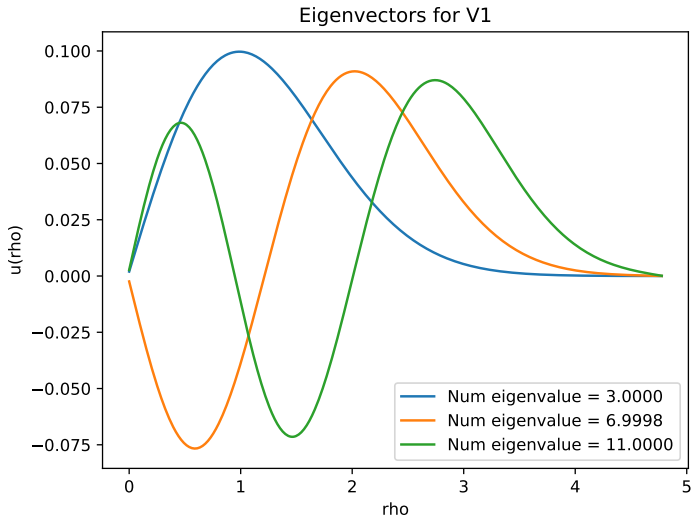

Figure 4: The eigenvectors, $u(\rho)$, as a function of absolute position, ρ, for the three lowest eigenvalues in the 3D quantum dots problem for one electron, using Jacobi's method, $n = 400$, $\rho_{max} = 4.6$.

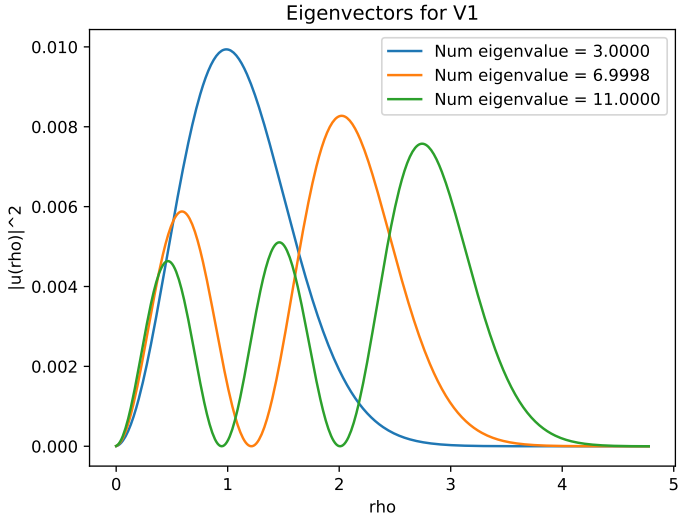

Figure 5: The eigenvectors squared, $|u(\rho)|^2$, as a function of absolute position, ρ, for the three lowest eigenvalues in the 3D quantum dots problem for one electron, using Jacobi's method, $n = 400$, $\rho_{max} = 4.6$.

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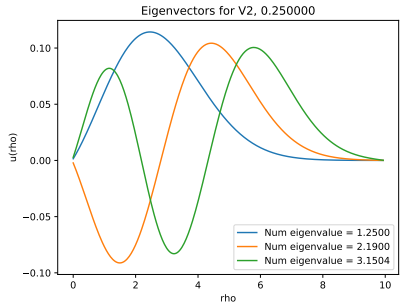
3.5 Quantum Dots in three dimensions - two electrons

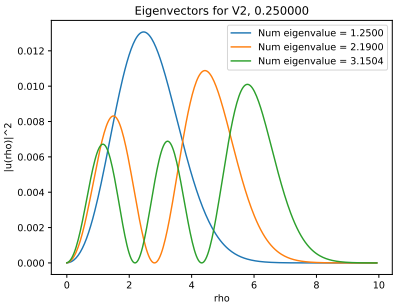
The following figures below present the repulsive Coulomb interaction of two electrons in a varying harmonic oscillator. As above, the ground state and two excited states are plotted. ρ now represents the position of one electron relative to the other one. Computation showed that the appropriate boundary changed with ω_r. Figure 6a displays the results for $\omega = 1/4$, $\rho_{max} = 10$, figure 6c for $\omega = 1/20$, $\rho_{max} = 20$, and figure 6e for $\omega = 1/54.7386$, $\rho_{max} = 30$. The matrix size was chosen to be $n = 300$.
Table 1 summaries the results for the ground state by displaying both the analytical and Jacobi eigenvalues for the different frequencies. Finally, we plotted $u(\rho)^2$ (figures 6b, 6d, 6f) which is proportional to the probability density, $\psi(\rho)$.

Table 1: 3D Quantum dots - two electrons: Analytical, λ_a, and numerical,λ_n, (Jacobi method: $\rho_{max1} = 9$, $\rho_{max2} = 20$, $\rho_{max3} = 30$ and $n = 300$) lowest eigenvalues for given frequency, w_r. Analytical values taken from ref. [4].

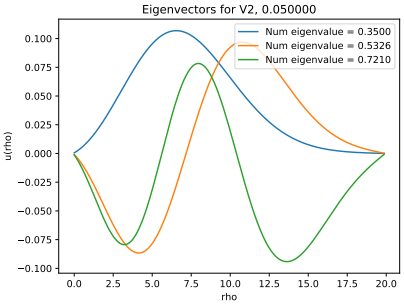
ω_r	λ_a	λ_n
1/4	1.250	1.250
/20	0.350	0.350
1/54.7380	0.164	0.164



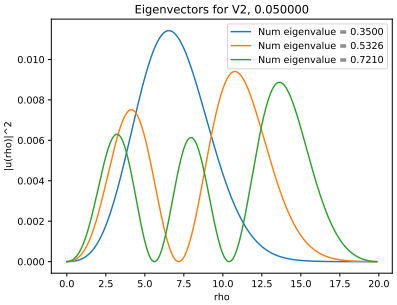
(a) $u(\rho)$ for $\omega_r = 1/4$



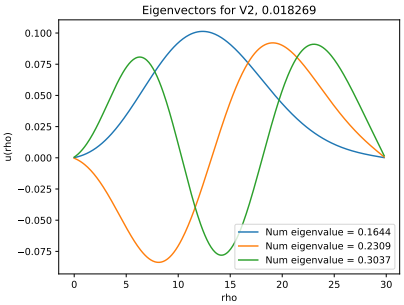
(b) $|u(\rho)|^2$ for $\omega_r = 1/4$



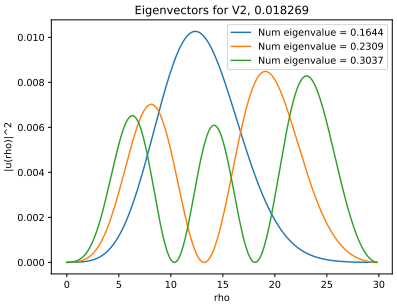
(c) $u(\rho)$ for $\omega_r = 1/20$



(d) $|u(\rho)|^2$ for $\omega_r = 1/20$



(e) $u(\rho)$ for $\omega_r = 1/54.7386$



(f) $|u(\rho)|^2$ for $\omega_r = 1/54.7386$

Figure 6: 3D Quantum dots - two electrons: Figures on the left showing the three lowest eigenvectors, $u(\rho)$, as a function of relative position (ρ) using the Jacobi algorithm, $n = 300$ and varying frequencies ω_r. Figures on the right show corresponding probability density, $|u(\rho)|^2$.

4 Discussion

4.1 Convergence Rate

As described in section 2.6, we expected that the convergence rate for the Jacobi method is proportional to n^2. The results match these expectations, indicating that the implementation was successful. The iterations is stopped either by a predetermined number of max iterations (given as n^3) or by a tolerance factor depending on which limit it reaches first. The tolerance factor, ϵ, is set to 10^{-8}. As the convergence rate is proportional to n^2, it is the tolerance factor terminating the iteration.
Further investigations could include lowering the tolerance factor and the number of max iterations. Limitations due to machine precision must then also be taken into account.

4.2 CPU time

Generally, more time is needed to solve the buckling spring if the dimensionality of the matrix increases. That is reasonable.
Moreover, the measured time is affected by the PC's granularity, temperature of the processor, number of chores the CPU is processing and so forth. If the time required for solving is very short, these inaccuracies have a greater impact. In other words, short time measurements are not so informative, since the precision is limited. This might explain the jump around $n = 50$. The second degree polynomial fit to the data points show that the CPU run time increases by $O(n^2)$, which is expected based on how the number of iterations increases.
However, the measurement only goes til $n = 200$. For the three physical problems, we used $n = 300 - 400$. For further investigation, the time behavior for large matrices should be observed.
In comparison, computations using the armadillo algorithm almost takes no time.

4.3 Buckling spring

First, the overlap of the eigenvectors calculated by Jacobi with those calculated by Armadillo shows that the implementation was performed correctly. The change in sign for $\lambda_3 = 39.4770$ is not a calculation error, but is based on the fact that eigenvectors can show either in the plus or minus direction.
The eigenvector $u(\rho)$ represents the displacement of the spring in the y-direction. For the ground state, $\lambda_1 = 9.8695$, $u(\rho)$ has the form of half of a sine-period. That is, the function has no node. For every excitation (here increase of the force), there is one more node. Consequently, $\lambda_2 = 39.4770$ has one node (one sine period) and $\lambda_3 = 88.8190$ has two.
If a force is applied on one end of the spring, the spring starts to bend in the middle. This deformation is reflected in the sine-top for λ_1. As more force is applied, the deformation will increase. Consequently, we get more nodes.

4.4 Quantum Dots in three dimensions - one electron

Figure 4 shows the ground state and two excited states for an electron which is captured in an harmonic oscillator potential. As in the buckling spring case, the ground state has zero nodes. For every excitation there is one more node and the extreme points are shifted to the right. We start with looking at the ground state.
As ρ represents the absolute position of the electron, $|u|^2$ presents the probability density (figure 5). For the ground state, the electron is most likely located at $\rho \approx 1.2$. The likelihood of finding the electron at $\rho > 3$ is practically zero. This is plausible. The electron has a little kinetic energy and can move to a certain extend in the potential well. However, its kinetic energy is limited and it is thus trapped in the potential well. Moreover, the total probability of finding the electron at a specific location must be 1.
If the electron becomes excited, it has more kinetic energy. Hence, it can move more freely, but is still trapped. Consequently, the probability-top, now reduced in size, shifts to the right. "To compensate", there is one more top, but much less in size, closer to origo. This is due to the additional node. Nodes indicate regions where an electron has zero probability of being found. Similarly for the second excited state, there are three tops. Generally, the probability of finding an electron farther away from origo increases with excitation.

4.5 Quantum Dots in three dimensions - two electrons

This case has a similar interpretation as the one electron case. What is changing it that ρ now represents the relative distance between the two electrons and ω_r determines the strength of the potential well. Furthermore, the electrons experience a repulsive Coulomb force. Table 1 shows that the computed eigenvalues match with the analytical ones. This indicates that the implementation was successful. As the the frequency decreases, so does the eigenvalue which is proportional to the relative energy.
Continuing with figure 6a and figure 6b, the ground state has zero nodes. The most probable distance is $\rho \approx 6$. As the electrons get excited, they have more kinetic energy and are statistically seen further apart. The first node, at $\rho \approx 3$, is a distance of zero probability.
For the figures 6c and 6d, the potential well becomes broader, since ω decreases. Consequently, the electrons have more space and their average distance increases. The same applies to figures 6e and 6d. Here, the most probable distance for the ground state is $\rho \approx 14$.
Further, the repulsive Coulomb force ensures that the probability of finding the two electrons attached to one another is zero.

5 Conclusion

We have looked at three physical problems by using the Jacobi method: buckling spring, 3D quantum dots for one and two electrons. Results have shown that

the Jacobi method is quite ineffective. Iterations are proportional to n^2 and for a matrix dimension between $50 - 200$, the run time is also proportional to n^2. Solving the equations with Armadillo almost took no time. Thus, future work should include making the code more efficient. It could be useful to use another, more efficient method. The Householder method, for example, is a popular and well-functioning alternative.
In all three physical problems, the analytical results match well with the Jacobi ones. The Jacobi method is therefore a correct functioning algorithm.
The buckling spring problem modeled how the spring is deformed if a force is applied. Computations were done for $\rho \in [0, 1]$ and $n = 200$ and plotting the three lowest eigenvectors. The more force is applied, the greater is the deformation. Further investigation could include varying the applied force both in strength and direction.
Going over to the quantum mechanical problems, the results for the one electron case showed the behavior of a trapped electron in an harmonic oscillator. The matrix dimension must be increased to $n = 400$ and the interval changed to $\rho \in [0, 4.6]$. The more excited the electron becomes, the more kinetic energy it has, the further away from origo it is probable to find.
Adding Coulomb interactions and varying the strength of the harmonic oscillator potential, we computed the relative distance between two electrons with $n = 300$ and $\rho \in [0, \rho_{max}]$ ($\rho_{max1} = 10, \rho_{max1} = 20, \rho_{max1} = 30$). The Coulomb force ensures that the electrons do not touch one another. A weaker, that is broader, harmonic oscillator potential increases the average distance between the electrons. In future work, the accurate interaction of ρ_{max} and n could be studied more closely.
Generally, the dimension of the initial matrix and the the observed interval must be chosen carefully in order to get correct results.

6 Appendix

6.1 Discretization as an eigenvalue problem

A second order differential equation, such as (1), can be written as a linear set of equations of the form

$$\mathbf{Au} = \lambda \mathbf{u},$$

where $\mathbf{A}$ is an $n \times n$ tridiagonal matrix and λ is an eigenvlaue corresponding to the eigenvector, $\mathbf{v}$.
Following on from eq. 4, the set of equation for $\lambda_i \mathbf{u_i}$ is given by

$$\frac{1}{h^2}(-u_{i+1} - u_{i-1} + 2u_i) + V_i u_i = \lambda_i \mathbf{u_i} \tag{52}$$

Rearranging the equation gives

$$\frac{1}{h^2}(-u_{i-1} + 2u_i - u_{i+1}) + V_i u_i = \lambda_i \mathbf{u_i} \tag{53}$$

Determining the equations for the boundary condition, $i = 0$ holds

$$\begin{aligned} \frac{1}{h^2}(-u_0 + 2v_1 - u_2) + V_1 u_1 &= \lambda_i \mathbf{u_i} \\ \frac{1}{h^2}(0 + 2u_1 - u_2) + V_1 u_1 &= \lambda_i \mathbf{u_i} \end{aligned} \tag{54}$$

since $v_0 = 0$. Given $v_{n+1} = 0$, similarly for $i = n$ applies

$$\begin{aligned} \frac{1}{h^2}(-u_{n-1} + 2u_n - u_{n+1}) + V_n u_n &= \lambda_i \mathbf{u_i} \\ \frac{1}{h^2}(-u_{n-1} + 2u_n - 0) + V_n u_n &= \lambda_i \mathbf{u_i} \end{aligned} \tag{55}$$

A combination of the above equations results in

$$\frac{1}{h^2}(2u_1 - u_2) + V_1 u_1 = \lambda_i \mathbf{u_i} \tag{56}$$

$$... \tag{57}$$

$$\frac{1}{h^2}(-u_{i-1} + 2u_i - u_{i+1}) + V_i u_i = \lambda_i \mathbf{u_i} \tag{58}$$

$$... \tag{59}$$

$$\frac{1}{h^2}(-u_{n-1} + 2u_n) + V_n u_n = \lambda_i \mathbf{u_i} \tag{60}$$

Thus, there are $n - 1$ equations that must be computed ($i \in [1, n-1]$). The set of equations can be rewritten in matrix-form, where $\mathbf{A} \in \mathbb{R}^{n \times n}$ and $\mathbf{u}, \lambda \in \mathbb{R}^n$

$$\begin{bmatrix} d & a & 0 & \dots & \dots & \dots \\ a & d & a & \dots & \dots & \dots \\ & a & d & a & \dots & \dots \\ & \dots & \dots & \dots & \dots & \dots \\ & & & a & d & a \\ & & & & a & d \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \dots \\ \dots \\ \dots \\ u_n \end{bmatrix} = \begin{bmatrix} \lambda_1 \mathbf{u_1} \\ \lambda_2 \mathbf{u_2} \\ \dots \\ \dots \\ \dots \\ \lambda_{n-1} \mathbf{u_{n-1}} \end{bmatrix}.$$

The diagonal elements are defined as $d = 2/h^2 + V_i$ and the non-diagonal ones as $a = -1/h^2$.

6.2 Quantum dots in three dimensions - Electron's energy

For one electron, given an oscillator frequency, ω, its principal quantum number, n, and an orbital momentum,l, its energy states are

$$E_{nl} = \hbar\omega \left(2n + l + \frac{3}{2}\right), \quad n = 0, 1, 2, \dots, \; l = 0, 1, 2 \dots \tag{61}$$

References

[1] Morten Hjorth-Jensen. *Computational Physics Lectures: Eigenvalue problems*. Sept. 2017. URL: http://compphysics.github.io/ComputationalPhysics/doc/pub/eigvalues/html/eigvalues.html. (accessed: 24.09.2020).

[2] *Jacobi Method: Eigenvalues and Eigenvectors*. June 2020. URL: https://www.patnauniversity.ac.in/e-content/science/physics/MScPhy58.pdf. (accessed: 17.09.2020).

[3] *Lecture Notes for numerical linear algebra*. June 2017. URL: https://www.uio.no/studier/emner/matnat/math/MAT-INF4130/h17/book2017.pdf. (accessed: 25.09.2020).

[4] M. Taut. "Two electrons in an external oscillator potential: Particular analytic solutions of a Coulomb correlation problem". In: *Physical Review 8* 48.5 (Nov. 1993). URL: http://prola.aps.org/abstract/PRA/v48/i5/p3561_1. (accessed: 24.09.2020).