Project 2

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1. Abstract

First study a buckling beam problem as a classical wave function problem in one dimension. Thereafter we extend the problem to quantum mechanics where electrons move in a three dimensional harmonic oscillator potential.

2. Introduction

This project aims to look at different numerical methods for solving eigenvalue problems, which is relevant in a lot areas of physics. In this project we will also explore the eigenvalue solver's value specifically, with a quantum mechanics problem.

We will solve the following equation:

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

where ρ and λ are the scaled values from a given differential equation representing a physical system.

3. Theory and technicalities

3.1 The problem

In this project, we are considering two wave function problems in one dimension. Generally, the differential equation we are to solve can be written like this:

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

This equation can be applied to both problems by making ρ and λ appropriate scaled values for the system in question.

Buckling beam

For the buckling beam, we are solving this differential equation:

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

where - the length of the beam is L. - $x \in [0, L]$ denotes the distance along the beam. - $u(x)$ is the vertical displacement in y -direction.

γ, F and L are known variables. We say that the scaled value $\rho = \frac{x}{L}$,making the variable ρ defined in $[0, 1]$. The boundary conditions for the scaled function $u(\rho)$ are now $u(0) = u(1) = 0$ - nice and general.

We can now rewrite 2 as:

$$-\frac{d^2u(\rho)}{d\rho^2} = \lambda u(\rho), \qquad \lambda = \frac{FL^2}{R}.$$

Quantum case

In the quantum case of the differential equation, we have one or two electrons as quantum dots in a 3-dimensional space, both stuck in a harmonic oscillator potential. They repel eachother by the static Coloumb interaction and we assume spherical symmetry. Their dynamics are represented by the radial part of the Schrödinger equation:

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

where $V(r)$ is the harmonic oscillator potential $\frac{1}{2}kr^2$ with $k = m\omega^2$ and E is the energy of the harmonic oscillator. The quantum number l is the orbital momentum of the electron, the oscillator frequency is ω and its energies are:

$$E_{nl} = \hbar\omega\left(2n + l + \frac{3}{2}\right), \qquad n = 0, 1, 2, ..., \qquad l = 0, 1, 2, ...$$

The radial position has boundary conditions $u(0) = u(\infty) = 0$. Since this is already transformed to spherical coordinates, we have $r \in [0, \infty)$. If we substitute $R(r) = \frac{1}{r}u(r)$ we get

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

Moving on, we introduce a dimensionless variable ρ which contains a variable α which we can define later.

If $\rho = \frac{1}{\alpha}r$ the equation reads:

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

Multiplying both sides by $2m\alpha^2/\hbar^2$ we get

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

We can now fix the constant α to eliminate all the constants

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

If we now define

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

the Schroedinger's equation can be rewritten as

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

which is solvable by an eigenvalue solver. The difference this time, however, is the added potential $\rho^2 u(\rho)$.

3.2 Orthogonal transformations

A unitary matrix $\mathbf{Q}$ has this property:

$$\mathbf{Q}^\dagger\mathbf{Q} = \mathbb{I} \Rightarrow \mathbf{Q}^\dagger = \mathbf{Q}^{-1}$$

where $\mathbb{I}$ is the identity.

Unitary transformations are key to the method we are implementing, so we need to make sure that it preserves the orthogonality eigenvectors we apply it on. Our starting basis being orthogonal is more formally written like this:

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

Applying our unitary matrix on these, transforms them into a new basis

$$\mathbf{w}_i = \mathbf{Q}\mathbf{v}_i.$$

Multiplying the above equation from the left with

$$\mathbf{w}_j^T = (\mathbf{Q}\mathbf{v}_j)^T$$

we get

$$\mathbf{w}_j^T \mathbf{w_i} = (\mathbf{Q}\mathbf{v}_j)^T \mathbf{Q}\mathbf{v}_i$$

$$\mathbf{w}_j^T \mathbf{w_i} = \mathbf{v}_j^T \mathbf{Q}^T \mathbf{Q}\mathbf{v}_i$$

Since $\mathbf{Q^T Q} = \mathbb{I}$,

$$\mathbf{w}_j^T \mathbf{w_i} = \mathbf{v}_j^T \mathbf{v_i} = \delta_{ij}.$$

This means our unitary transformation preserves the orthogonality of our basis.

3.3 Jacobi's method

The Jacobi eigenvalue method is an iterative method for finding eigenvalues. It is based on the idea of doing a number of unitary basis transformations on the matrix in question, with the goal of diagonalizing it.

$$\mathbf{Q}_n^\dagger \mathbf{Q}_{n-1}^\dagger ... \mathbf{Q}_1^\dagger \mathbf{A} \mathbf{Q}_1 ... \mathbf{Q}_{n-1} \mathbf{Q}_n = \mathbf{D},$$

where $\mathbf{A}$ is the starting matrix, $\mathbf{Q}_i$ are unitary matrices and $\mathbf{D}$ is diagonal, containing the eigenvalues.

Jumping back to our original differential equation 1,

Our differential equation can now be discretised into an eingenvalue problem. Using the following expression for the second derivative (from Project 1) where stepsize = h defined from the max and min value of ρ, respectively ρ_N and ρ_0.

$$u'' = \frac{u(\rho+h) - 2u(\rho) + u(\rho-h)}{h^2} - O(h^2), \qquad h = \frac{\rho_N - \rho_0}{N}$$

N: number of integration points.

Value of ρ in point i:

$$\rho_i = \rho_0 + ih \qquad i = 1, 2, \ldots, N$$

Then our equation can be rewritten for the new ρ_i

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

Compact:

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

Finally we can rewrite it as an eigenvalue problem

$$\mathbf{Au} = \lambda \mathbf{u}, \tag{3}$$

where

$$\mathbf{A} = \begin{bmatrix} d & a & 0 & 0 & \ldots & 0 & 0 \\ a & d & a & 0 & \ldots & 0 & 0 \\ 0 & a & d & a & 0 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & \ldots & \ldots & \ldots & a & d & a \\ 0 & \ldots & \ldots & \ldots & \ldots & a & d \end{bmatrix} \qquad \text{and} \qquad \mathbf{u} = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \ldots \\ u_{N-2} \\ u_{N-1} \end{bmatrix}$$

The endpoints, u_0 and u_N, are not included, and we will set $d = \frac{2}{h^2}$ and $a = -\frac{1}{h^2}$.

Now we can solve our equation numerically using Jacobi's method and compare with the analytical eingenvalues:

$$\lambda_i = d + 2a\cos(\frac{j\pi}{N+1}) \qquad j = 1, 2, \ldots, N. \tag{4}$$

In order to solve equation 3 we will implement Jacobi's rotation algorithm. But first we have to do the following: - Diagonalize a matrix with a given size($N \times N$).

- Use armadillos functions for diagonalizing. - Find analytical eigenvalues by 4 for comparison with the numerical ones.

In our Jacobi method we define the following:

$$\tan\theta = t = s/cs = \sin\theta c = cos\theta \cot 2\theta = \tau = \frac{a_{ll} - a_{kk}}{2a_{kl}}$$

We define θ so all non diagnoal elements of the transformed matrix become non-zero. Since

$$\cot 2\theta = \frac{1}{2}(\cot\theta - \tan\theta)$$

We can rewrite as..

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

giving

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

Then

$$c = \frac{1}{\sqrt{1+t^2}} \quad \text{and} \quad s = tc$$

kilde til oppgave 2 a): http://www.math.harvard.edu/archive/21b_spring_08/handouts/orthomatrix.pdf

Our method applied

The compact discretized Schroedinger equation will be

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

where $V_i = \rho_i^2$ and h is the steplength. From this it is clear that on tridiagonal matrix form it is written

$$\begin{pmatrix} d_i & e_i & 0 & \dots & \dots & \dots & 0 \\ e_i & d_i & e_i & 0 & \dots & \dots & 0 \\ 0 & e_i & d_i & e_i & 0 & \dots & 0 \\ \vdots & 0 & \ddots & \ddots & \ddots & & \vdots \\ \vdots & \vdots & & 0 & e_i & d_i & e_i \\ 0 & \dots & \dots & \dots & 0 & e_i & d_i \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{N-2} \\ u_{N-1} \end{pmatrix} = \lambda \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{N-2} \\ u_{N-1} \end{pmatrix}$$

with the diagonal elements $d_i = \frac{2}{h^2} + V_i$ and the non-diagonal elements $e_i = -\frac{1}{h^2}$.

It is now clear that the eigenvalue solver we made will be able to find these eigenvalues. However it will have to be tweaked by finding a sufficient number

of integration points, N and an approximation of ρ_{max} to infinity that yields eigenvalues close enough to the analytical ones of which the first four is $\lambda = 3, 7, 11, 15$.

With these eigenvalues it is possible to calculate the energy and position of the electron, but we will not demonstrate that here. We will instead investigate what number of integration points, N, and what approximation of infinity we can use to get sufficiently correct eigenvalues.

To do this we fix $\rho_{max} = 10$ and find the average deviation of our calculated ones from the analytical ones for $N = 100, 200, 300, 400$ and plot the error and time versus the number of integration points. This can be found in the d branch in *Code/main.cpp*

Then we fix the number of integration points to $N = 200$ and calculate the average error for the approximations $\rho_{max} = 4, 5, 6, 7, 8, 9, 10, 11$ and plot the error and time versus the approximation of ρ_{max}. This can be found in the d branch in *Code/main_rho.cpp*

Results

Quantum mechanics eigenvalue calculations

The investigation of a sufficient amount of integration points, N gave us the plot shown in figure **??**fig:int-points).

The investigation of the best approximation to infinity gave us the plot shown in

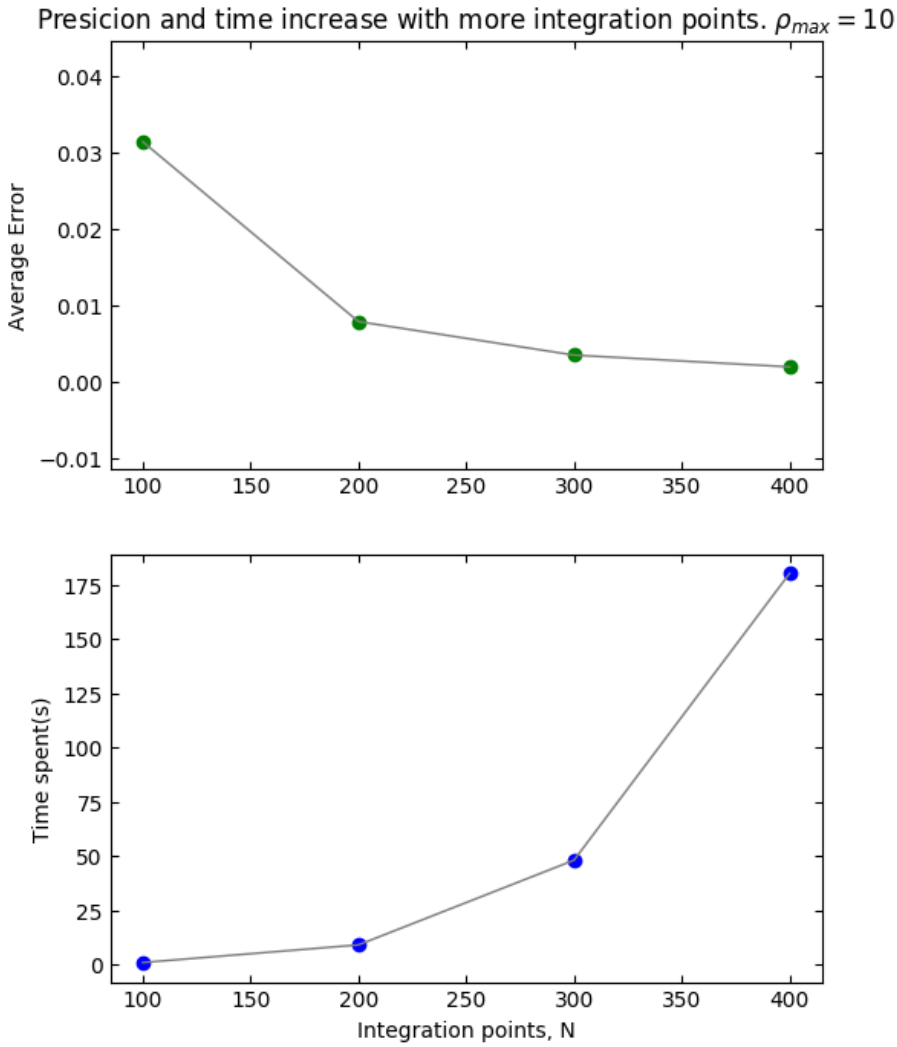

Figure 1: Shows time spent and average error vs number of integration points, N

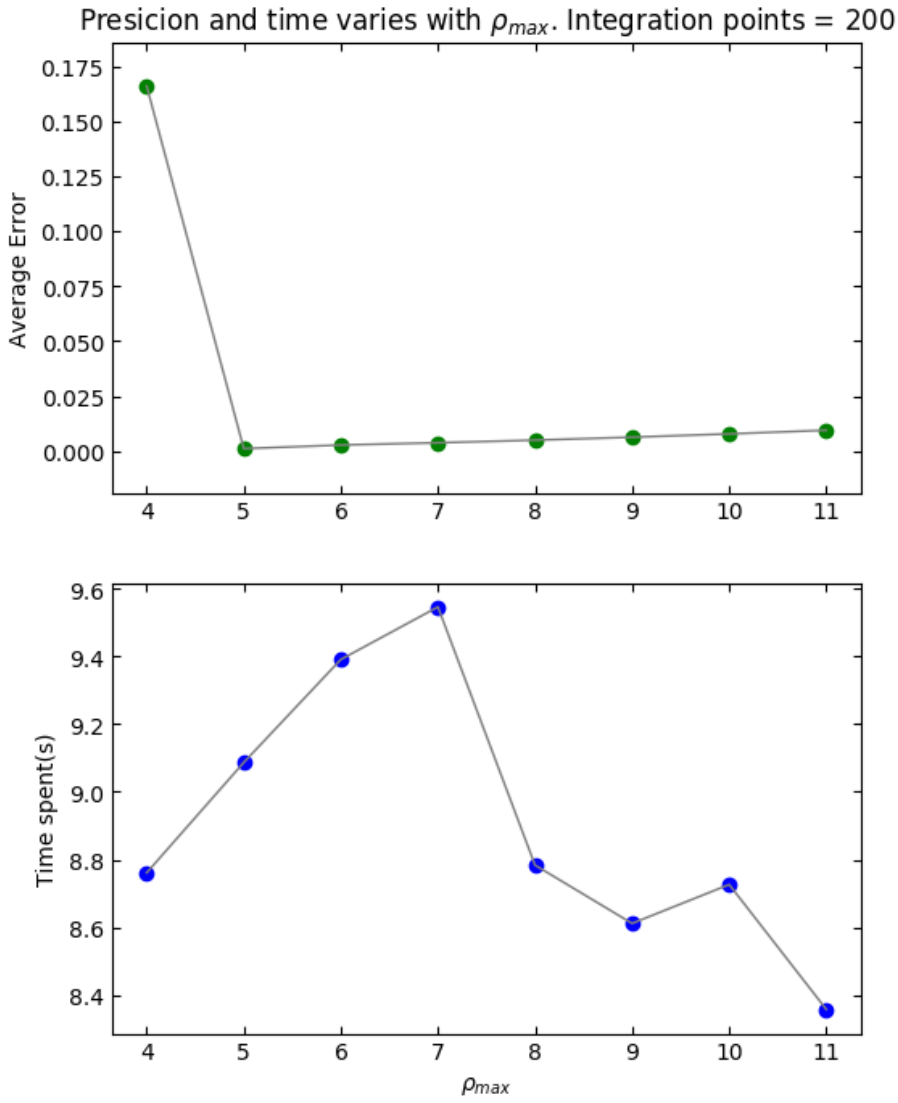

figure **??**fig:rho-approx).
It is also worth noting that all these graphs are reproducible, except the time graph of the approximation of ρ_{max} which were very different every time.

Discussion

Quantum mechanics eigenvalue calculations

From the figures presented in the results we see that while a higher number of integration points yields better results, a big downside is that the time spent

also increases.

With the changing of ρ_{max} we see that first the error decreases, but after $\rho_{max} = 5$ we actually start to see an increase in error again. This might be because a higher ρ_{max} gives a bigger step-size which again gives lower numbers on the off-diagonal elements, which in turn yields a lower amount of Jacobi rotations before the off-diagonal elements are below the tolerance for being called zero.

The time spent on the calculations seem pretty random and that is probably because the changing of ρ_{max} doesn't make the computer do any more or less work, it simply changes the numbers. The fluctuations might therefore just be that the computer has different background tasks running at different times.