Eigenvalue problem, from the equations of a buckling beam to Shroedinger'equation for two electrons in a three-dimentional harmonic oscillator well

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In this project we have investigated the eigenvalue problem for a buckling beam as well as Schrodinger's equation for one and two electrons. Jacobi's method was used to find the eigenvalues of the matrices. The method was easy to implement and gave the correct eigenvalues up to four decimals for a 200×200 matrix. It was, however, much slower than eg. Armadillo's *eigsys* function. For two electrons in a potential well, we saw that an increased value of the potential would also increase the eigenvalue for that system.

I. INTRODUCTION

In this project, a thorough investigation of the eigenvalue problem will be conducted. We will start with the two-point boundary value problem of a buckling beam or a spring fastened at both ends. This is one of the problems which has analytical solutions. Thereafter, by simply adding a new variable along the diagonal elements, we can study quantum mechanical problems. In particular, we will study the harmonic oscillator problem in three dimensions, with one or two electrons. For the latter case we can study the role of the repulsive Coulomb interaction and extract interesting physics results. For selected frequencies, this interacting two-electron problem exhibits analytical solutions, one of the few cases of an interacting system where we can find analytical solutions. See M. Taut, 1993 [3], for the derivation of analytical expressions for the eigenpairs. To solve the eigenvalue problems numerically, we will use a solver based on Jacobi's method. Unit tests will also be done in this project, using Catch for C++.

II. THEORY

A. Buckling beam problem

We start by looking at the buckling beam problem, i.e. a classical wave function in one dimension. Starting with the following differential equation,

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

where $u(x)$ is the vertical displacement of the beam in the y direction. The beam has length L, $x \in [0, L]$ and F is a force applied at $(L, 0)$ in the direction towards the origin. The parameter γ is a constant defined by properties like the rigidity of the beam. We apply so-called Dirichlet boundary conditions and set $u(0) = u(L) = 0$.

In this specific case two of the parameters γ, F and L are known. As an example, assume we know F and L. Then the eigenvalue problem we set up below will allow us to find γ.

We define a dimensional variable $\rho = \frac{x}{L}$, meaning that we have $\rho \in [0, 1]$.By reordering the equation as

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

with $\lambda = FL^2/\gamma$ we have an equation that when discretized, becomes an eigenvalue problem. This is done in section III.

A unitary transformation preserves the orthogonality of the obtained eigenvectors. We consider first a basis of vectors $\mathbf{v}_i$,

$$\mathbf{v}_i = \begin{bmatrix} v_{i1} \\ \vdots \\ \vdots \\ v_{in} \end{bmatrix}$$

By assuming that the basis is orthogonal,

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

we can show that an orthogonal or unitary transformation

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

preserves the dot product and orthogonality. We now have the following

$$\mathbf{w}_j^T \mathbf{w}_i = (\mathbf{U}\mathbf{v}_i)^T \mathbf{U}\mathbf{v}_i = \mathbf{U}^T \mathbf{v}_i^T \mathbf{U}\mathbf{v}_i.$$

Knowing that $\mathbf{U}^T\mathbf{U} = \mathbf{I}$, where $\mathbf{I}$ is the identity matrix, we get the following by using the

$$= \mathbf{v}_i^T \mathbf{I} \mathbf{v}_j = \delta_{ij}, \tag{2}$$

where δ_{ij} is the Kronecker delta. The orthogonality and dot product is therefore conserved.

B. Jacobi's method

In order to solve the matrix given in equation 7, we need to use Jacobi's method. We we define the quantities $\tan\theta = t = s/c$, with $s = \sin\theta$ and $c = \cos\theta$ and

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

We can then define the angle θ so that the non-diagonal matrix elements of the transformed matrix a_{kl} become non-zero and we obtain the quadratic equation (using $\cot 2\theta = 1/2(\cot\theta - \tan\theta)$

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

resulting in

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

and c and s are easily obtained via

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

and $s = tc$.

C. One electron in three dimensions

By assuming that some electrons move in a three-dimensional harmonic oscillator potential and repel each other via the static Coulomb interaction, we can implement quantum mechanics to our matrix-problem. We assume spherical symmetry and look at the solution of the radial part of Schroedinger's equation for one electron. This equation reads

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

By substituting $R(r) = (1/r)u(r)$, inserting the dimensionless variable $\rho = (1/\alpha)r$ and using the potential $V(\rho) = (1/2)k\alpha^2\rho^2$, this can be rewritten as

$$-\frac{d^2}{d\rho^2}u(\rho) + \rho^2 u(\rho) = \lambda u(\rho). \tag{3}$$

For the complete derivation of this expression, see the Appendix in section VI A.

This is the first equation to solve numerically. In three dimensions the eigenvalues for $l = 0$ for our scaling are expected to be $\lambda_0 = 3, \lambda_1 = 7, \lambda_2 = 11, \lambda_3 = 15$, Jensen, M.H.[1]. These will be used for comparison for our own algorithm.

D. Two electrons in three dimensions

We will now study two electrons in a harmonic oscillator well which also interact via a repulsive Coulomb interaction. Starting with the single-electron equation written as

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}u(r) + \frac{1}{2}kr^2u(r) = E^{(1)}u(r),$$

where $E^{(1)}$ stands for the energy with one electron only. For two electrons with no repulsive Coulomb interaction, we have the following Schrodinger's equation

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

Where $u(r_1, r_2)$ is the two-electron wave function and $E^{(2)}$ represent the two-electron energy. By introducing a relative coordinate, inserting the wave function $u(r, R) = \psi(r)\phi(R)$, the sum of the relative energy and the repulsive Coulomb interaction, we are left with the following expression

$$-\frac{d^2}{d\rho^2}\psi(\rho) + \omega_r^2\rho^2\psi(\rho) + \frac{1}{\rho} = \lambda\psi(\rho). \tag{4}$$

The complete derivation of this expression, can be found in Appendix in section VI B. Here we treat ω_r as a parameter which reflects the strength of the oscillator potential. We will study the cases $\omega_r = 0.01$, $\omega_r = 0.5$, $\omega_r = 1$, and $\omega_r = 5$ for the ground state only, since it is the lowest-lying state.

With no repulsive Coulomb interaction we should get a result which corresponds to the relative energy of a non-interacting system. Similarly for the single electron, we are only interested in the ground state with $l = 0$. We omit the center-of-mass energy.

III. METHOD

The programs can be found in our github repository [2].

A. Wavefunction in one dimension

We use the same expression for the second derivative of a function u as we did in project 1, namely

$$u'' = \frac{u(\rho+h) - 2u(\rho) + u(\rho-h)}{h^2} + O(h^2), \tag{5}$$

where h is our step. Next we define minimum and maximum values for the variable ρ, $\rho_{\min} = 0$ and $\rho_{\max} = 1$, respectively. With a given number of mesh points, N, we define the step length h as, with $\rho_{\min} = \rho_0$ and $\rho_{\max} = \rho_N$,

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

The value of ρ at a point i is then

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

We can rewrite the differential equation for a value ρ_i as

$$-\frac{u(\rho_i+h) - 2u(\rho_i) + u(\rho_i-h)}{h^2} = \lambda u(\rho_i), \tag{6}$$

or in a more compact way as

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

Following our approach from project 1, we can rewrite this equation in a more a general form, but now as an eigenvalue problem, that is

$$\begin{bmatrix} d & a & 0 & 0 & \ldots & 0 & 0 \\ a & d & a & 0 & \ldots & 0 & 0 \\ 0 & a & d & a & 0 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & \ldots & \ldots & \ldots & a & d & a \\ 0 & \ldots & \ldots & \ldots & \ldots & a & d \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \ldots \\ u_{N-2} \\ u_{N-1} \end{bmatrix} = \lambda \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \ldots \\ u_{N-2} \\ u_{N-1} \end{bmatrix}. \tag{7}$$

As in project 1, we have not included the endpoints u_0 and u_N. We have defined $d = 2/h^2$ and the non-diagonal ones as $a = -1/h^2$. This eigenvalue problem has analytical eigenpairs, with eigenvalues given as

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

B. Adding a harmonic oscillator potential

Next, we assume that the electrons move in a harmonic oscillator potential in three dimensions. We implement this to our algorithm by adding the potential on equation (6), which for one electron gives:

$$-\frac{u(\rho_i+h)-2u(\rho_i)+u(\rho_i-h)}{h^2}+\rho_i^2u(\rho_i)=\lambda u(\rho_i) \quad (8)$$

and in a more compact way:

$$-\frac{u_{i+1}-2u_i+u_{i-1}}{h^2}+\rho_i^2u_i=\lambda u_i \quad (9)$$

We implement this by adding ρ^2 to the diagonal elements in our matrix A.

For two electrons we also have a repulsive Coloumb interaction, given by equation 4 which can be implemented in our algorithm by adding the potential $\omega_r^2\rho^2+1/\rho$ to the diagonal elements.

C. Implementing Jacobi's algorithm

Jacobi's method is an iterative algorithm to find the eigenvalues of a symmetric matrix A. This is done by rotating the rows and columns in such a way that all of the offdiagonal elements are eliminated.

We will implement this by creating a function to find the largest offdiagonal element and then a function to rotate around this element's row and coloumn.

Each rotation requires 4n operations and one needs typically $3n^2$ - $5n^2$ rotations to zero out non-diagonal elements. See M. Jensen 2015 [1]. This results in a total of $12n^3$ - $20n^3$ floating point operations (FLOPS).

D. Unit tests

We will implement unit tests in our code to test different parts of our program. This is done utilizing Catch. First, we will test our maximum offdiagonal elements function. This is done by comparing the computed results with analytical for a small matrix. The second unit test we will implement is a test to see if our computed eigenvalues matches the eigenvalues we get using armadillo.

IV. RESULTS

We tested our program for different grid points n and evaluated the time and number of iterations needed to diagonalize a tridiagonal matrix. In the following matrix we listed these results along with the expected number of iterations.

Grid points n	Expected no. of iterations	No. of iterations
5	75-125	37
20	1200-2000	767
100	30 000-50 000	20301
200	120 000-200000	81856

TABLE I: *Table of the grid point numbers n with number of iterations when rotating the matrix with Jacobi's method, as described in section III C. The expected number of iterations are calculated by using n and the formula from the said section, while the actual number of iterations were computed directly from the algorithm.*

Grid points n	time, armadillo [s]	time, jacobis method [s]
5	0.01071	0.000279
20	0.003059	0.004151
100	0.00331	0.748001
200	0.002849	10.7683

TABLE II: *Table of the grid point numbers n and time used while rotating the matrix with Jacobi's method, as described in section III C. Also the time used when utilize Armadillos eigsym-method.*

We computed the eigenvalues for the harmonic oscillator in three dimension for one electron. The best value we obtained for ρ_{max} and number of grid points n were $\rho_{max}=4.5$ and $n=200$. The first four values are listed in the table below, together with the analytical values.

Expected eigenvalues, λ	Computed eigenvalues, λ
3	2.99984
7	6.99934
11	11.0038
15	15.0839

TABLE III: *Table of eigenvalues λ calculated by Jacobi's method, see section II C. The method is described in section III C, and the expected eigenvalues are given in section II B. One can see that for the lowest state, Jacobi's method is has produced values which, for up to four leading digits after the decimal point, are a close to the expected value.*

We also computed eigenvalues for two electrons in a potential with repulsive forces as a function of the oscillator parameter ω_r. Below is a table of the results for the lowest state.

ω_r	λ_0
0.01	0.986362
0.5	2.23599
1.0	4.05771
5	17.4446

TABLE IV: *Table of eigenvalues for two electron system, see section II D. Eigenvalues λ given with different oscillating potential parameter ω_r. Here we have computed a grid with $n=200$ and a $\rho_{max}=4.5$.*

V. DISCUSSION

The number of iterations for different grid points is listed in table I, along with expected number of iterations. We

can see that the expected number is generally larger than the actual number of iterations in our program. This is a consequence of our matrix being tridiagonal and not dense. With a tridiagonal matrix, all elements are already zero except for three diagonal coloumns.

The time it took to find the eigenvalues is listed in table II. For $n = 5$ the Jacobi rotation was faster than the Armadillo function. But with more grid points, the Jacobi rotation became much slower, and at 200 grid points spent nearly 11 seconds. This is as one would expect, as the number of FLOPS goes as $\propto n^3$, as described in section III C. The Armadillo function only used 0.003 seconds to find the eigenvalues for the same number of grid points.

We also computed the eigenvalues of one electron in a harmonic oscillator well, these are given in table III. These are found by using Jacobi's method, as discussed earlier. To find a value close to the exact eigenvalue, a number of ρ_{max}-values were tested. The best fit were when we had a relatively large matrix, $n = 200$ and a $\rho_{max} = 4.5$. When fitting the program for two electrons, an extra potential was added to the existing one. Since the electrons repel each other, the oscillator potential ω_r can affect the eigenvalues of both electrons. By looking at table IV, one can see that for an increasing ω_r the eigenvalues for the ground state also increase. This is consistent with quantum mechanics, which expects that an increased potential strength also increases energy eigenstates.

In this project, we also did some unit tests. This is a good way to approach code writing, as we are then able to find and localize errors from different parts of our code. Our tests were relatively simple, and we weren't able to detect the errors we encountered when adding a potential to our matrix. It was however a good introduction to Catch as a unit test framework.

VI. CONCLUSION

We have in this project calculated eigenvalues for three different cases. First we found the eigenvalues for a tridiagonal Toeplitz matrix, and compared Jacobi's method with Armadillo's *syseig*. It was shown that Jacobi's method is much slower when handling large matrices than Armadillo. Jacobi's method is a brute force method, which is easy to implement and gives the correct answers, but is very slow.

When introducing Shroedinger's equation to find eigenvalues of two different cases, first for one electron and then for two electrons, we saw that Jacobi's method can be impleded to give the correct eigenvalues. And for the second case, with the oscillating potential, we saw that an increased potential gives an increased eigenvalue.

REFERENCES

[1] Jensen, M. H. (2015). Computational physics, lecture notes fall 2015. `https://github.com/CompPhysics/ComputationalPhysics/blob/master/doc/Lectures/lectures2015.pdf`, Retrieved 6.9.2019.

[2] Jessie H. K. Warraich, Christina Knudsen (2019). Project 2.

[3] Taut, M. (1993). Two electrons in an external oscillator potential: Particular analytic solutions of a coulomb correlation problem. *Physical Review A*, 48(5):3561–3566.

APPENDIX A:

A. Derivation of Schrodinger's equation for one electron

We begin with the following expression for the Schrodinger equation

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

In our case $V(r)$ is the harmonic oscillator potential $(1/2)kr^2$ with $k=m\omega^2$ and E is the energy of the harmonic oscillator in three dimensions. The oscillator frequency is ω and the energies are

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

with $n=0,1,2,\dots$ and $l=0,1,2,\dots$.

Since we have made a transformation to spherical coordinates it means that $r\in[0,\infty)$. The quantum number l is the orbital momentum of the electron. Then we substitute $R(r)=(1/r)u(r)$ and obtain

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

The boundary conditions are $u(0)=0$ and $u(\infty)=0$.

We introduce a dimensionless variable $\rho=(1/\alpha)r$ where α is a constant with dimension length and get

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

We will set in this project $l=0$. Inserting $V(\rho)=(1/2)k\alpha^2\rho^2$ we end up with

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

We multiply thereafter with $2m\alpha^2/\hbar^2$ on both sides and obtain

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

The constant α can now be fixed so that

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

By defining

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

we can rewrite Schrodinger's equation as

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

B. Derivation of Schrodinger's equation for two electrons

For two electrons with no repulsive Coulomb interaction, we have the following Schroedinger equation

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

Where $u(r_1, r_2)$ is the two-electron wave function and $E^{(2)}$ represent the two-electron energy. With no interaction this can be written out as the product of two single-electron wave functions, that is we have a solution on closed form. We introduce the relative coordinate $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and the center-of-mass coordinate $\mathbf{R} = 1/2(\mathbf{r}_1 + \mathbf{r}_2)$. With these new coordinates, the radial Schrodinger equation reads

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

The equations for r and R can be separated via the ansatz for the wave function $u(r, R) = \psi(r)\phi(R)$ and the energy is given by the sum of the relative energy E_r and the center-of-mass energy E_R, that is

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

We add then the repulsive Coulomb interaction between two electrons, namely a term

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

with $\beta e^2 = 1.44$ eVnm.

Adding this term, the r-dependent Schroedinger equation becomes

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

This equation is similar to the one we have in section VI A, so we can introduce the dimensionless variable $\rho = r/\alpha$.

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

We want to manipulate this equation further to make it as similar to the case with one electron as possible. We define a new 'frequency'

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

and fix the constant α by requiring

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

Defining

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

we can rewrite Schroedinger's equation as

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