Cool Title

Project 2, FYS-3150

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All source codes can be found at: `https://github.com/inakbk/Project_1.git` in the folders `exercise_b` and `exercise_d`.

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Abstract

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1 Motivation and purpose

The aim of this project is to solve Schrödinger's equation for two electrons in a three-dimensional harmonic oscillator well with and without a repulsive Coulomb interaction. Your task is to solve this equation by reformulating it in a discretized form as an eigenvalue equation to be solved with Jacobi's method. –>code which implements Jacobi's method.

Electrons confined in small areas in semiconductors, so-called quantum dots, form a hot research area in modern solid-state physics, with applications spanning from such diverse fields as quantum nano-medicine to the contruction of quantum gates. You can read about quantum dots at `http://en.wikipedia.org/wiki/Quantum_dot`, which also contains links to several scientific articles. A recent article of interest is the review by Semonin *et al* in Materials Today, volume 15, page 508 (2012).

In this article we will let two electrons move in a three-dimensional harmonic oscillator potential that repel each other via the Coulomb interaction. Throughout this paper we will assume spherically symmetry and let the angular momentum be $l = 0$. Before solving the problem for two electrons we will look at one electron in a harmonic oscillator potential.

To solve the Schrödinger's equation for one electron(and two??) we will have to transformed the equations into a matrix eigenvalue problem. When we have rewritten the problem we will use Jacobi's rotation algorithm to find the solutions.

Together with linear equations and least squares, the third major problem in matrix computations deals with the algebraic eigenvalue problem. Here we limit our attention to the symmetric case. We focus in particular similarity transformations, –> Jacobi [1]

2 Solving eigenvalueproblems using similarity transformations

Let us assume that we have the eigenvalue problem

$$\mathbf{A}\mathbf{x}^{(\mathbf{v})} = \lambda \mathbf{x}^{(\mathbf{v})}$$

where $\lambda^{(v)}$ are the eigenvalues and $\mathbf{x}^{(\mathbf{v})}$ the corresponding eigenvectors.[2] Assuming that the matrix $\mathbf{A}$ is real and symetric we can use the Jacobi rotation algoritm to solve the eigenvalue problem. First we will describe the use of similarity tansformations in general and then the Jacobi rotation algorithm in detail.

[1] sitert fra lectures2015 p. 225

[2] The introduction to this section is based on the lecturenotes"lectures2015.pdf"

Let $\mathbf{D}$ be the diagonal matrix with the eigenvalues of $\mathbf{A}$ on the diagonal:

$$\mathbf{D} = \begin{pmatrix} \lambda_1 & 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & \lambda_3 & 0 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & \dots & \lambda_{n-1} & 0 \\ 0 & \dots & \dots & \dots & \dots & 0 & \lambda_n \end{pmatrix} \tag{1}$$

We say that a matrix $\mathbf{B}$ is a similarity transform of $\mathbf{A}$ if

$$\mathbf{B} = \mathbf{S^T A S}$$

Where $\mathbf{S}$ is a unitary matrix so $\mathbf{S^T S} = \mathbf{S^{-1} S} = \mathbf{I}$. The point of this is that the matrix $\mathbf{B}$ has the same eigenvalues as $\mathbf{A}$. Since $\mathbf{A}$ is real and symetric there exists a real orthonogal matrix $\mathbf{S}'$ such that:

$$\mathbf{S'^T A S'} = \mathbf{D}$$

So the strategy is then to perform a series of similarity transformations on the original matrix $\mathbf{A}$ so that the matrix reduces to the diagonal matrix $\mathbf{D}$ with the eigenvalues on the diagonal:

$$\mathbf{S_N^T \dots S_1^T A S_1^T \dots S_N} = \mathbf{D}$$

where $\mathbf{S_N \dots S_1} = \mathbf{S}'$. This must be done on both sides of the equation. Only one transformation is given by:

$$(\mathbf{S^T A S})(\mathbf{S^T x}) = \lambda \mathbf{S^T x}$$
$$\mathbf{B}(\mathbf{S^T x}) = \lambda(\mathbf{S^T x})$$

using that $\mathbf{S}$ is unitary. We see that the eigenvalue of $\mathbf{B}$ is the same as for $\mathbf{A}$, but the eigenvector is changed to $\mathbf{S^T x}$.

2.1 Numerical method: Jacobi's rotation algorithm

We will now see how we can find the eigenvalues of a real and symetric matrix $\mathbf{A}$ by using the Jacobi's rotation algoritm, or Jacobi's method.

The Jacobi's method introduces the $(n \times n)$ unitary orthogonal transformation matrix

$$\mathbf{S} = \begin{pmatrix} 1 & 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 1 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & \cos\theta & 0 & 0 & \dots & \sin\theta \\ 0 & 0 & 0 & 1 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & \dots & 1 & 0 \\ 0 & \dots & -\sin\theta & \dots & \dots & 0 & \cos\theta \end{pmatrix} \tag{2}$$

that performs a plane rotation around an angle θ in the Euclidean n-dimentional space. For simpler notation we define the quantities $\tan\theta = t = s/c$, with $s = \sin\theta$ and $c = \cos\theta$. The elements of the matrix $\mathbf{S}$ that differ from zero is given by the indexes k, l:

$$s_{kk} = s_{ll} = c, \quad s_{kl} = -s_{lk} = -s, \quad s_{ii} = 1$$

where $i \neq k$, $i \neq l$ and i, j are the indexes of the matrix. Then the similarity transformation

$$\mathbf{B} = \mathbf{S^T A S}$$

can be written on component form as:

$$\begin{aligned}
b_{ii} &= a_{ii} \\
b_{ik} &= ca_{ik} - sa_{il} \\
b_{il} &= ca_{il} - sa_{ik} \\
b_{kk} &= c^2 a_{kk} - scsa_{kl} + s^2 a_{ll} \\
b_{ll} &= c^2 a_{ll} + 2csa_{kl} + s^2 a_{kk} \\
b_{kl} &= cs(a_{kk} - a_{ll}) + (c^2 - s^2) a_{kl}
\end{aligned}$$

We want to choose the angle θ so that all the non-diagonal matric elements becomes zero, that is $b_{kl} = 0$. Introducing a new variable τ dependent on k, l:

$$\begin{aligned}
b_{kl} = cs(a_{kk} - a_{ll}) + (c^2 - s^2) a_{kl} = 0 \\
\Rightarrow \frac{a_{ll} - a_{kk}}{a_{kl}} = \frac{c^2 - s^2}{cs} = \frac{2\cos 2\theta}{\sin 2\theta} = 2\cot 2\theta \\
\Rightarrow \tau = \cot 2\theta = \frac{a_{ll} - a_{kk}}{2a_{kl}}
\end{aligned}$$

Then $b_{kl} = 0$ can be written as a second order equation

$$\begin{aligned}
2\tau = \frac{c^2 - s^2}{cs} = \frac{c^2}{cs} - \frac{s^2}{cs} = \frac{1}{t} - t \\
\Rightarrow 2\tau t = 1 - t^2 \\
\Rightarrow t^2 + 2\tau t - 1 = 0
\end{aligned}$$

with the solution

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

We obtain c ans s from

$$\begin{aligned}
c^2 + s^2 = 1 \\
\Rightarrow c = \frac{1}{\sqrt{1 + t^2}},
\end{aligned}$$

and using that $s = tc$.

But which of the roots of t should we choose? To make shure that the the similarity transformation does not make bigger changes to the other elements of $\mathbf{A}$ while making another element zero we minimize the difference between the matrices $\mathbf{B}$ and $\mathbf{A}$ by letting $|\theta| \leq \pi/4$. This also makes shure that the iterations goes faster toward the solution, else the iterations might not converge at all after a reasonable number of iterations.

Separating the inequality gives $\theta \leq \pi/4$ and $\theta \geq -\pi/4$. Starting with the first inequality:

$$\begin{aligned}
\theta = \arctan t \leq \pi/4 \\
t \leq \tan(\pi/4) = 1
\end{aligned}$$

and

$$\begin{aligned}\theta = \arctan t &\geq -\pi/4 \\ t &\geq \tan(-\pi/4) = -1\end{aligned}$$

so we see that $|t| \leq 1 \Rightarrow -\tau \pm \sqrt{1+\tau^2} \leq 1$. If we look at the case where $\tau > 0$ and try the positive root of t we see that:

$$\begin{aligned}-\tau + \sqrt{1+\tau^2} &\leq -|\tau| + 1 + |\tau| = 1 \\ &\Rightarrow t \leq 1 \Rightarrow \theta \leq \pi/4\end{aligned}$$

must be satisfied.

If we then try the case when $\tau < 0$ and the negative root of t we see that:

$$\begin{aligned}-\tau - \sqrt{1+\tau^2} = |\tau| - \sqrt{1+\tau^2} &\geq |\tau| - (1 + |\tau|) = -1 \\ &\Rightarrow t \geq -1 \Rightarrow \theta \geq -\pi/4\end{aligned}$$

must be satisfied. So the choice of the root of t is dependent on τ. When $\tau > 0$ we choose the positive root, and when $\tau < 0$ we choose the negative root to make shure that $|\theta| \leq \pi/4$ is satisfied.

The Jacobi algorithm can then be described as follows:

1. Find the indexes k, l of the maximum element of the matrix $\mathbf{A}$.
2. Obtain c and s, the matrix elements of $\mathbf{S}$, given by k, l.
3. Calculate the similarity transformation $\mathbf{B} = \mathbf{S^T A S}$.
4. Start on [1.] again, setting $\mathbf{A} = \mathbf{B}$, untill all off-diagonal elements are esentially zero (less than a given threshold). When the iterations stop the eigenvalues are given by the matrix $\mathbf{D} = \mathbf{B}$.

We see that all information needed to perform a Jacobi rotation is given by the indexes k, l of the maximum elements of $\mathbf{A}$.

3 Physics 1: One electron in a three-dimensional harmonic oscillator potential.

3.1 Rewriting the Schrödinger's equation to a dimensionless form

We look at the Schödinger's equation for one electron at a radius $r \in [0, \infty)$ in a harmonic oscillator potential given by:

$$V(r) = (1/2)kr^2$$

where $k = m\omega^2$ and ω is the oscillator frequence. The energy E of the harmonic oscillator in three dimensions is given by:

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

with $n = 0, 1, 2, \ldots$ and $l = 0, 1, 2, \ldots$ is the orbital momentum of the electron.

We are only interested in the solution of the radial part of the Schrödinger equation given by

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} - \frac{l(l+1)}{r^2}\right)R(r) + V(r)R(r) = ER(r). \tag{3}$$

We then use the substitution $R(r) = (1/r)u(r)$ 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 will modify equation 3 further by introducing a dimensionless variable $\rho = (1/\alpha)r$ where α is a constant with dimension length and get

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

Now inserting $l = 0$ and the rewritten potential $V(\rho) = (1/2)k\alpha^2\rho^2$ we obtain:

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

and then multiply by $2m\alpha^2/\hbar^2$ on both sides

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

We fix the constant α so that

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

and then define

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

Finally equation 3 can be written as

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

which is the equation we want to solve numerically. We know[3] that this equation has the eigenvalues $\lambda_0 = 3, \lambda_1 = 7, \lambda_2 = 11, \ldots.$ for $l = 0$. These analytical values will be used to test the precition of the numerical method.

[3] This is given in the assignment text for Project 2, FYS3150..

3.2 Discretizing the Schrödingers equation to solve numerically.

We will now rewrite the Schrödingers equation on a discretized form to be able to solve it as an matrix eigenvalue problem.

We use the expression for the second derivative of the function $u(\rho)$

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

where h is our step. We define the minimum and maximum values for the variable ρ, $\rho_{\text{min}} = 0$ and ρ_{max} so that:

$$h = \frac{\rho_{\text{max}} - \rho_{\text{min}}}{n_{\text{step}}}.$$

where n_{step} is a given number of steps. Since $\rho \propto r$ and $r \in [0, \infty)$ the maximum value of ρ should be $\rho_{\text{max}} = \infty$. But we cannot set a infinite value when computing the solution numerically. We will therefore have to choose a significally large enough ρ that give stable results for different n_{step} (test noe noe ??)

We can then define an arbitrary value of ρ as

$$\rho_i = \rho_{\text{min}} + ih \qquad i = 0, 1, 2, \dots, n_{\text{step}}$$

so that the Schrödinger equation for ρ_i reads

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

or in a more compact way with the harmonic oscillator potential $V_i = \rho_i^2$:

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

Then we can define first the diagonal matrix element

$$d_i = \frac{2}{h^2} + V_i,$$

and the non-diagonal matrix element:

$$e_i = -\frac{1}{h^2}.$$

We observe that in this case all the non-diagonal matrix element is given by a constant, so we can denote them all as $e = -\frac{1}{h^2}$ instead. (insert e og ikke ei hele veien??)

With these definitions the Schrödinger equation (4) takes the following form

$$d_i u_i + e_{i-1} u_{i-1} + e_{i+1} u_{i+1} = \lambda u_i, \tag{6}$$

where u_i is unknown. This can be written as a matrix eigenvalue problem

$$\begin{pmatrix} d_1 & e_1 & 0 & 0 & \dots & 0 & 0 \\ e_1 & d_2 & e_2 & 0 & \dots & 0 & 0 \\ 0 & e_2 & d_3 & e_3 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & \dots & d_{n_{\text{step}}-2} & e_{n_{\text{step}}-1} \\ 0 & \dots & \dots & \dots & \dots & e_{n_{\text{step}}-1} & d_{n_{\text{step}}-1} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \dots \\ \dots \\ \dots \\ u_{n_{\text{step}}-1} \end{pmatrix} = \lambda \begin{pmatrix} u_1 \\ u_2 \\ \dots \\ \dots \\ \dots \\ u_{n_{\text{step}}-1} \end{pmatrix} \tag{7}$$

The solutions are known via the boundary conditions at $i = n_{\mathrm{step}}$ and at the other end point, for ρ_0, which is zero in both cases. The goal is to use Jacobi's algoritm to solve equation 6.

How many points n_{step} do you need in order to get the lowest three eigenvalues with four leading digits? Remember to check the eigenvalues for the dependency on the choice of ρ_{max}.

How many similarity transformations are needed before you reach a result where all non-diagonal matrix elements are essentially zero? Try to estimate the number of transformations and extract a behavior as function of the dimensionality of the matrix.

You can check your results against the code based on Householder's algorithm, *tqli* in the file lib.cpp. Alternatively, you can use the Armadillo function for solving eigenvalue problems.

Comment your results (here you could for example compute the time needed for both algorithms for a given dimensionality of the matrix).

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4 Physics 2: Two electrons in a three-dimensional harmonic oscillator potential.

4.1 W. coulomb

4.2 W.o. coulomb

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c) We will now study two electrons in a harmonic oscillator well which also interact via a repulsive Coulomb interaction. Let us start 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 Schrödinger equation

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

Note that we deal with a two-electron wave function $u(r_1, r_2)$ and two-electron energy $E^{(2)}$.

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 Schrödinger 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 Schrödinger equation becomes

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

This equation is similar to the one we had previously in (a) and we introduce again a dimensionless variable $\rho = r/\alpha$. Repeating the same steps as in (a), we arrive at

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

We want to manipulate this equation further to make it as similar to that in (a) as possible. We define a 'frequency'

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

and fix the constant α by requiring

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

or

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

Defining

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

we can rewrite Schrödinger's equation as

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

We treat ω_r as a parameter which reflects the strength of the oscillator potential.

Here 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, that is the lowest-lying state.

With no repulsive Coulomb interaction you should get a result which corresponds to the relative energy of a non-interacting system. Make sure your results are stable as functions of ρ_{max} and the number of steps.

We are only interested in the ground state with $l = 0$. We omit the center-of-mass energy.

You can reuse the code you wrote for (a), but you need to change the potential from ρ^2 to $\omega_r^2\rho^2 + 1/\rho$.

Comment the results for the lowest state (ground state) as function of varying strengths of ω_r.

For specific oscillator frequencies, the above equation has answers in an analytical form, see the article by M. Taut, Phys. Rev. A 48, 3561 - 3566 (1993). The article can be retrieved from the following web address `http://prola.aps.org/abstract/PRA/v48/i5/p3561_1`.

d) In this exercise we want to plot the wave function for two electrons as functions of the relative coordinate r and different values of ω_r. With no Coulomb interaction you should have a result which corresponds to the non-interacting case. Plot either the function itself or the probability distribution (the function squared) with and without the repulsion between the two electrons. Varying ω_r, the shape of the wave function will change.

   We are only interested in the wave function for the ground state with $l = 0$ and the two first excited states with the same symmetry and omit again the center-of-mass motion.

   You can choose between three approaches; the first is to use the existing *tqli* function. Here the eigenvectors are obtained from the matrix $z[i][j]$, where the index j refers to eigenvalue j. The index i points to the value of the wave function in position ρ_j. That is, $u^{(\lambda_j)}(\rho_i) = z[i][j]$.

   The eigenvectors are normalized. Plot then the normalized wave functions for different values of ω_r and comment the results.

   Another alternative is to add a piece to your Jacobi routine which also returns the eigenvectors. This is the more difficult part. You will also need to normalize the eigenvectors.

   Finally, the armadillo function *eig_ sys* can be used to find eigenvalues and eigenvectors.

e) Here you are asked to implement unit tests in either your C++ program or your Fortran program. For C++ users, please follow the guidelines on how to install unit tests with c++ on the webpage. For Fortran user, the software package Fortran Unit Test Framework (FRUIT), `sourceforge.net/projects/fortranxunit`. These issues will be discussed in more detail at the lab and lectures during week 38.

f) This exercise is optional and is meant more as a challenge. Implement the iterative Lanczos' algorithm discussed in the lecture notes and compute the lowest eigenvalues as done in exercise c) above. Compare your results and discuss faults and merits of the iterative method versus direct methods like Jacobi's method.