Quantum dots in three dimensions

FYS3140 – Project 2

[github.com/henrikx2/FYS3150](https://github.com/henrikx2/FYS3150)

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# Abstract

In this report, the eigenvalue problem of a system with electrons in a harmonic oscillator potential is explored. The well known and stable Jacobi’s rotation method is used to diagonalize the Hamiltonian matrix into an eigenvalue matrix. The equilibrium between calculation speed and decimal precision of the eigenvalues are discussed as a function of step size, interval length and numbers of iterations.

# Introduction

The experiment aims to solve the general eigenvalue equation of the type

Where is going to be the Hamiltonian operator of the harmonic oscillator well potential and is the energy eigenvalue of the given state .

The equation is solved by firstly; constructing a tridiagonal Hamiltonian matrix. This matrix is derived by simplifying the Schroedinger’s equation for one or two electrons in the HO potential and making it dimensionless. Then, the matrix is processed with orthogonal transformation through Jacobi’s rotation algorithm. This reveals a diagonal matrix with the eigenvalues of the Hamiltonian at its diagonal. The eigenvalues are then compared to the analytic eigenvalues. Lastly, the ground state of the system’s dependence on Coulomb interactions and varying HO potential will be explored.

# Theory

## One electron in the HO potential

The solution to the radial part of the Schroedinger’s equation for one electron in the HO potential is given as

|  |  |  |
| --- | --- | --- |
|  |  | (1) |

Where is the HO potential with and , is the wavefunction and is the energy of the harmonic oscillator. The energies can be written as a function of the frequency as

|  |  |  |
| --- | --- | --- |
|  |  | (2) |

Where is the principal quantum number and is the angular momentum quantum number of the electron. Substituting , Eq. 1 becomes

|  |  |  |
| --- | --- | --- |
|  |  | (3) |

Where the Dirichlet boundary conditions give and . To make the Eq. 3 dimensionless, it is rewritten as a function of the dimensionless variable where has dimensions length. The HO potential is then given . This project only concentrates only on a system where , which simplifies Eq. 3 to

|  |  |  |
| --- | --- | --- |
|  |  | (4) |

To make Eq. 4 suitable for solving numerically, it is multiplied by , so that

|  |  |  |
| --- | --- | --- |
|  |  | (5) |

Which is further manipulated with the condition

|  |  |  |
| --- | --- | --- |
|  |  | (6) |

So that defining

|  |  |  |
| --- | --- | --- |
|  |  | (7) |

Gives the simplified Schroedinger’s equation which is to be solved as

|  |  |  |
| --- | --- | --- |
|  |  | (8) |

The analytical eigenvalues of this equation are

Since the maximum value cannot be set to , this will be varying as to get the most correct energies. The values of is defined . The number of mesh points are given as and the step length reads

|  |  |  |
| --- | --- | --- |
|  |  | (9) |

Which in turn gives the expression for the value of at a given iteration as

|  |  |  |
| --- | --- | --- |
|  |  | (10) |

An approximation to the 2nd derivative can be expressed

|  |  |  |
| --- | --- | --- |
|  |  | (11) |

Using Eq. 11 and the HO potential to describe the discrete case of the Schroedinger’s equation as

|  |  |  |
| --- | --- | --- |
|  |  | (12) |

It is easy to notice the tridiagonal matrix equation where the matrix is defined as follows

In other words, the diagonal elements and the non-diagonal elements are denoted as

|  |  |  |
| --- | --- | --- |
|  |  | (13) |
|  |  | (14) | |

## Two electrons in the HO potential

In the case of two electrons in the HO well, the Coulomb interaction between these two must be accounted for. The standard Schroedinger’s equation for one electron in a HO potential well is as before

|  |  |  |
| --- | --- | --- |
|  |  | (15) |

Where is the energy of the system with only one electron. Now, adding the other electron (but no Coulomb interactions) the equation reads

|  |  |  |
| --- | --- | --- |
|  |  | (16) |

Now, using relative coordinate and center-of-mass coordinate , the Shroedinger equation becomes

|  |  |  |
| --- | --- | --- |
|  |  | (17) |

Separating and can be done using the ansatz for the separation of the wave function , where det energy is a sum of the relative and the center-of-mass energy given by .

The Coulomb interactions between the electrons is given by the expression

|  |  |  |
| --- | --- | --- |
|  |  | (18) |

In which the constant . This can be added to the part of the equation

|  |  |  |
| --- | --- | --- |
|  |  | (19) |

By making Eq. 19 dimensionless by the same steps as in 2.1, the equation reads

|  |  |  |
| --- | --- | --- |
|  |  | (20) |

To make Eq. 20 “identical” to Eq. 8, a new “frequency” is defined as

|  |  |  |
| --- | --- | --- |
|  |  | (21) |

Where the parameter mirrors the strength of the HO potential. Furthermore

|  |  |  |
| --- | --- | --- |
|  |  | (22) |

Such that

|  |  |  |
| --- | --- | --- |
|  |  | (23) |

And the eigenvalue

|  |  |  |
| --- | --- | --- |
|  |  | (24) |

So that the final Schroedinger’s equation reads

|  |  |  |
| --- | --- | --- |
|  |  | (25) |

The diagonal in the tridiagonal matrix is now defined (the off-diagonals stay the same)

|  |  |  |
| --- | --- | --- |
|  |  | (26) |

If there where not to be a Coulomb interaction between the two particles, the would be just like the one in the singe electron system, but with and hence defined as:

## Preservation of orthogonality

For the method described in section 3 to work, it is essential to prove that a unitary transformation preserves the dot product and the orthogonality of vectors in a basis. Consider the orthogonal basis

For a matrix U to be unitary it must have the property . Consider the transformation . The dot product is then

Hence, the orthogonal/unitary transformation preserves the orthogonality.

# Methods

## Jacobi’s rotation algorithm

Jacobi’s rotation algorithm evolves around performing an orthogonal transformation with a rotation matrix of the type

Which has the property and performs a rotation of angle in the Euclidean space. The elements of that are not zero are given as

The algorithm is used to transform a symmetric matrix into a diagonal matrix where the diagonal consists of the eigenvalues. This diagonalization is performed by doing the orthogonal transformation several times, so that the off-diagonal elements converge to zero.

Defining and a 2x2 system would look like this

The requirement that implies that

Where it’s easy to see that if the off-diagonal element , then , which implies that and , or in other words; no rotation needed as off-diagonals is close to zero. Next, defining

A quadratic equation can be derived from the relation so that

|  |  |  |
| --- | --- | --- |
|  |  | (27) |

From the relation , and are defined as

The equations for the new matrix elements when iterating are

This gives a new matrix , on which the same procedure is done until it’s off-diagonal elements are under a certain tolerance

## Code structure

1. Build the matrix A by implementing the diagonal elements from the corresponding problem in section 2.
2. Find the off-diagonal element with the largest absolute value and assign its matrix index to and .
3. Calculate , and .
4. Calculate the 6 equations with the obtained and and update the matrix A.
5. Repeat until off-diagonal elements are lower than the specified tolerance.

## Running the calculations

To run the calculations using the provided source code in the git repository, it is required to have Python 3 with the NumPy, matplotlib and tabulate packages installed. Run the calculations by executing main.py and follow the UI in terminal.

# Results and discussion

## Single electron

## Two electrons

# Conclusion

## 

# Appendix

## Optimal and number of iterations

The most optimal and values to achieve eigenvalues of 4 decimal precision is described in Table 6.1.1. These are calculated by trying different values.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | **Single electron** | | **Two electrons** | | **Two electron with potential** | |
| **Eigenvalues:** |  |  |  |  |  |  |
| 3 | 3 | 325 |  |  |  |  |
| 7 | 3.7 | 337 |  |  |  |  |
| 11 | 4.2 |  |  |  |  |  |

# References

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