FYS4150 - Project 1

Vegard Rønning & Heine H. Ness & Sindre R. Bilden

University of Oslo

vegard.ronning@fys.uio.no ; h.h.ness@fys.uio.no ; s.r.bilden@fys.uio.no

github.com/sindrerb/FYS4150-Collaboration/tree/master/Doc/Project2

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Abstract

As tracers in medicine or qubits in quantum computing, quantum dots usages are hot topics in science. One advantage of quantum dots are their discrete energy levels wich may be tuned by existing technology and knowledge. As a one particle problem, the quantum dot may be solved analytcally as a particle in a three dimentional harmonic oscillator potential (HO), but the solution is almost impossible to find once multiple particles are confined in one single quantum dot. This project takes advantage of nummerical methods to solve the eigenvalue problem of two electrons in a quantum dot and examines the impact of columb interactions on the system. The results shows that the impact of the columb interactions are higher as the potential grows wider.

I. Introduction

Quantum dots are promising fields of science with many different usages. As a single particle system, the quantum dot is possible solve analytically by approximating it to a three dimentional harmonic oscillator potential. Once the system is introduced to two or more paricles, it turns very complex and it is often not possible to solve analytically in the same way as for a single particle system. By Jacobi's method, a close approximation may be achieved, and may be used to confirm experimental results or used as an experiment by itself. This project consists of two main parts where the first is writing an Jacobi's method to an algorithm that solves the Shroedinger equation (SE) numerically for a one particle in a three dimensional harmonic oscillator(HO) potential. The algorithm will be controlled to analytical results before proceeding to the second part wich is to introduce a second particle and solve the system with and without Coulomb interactions. The impact of columb interactions is then calculated by studying the energy differnce between the interacting and the non interacting case.

II. Methods

i. Jacobi's method

The Jacobi's method is a iterative method wich uses Jacobi's rotation matrix $\hat{S}$ a number of times to turn a symmetric, hermittian matrix $\hat{A}$ to a diagonal matrix $\hat{D}$.

$$\hat{S}^T\hat{A}\hat{S} = \hat{S}_n^T\hat{S}_{n-1}^T\cdots\hat{S}_1^T\hat{A}\hat{S}_1\cdots\hat{S}_{n-1}\hat{S}_n = \hat{D}$$

The rotation matrix $\hat{S}_i$, where $i = 1, 2\cdots n$, has the form of an identity matrix with $c = \cos(\theta)$ and $s = \sin(\theta)$ in a symmetric fashion inside depending on which two elements in $\hat{A}$ is to be rotated. n depends on the number of rotations needed to transform $\hat{A}$ to $\hat{D}$.

$$\hat{S} = \begin{bmatrix} 1 & 0 & & \cdots & & & 0 \\ 0 & \ddots & & & & & \\ & & c & \cdots & s & & \\ \vdots & & \vdots & \ddots & \vdots & & \vdots \\ & & -s & \cdots & c & & \\ & & & & & \ddots & 0 \\ 0 & & & \cdots & & 0 & 1 \end{bmatrix}$$

In this assignment we will use Jacobi's method to solve a eigenvalue problem. The eigenvalues (λ) are preserved using the this method but the eigenvectors are generally not, only the orthogonality of the eigenvectors are preserves. The eigenvalue problem $\hat{A}\vec{x} = \lambda\vec{x}$ then becomes

$$(\hat{S}^T\hat{A}\hat{S})(\hat{S}^T\vec{x}) = (\hat{S}^T\lambda\hat{S})(\hat{S}^T\vec{x})$$
$$\hat{D}(\hat{S}^T\vec{x}) = \lambda(\hat{S}^T\vec{x})$$

If $\hat{A}$ is composed of elements a_{ij} and matrix $\hat{B}$ of elements b_{ij}. One rotation $\hat{S}_i^T\hat{A}\hat{S}_i = \hat{B}$ can be done with an algorithm.

First the largest non-diagonal element a_{kl} has to be located then the element will be set to zero. Since the matrix is symmetric the element a_{lk} will be subject to the same operation.

$$b_{kl} = b_{lk} = (a_{kk} - a_{ll})cs + a_{kl}(c^2 - s^2) = 0$$

The equation $(a_{kk} - a_{ll})cs + a_{kl}(c^2 - s^2) = 0$ is solved rewriting the equation using $\Gamma = \frac{a_{ll}-a_{kk}}{2a_{kl}}$ and $t = \frac{s}{c} = \tan(\theta)$ to get the second order polynomial $t^2 + 2\Gamma t - 1 = 0$. This gives solutions for the trigonometrical expessions. $t = -\Gamma \pm \sqrt{1+\Gamma^2}$, $s = tc$ and $c = \frac{1}{\sqrt{1+\Gamma^2}}$. To avoid problems where Γ gets large and possible loss of numerical presission we rewrite $t = \frac{1}{\Gamma+\sqrt{1+\Gamma^2}}$.

Rotation algorithm is solved with the previously given solutions for t,c and s by a simple algorithm.

$$\begin{aligned}
b_{ii} &= a_{ii} && |i \neq k, l \\
b_{ik} &= a_{ik}c - a_{il}s && |i \neq k, l \\
b_{il} &= a_{il}c + a_{ik}s && |i \neq k, l \\
b_{kk} &= a_{kk}c^2 - 2a_{kl}cs + a_{ll}s^2 \\
b_{ll} &= a_{ll}c^2 + 2a_{kl}cs + a_{kl}s^2 \\
b_{kl} &= b_{lk} = 0
\end{aligned}$$

Here $i = 1, 2 \cdots n$ is the iteration variable and k and l are parameter belonging to the element in rtotation.

ii. Abel-Ruffini Impossiobility Theorem

The eigenvalue problem $\det(\hat{A} - \lambda\hat{I})\vec{x} = 0$ of a matrix $\hat{A} \in \mathbb{C}^{n\times n}$ is basically a problem of finding the roots of a polynomial $P(\lambda)$.

$$P(\lambda) = \prod_{i=1}^{n}(\lambda_i - \lambda)$$

The Abel-Ruffinis impossibility theorem states that not all polynomials og degree $n \geq 5$ can not be solved using roots alone and the solutions for these cases can only be approximated. [1]

This implies that matrices $\hat{A}$ of large dimensions has to be solved numerically and it is only possible to get an approximation for the eigenvalues with a chosen degree of accuracy within the boundaries of the computer.

iii. Unit tests

A unit test is a small piece of code that tests parts of a program for calculation errors. This to ensure that the program runs as expected and delivers correct results throughout the program. The unit tests we have used in this assignment are as follows.

Orthogonality test

The Jacobi method preforms orthogonal or unitary transformations to the matrix it operates on. That means the orthogonality of each column in a matrix $\hat{A}$ is conserved.

If $\hat{A}$ is a orthogonal matrix with orthogonal column vectors $\hat{A} = [\vec{a_1}\vec{a_2}\cdots\vec{a_n}]$ the dot product of any column vector can be described by a Kronecker delta δ_{ij}.

$$\vec{a_i}^T\vec{a_j} = |a_i|^2\delta_{ij} = \begin{cases} |a_i|^2 | i = j \\ 0 \quad | i \neq j \end{cases}$$

For a transformation done by a matrix $\hat{S}$ to be unitary any column all vectors $\vec{w}_i$ produced by the transformation $\hat{S}\vec{v}_i = \vec{w}_i$ must also be orthogonal.

$$\vec{w_i}^T\vec{w}_j = (\hat{S}\vec{v}_i)^T\hat{S}\vec{v}_j = \hat{S}^T\vec{v_i}^T\hat{S}\vec{v}_j = \vec{v_i}^T\hat{S}^T\hat{S}\vec{v}_j = \vec{v}_i\vec{v}_j = \delta_{ij}$$

Normality test

Since the Jacobi method preforms unitary transformations to the matrix it operates on, the normality is conserved if the columns of $\hat{A}$ is normalized.

This project is using Jacobi rotation on the identity matrix wich is normalized by definition. Introducing the criteria

$$col_i(\hat{A})^T \cdot col_i(\hat{A}) = 1$$

gives a brief indication of the conservation of normality wich is important for the interpretation of the wavefunction.

III. Implementation

A quantum dot may be approximated to a three dimentional HO-potential. By assuming shperical symmetry the radial part the SL may be rewritten to

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

Where the potential $V(r)$ is known by the HO-potential $\frac{1}{2}kr^2$, with $k = m\omega^2$ and the quantum number l describe the orbital momentum of the electron. The energies and oscillator frequency is given by

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

where $n \in \mathbb{N}$, $l \in \mathbb{N}$ and $r \in [0, \infty)$. By rewriting $R(r)$ as $rR(r) = u(r)$ we get

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

The expression can be further simplified by introducing the dimensionless variable $\rho = \frac{1}{\alpha}r$, setting $V(\rho) = \frac{1}{2}k\alpha^2\rho^2$, multiply with $\frac{2m\alpha^2}{\hbar^2}$ and set $l = 0$ so that

$$-\frac{d^2}{d\rho^2}u(\rho) + \underbrace{\frac{mk}{\hbar^2}\alpha^4}_{I}\rho^2 u(\rho) = \underbrace{\frac{2m\alpha^2}{\hbar^2}E}_{II}u(\rho)$$

and finally setting I $= 1$ and defining II $= \lambda$ the final form of the SL for one electron in a HO-potential can be written as

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

Equation 1 may be discretized and solved numerically as a matrix eigenvalue problem were $V_i = \rho_i^2$.

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

Two particle system

By introducing another electron to the system, the system includes two particles in the potential and the interactions between them. SE for two electrons with no Coulomb interactions can be written as

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}k(r_1^2 + r_2^2)\right)u(r_1, r_2) = Eu(r_1, r_2)$$

This can be rewritten by introducing the relative coordinate $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and the center-of-mass(COM) coordinate $\mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$. The radial SE is then

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

The ansatz for the wavefunction $u(r, R) = \psi(r)\phi(R)$ makes it possible to separate the equation for $\mathbf{r}$ and $\mathbf{R}$ so that the energy is the sum of the relative energy and the COM-energy($E = E_r + E_R$). Taking the repulsive Coulomb interaction

$$V_(r_1, r_2) = \frac{\beta e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} = \frac{\beta e^2}{r}, \quad \beta e^2 = 1.44 \text{ eVnm}$$

in to account the r-dependent part of the SE can be written as

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

By now introducing the dimensionless variable $\rho=\frac{r}{\alpha}$ and repeating the same steps as for the one electron case we get

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

To further simplify the equation we introduce the new frequency

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

Setting I $=1$ and II $=\lambda$ we arrive at the final form of SE for the two electron case

$$-\frac{d^2}{d\rho^2}\psi(\rho)+\omega_r^2\rho^2\psi(\rho)+\frac{1}{\rho}\psi(\rho)=\lambda\psi(\rho) \quad (3)$$

Like equation 1, equation 3 may be discretized into

$$-\frac{u_{i+1}-2u_i+u_{i-1}}{h^2}+V_iu_i=\lambda u_i \qquad (4)$$

Were the new potential $V_i=\omega_r^2\rho_i^2+\frac{1}{\rho}$. Both equation 2 and 4 may be rewritten to $\hat{H}\hat{u}=\lambda\hat{u}$ were $\hat{H}$ is a tridiagonal matrix with center diagonal $d_{ii}=\frac{2}{h^2}+V_i$ and the upper diagonal equal to the lower diagonal equal to $e_{ij}=\frac{-1}{h^2}$. Theese matrix eigenvalue problems may be solved by Jacobi's method.

Tests of conserved orthogonality and normality was done on a one electron system to ensure that the algorithm was correct, sample-matrices was written to a file and later tested for conserved orthogonality and normality. Later a convergence test of the number of iterations was done to weight the accuaracy and computational time. The algortihm was set to solve the schroedinger equation for a two particle system with ω_r equal to $0.01, 0.5, 1$ and 5. Both with and without columb interactions.

IV. Results and discussion

The jacobian method requires many iterations in order to reach a satisfying accuaracy of the energies. Table 1 from the convergence test of meshpoints indicates that $N=500$ is a minimum requirement for a four digit accuaracy but results also in a high computational time. Figure 1 shows the number of iterations for a given set of meshpoints, assumed to be proportional to computation time. A number of meshpoints $N=400$ results in a accuaracy to approximately the third digit, wich is thought to be accuarate enough for the purpose of this experiment while reducing the computational time drastically.

N	λ_0	λ_1	λ_2
10	2.68672	6.11302	11.0574
50	2.98745	6.93692	10.8453
100	2.99687	6.98432	10.9617
200	2.99916	6.99610	10.9904
300	2.99961	6.99828	10.9958
400	2.99986	6.99903	10.9976
500	2.99993	6.99937	10.9986

Table 1: *Table showing the three lowest computed eigenvalues λ with N meshpoints, in comparment to the exact $\lambda_0=3$,$\lambda_1=7$ and $\lambda_2=11$.*

Results from the computation of the two particle systems is given in Figure $3-8$, where it is a clear correspondance between the ω_r and the columb interactions. A high ω_f results in a narrow potential and a confinement of the electrons, in this narrow potential the columb interactions was thought to give a great impact on the wavefunction but Figure 8 contradicts this hypothesis. Figure 3 does also show an unexpected behaviour where the columb interaction has a greater impact in the electrons than expected. A relation between the energies of the systems with and without columb interaction is given in Table 2. The behaviour may be explained by the fact that $V_{Columb}=\frac{\beta}{r}$ diverge while r goes to zero. In a narrow potential, the columb interactions is large but does not overpower the confinement of the potential.

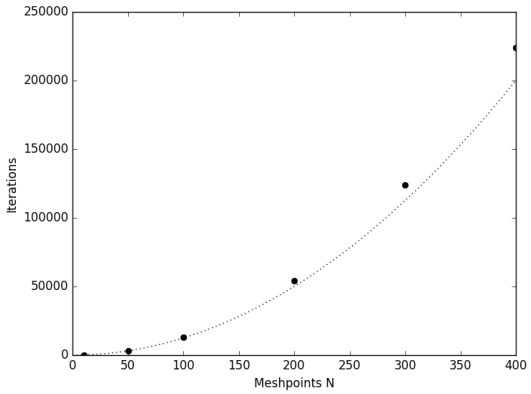

Figure 1: *Graph over the number of iterations for a given set of meshpoints N. The red line is proportional to N^2 as comparement.*

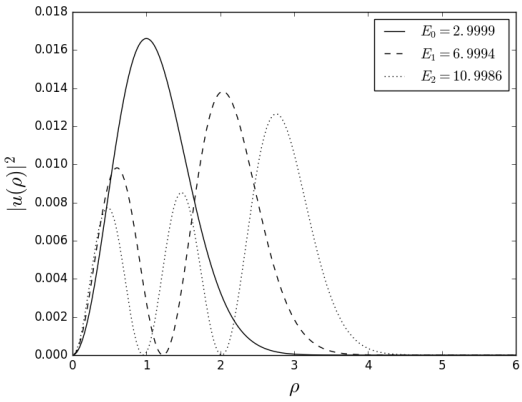

Figure 2: *The first three eigenstates with their respective eigenstates in a harmonic oscillator with one particle, computed with $N = 500$ meshpoints.*

ω_r	Interaction	No Interaction	Impact
0.01	0.105	0.030	0.72
0.25	1.250	0.750	0.40
0.50	2.230	1.500	0.33
1.00	4.058	3.000	0.26
2.50	9.211	7.500	0.19
5.00	17.448	15.000	0.14

Table 2: *Table showing the energy of the ground state in a two particle system with and without columb interactions. The impact is defined by the energy difference of the systems divided by the energy of the interacting system. The energies are rounded to the third digit.*

While widening the potential, the confinement decreases more rapidly than the columb interactions.

V. Summary and Conclusion

A nummerical experiment is been done where the schroedinger equation is solved iteratively by Jacobi's method. The algortihm is first compared to exact results of a simple system before calculating more complex systems. The results of Table 2 it is clear that the impact of the columb interaction on a system increases as the potential is widening.

This may help to used to design quantum dots able to contain more than one electron wile still knowing roughly the energies of the electrons.

References

[1] Morten Hjorth-Jensen. *Computational Physics Lecture Notes Fall 2015*. Department of physics, university of Oslo, 2015.

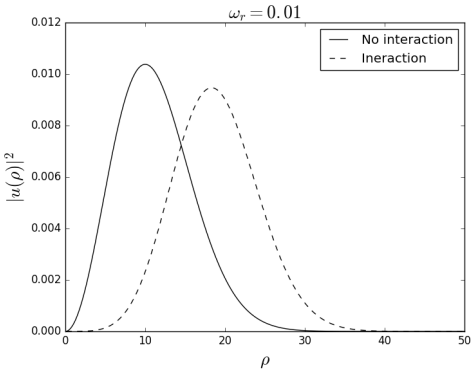

Figure 3: *Comparison of the wavefunction with and without columb interactions in a HO-potential where* $\omega_r = 0.01$

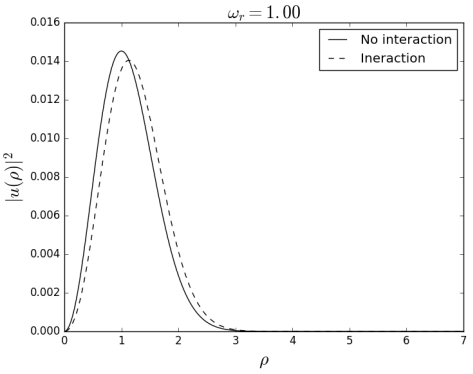

Figure 6: *Comparison of the wavefunction with and without columb interactions in a HO-potential where* $\omega_r = 1.00$

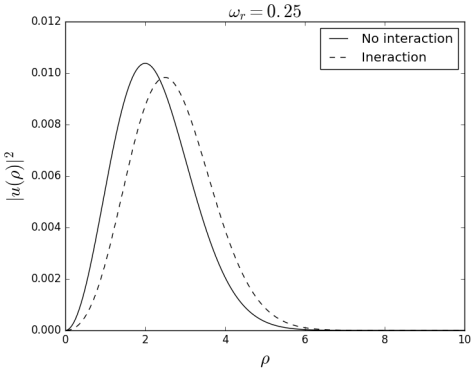

Figure 4: *Comparison of the wavefunction with and without columb interactions in a HO-potential where* $\omega_r = 0.25$

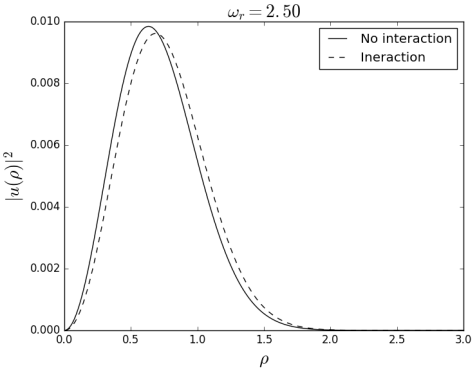

Figure 7: *Comparison of the wavefunction with and without columb interactions in a HO-potential where* $\omega_r = 2.50$

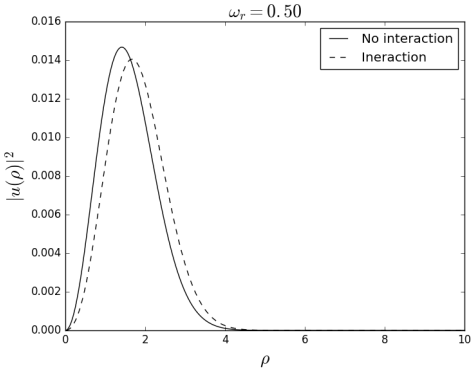

Figure 5: *Comparison of the wavefunction with and without columb interactions in a HO-potential where* $\omega_r = 0.5$

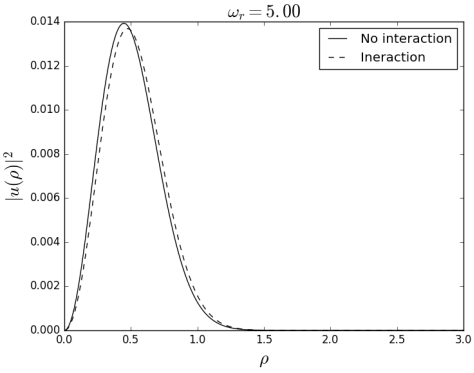

Figure 8: *Comparison of the wavefunction with and without columb interactions in a HO-potential where* $\omega_r = 5.00$