FYS3150/4150 - Project 2
Nummerical methods for solving Schröedinger equation for two different potentials

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Abstract

In this project we have solved Schröedinger equation for both interacting and non- interacting case. The potential we choosed is the harmonic oscillator and the cloumb potential. When increasing the angular frequency in the harmonic oscillator the harmonic oscillator well is narrower and starts to dominate the coloumb potential. Thus showing that for large ω_r the interacting force becomes neglible. For this project we used the jacobi method and armadillos eigenvalue solver. Comparing these two methods, we found out that armadillos solver is more effiecient and easier to use.

Contents

1 Introduction:

In this project we will be solving Schröedingers equation for two electrons for two different cases: Non and interacting case. For this we will be using cloumb potential with the harmonic oscillator potential well (interacting case), and harmonic oscillator alone (non-interacting). The motivation behind this project is to show when the angular frequency in harmonic oscillator increases the coloumb potential becomes more and more neglible. Due to the depth of the harmonic oscillator well is shrinked. Today such topic is highly active reasch field in solid state physics (semi-conductors, etc..) for different purposes. Some of this purposes is presented in [Loss and Divicenzo, 1998].

This problem can be turned into a eigenvalue problem and can be easily be solved by using different types of nummerical methods. For this project we will be using jacobi's method and armadillos built-in function and benchmark those two methods against each other.

2 Theoretical Model:

2.1 Jacobi rotation:

Jacobi rotation or the so called Jacobis algorithm, is a alogirthm which turns any given matrix $\mathbf{A}$ into a diagonal matrix $\mathbf{A_D}$. This is done by multiplying a set of orthogonal transformation $\mathbf{J}_i$, N times until a diagonal matrix is formed. Thus each time $\mathbf{J}_i$ is multiplied an entry in $\mathbf{A}$ is zeroed out.

$$\mathbf{A_D} = \mathbf{J}_N^T ....\mathbf{J}_1^T \mathbf{A}\mathbf{J}_1 ....\mathbf{J}_N \tag{1}$$

A more detailed expalination is provided here [Hjorth-Jensen, 2015]. Since $\mathbf{J}_i$ is a orthogonal transformation matrix it preserves the properties and the eigenvalues of $\mathbf{A}$. Thus, this method is a outstanding method to calculate the eigenvalues for a any given matrix due to its simplicity, but slow compared to algorithms (this will be discussed in detailed later). Since $\mathbf{A}_D$ is a diagonal matrix the eigenvlaues is along the diagonal:

$$\mathbf{A}_D = \begin{pmatrix} \lambda_1 & ... & .... & 0 & ... & 0 \\ 0 & \lambda_2 & ... & ... & ... & . \\ . & . & \lambda_3 & ... & ... & . \\ . & .. & . & \lambda_4 & ... & . \\ . & .. & ... & . & ... & 0 \\ 0 & .. & ... & ... & 0 & \lambda_N \end{pmatrix} \tag{2}$$

Where λ_i is the eigenvalues of matrix $\mathbf{A}$ and $\mathbf{A}_D$.

2.1.1 Properties of orthogonal transformation:

We will now show that the orthogonal transformation preserves the dot product and orthogonality. Consider a orthonormal vector $\mathbf{v}$ and transformation matrix $\mathbf{J}$. This orthogonal transformation matrix has the property:

$$\mathbf{J}^T = \mathbf{J}^{-1} \tag{3}$$

Notice that our orthonormal vectors form a basis $\mathcal{B} = \{\mathbf{v}\}$, thus $v_i^T v_j = \delta_{ij}$, where δ_{ij} is the kronecker delta . Further we will consider a vector $\mathbf{w} = \mathbf{J}\mathbf{v}$. The question is: "What will happen if we take the dot product of $\mathbf{w}$ with itself?". Consider the following:

$$\mathbf{w}\cdot\mathbf{w} = w_i^T w_j = (\mathbf{J}v_i)^T \mathbf{J}v_j = v_i^T \mathbf{J}^T \mathbf{J} v_j = v_i^T \mathbf{J}^{-1}\mathbf{J} v_j = v_i^T v_j = \delta_{ij} \tag{4}$$

Thus:

$$\mathbf{w}\cdot\mathbf{w} = w_i^T w_j = \delta_{ij} \tag{5}$$

2.2 Schröedinger Equation:

As previously mentioned we will be solving the three dimensional Schröedinger equation for harmonic oscillator and the coloumb potential:

$$V(r) = \frac{1}{2} m\omega^2 \mathbf{r}^2 \tag{6}$$

Where $\mathbf{r}$ is the position vector for center of mass for the electrons and ω is the frequency. We are going to define the potential as following.

$$V(r) = \frac{1}{2}k\mathbf{r}^2 \tag{7}$$

The constant k defines the steepness of the well. The coloumb potential:

$$V(r) = \frac{q}{4\pi\epsilon_0 r} \tag{8}$$

The time independent Schröedinger equation is mathematically defined as:

$$\frac{\hbar^2}{2m}\nabla^2\Psi + V(r)\Psi = E\Psi \tag{9}$$

Since the potential is radially symmetric, the angular part can be dropped. Thus:

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}r^2\frac{\mathrm{d}}{\mathrm{d}r} - \frac{l(l+1)}{r^2}\right)R(r) + V(r)R(r) = ER(r) \tag{10}$$

Where l is the oribtal angular momentum and E is the energy in the system. Doing the following substituion $R(r) = u(r)/r$ ([Griffiths, 2016]) we can rewrite our equation to:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}u(r) + \left(V(r) + \frac{l(l+1)}{r^2}\frac{\hbar^2}{2m}\right)u(r) = Eu(r) \tag{11}$$

We will now introduce a dimensionless distance variable $\rho = r/\alpha$ where α has dimension length. After some algebra, the Schröedinger equation can then be formulated as (in this project [Hjorth-Jensen, 2018] we have choosen to set $l = 0$):

$$-\frac{d^2}{d\rho^2}u(\rho) + V(\rho)u(\rho) = \lambda u(\rho) \tag{12}$$

where λ is the dimensionless energy eigenvalues defined as:

$$\lambda = \frac{2m\alpha^2}{\hbar^2}E \tag{13}$$

Note that:

$$\alpha^4 = \frac{\hbar^2}{mk} \tag{14}$$

The potential will look like: Non-interacting:

$$V_{HarmonicOscillator}(\rho) = \omega_r\rho^2 \tag{15}$$

where ω_r is the characteristic frequency defined in ([Hjorth-Jensen, 2018]) interacting:

$$V = V_{HarmonicOscillator}(\rho) + V_{Coloumb}(\rho) = \omega_r\rho^2 + 1/\rho \tag{16}$$

2.3 Schröedinger's equation and the eigenvalue problem:

Recall from previous the reformulation of Schröedingers equation:

$$-\frac{d^2}{d\rho^2}u(\rho) + V(\rho)u(\rho) = \lambda u(\rho) \tag{17}$$

This can be turned into a eigenvalue problem. We will now define a vector $\mathbf{u}$, a square diagonal matrix $\mathbf{V}$ (with the potentials on its diagonal element). The derivative operator can be written as toeplitz matrix $\mathbf{T}$ with $2/h^2$ on its main diagonal and $-1/h^2$, where h is the stepsize.

$$\underbrace{(\mathbf{T}+\mathbf{V})}_{\mathbf{A}}\mathbf{u}(\rho) = \lambda\mathbf{u}(\rho) \tag{18}$$

where we will define the main, upper and lower diagonal as:

$$d_i = \frac{2}{h^2} + V_i \qquad e_i = -\frac{1}{h^2} \tag{19}$$

Thus this can be discretized, and will have following look:

$$d_i u_i + e_{i-1}u_{i-1} + e_{i+1}u_{i+1} = \lambda u_i \tag{20}$$

2.4 boundary conditions:

In this project we will be solving the Schröedinger equation for Dirichlet boundaries. For $u_0 = u_N = 0$ we have:

$$(d_1 - \lambda)u_1 + e_2 u_1 = 0 \tag{21}$$

$$(e_{N-1} + e_{N+1})u_1 = 0 \tag{22}$$

This means we can remove these values the rows and coloumns and simply add zero on the top and bottom on the eigenvector.

3 Method

3.1 Algorithm

To study different situations of electrons in a harmonic oscillator potential, we had to develope Jacobi method algorithm (which is heavily inspired by the code found in [Hjorth-Jensen, 2015]). The pseudo code of the transformations is (see github repository for all the source codes implemented with c++)

```
while(biggest_of_diagonal < eps AND iterations < max_iterations)
 JacobiRotation(A, k, l)
 FindMaxOffDiagonal(A, k, l)
```

The idea behind this algorithm is to perform the rotation on the biggest off diagonal element in the matrix A, which has index k and l. After every rotation, we are updating the indexes with *FindMaxOffDiagonal*. Diagonalization is done when the biggest off diagonal element is smaller than given *eps*, which is an approximation to zero.

3.2 Unit tests

We applied both of the functions shown in the pseudo code on a small test matrices, to ensure that our algorithm is working the way we want it to before we moved on the bigger matrices to solve quantum problems. First, we checked the *FindMaxOffDiagonal* by simply checking if it returned the correct value

```
    find_max_offdiag(A,k,l,n);

if((abs((A(l,k))-(abs(biggest_element))) < eps) && (k == 2) && (l == 1))
    {
```

```
        //PASSED
    }
    else{
        cout << "Finding max offdiag element test FAILED - need to check the
             find_max_offdiag function" << endl;
        exit(1);
    }
```

where *biggest_element* is the biggest value placed on the off-diagonal in the test matrix.

To test the *JacobiRotation* we had to implement the whole algorithm (together with *FindMaxOffDiagonal* as shown in pseudo code above) to be able to check

1. eigenvalues produced by code against the analytical eigenvalues
2. orthogonality of the eigenvectors produced
3. symmetry conversation of a test matrix

3.3 Parameters

After passing all of the tests, we were ready to solve quantum problems. We were interested in two scenarios, one and two electrons in a potential well. With only one electron we had harmonic oscillator potential. With two electrons we had to add the Coulomb repulsive force between the particles. We were interested to study how the eigenfunction will behave with different ω_r in range between 0.01 to 5.0.

In addition we needed to find a good nummerical fit to approximate $\rho_{max} = \infty$ to match a given range of ω_r. We chose $\rho_{max} = 40$ for $\omega_r = 0.01$ and $\rho_{max} = 5$ for $\omega_r = \{0.5, 1.0, 5.0\}$.

4 Results

4.1 Efficiency

As we can see in section 3.1, Jacobi transformation algorithm does operate under two main conditions in the *while* loop, either the maximum off-diagonal element will be approximately zero or we exceed given transformation limit. Diagonalization of our matrix, depends on the matrix itself and it's dimensionality. The graph below shows number of rotations needed to diagonalize matrices with different dimensions.

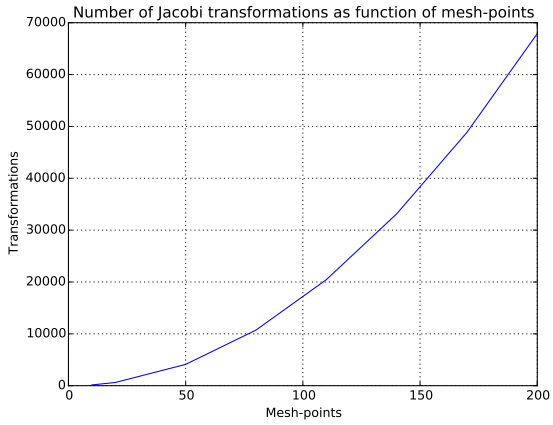


Figure 1

The time consumption compared with in-build armadillo function to find eigenpairs is significant.

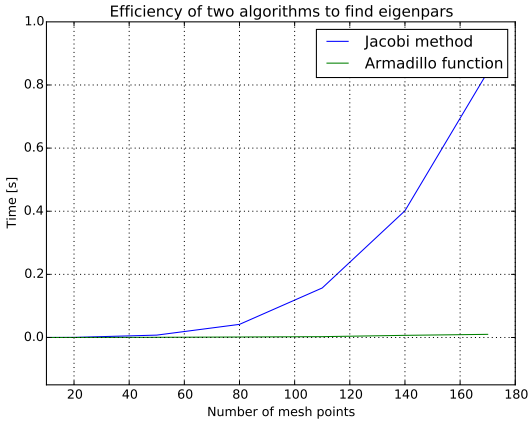
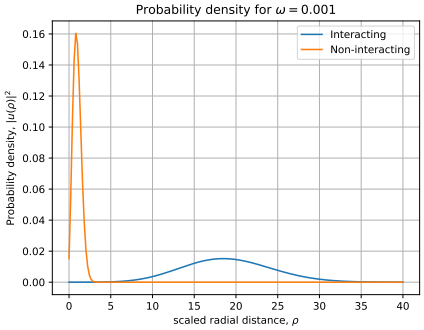
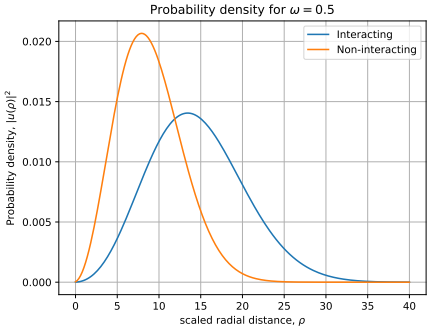


Figure 2

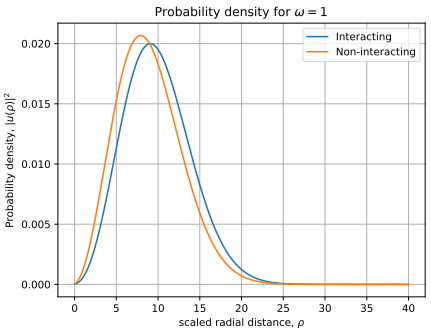
4.2 Ground state eigenfunctions



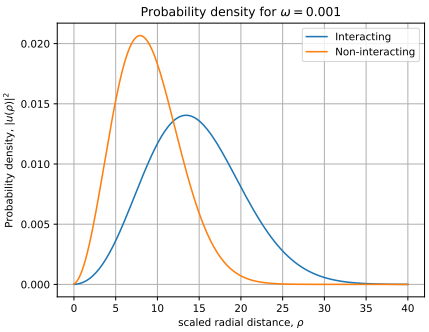
(a) $\omega_r = 0.01$



(b) $\omega_r = 0.5$



(c) $\omega_r = 1$



(d) $\omega_r = 5$

Figure 3: This following four plots shows how the probability density of the ground state eigenfunction varies, when tweaking the frequency ω_r. Here we have squared the groundstate eigenfunction and plotted against the gridpoints used.

5 Discussion

5.1 Efficiency

Diagonalization of a given matrix using Jacobi method depends on the matrix itself. Even if we set the limit of transformations to be infinity, some of the matrices does not converge to diagonal matrix, because off-diagonal elements never become zero or close to zero. This can happen in cases where off-diagonal elements which are already close to zero after a few transformations, become non-zero again after next transformation which aims to zero out a different off-diagonal element. In these cases we will never get a diagonalized matrix.

Armadillo in-build function to solve eigenproblems is optimalized and runs very quickly even if dimension of a matrix increases. This is why we used armadillo to get our eigenvectors which we used to plot ground state eigenfunctions. Second reason is that armadillo gives sorted output pairs of eigenvalues and eigenvectors. If we would like to use Jacobi method to plot ground state eigenfunction, we would have to use few more FLOPS and iterations to find the row index of absoulte value of the smalles smallest diagonal element (eigenvalue). This index corresponds to the column index in eigenvector matrix.

5.2 Groundstate eigenfunctions

As expected when increasing the frequency of the harmonic oscillator the gap between the electrons are narrower. For the interacting case we see that when this parameter ω_r is increased, the harmonic potential dominates the coloumb potential. In graph (d) in (3) we see that this is not true, but it should be almost overlap of those two graphs, but this is due to some error when some files are produced. Thus when increasing ω_r the harmonic potential becomes more and more dominant in the interacting case. This can be seen when equating the coloumb potential and harmonic oscillator. The relation between the distance and frequency is given by:

$$\rho < \omega_r^{-1/3} \tag{23}$$

For the non interacting case we see that the width of the potential becomes narrower thus the electrons oscillator closer relative to each other. The eigenfunctions and its corresponding eigenvalue was found by using c++ library armadillo, due its efficiency (compared to jacobis method which is significantly slower) and sorting the eigenfunctions with is correspongding eigenvalue.

6 Conclusion

In this project we solved Schröedingers equation for two different potentials. As it turns out for the interacting case when presenting the coloumb potential. The electrons gets closer as we increase the frequency ω_r, this is because the coloumb potenial is dominated by the harmonic potential. By using intuition this make sense since the gap in the harmonic potential is getting narrower.

For the nummerical part: The jacobi method we used was nummerically stable but slow and tedious compared to armadillos matrix equation solver. Note that (as mentioned previously) the groundstate eigenfunctions were found by using armadillo, this is due to efficiency and that armadillo sorts eigenfunction with its correspong eigenvalue.

6.1 For future work

- we can look deeper into our code and find why the last plot in the probability density is not overlaping
- comparing the nummerical solution and analytical solution found in [Taut, 1993]

References

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[Loss and Divicenzo, 1998] Loss, D. and Divicenzo, D. (1998). Quantum computations with quantum dots. *Phys.Rev A*, 57(120).

[Taut, 1993] Taut, M. (1993). Two electrons in an external oscillator potential: Particular analytical solutions of a coloumb correlation problem. *Phys rev.*, A 48(3561).