

Project2 Fys3150

Håkon Kristiansen and Stian Goplen

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Abstract

First we rewrite the radial Schrödinger equation (SE) for one electron with the harmonic oscillator potential, and the SE for two electrons with repulsive Coulomb interaction as eigenvalue problems. Then we introduce a discretization for the problem. We outline Jacobi's rotation algorithm (JRA) for solving the discrete problem. We compare the computed eigenvalues with known analytic eigenvalues for one electron with harmonic oscillator potential. Further we estimate the time complexity of JRA. We present numerical solutions of the SE for both one and two electrons. Finally we give a brief explanation of how to reproduce our results.

1 Schrödinger's equation

We want to rewrite the SE as an eigenvalue problem for one and two electrons. We assume that the electrons move in a three-dimensional oscillator potential and repel each other via the static Coulomb interaction. Further we assume spherical symmetry.

1.1 One electron with harmonic oscillator potential

At first we are interested in the solution of the radial part of the SE for one electron given by:

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

$V(r) = \frac{1}{2}kr^2$ is the harmonic oscillator potential with $k = m\omega^2$ where ω is the oscillator frequency. E is the energy of the harmonic oscillator in three dimensions, and is given by:

$$E_{nl} = \hbar\omega \left(2n + l + \frac{3}{2} \right), \quad l, n = 0, 1, 2, \dots$$

Spherical coordinates $\rightarrow r \in [0, \infty)$ and the quantum number l is the orbital momentum of the electron. We use the substitution $R(r) = \frac{1}{r}u(r)$ and insert it into 1, obtaining:

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

The boundary conditions are given as:

$$u(0) = 0, \quad u(\infty) = 0.$$

Next we define a dimensionless variable $\rho = \frac{1}{\alpha}r$ where α is a constant with dimension length. Inserting this in 2 gives:

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

We are only interested in the case where $l = 0$ and we now insert $V(\rho) = \frac{1}{2}k\alpha^2\rho^2$ and multiply with $\frac{2m\alpha^2}{\hbar^2}$ on both sides. Then we have

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

Define $\lambda = \frac{2m\alpha^2 E}{\hbar^2}$ and fix α such that

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

Finally the SE reads

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

1.2 Two electrons with repulsive Coulomb interaction

The SE for two electrons with no repulsive Coulomb interaction is given by

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr_1^2} - \frac{\hbar^2}{2m}\frac{d^2}{dr_2^2} + \frac{1}{2}kr_1^2 + \frac{1}{2}kr_2^2\right)u(r_1, r_2) = E^{(2)}u(r_1, r_2), \quad (4)$$

where $u(r_1, r_2)$ is a two-electron wave function, and $E^{(2)}$ is the two-electron energy. Next we introduce the relative coordinates $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and the center-of-mass coordinates $\mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$. Then we have

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

We can separate the equations for r and R using separation of variables with $u(r, R) = \psi(r)\phi(R)$ and $E^{(2)} = E_r + E_R$.

The Coulomb interaction between two electrons is given by

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

Adding this term to the r -dependent SE gives

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

Let $\rho = \frac{r}{\alpha}$ be a dimensionless variable. Note that we interpret ρ as the distance between the two electrons. Then we have

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

Next we define

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

and fix α such that

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

Define

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

and insert it into the above equation, we arrive at

$$-\frac{d^2}{d\rho^2}\psi(\rho) + \left(\omega_r^2\rho^2 + \frac{1}{\rho}\right)\psi(\rho) = \lambda\psi(\rho), \quad (5)$$

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

1.3 Discretization

We want to solve 3 and 5 numerically. Note that they are both on the form

$$-u''(\rho) + V(\rho)u(\rho) = \lambda u(\rho) \quad (6)$$

where $V(\rho) = \rho^2$ and $V(\rho) = \omega_r^2\rho^2 + \frac{1}{\rho}$ respectively. For the second derivative we use the standard approximation

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

where h is our step length. We have to define minimum and maximum values for ρ , $\rho_{min} = 0$ and ρ_{max} . Since we cannot set $\rho_{max} = \infty$ we have to run the program for different values of ρ_{max} . Next we define

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

where n_{step} is the number of discretization points. Let

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

Then 6 can be written as

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

or

$$-\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + V_i u_i = \lambda u_i, \quad i = 1, 2, \dots, n_{step}-1.$$

The boundary conditions $u(0) = 0$ and $u(\infty) = 0$ gives $u_0 = 0$ and $u_{n_{step}} = 0$. This can now be written as

$$A\mathbf{u} = \lambda\mathbf{u}$$

where A is a symmetric tridiagonal $(n-1)(n-1)$ matrix.

$$\mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \\ \dots \\ \dots \\ u_{n_{step}-1} \end{pmatrix}$$

and

$$A = \begin{pmatrix} d_1 & e_1 & 0 & 0 & \dots & 0 & 0 \\ e_1 & d_2 & e_2 & 0 & \dots & 0 & 0 \\ 0 & e_2 & d_3 & e_3 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & \dots & d_{n_{\text{step}}-2} & e_{n_{\text{step}}-1} \\ 0 & \dots & \dots & \dots & \dots & e_{n_{\text{step}}-1} & d_{n_{\text{step}}-1} \end{pmatrix}$$

The elements on the main diagonal is

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

and the off-diagonal elements are

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

The SE for both the one-electron and the two-electron case is now reduced to an eigenvalue problem which can be solved numerically where the only difference between the two is the potential V_i . In order to do so we use JRA.

2 Numerical solution to the eigenvalue problem

Above we show that the SE can be written as an eigenvalue problem

$$A\mathbf{u} = \lambda\mathbf{u}$$

where A is tridiagonal, real and symmetric. There is a result¹ that says that if A is real and symmetric there exists a real orthogonal matrix, S , such that

$$S^T A S = \text{diag}(\lambda_1, \dots, \lambda_n).$$

2.1 Similarity transformations

We say that a matrix B is a similarity transform of A if

$$B = S^T A S, \quad S^T S = S^{-1} S = I,$$

with the convenient property that B and A have the same eigenvalues since

$$\begin{aligned} A\mathbf{x} &= \lambda\mathbf{x} \\ (S^T A S)(S^T \mathbf{x}) &= \lambda(S^T \mathbf{x}) \\ B(S^T \mathbf{x}) &= \lambda(S^T \mathbf{x}). \end{aligned}$$

Note that even though A and B have the same eigenvalues the eigenvectors are different, where \mathbf{x} are the eigenvectors of A , and $S^T \mathbf{x}$ are the eigenvectors of B .

¹page214 Morten Hjort-Jensen Computational Physics lecture notes fall 2014

2.2 Jacobi's rotation algorithm

In JRA the idea is to use a series of similarity transformations such that A becomes diagonal. More specifically

$$S_N^T S_{N-1}^T \dots S_1^T A S_1 \dots S_{N-1} S_N = D = \text{diag}(\lambda_1, \dots, \lambda_n).$$

Say we want the elements $((k,l),(l,k))$ of A to be zero. Then the non-zero elements of $S_i, i = 1, \dots, N$ are given by

$$\begin{aligned} s_{kk} &= s_{ll} = \cos(\theta) \\ s_{kl} &= -s_{lk} = -\sin(\theta) \\ s_{ii} &= 1, \quad i \neq k, \quad i \neq l. \end{aligned}$$

Here S is orthogonal and $S^T = S^{-1}$. S performs a plane rotation around an angle θ in Euclidean n -space. Then $B = S^T A S$ results in

$$\begin{aligned} b_{ii} &= a_{ii}, \quad i \neq k, \quad i \neq l \\ b_{ik} &= a_{ik} \cos(\theta) - a_{il} \sin(\theta), \quad i \neq k, \quad i \neq l \\ b_{il} &= a_{il} \cos(\theta) + a_{ik} \sin(\theta), \quad i \neq k, \quad i \neq l \\ b_{kk} &= a_{kk} \cos^2(\theta) - 2a_{kl} \cos(\theta) \sin(\theta) + a_{ll} \sin^2(\theta) \\ b_{ll} &= a_{ll} \cos^2(\theta) + 2a_{kl} \cos(\theta) \sin(\theta) + a_{kk} \sin^2(\theta) \\ b_{kl} &= b_{lk} = (a_{kk} - a_{ll}) \cos(\theta) \sin(\theta) + a_{kl} (\cos^2(\theta) - \sin^2(\theta)). \end{aligned}$$

We want to choose θ such that all b_{kl} becomes zero, thus

$$b_{kl} = b_{lk} = (a_{kk} - a_{ll}) \cos(\theta) \sin(\theta) + a_{kl} (\cos^2(\theta) - \sin^2(\theta)) = 0,$$

which results in

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

Using $\cot(2\theta) = \frac{1}{2}(\cot(\theta) - \tan(\theta))$ gives

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

where $\tau = \cot(2\theta)$ and $t = \tan(\theta)$. The solutions to the above equation is given by

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

Note that $t = \frac{s}{c}$ and $c = \frac{1}{\sqrt{1+t^2}}$, where $c = \cos(\theta)$ and $s = \sin(\theta)$. We now want to choose c such that the difference between B and A with respect to the Frobenius norm

$$\|B - A\|_F^2 = 4(1 - c) \sum_{i=1, i \neq k, l} (a_{ik}^2 + a_{il}^2) + \frac{2a_{kl}^2}{c^2}$$

is minimized. In order to achieve this we choose the smaller of the roots of t . If $\tau < 0$ the smallest root is

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

and if $\tau > 0$ the smallest root is

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

With t being the smaller of the roots we have

$$|t| \leq 1 \Rightarrow |c| \leq \frac{1}{\sqrt{2}} \Rightarrow |\theta| \leq \frac{\pi}{4}$$

which has the effect that $\|B - A\|_F^2$ is minimized. We repeat this process until the off-diagonal norm of A is less than some small prefixed ϵ , i.e we want

$$off(A) = \sqrt{\sum_{i=1}^n \sum_{j=1, j \neq i}^n |a_{ij}|^2} < \epsilon.$$

Then finally the eigenvalues is just the elements on the diagonal of the transformed matrix A . In order to obtain the eigenvectors we note that

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

where $S^T \mathbf{x}$ is the eigenvector of B . Let

$$\mathbf{y} = S^T \mathbf{x}$$

then

$$\mathbf{x} = S\mathbf{y}.$$

If $B = diag(\lambda_1, \dots, \lambda_n)$ then the eigenvector \mathbf{y}_j corresponding to λ_j , $j = 1, \dots, n$ is given by

$$\mathbf{y}_j = (0, 0, \dots, 0, 1, 0, \dots, 0)$$

where the non-zero element is at position j . Let

$$\begin{aligned} R_0 &= I \\ R_1 &= S_1 R_0 \\ R_2 &= S_2 R_1 \\ &\vdots \\ R_N &= S_N R_{N-1} \end{aligned}$$

where the new elements of R are given by

$$r_{ik} = cr_{ik} - sr_{il}$$

and

$$r_{il} = cr_{il} + sr_{ik}$$

with $i \neq k$, $i \neq l$. Then the eigenvectors of the transformed matrix A is just the columns of R_N . Hence JRA can be summarized as follows:

Choose a tolerance ϵ , i.e $\epsilon = 10^{-8}$
While $\max(a_{ij}^2 > \epsilon)$:
Choose the largest non-diagonal element to set to zero
 $|a_{kl}| = \max_{i \neq j} |a_{ij}|$.
Compute τ , t , s and c
Compute $B = S(k, l, \theta)^T A S(k, l, \theta)$
Compute $R_{new} = S(k, l, \theta) R$
Repeat until $\max(a_{ij}^2 \leq \epsilon)$.

3 Results and discussion

3.1 Stability

First we solve eq.3 numerically. In three dimensions, the first three eigenvalues for $l = 0$ are given exactly by

$$\lambda_1 = 3, \lambda_2 = 7, \lambda_3 = 11.$$

Table 1: Results for solving the one-electron case with $\rho_{max} = 5$ and $\epsilon = 10^{-8}$. $\lambda_{i,c}$ denotes the computed eigenvalues for different values of n_{step} .

$n_{step} = 150$	$\lambda_{1,c} = 2.99965$	$\lambda_{2,c} = 6.99827$	$\lambda_{3,c} = 10.99596$
$n_{step} = 160$	$\lambda_{1,c} = 2.99969$	$\lambda_{2,c} = 6.99848$	$\lambda_{3,c} = 10.99647$
$n_{step} = 170$	$\lambda_{1,c} = 2.99973$	$\lambda_{2,c} = 6.99865$	$\lambda_{3,c} = 10.99690$
$n_{step} = 180$	$\lambda_{1,c} = 2.99976$	$\lambda_{2,c} = 6.99808$	$\lambda_{3,c} = 10.99725$
$n_{step} = 190$	$\lambda_{1,c} = 2.99978$	$\lambda_{2,c} = 6.99892$	$\lambda_{3,c} = 10.99756$
$n_{step} = 200$	$\lambda_{1,c} = 2.99980$	$\lambda_{2,c} = 6.99903$	$\lambda_{3,c} = 10.99781$

We see from Table1 that the computed eigenvalues are equal to the exact values up to 4 leading digits when $n_{step} \geq 170$.

We want to check that the results are stable with respect to the choice of ρ_{max} . Remember that

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

with $\rho_{min} = 0$. This is just

$$h = \frac{\rho_{max}}{n_{step}}$$

We now fix h . Then

$$n_{step} = \frac{\rho_{max}}{h}$$

The precision of the algorithm is dependent on h and ρ_{max} . If h was not fixed the algorithm would favourize small ρ_{max} and large n_{step} . By fixing h we can now check the stability of the computed eigenvalues with respect to ρ_{max} .

Table 2: Results for solving the one-electron case with $h = 0.05$ and $\epsilon = 10^{-8}$ for different values of ρ_{max} . Again $\lambda_{i,c}$ denotes the computed eigenvalues.

$\rho_{max} = 1$	$\lambda_{1,c} = 10.13087$	$\lambda_{2,c} = 39.47574$	$\lambda_{3,c} = 87.52265$
$\rho_{max} = 2$	$\lambda_{1,c} = 3.52820$	$\lambda_{2,c} = 11.14882$	$\lambda_{3,c} = 23.42725$
$\rho_{max} = 3$	$\lambda_{1,c} = 3.01138$	$\lambda_{2,c} = 7.32337$	$\lambda_{3,c} = 12.92549$
$\rho_{max} = 4$	$\lambda_{1,c} = 2.99925$	$\lambda_{2,c} = 6.99947$	$\lambda_{3,c} = 11.06874$
$\rho_{max} = 5$	$\lambda_{1,c} = 2.99922$	$\lambda_{2,c} = 6.99609$	$\lambda_{3,c} = 10.99066$
$\rho_{max} = 6$	$\lambda_{1,c} = 2.99922$	$\lambda_{2,c} = 6.99609$	$\lambda_{3,c} = 10.99046$
$\rho_{max} = 7$	$\lambda_{1,c} = 2.99922$	$\lambda_{2,c} = 6.99609$	$\lambda_{3,c} = 10.99046$
$\rho_{max} = 8$	$\lambda_{1,c} = 2.99922$	$\lambda_{2,c} = 6.99609$	$\lambda_{3,c} = 10.99046$

We see from Table2 that if ρ_{max} is too small we just get nonsense, and that for $\rho_{max} \geq 5$ we get the desired eigenvalues and the results are stable.

3.2 Transformations and time complexity

We now want to investigate how many similarity transformations we need to do before all non-diagonal elements are essentially zero. Setting $\rho_{max} = 5$ and $\epsilon = 10^{-8}$ and running the code for different matrix sizes we get the following results.

n_step vs number of similarity transformations with rho_max=15, eps=1.0e-8

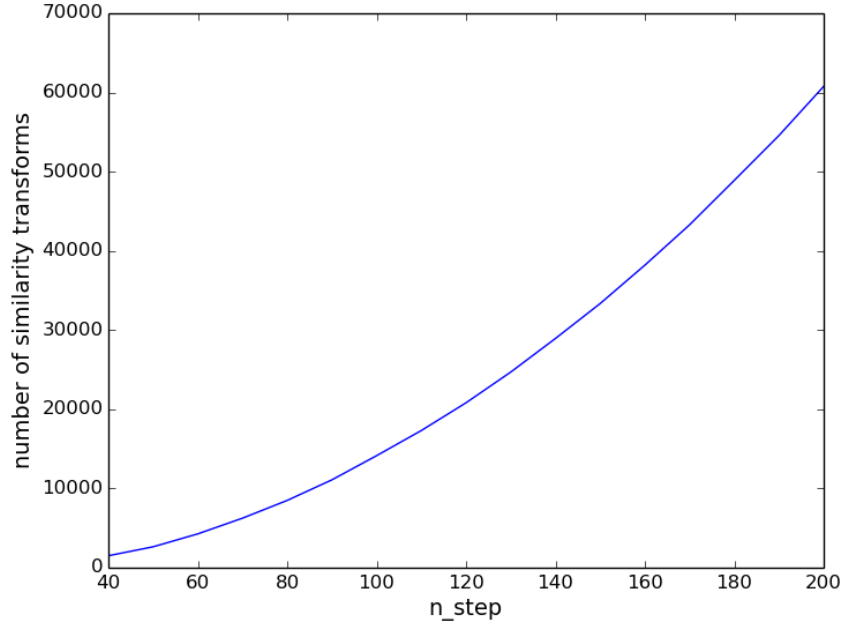


Figure 1: Plot showing how many similarity transformations which is needed before all non-diagonal elements are essentially zero for different matrix sizes.

According to Jensen² the number of transformations needed are typically $3n^2 - 5n$ and the total number of operations are $12n^3 - 20n^2$. We see from Figure 1 that if we double the matrix size the number of transformations increases by a factor of four, indicating that

$$S(n_{step}) = cn_{step}^2, \quad c \in \mathbb{R},$$

where S is the number of similarity transformations needed before all non-diagonal elements are essentially zero. This is in agreement with what we would expect.

Furthermore we want to compare the runtime of JRA with Armadillo's eigensolver(eig_sym(A)).

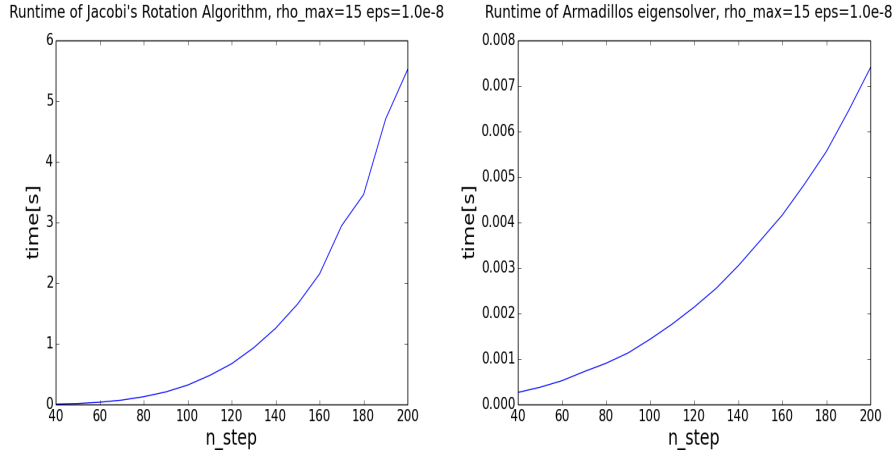


Figure 2: Plots showing the runtime of JRA and armadillo's eigensolver for different matrix sizes.

If we look at the left plot we see that if we double the size of the matrix, the runtime of JRA goes up by a factor of eight. This indicates that the time complexity is of $O(n^3)$, which corresponds with the result given by Jensen. Looking at the right plot we see that doubling the size of the matrix increases the runtime of armadillo's eigensolver by a factor of four, indicating a time complexity of $O(n^2)$. Compared to armadillo's eigensolver the efficiency of JRA is abysmal.

3.3 Solution for one electron with harmonic oscillator potential

We have plotted the ground state solutions to the radial SE for one electron and the corresponding potential, $V(\rho) = \rho^2$. The potential, V , defines the strength of the force pushing the electron towards the center of the sphere. Since $F = -\frac{dV}{d\rho} = -\rho$, $\rho \geq 0$ the force always acts towards the center of the sphere. $|u(\rho)|^2$ is interpreted as the probability of the electron being a distance ρ from the center. If we look at the classical model we expect the electron to

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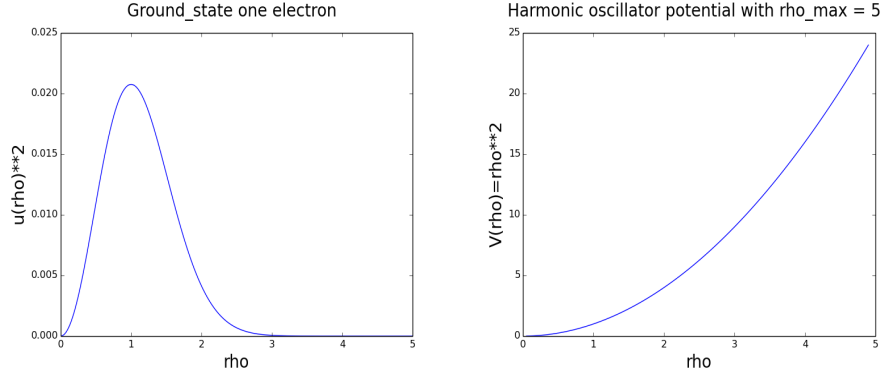


Figure 3: Ground state solution for one electron with harmonic oscillator potential

be at the point where the potential is at its minimum. But in our plot we see that the highest probability is slightly to the right of $V_{min}(\rho)$. This might be because the electron has quantized energy and will never reach the equilibrium point we would expect from the classical case.

3.4 Solution for two electrons with Coulomb interaction

3.4.1 Ground state

Below we have plotted the ground state solutions to the radial SE for two electrons and the corresponding potentials, $V(\rho) = \omega_r^2 \rho^2 + \frac{1}{\rho}$, for $\omega_r = \{0.01, 0.5, 1, 5\}$. The physical interpretation for the potential, V , is that the $\omega_r^2 \rho^2$ term is the force from the well pushing the electrons together, and the $\frac{1}{\rho}$ term is the repulsion between the electrons. $|u(\rho)|^2$ is interpreted as the probability of the electrons being a distance ρ apart.

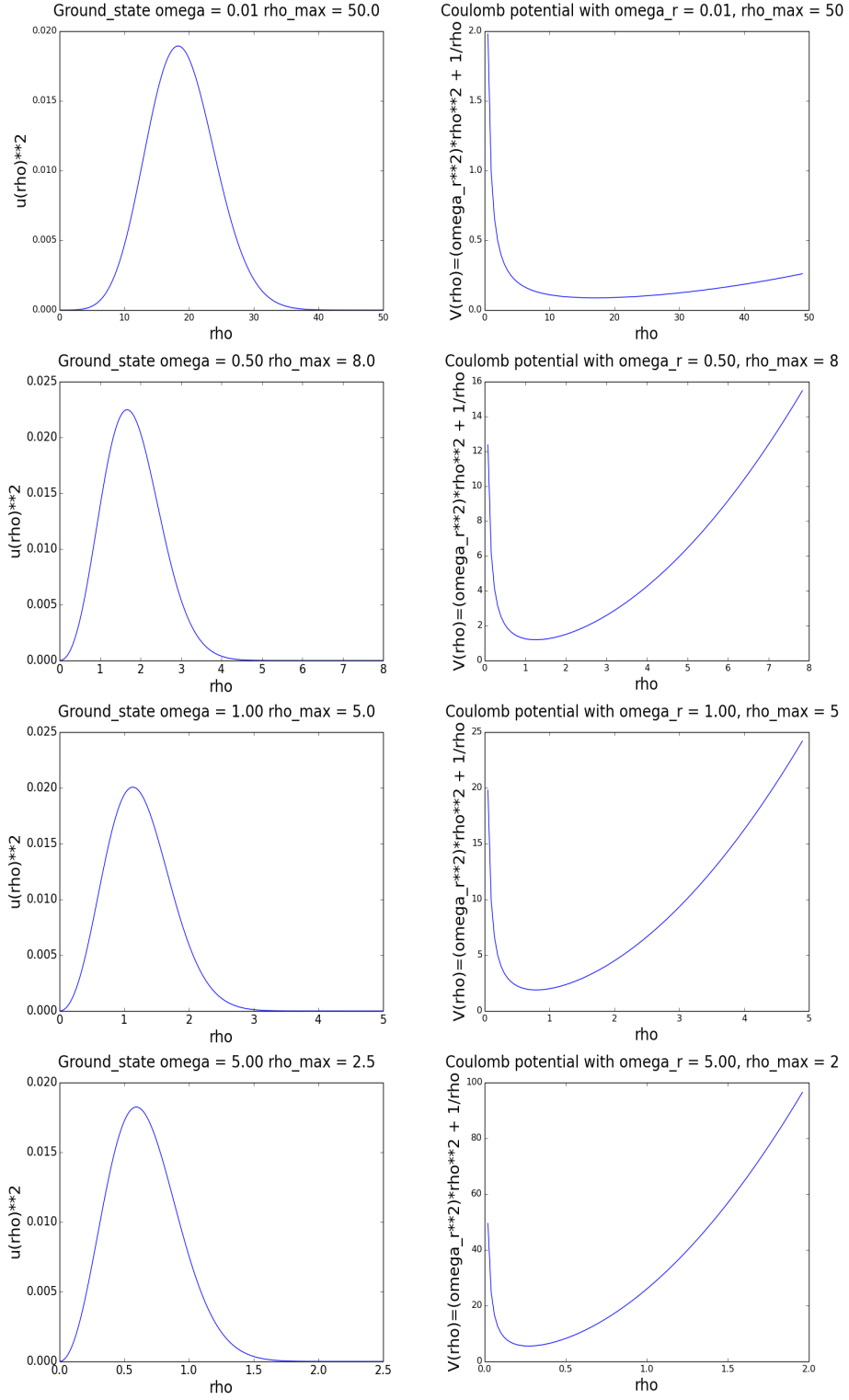


Figure 4: Ground state for specific ω_r with corresponding potential.

We see from the plots that the smaller ω_r is, the more probable it is that the electrons are further apart. This is due to the fact that the smaller ω_r is, the more the $\frac{1}{\rho}$ term will affect the potential. On the other hand, if ω_r gets larger, the $\omega_r^2 \rho^2$ term dominates and the electrons will be pushed closer together. In order for the repulsive force to overcome the force from the well we must demand that

$$\frac{1}{\rho} > \omega_r^2 \rho^2$$

or said differently

$$\rho < \frac{1}{\omega_r^{\frac{2}{3}}}.$$

Then its clear that for smaller ω_r the repulsive force contributes more to the potential than for larger ω_r . Note that the shape is similar in all the plots. We also see that the most probable distance between the electrons is slightly larger than the distance which gives the minimum value of the potential. This again might be because the electrons have quantized energy.

3.4.2 First excited state

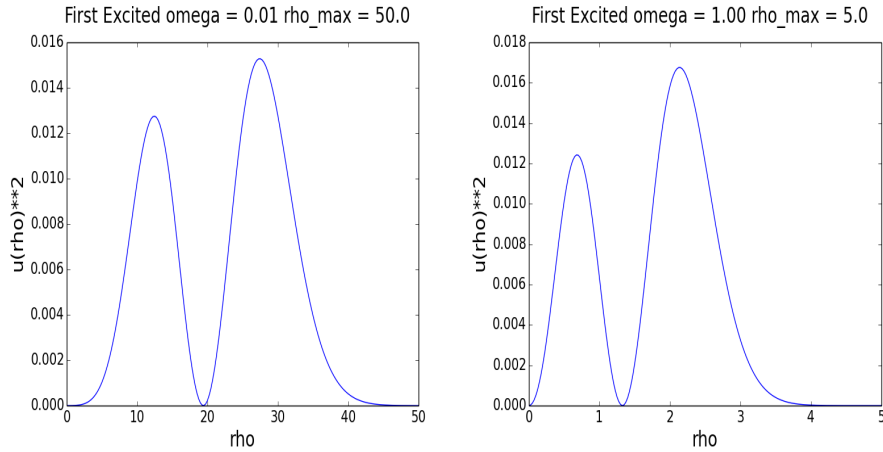


Figure 5: First excited

What we see here is that the shape of the graph is the same for different ω_r . The difference from the ground state is that there are some intermediate distances between the electrons which are not at all likely to occur. We have two global maximum points of $|u(\rho)|^2$ where the one to the right is always larger.

3.4.3 Second excited state

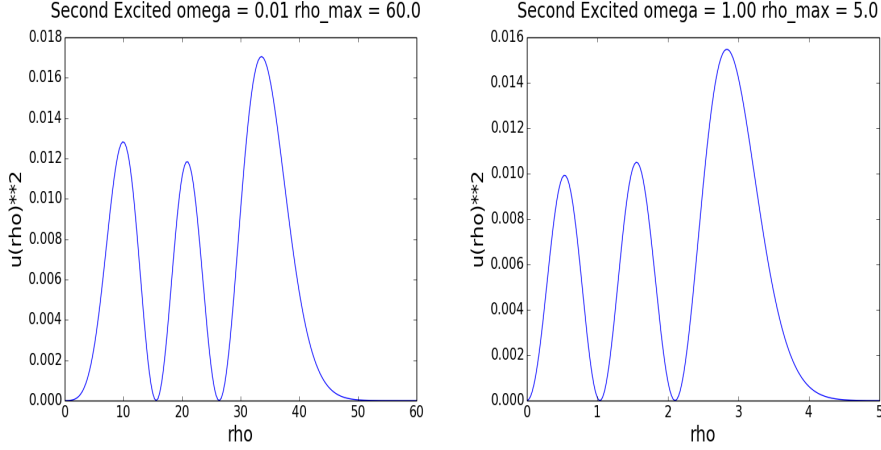


Figure 6: Second excited

Again the shapes of the curves are similar but now we have three global maximums and two intermediate distances with approximately zero probability. We would expect this tendency to continue for higher energy levels.

4 Conclusion

We have seen that for one electron with harmonic oscillator potential the first three computed eigenvalues are equal to the analytic eigenvalues up to four leading digits if $n_{step} \geq 170$. The computed eigenvalues are stable with respect to ρ_{max} and $h = 0.05$ if $\rho_{max} \geq 5$. We have estimated that the number of similarity transformations needed to reduce the non-diagonal elements of A to less than 10^{-8} is of $O(n^2)$. We have also estimated that the total number of operations needed to solve the eigenvalue problem is of $O(n^3)$ and seen that armadillo's eigensolver is faster by a factor of n . We have presented numerical solutions to the SE for one electron with harmonic oscillator potential, and two electrons with Coulomb interaction. For two electrons we have seen that small oscillator frequencies, ω_r , gives a higher probability for the electrons being further apart than if ω_r is large.

5 Appendix

5.1 Reproduction of results

In the github link provided at the top there is a file called main.cpp which contains the main program written in C++ where we have implemented JRA for solving the one and two-electron cases. It also contains several python scripts which run the main program in order to obtain the different results. To obtain the results presented above, run the following scripts:

Table1, Figure1 and Figure2: run_version2.py
Table2: run_version1.py
Figure3: plot_one_electron.py
Figure4, Figure5, Figure6: run_version3.py
The Coulomb potentials: coulombpotplot.py
The harmonic oscillator potential: plotharmonicpot.py