

Project 1 in FYS4411: Computational Physics 2

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Abstract

In the exploration of a quantum dot system consisting of electrons in a two-dimensional harmonic oscillator, we have found the ground state energy E_0^{HF} of a many-body system using the Hartree-Fock method. By including spin-degrees of freedom, we've acquired additional degeneracies for each filled shell in the harmonic oscillator. By including spin d.o.f., we find that the number of electrons for each filled shell correspond to *magic numbers*, $A = 2, 6, 12, 20$ and so on - which is the number of electrons we've run our simulation for. When comparing with other papers on the topic which have used different approaches and methods [2], we find our numbers to converge for similar values. Further, instabilities in the Hartree-Fock method are discussed. Overall, the program developed [3] methods used should be suitable for future projects.

1 Introduction

For this project our main task was to explore interacting systems of electrons in two dimensions, quantum dots. Such systems have a wide range of applications, as they can For exploring such systems, we were to employ the Hartree-Fock method. The Hartree-Fock method allows us to find the ground state of a given Hamiltonian for a many particle system. As for our case, we have looked at electrons confined in a harmonic oscillator potential where every shell up to a chosen limit has been filled. By doing this, we have that the number of electrons confine to *magic numbers*, $A = 2, 6, 12, 20, 30$ and so on. With different electron numbers, we will explore composite systems of electrons with different single particle state energies, ω .

In order to present my results, I will begin repeating the physics and mathematics involved in this project, and finally go through the Hartree-Fock algorithm. Much of the theory presented will can also be found in

the compendium used as lecture notes [1]. The journey will start with the Hamiltonian.

2 Theory

The full Hamiltonian for our quantum dot system is on the form

$$H = H_0 + H_I$$

$$= \sum_{i=1}^A \left(-\frac{1}{2} \nabla_i^2 + \frac{1}{2} \omega^2 r_i^2 \right) + \sum_{i<j}^A \frac{1}{r_{ij}} \quad (1)$$

$$= \sum_{i=1}^A \hat{h}_{i,0} + \sum_{i<j}^A V(r_{ij}), \quad (2)$$

with atomic units $\hbar = c = e = m_e = 1$. The energy results will be denoted as a.u. The first part H_0 is the unperturbed Hamiltonian, consisting of the kinetic energy and the harmonic oscillator potential. The r_{ij} is defined as $r_{ij} = \sqrt{\mathbf{r}_1 - \mathbf{r}_2}$, while the r_i is defined as $r_i = \sqrt{r_{ix}^2 + r_{iy}^2}$. The harmonic oscillator potential has a oscillator frequency ω . The sums run over all particles A . For our usage will A indicate particles below the Fermi level. We will be using the Born-Oppenheimer approximation, which means we will for all intents and purposes ignoring the nucleus in our calculations.

An unperturbed two dimensional harmonic oscillator have energies given as

$$\epsilon_{n_x, n_y} = \omega(n_x + n_y + 1) \quad (3)$$

The wave function solution for a harmonic oscillator is given by the Hermite polynomials,

$$\phi_{n_x, n_y}(x, y) = A H_{n_x}(\sqrt{\omega}x) H_{n_y}(\sqrt{\omega}y) \exp(-\omega(x^2 + y^2)/2) \quad (4)$$

The A is in this case a normalization constant.

As is evident in our calculations later on, we will be using polar coordinates to describe our system. Doing this changes our quantum numbers from n_x and n_y to n and m , and the energies is now given by

$$\epsilon_{n, m} = \omega(2n + |m| + 1) \quad (5)$$

2.1 Harmonic oscillator basis

Given that we are looking at a harmonic oscillator and are including spin degrees of freedom, we will have a basis where each level has a degeneracy corresponding of $d(n) = 2n$, where n is the shell we are looking at. Writing out the first few shells, we get

Shell number	(n, m)	Energy	Degeneracy	N
1	$(0, 0)$	$\hbar\omega$	2	2
2	$(0, -1), (0, 1)$	$2\hbar\omega$	4	6
3	$(0, -2), (1, 0), (0, 2)$	$3\hbar\omega$	6	12
4	$(0, -3), (1, -1), (1, 1), (0, 3)$	$3\hbar\omega$	8	20

Table 1: The first few single particle states configurations of a 2D harmonic oscillator in polar coordinates. The energy is calculated using equation (5).

2.2 Hartree-Fock

Before we start deriving the Hartree-Fock equations, let us restate a few of the approximations and assumptions we make. As already mentioned - the Born-Oppenheimer approximation is assumed. We will also assume that the entire system can be described by a single Slater determinant. We begin by setting up the functional for the ground state energy which we are to minimize,

$$E_0 \leq E[\Phi] = \int \Phi^* \hat{H} \Phi d\tau. \quad (6)$$

with $d\tau = d\mathbf{r}_1 d\mathbf{r}_2 \dots d\mathbf{r}_A$ and Φ as a wave function we wish to use to minimize the energy for. Inserting for the Hamiltonian we set up earlier (2), we get

$$E[\Phi] = \int \Phi^* H_0 \Phi d\tau + \int \Phi^* H_I \Phi d\tau$$

We start by looking at the first term. Using the permutation operator (21), we can write out the Slater determinants as defined in the appendix (equation (22)),

$$\begin{aligned} \int \Phi^* H_0 \Phi d\tau &= \int \sqrt{A!} \hat{A} \Phi_H^* \hat{H}_0 \sqrt{A!} \hat{A} \Phi_H d\tau \\ &= A! \int \hat{A} \Phi_H^* \hat{H}_0 \hat{A} \Phi_H d\tau \end{aligned}$$

We can now make use of the properties of the anti-symmetrization operator,

$$[\hat{H}_0, \hat{A}] = [\hat{H}_I, \hat{A}] = 0 \quad (7)$$

and $\hat{A}^2 = \hat{A}$. Using the definition of the anti-symmetrization operator given in equation (21), we get

$$\begin{aligned} & A! \int \hat{A} \Phi_H^* \hat{H}_0 \hat{A} \Phi_H d\tau \\ &= \sum_P (-1)^P \int \Phi_H^* \hat{H}_0 \hat{P} \Phi_H d\tau \\ &= \sum_{i=1}^A \sum_P (-1)^P \int \Phi_H^* \hat{H}_0 \hat{P} \Phi_H d\tau \\ &= \sum_{i=1}^A \sum_P (-1)^P \int \prod_r \psi_r^*(\mathbf{r}_r) \hat{H}_0 \hat{P} \prod_s \psi_s(\mathbf{r}_s) d\tau \\ &= \sum_{i=1}^A \sum_P \prod_r \prod_s (-1)^P \int \psi_r^*(\mathbf{r}_r) \hat{H}_0 \hat{P} \psi_s(\mathbf{r}_s) d\tau \end{aligned}$$

We see that due to the fact that we have orthogonality, all instances where two or more particles are switched will vanish. This then removes the products and the permutation summation. Instead, we are left with a sum over all the different particle states,

$$\sum_{\mu=1}^A \int \psi_\mu^*(\mathbf{r}_i) \hat{H}_0 \psi_\mu(\mathbf{r}_i) d\mathbf{r}_i$$

Using Dirac notation, we simplify further,

$$\begin{aligned} \int \Phi^* H_0 \Phi d\tau &= \sum_{\mu=1}^A \int \psi_\mu^*(\mathbf{r}_i) \hat{H}_0 \psi_\mu(\mathbf{r}_i) d\mathbf{r}_i \\ &= \sum_{\mu=1}^A \langle \mu | \hat{h}_0 | \mu \rangle \end{aligned} \quad (8)$$

Now that we have massaged the non-interacting Hamiltonian into a more manageable expression, it is only fair to do the same with the interacting

Hamiltonian, \hat{H}_I .

$$\begin{aligned}
\int \Phi^* H_I \Phi d\tau &= \sum_{i < j}^A \int \Phi^* V(r_{ij}) \Phi d\tau \\
&= A! \sum_{i < j}^A \int \Phi_H^* \hat{A} V(r_{ij}) \hat{A} \Phi_H d\tau \\
&= \sum_{i < j}^A \sum_P (-1)^P \int \Phi_H^* \frac{1}{r_{ij}} \hat{P} \Phi_H d\tau
\end{aligned}$$

We now have to do some thinking. We can start by realizing that the \hat{P} operator switches two particles, such that e.g. $\hat{P}\psi_\alpha(\mathbf{r}_1)\psi_\beta(\mathbf{r}_2) = \psi_\alpha(\mathbf{r}_2)\psi_\beta(\mathbf{r}_1)$. If we now write out the sum for the exchanged elements, we get

$$\int \Phi^* H_I \Phi d\tau = \sum_{i < j}^A \left[(-1)^0 \int \Phi_H^* \frac{1}{r_{ij}} \Phi_H d\tau + (-1)^1 \int \Phi_H^* \frac{1}{r_{ij}} P_{ij} \Phi_H d\tau + \dots \right]$$

Due to the orthogonality of the wave functions, we will have that only the terms with one permutation and no permutations will survive the summation. Further, we have that only permutations involving particles considered by the potential $V(r_{ij})$, will survive the permutation and orthogonality requirement. This simplifies our expression to

$$\begin{aligned}
\int \Phi^* H_I \Phi d\tau &= \sum_{i < j}^A \int \Phi_H^* \frac{1}{r_{ij}} (1 - P_{ij}) \Phi_H d\tau \\
&= \frac{1}{2} \sum_{\mu=1}^A \sum_{\nu=1}^A \int \psi_\mu^*(\mathbf{r}_i) \psi_\nu^*(\mathbf{r}_j) \frac{1}{r_{ij}} (1 - P_{ij}) \psi_\mu(\mathbf{r}_i) \psi_\nu(\mathbf{r}_j) d\mathbf{r}_i d\mathbf{r}_j \\
&= \frac{1}{2} \sum_{\mu=1}^A \sum_{\nu=1}^A \left[\int \psi_\mu^*(\mathbf{r}_i) \psi_\nu^*(\mathbf{r}_j) \frac{1}{r_{ij}} \psi_\mu(\mathbf{r}_i) \psi_\nu(\mathbf{r}_j) d\mathbf{r}_i d\mathbf{r}_j \right. \\
&\quad \left. - \int \psi_\mu^*(\mathbf{r}_i) \psi_\nu^*(\mathbf{r}_j) \frac{1}{r_{ij}} \psi_\nu(\mathbf{r}_i) \psi_\mu(\mathbf{r}_j) d\mathbf{r}_i d\mathbf{r}_j \right] \\
&= \frac{1}{2} \sum_{\mu=1}^A \sum_{\nu=1}^A [\langle \mu\nu | \hat{v} | \mu\nu \rangle - \langle \mu\nu | \hat{v} | \nu\mu \rangle] \\
&= \frac{1}{2} \sum_{\mu=1}^A \sum_{\nu=1}^A \langle \mu\nu | \hat{v} | \mu\nu \rangle_{AS}
\end{aligned}$$

In the last equation we used Dirac notation similar to what that were seen in (8). We now have all we need to write the full energy functional,

$$\begin{aligned}
E[\Phi] = & \sum_{\mu=1}^A \int \psi_{\mu}^*(\mathbf{r}_i) \hat{H}_0 \psi_{\mu}(\mathbf{r}_i) d\mathbf{r}_i \\
& + \frac{1}{2} \sum_{\mu=1}^A \sum_{\nu=1}^A \left[\int \psi_{\mu}^*(\mathbf{r}_i) \psi_{\nu}^*(\mathbf{r}_j) \frac{1}{r_{ij}} \psi_{\mu}(\mathbf{r}_i) \psi_{\nu}(\mathbf{r}_j) d\mathbf{r}_i d\mathbf{r}_j \right. \\
& \left. - \int \psi_{\mu}^*(\mathbf{r}_i) \psi_{\nu}^*(\mathbf{r}_j) \frac{1}{r_{ij}} \psi_{\nu}(\mathbf{r}_i) \psi_{\mu}(\mathbf{r}_j) d\mathbf{r}_i d\mathbf{r}_j \right]
\end{aligned} \tag{9}$$

Written in a compact form of notation, this is

$$E[\Phi] = \sum_{\mu=1}^A \langle \mu | \hat{h}_0 | \mu \rangle + \frac{1}{2} \sum_{\mu=1}^A \sum_{\nu=1}^A \langle \mu \nu | \hat{v} | \mu \nu \rangle_{AS} \tag{10}$$

We can now expand this function in a new basis, ψ . ψ is given by an orthogonal basis ϕ

$$\psi_p = \sum_{\lambda} C_{p\lambda} \phi_{\lambda} \tag{11}$$

where the λ runs over all the single particle states $\alpha, \beta, \dots, \nu$. In theory, this is an infinite basis. We will however make due with N single particle states, defined at a certain cutoff-shell. We can now relabel the energy functional indices from μ, ν to i, j , meaning all running over all our particles. Greek letters now run over all single particle states.

$$E[\Phi] = \sum_{i=1}^A \sum \langle i | \hat{h}_0 | i \rangle + \frac{1}{2} \sum_{i,j=1}^A \langle ij | \hat{v} | ij \rangle_{AS}$$

We can use that the wave functions can be written in a orthogonal basis (see equation (11)), which further reduces this to

$$\begin{aligned}
E[\Phi] = & \sum_{i=1}^A \sum_{\alpha\beta}^N C_{i\alpha}^* C_{i\beta} \epsilon_{\alpha} \langle \alpha | \hat{h}_0 | \beta \rangle \\
& + \frac{1}{2} \sum_{ij}^A \sum_{\alpha\beta\gamma\delta}^N C_{i\alpha}^* C_{j\beta}^* C_{i\gamma} C_{j\delta} \langle \alpha\beta | \hat{v} | \gamma\delta \rangle_{AS}
\end{aligned} \tag{12}$$

We now wish to minimize this equation, and we do so by introducing Lagrangian multipliers. We wish the Lagrangian multipliers to adhere to the orthogonality given by two particle states,

$$\langle a|b\rangle = \sum_{\alpha\beta} C_{a\alpha}^* C_{a\beta} \langle \alpha|\beta\rangle = \sum_{\alpha\beta} C_{a\alpha}^* C_{a\beta} \delta_{\alpha\beta} = \sum_{\alpha} C_{a\alpha}^* C_{a\alpha}$$

With the Lagrangian multiplier being $\sum_{i=1}^A \epsilon_i$, we get the function we need to minimize to be

$$E[\Phi] - \sum_{i=1}^A \epsilon_i \sum_{\alpha}^N C_{i\alpha}^* C_{i\alpha}$$

with N being the total number of single particle states. Minimizing with respect to $C_{k\alpha}^*$, with k indicating a single particle state below the Fermi level. We get

$$\frac{d}{dC_{k\alpha}^*} \left[E[\Phi] - \sum_{i=1}^A \epsilon_i \sum_{\alpha}^N C_{i\alpha}^* C_{i\alpha} \right] = 0$$

Inserting for $E[\Phi]$ and recalling from tensor analysis that $\frac{dx_i}{dx_j} = \delta_{ij}$, we get

$$\begin{aligned} \frac{d}{dC_{k\alpha}^*} \left\{ \sum_{i=1}^A \sum_{\alpha\beta}^N C_{i\alpha}^* C_{i\beta} \langle \alpha|\hat{h}_0|\beta\rangle + \frac{1}{2} \sum_{ij}^A \sum_{\alpha\beta\gamma\delta}^N C_{i\alpha}^* C_{j\beta}^* C_{i\gamma} C_{j\delta} \langle \alpha\beta|\hat{v}|\gamma\delta\rangle_{AS} \right. \\ \left. - \sum_{i=1}^A \epsilon_i \sum_{\alpha}^N C_{i\alpha}^* C_{i\alpha} \right\} = 0 \end{aligned}$$

While the first sum is trivial to take the derivative of, the second derivation of the second part is slightly more involved(hello, tensor chain-rule). It goes

as follow,

$$\begin{aligned}
& \frac{d}{dC_{k\alpha}^*} \left\{ \frac{1}{2} \sum_{ij}^A \sum_{\alpha\beta\gamma\delta}^N C_{i\alpha}^* C_{j\beta}^* C_{i\gamma} C_{j\delta} \right\} \\
&= \frac{1}{2} \left\{ \sum_{ij}^A \sum_{\alpha\beta\gamma\delta}^N (\delta_{ki} \delta_{\alpha\alpha} C_{j\beta}^* C_{i\gamma} C_{j\delta} + \delta_{kj} \delta_{\alpha\beta} C_{i\alpha}^* C_{i\gamma} C_{j\delta}) \right\} \\
&= \frac{1}{2} \left\{ \sum_j^A \sum_{\beta\gamma\delta}^N C_{j\beta}^* C_{k\gamma} C_{j\delta} + \sum_i^A \sum_{\beta\gamma\delta}^N C_{i\beta}^* C_{i\gamma} C_{k\delta} \right\} \\
&= \frac{1}{2} \left\{ \sum_j^A \sum_{\beta\gamma\delta}^N C_{j\beta}^* C_{k\gamma} C_{j\delta} + \sum_j^A \sum_{\beta\delta\gamma}^N C_{j\beta}^* C_{j\delta} C_{k\gamma} \right\} \\
&= \sum_j^A \sum_{\beta\gamma\delta}^N C_{j\beta}^* C_{k\gamma} C_{j\delta}
\end{aligned}$$

Note that the sum over α also disappeared due to the tensor derivative. In any case, our result becomes

$$\sum_{\beta}^N C_{k\beta} \langle \alpha | \hat{h}_0 | \beta \rangle + \sum_j^A \sum_{\beta\gamma\delta}^N C_{j\beta}^* C_{k\gamma} C_{j\delta} \langle \alpha\beta | \hat{v} | \gamma\delta \rangle_{AS} = \epsilon_k^{HF} C_{k\alpha}$$

We can now change dummy variables in the second term, $\beta \leftrightarrow \gamma$.

$$\sum_{\beta}^N C_{k\beta} \langle \alpha | \hat{h}_0 | \beta \rangle + \sum_j^A \sum_{\gamma\beta\delta}^N C_{j\gamma}^* C_{k\beta} C_{j\delta} \langle \alpha\gamma | \hat{v} | \beta\delta \rangle_{AS} = \epsilon_k^{HF} C_{k\alpha}$$

Also relabeling $k \leftrightarrow i$ and moving the sum over β outside, gives us

$$\sum_{\beta}^N \left\{ \langle \alpha | \hat{h}_0 | \beta \rangle + \sum_j^A \sum_{\gamma\delta}^N C_{j\gamma}^* C_{j\delta} \langle \alpha\gamma | \hat{v} | \beta\delta \rangle_{AS} \right\} C_{i\beta} = \epsilon_i^{HF} C_{i\alpha}$$

Assuming the basis is orthogonal, we can define the Hartree-Fock matrix,

$$h_{\alpha\beta}^{HF} = \epsilon_{\alpha} \delta_{\alpha\beta} + \sum_j^A \sum_{\gamma\delta}^N C_{j\gamma}^* C_{j\delta} \langle \alpha\gamma | \hat{v} | \beta\delta \rangle_{AS} \quad (13)$$

Using the density matrix as defined in equation (17), we can further simplify this to

$$h_{\alpha\beta}^{HF} = \epsilon_{\alpha}\delta_{\alpha\beta} + \frac{1}{2} \sum_{\gamma\delta}^N \rho_{\gamma\delta} \langle \alpha\gamma | \hat{v} | \beta\delta \rangle_{AS} \quad (14)$$

The interaction part is a four dimensional integral that can be written as

$$\langle \alpha\gamma | \hat{v} | \beta\delta \rangle = \int \Psi_{\alpha}^*(\mathbf{r}_i) \Psi_{\gamma}^*(\mathbf{r}_j) V(r_{ij}) \Psi_{\beta}(\mathbf{r}_i) \Psi_{\delta}(\mathbf{r}_j) d\mathbf{r}_i d\mathbf{r}_j \quad (15)$$

and thus stored as a N^4 matrix, with indices corresponding to different single particle states. With from these definitions, we get the following equation

$$h_{\alpha\beta}^{HF} C_{i\beta} = \epsilon_i^{HF} C_{i\alpha}, \quad (16)$$

which we immediately recognize as an Eigenvalue problem. We now have all the ingredients we need to formulate the Hartree-Fock algorithm.

2.2.1 Density matrix calculation

In equation the Hartree-Fock matrix (13), we can pre-calculate the $C_{j\gamma}^* C_{j\delta}$. This gives us the density matrix, ρ ,

$$\rho_{\gamma\delta} = \sum_{j=1}^A C_{\gamma j}^* C_{\delta j} \quad (17)$$

2.2.2 Hartree-Fock ground state energy

In order to find the correct expression for the Hartree-Fock ground state energy, we remind ourselves how the \hat{h}^{HF} Hamiltonian is defined as following,

$$\hat{h}^{HF} = \hat{h}_0 + \hat{u}^{HF},$$

where \hat{u}^{HF} is the Hartree-Fock potential. From our energy functional (10), we have

$$E_0^{HF} = \sum_{i=1}^A \langle i | \hat{h}_0 | i \rangle + \frac{1}{2} \sum_{i=1}^A \sum_{j=1}^A \langle ij | \hat{v} | ij \rangle_{AS}$$

By recalling that \hat{u}^{HF} is defined as

$$\langle i | \hat{u}^{HF} | i \rangle = \sum_{j=1}^N \langle ij | \hat{v} | ij \rangle_{AS}$$

Also remembering that $\hat{h}^{HF} = \hat{h}_0 + \hat{u}^{HF}$, we can add and subtract \hat{u}^{HF} ,

$$\begin{aligned}
E_0^{HF} &= \sum_{i=1}^A \langle i | \hat{h}_0 | i \rangle + \frac{1}{2} \sum_{i=1}^A \sum_{j=1}^A \langle ij | \hat{v} | ij \rangle_{AS} + \sum_{i=1}^A \langle i | \hat{u}^{HF} | i \rangle - \sum_{i=1}^A \langle i | \hat{u}^{HF} | i \rangle \\
&= \sum_{i=1}^A \langle i | \hat{h}^{HF} | i \rangle + \frac{1}{2} \sum_{i=1}^A \sum_{j=1}^A [\langle ij | \hat{v} | ij \rangle_{AS} - \langle ij | \hat{v} | ij \rangle_{AS}] \\
&= \sum_{i=1}^A \epsilon_i^{HF} - \frac{1}{2} \sum_{i=1}^A \sum_{j=1}^A \langle ij | \hat{v} | ij \rangle_{AS}
\end{aligned}$$

Inserting for the basis transformation as seen in equation (11), we get the following equation for the Hartree-Fock ground state energy

$$E_0^{HF} = \sum_{i=1}^A \epsilon_i^{HF} - \frac{1}{2} \sum_{i,j=0}^A \sum_{\alpha\beta\gamma\delta}^N C_{i,\alpha}^* C_{i,\beta}^* C_{j,\gamma} C_{j,\delta} \langle \alpha\gamma | \hat{v} | \beta\delta \rangle_{AS} \quad (18)$$

2.2.3 Hartree-Fock algorithm

In order to find a energy minimum for the energy functional (10), we have to solve this problem in an iterative way. The algorithm will run till the convergence criteria is met. That is, the previous single particle energies does not change significantly from the previous single particle energy values.

$$\frac{\sum_i^N |\epsilon_i^n - \epsilon_i^{n-1}|}{N} \leq \lambda, \quad (19)$$

where $\lambda = 10^{-10}$ and n symbolizes the current Hartree-Fock iteration.

Algorithm 1 Hartree-Fock. Number of Hartree-Fock iterations given by number of times step 4-6 is repeated.

- 1: Set the interaction matrix $\langle \alpha\gamma | \hat{v} | \beta\delta \rangle$, as given by equation (15), as a function of shells.
 - 2: Set up the C matrix as a identity matrix.
 - 3: Set up the density matrix ρ as seen in equation (17).
 - 4: Calculate the $h_{\alpha\beta}^{HF}$ matrix accordingly to equation (14).
 - 5: Solve the Eigenvalue problem as given by equation (16).
 - 6: With the new C-matrix found by solving the Eigenvalue problem, recalculate te ρ -matrix in equation (17).
 - 7: Repeat 4-6 till convergence criteria of equation (19) is met.
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When the algorithm has run its due course (and hopefully converged), we can then calculate the Hartree-Fock ground state energy based on equation (18).

3 Implementation

For solving this many-body problem, I implemented the Hartree-Fock algorithm 1 in C++. The code can be found by following the GitHub address given in the reference section [3].

3.1 Unit tests and verification

In order to verify our results, three different unit tests were performed.

3.1.1 Hartree-Fock method for unperturbed Hamiltonian

For this unit test, we are checking that the Hartree-Fock algorithm returns the unperturbed result if the Coulomb interaction is zero. The program converged after a single Hartree-Fock iteration for all values tested. The test was run for electron numbers of 2, 6, 12 and 20, shells from 3 to 8 and $\omega = 1.0$ a.u.

3.1.2 Preservation of degeneracy

The test performed here is to check that degeneracies are preserved throughout the Hartree-Fock method. That is, although the states become mixed through the Hartree-Fock method, we still have degenerate states. The test was run for electron numbers of 2, 6, 12 and 20, shells from 3 to 6 and $\omega = 1.0$ a.u.

3.1.3 Preservation of unitarity

Here we are checking that the C -matrix remains unitary throughout the calculations. Tests were performed with $\omega = 1.0$ a.u., electron numbers of 2, 6, 12 and 20 and 3 up to 7 shells.

4 Results

I perform calculations for primary three different values of ω , $\omega = 0.28$ a.u., $\omega = 0.5$ a.u. and $\omega = 1.0$ a.u. The number of atoms equal filled up shells,

that is they follow so-called *magic numbers*, $A = 2, 6, 12, 20$. Further, we run for different number of shells. The maximum Hartree-Fock iterations allowed were set to be 500.

Table 2: Results for $\omega = 1.0$ a.u. The first four columns show energies for different numbers of electrons. [†] the method converged after one iteration. * the method reached maximum Hartree-Fock iterations. All values are in atomic units a.u.

Shells	$A = 2$	$A = 6$	$A = 12$	$A = 20$
3	3.16269	21.5932	73.765549	
4	3.162691	20.766919	70.673849	177.963300 [†]
5	3.161921	20.748402	67.569930	159.972600*
6	3.161921	20.720257	67.296869	161.339720
7	3.161909	20.720132	66.934745	159.958720
8	3.161909	20.719248	66.923094	158.400170
9	3.161909	20.719248	66.912244	128.780950*
10	3.16191	20.7192	66.912035	158.01767
11		20.7192	66.911365	158.01028

Table 3: Results for $\omega = 0.5$ a.u. The first four columns show energies for different numbers of electrons. [†] the method converged after one iteration. * the method reached maximum Hartree-Fock iterations. All values are in atomic units a.u.

Shells	$A = 2$	$A = 6$	$A = 12$	$A = 20$
4	1.799856	12.357471	43.422400	113.412650 [†]
5	1.799748	12.325128	41.108851	99.747163*
6	1.799748	12.271499	40.750512	99.754600
7	1.799745	12.271375	40.302719	84.490335*
8	1.799745	12.271361	40.263752	57.308726*
9	1.799743	12.271337	40.216688	45.346529*

Table 4: Results for $\omega = 0.28$ a.u. The first four columns show energies for different numbers of electrons. [†] the method converged after one iteration. * the method reached maximum Hartree-Fock iterations. All values are in atomic units a.u.

Shells	$A = 2$	$A = 6$	$A = 12$	$A = 20$
4	1.141775	8.139719	29.621422	79.220310 [†]
5	1.141741	8.095876	27.596111	72.011644
6	1.141741	8.021956	23.616786*	67.907357
7	1.141717	8.020571	21.148806*	52.492447*
8	1.141717	8.019625	17.713336*	30.422769*
9	1.141713	8.019611	16.710103*	21.086059*

Table 5: Results for $\omega = 0.1$ a.u. The first four columns show energies for different numbers of electrons. [†] the method converged after one iteration. * the method reached maximum Hartree-Fock iterations. All values are in atomic units a.u.

Shells	$A = 2$	$A = 6$	$A = 12$	$A = 20$
3	0.526903	4.435740	17.272337 [†]	
4	0.526903	4.019787	15.320991	43.303270 [†]
5	0.525666	3.963148	14.098239	38.031297
6	0.525666	3.870617	10.537292*	32.681662*
7	0.525635	3.863135	8.239137*	22.924841*
8	0.525635	3.852880	3.910698*	10.445496*
9	0.525635	3.852591	2.213794*	3.120504*
10	0.525635	3.852393	1.277939*	0.325672*

4.1 Unit tests and verification

The unit tests for having an unperturbed Hartree-Fock Hamiltonian and checking the preservation of unity in C -matrix both passed. An example of the results for the preservation of degeneracy can be seen in table 6 for six electrons and three shells.

Table 6: Single particle state energies ϵ_i^n for $\omega = 1.0$ a.u., three shells and 6 electrons before convergence ϵ_i^0 and after convergence ϵ_i^f . The Hartree-Fock method converged after 9 iterations.

Before ϵ_i^0 [a.u.]	After ϵ_i^f [a.u.]
1.0	4.87879
1.0	4.87879
2.0	5.71988
2.0	5.71988
2.0	5.71988
2.0	5.71988
3.0	6.86513
3.0	6.86513
3.0	6.86513
3.0	6.86513
3.0	7.24094
3.0	7.24094

5 Conclusions and discussions

The results that have been obtained in the tables for $\omega = 0.28$ a.u. (see 4), $\omega = 0.5$ a.u. (see 3) and $\omega = 1.0$ a.u. (see 2) can be compared with results in the article by M. Pedersen Lohne et al. [2] Upon doing so, we discover that our results appear to coincide rather well with the results obtained through diffusion Monte Carlo, although the results presented for the Hartree-Fock energies appear to be slightly larger. The cause of this is not necessarily that the program used contain errors, but rather the fact that it is a crude of the model.

The crudeness of the model is somewhat highlighted by the fact that we observe that the Hartree-Fock algorithm becomes unstable for low oscillator frequencies ω and large electron numbers. As seen in the tables for different ω -values(see table 2, 3, 4 and 5), we fail to reach convergence within the maximum of 500 Hartree-Fock iterations we have set. One reason for this may be that we oscillate between different local minima, which prohibit any quick convergence. Otherwise, we performed unit tests to check that our method is correctly implemented.

We also observe that when we have an equal number of states as particles, we have that the Hartree-Fock algorithm converges after only one iteration.

This is to be expected, as we should only have the need for a single iteration to "displace" the electron states.

Given that the Hartree-Fock potential is zero - that is there is no interaction, we should get convergence after a single Hartree-Fock iteration. This criteria is fulfilled for 2, 6, 12 and 20 electrons, shells from 3 to 8 and $\omega = 1.0$ a.u. Similar, our C -matrix test for unitarity were also passed. We have because of this and the similarity to the values obtained by the M. Pedersen Lohne et al. article [2] no reason not to think that the method is correctly implemented. For all values tested, the tests was passed.

From table 6 we see that we gain degenerate energy levels, although in a symmetric manner. An equal amount of energy levels are degenerate if you "split" the ground state energy level list in two by the middle of it. The number of energy states at each new shell or state never less than two, which is to be expected as we have included spin degrees of freedom. The reason for the symmetry in the degeneracy is something I would have liked to explore further, given there was time.

Reason for high rate of instability seen when the number of electrons increases as well for low ω values (see E_0^{HF} for 12 and 20 electrons in table 5 and 4) is something I would have liked to investigate if time was endless.

In the end, the goal for this project was to develop a program that can calculate the ground state energy for a quantum dot system consisting of electrons confined in a harmonic oscillator. Not only that, we are now also capable of retrieving the wave functions and their energies for the different states. Although the method has instabilities for certain configurations, it should hopefully be robust enough to be usable in later projects.

6 Appendix A: mathematical formulas

6.1 Slater determinants

A Slater determinant is an expression describing a multi-fermionic system in accordance to the Pauli principle. For system of A particles, we have

$$\Phi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A; \alpha, \dots, \sigma) = \frac{1}{\sqrt{A!}} \begin{vmatrix} \psi_\alpha(\mathbf{r}_1) & \dots & \psi_\alpha(\mathbf{r}_A) \\ \dots & \dots & \dots \\ \psi_\sigma(\mathbf{r}_1) & \dots & \psi_\sigma(\mathbf{r}_A) \end{vmatrix} \quad (20)$$

This can be written in a more compact form using the anti-symmetrization operator \hat{A} ,

$$\hat{A} = \frac{1}{A!} \sum_P (-1)^P \hat{P} \quad (21)$$

Combining the Slater determinant (20) with \hat{A} , we get

$$\begin{aligned} \Phi(\mathbf{r}_1, \dots, \mathbf{r}_A; \alpha, \dots, \nu) &= \frac{1}{\sqrt{A!}} \sum_P (-1)^P \hat{P} \psi_\alpha(\mathbf{r}_1) \dots \psi_\nu(\mathbf{r}_A) \\ &= \frac{1}{\sqrt{A!}} \sum_P (-1)^P \hat{P} \prod_s \psi_s(\mathbf{r}_s) \\ &= \sqrt{A!} \hat{A} \Phi_H, \end{aligned} \quad (22)$$

where Φ_H is the wave function that is being permuted according to its components.

6.1.1 Slater determinant products

We can now show that a new Slater determinant constructed from a previous basis and its Slater determinant can be written - in a somewhat short-hand notation - as

$$\Phi = C\Psi \quad (23)$$

We will now use p, q, \dots, u and $\alpha, \beta, \dots, \gamma$ together under the assumption that the Slater determinant is a $N \times N$ matrix. We get,

$$\begin{aligned} \Phi &= \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_p(\mathbf{r}_1) & \psi_p(\mathbf{r}_2) & \dots \\ \psi_q(\mathbf{r}_1) & \dots & \dots \\ \dots & \dots & \dots \\ \psi_u(\mathbf{r}_1) & \dots & \psi_u(\mathbf{r}_N) \end{vmatrix} \\ &= \frac{1}{\sqrt{N!}} \begin{vmatrix} \sum_\lambda C_{p\lambda} \phi_\lambda(\mathbf{r}_1) & \dots & \sum_\lambda C_{p\lambda} \phi_\lambda(\mathbf{r}_N) \\ \dots & \dots & \dots \\ \sum_\lambda C_{u\lambda} \phi_\lambda(\mathbf{r}_1) & \dots & \sum_\lambda C_{u\lambda} \phi_\lambda(\mathbf{r}_N) \end{vmatrix} \\ &= \frac{1}{\sqrt{N!}} \begin{vmatrix} (C_{p\alpha} \phi_\alpha(\mathbf{r}_1) + C_{p\beta} \phi_\beta(\mathbf{r}_1) + \dots + C_{p\gamma} \phi_\gamma(\mathbf{r}_1)) & \dots & \dots \\ \dots & \dots & \dots \\ (C_{u\alpha} \phi_\alpha(\mathbf{r}_1) + C_{u\beta} \phi_\beta(\mathbf{r}_1) + \dots + C_{u\gamma} \phi_\gamma(\mathbf{r}_1)) & \dots & \dots \end{vmatrix} \end{aligned}$$

We can now recognize the sum as a matrix multiplication product, and rewrite our expression to

$$\frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_p(\mathbf{r}_1) & \psi_p(\mathbf{r}_2) & \dots \\ \psi_q(\mathbf{r}_1) & \dots & \dots \\ \dots & \dots & \dots \\ \psi_u(\mathbf{r}_1) & \dots & \psi_u(\mathbf{r}_N) \end{vmatrix} = \begin{vmatrix} C_{p\alpha} & c_{p\beta} & \dots & C_{p\gamma} \\ C_{q\alpha} & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots \\ C_{u\alpha} & \dots & \dots & C_{u\gamma} \end{vmatrix} \\ \times \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_\alpha(\mathbf{r}_1) & \phi_\alpha(\mathbf{r}_2) & \dots & \phi_\alpha(\mathbf{r}_N) \\ \phi_\beta(\mathbf{r}_1) & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots \\ \phi_\gamma(\mathbf{r}_1) & \dots & \dots & \phi_\gamma(\mathbf{r}_N) \end{vmatrix}$$

And we have shown that the new Slater determinant can be shown as a product between the C matrix and the old Slater determinant.

6.2 Basis orthogonality

Given an basis seen in equation (11), and that ϕ_λ is an orthogonal basis, we can show from this that ψ_p also must be an orthogonal basis.

$$\begin{aligned} \langle \psi_p | \psi_q \rangle &= \int \left(\sum_{\lambda} C_{p\lambda}^* \phi_{\lambda} \right) \left(\sum_{\eta} C_{q\eta} \phi_{\eta} \right) d\mathbf{r}_i \\ &= \sum_{\lambda, \eta} C_{p\lambda}^* C_{q\eta} \int \phi_{\lambda} \phi_{\eta} d\mathbf{r}_i \\ &= \sum_{\lambda, \eta} C_{p\lambda}^* C_{q\eta} \delta_{\lambda\eta} \\ &= \sum_{\lambda} C_{p\lambda}^* C_{q\lambda} \end{aligned}$$

And thus we see that the new basis must be orthogonal.

References

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- [3] M. Vege. Project 1 github repository. [https://github.com/hmvege/
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