Project 1 in FYS4411: Computational Physics 2

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Abstract

NAN

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. The journey will start with the Hamiltonian

2 Theory

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

$$H = H_0 + H_I$$

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

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

with natural units $\hbar = c = e = m_e = 1$. 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 $r_i = \sqrt{r_{i_x}^2 + r_{i_y}^2}$. 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

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

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

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

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

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

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 degenerace 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	$(0,0)$	$h\omega$	2	2
2	$(0,-1), (0,1)$	$2h\omega$	4	6
3	$(0,-2), (1,0), (0,2)$	$3h\omega$	6	12
4	$(0,-3), (1,-1), (1,1), (0,3)$	$3h\omega$	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,

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

with $d\tau = d\mathbf{r}_1 d\mathbf{r}_2 \ldots d\mathbf{r}_A$ and Φ as a wave function 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)),

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

$$= A! \int \hat{A} \Phi_H^* \hat{H}_0 \hat{A} \Phi_H d\tau$$

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

$$[\hat{H}_0, \hat{A}] = [\hat{H}_I, \hat{A}] = 0 \tag{7}$$

3

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

$$
A! \int \hat{A}\Phi_H^* \hat{H}_0 \hat{A}\Phi_H d\tau
$$

$$
= \sum_P (-1)^P \int \Phi_H^* \hat{H}_0 \hat{P}\Phi_H d\tau
$$

$$
= \sum_{i=1}^{A} \sum_P (-1)^P \int \Phi_H^* \hat{P}\Phi_H d\tau
$$

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

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

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,

$$
\int \Phi^* H_0 \Phi d\tau = \sum_{\mu=1}^{A} \int \psi_\mu^*(\mathbf{r}_i) \hat{H}_0 \psi_\mu(\mathbf{r}_i) d\mathbf{r}_i
$$

$$
= \sum_{\mu=1}^{A} \langle \mu | \hat{h}_0 | \mu \rangle \tag{8}
$$

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, $\hat{H}_I$.

$$\int \Phi^* H_I \Phi d\tau = \sum_{i<j}^{A} \int \Phi^* V(r_{ij}) \Phi d\tau$$

$$= A! \sum_{i<j}^{A} \int \Phi_H^* \hat{A} V(r_{ij}) \hat{A} \Phi_H d\tau$$

$$= \sum_{i<j}^{A} \sum_P (-1)^P \int \Phi_H^* \frac{1}{r_{ij}} \hat{P} \Phi_H d\tau$$

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

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

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

$$\int \Phi^* H_I \Phi d\tau = \sum_{i<j}^{A} \int \Phi_H^* \frac{1}{r_{ij}} (1 - P_{ij}) \Phi_H d\tau$$

$$= \frac{1}{2} \sum_{\mu=1}^{A} \sum_{\nu=1}^{A} \int \psi_\mu^*(\mathbf{r}_i) \psi_\nu^*(\mathbf{r}_j) \frac{1}{r_{ij}} (1 - P_{ij}) \psi_\mu(\mathbf{r}_i) \psi_\nu(\mathbf{r}_j) d\mathbf{r}_i d\mathbf{r}_j$$

$$= \frac{1}{2} \sum_{\mu=1}^{A} \sum_{\nu=1}^{A} \left[\int \psi_\mu^*(\mathbf{r}_i) \psi_\nu^*(\mathbf{r}_j) \frac{1}{r_{ij}} \psi_\mu(\mathbf{r}_i) \psi_\nu(\mathbf{r}_j) d\mathbf{r}_i d\mathbf{r}_j \right.$$

$$\left. - \int \psi_\mu^*(\mathbf{r}_i) \psi_\nu^*(\mathbf{r}_j) \frac{1}{r_{ij}} \psi_\nu(\mathbf{r}_i) \psi_\mu(\mathbf{r}_j) d\mathbf{r}_i d\mathbf{r}_j \right]$$

$$= \frac{1}{2} \sum_{\mu=1}^{A} \sum_{\nu=1}^{A} \left[\langle \mu\nu | \hat{v} | \mu\nu \rangle - \langle \mu\nu | \hat{v} | \nu\mu \rangle \right]$$

$$= \frac{1}{2} \sum_{\mu=1}^{A} \sum_{\nu=1}^{A} \langle \mu\nu | \hat{v} | \mu\nu \rangle_{AS}$$

5

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,

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

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 $\alpha, \beta, \ldots, \nu$. 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

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

6

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

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

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

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

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

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

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

as follow,

$$\frac{d}{dC_{k\alpha}^*}\left\{\frac{1}{2}\sum_{ij}^{A}\sum_{\alpha\beta\gamma\delta}^{N}C_{i\alpha}^*C_{j\beta}^*C_{i\gamma}C_{j\delta}\right\}$$

$$=\frac{1}{2}\left\{\sum_{ij}^{A}\sum_{\alpha\beta\gamma\delta}^{N}(\delta_{ki}\delta_{\alpha\alpha}C_{j\beta}^*C_{i\gamma}C_{j\delta}+\delta_{kj}\delta_{\alpha\beta}C_{i\alpha}^*C_{i\gamma}C_{j\delta})\right\}$$

$$=\frac{1}{2}\left\{\sum_{j}^{A}\sum_{\beta\gamma\delta}^{N}C_{j\beta}^*C_{k\gamma}C_{j\delta}+\sum_{i}^{A}\sum_{\beta\gamma\delta}^{N}C_{i\beta}^*C_{i\gamma}C_{k\delta}\right\}$$

$$=\frac{1}{2}\left\{\sum_{j}^{A}\sum_{\beta\gamma\delta}^{N}C_{j\beta}^*C_{k\gamma}C_{j\delta}+\sum_{j}^{A}\sum_{\beta\delta\gamma}^{N}C_{j\beta}^*C_{j\delta}C_{k\gamma}\right\}$$

$$=\sum_{j}^{A}\sum_{\beta\gamma\delta}^{N}C_{j\beta}^*C_{k\gamma}C_{j\delta}$$

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,

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

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

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

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

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

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

$$h_{\alpha\beta}^{HF} C_{i\beta} = \epsilon_i^{HF} C_{i\alpha}, \tag{16}$$

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,

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

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

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

9

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 groundstate energy

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

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.

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

where $\lambda = 10^{-10}$ and n symbolises 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.

When the algorithm has run its due course(and hopefully converged), we can then calculate the Hartree-Fock groundstate energy based of 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 adress given in the reference section cite .

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. SKRIV

3.1.2 Preservation of degeneracy

The test performed here is to check that degeneracies are preserved throughout the Hartree-Fock method. That is, allthough the states becomes mixed through the Hartree-Fock method, we still have degenerate states. SKRIV

3.1.3 Preservation of unitarity

Here we are checking that the C-matrix remains unitary throughout the calculations. SKRIV

4 Results

I perform calculations for primary three different values of ω, $\omega = 0.28$, $\omega = 0.5$ and $\omega = 1.0$. 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.

Table 2: Results for $\omega = 1.0$. First four columns show energies for different numbers of electrons.

Shells	$A = 2$	$A = 6$	$A = 12$	$A = 20$
3	3.16269	21.5932	73.765549	0
4	3.16269	20.7669	70.673849	177.9633
5	3.16192	20.7484	67.569930	159.9726
6	3.16192	20.7203	67.296869	161.33972
7	3.16191	20.7201	66.934745	159.95872
8	3.16191	20.7192	66.923094	158.40017
9	3.16191	20.7192	66.912244	128.78095
10	3.16191	20.7192	66.912035	158.01767
11	0	20.7192	66.911365	158.01028

5 Conclusions and discussions

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

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

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

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

12

Table 3: Results for $\omega = 0.1$. First four columns show energies for different numbers of electrons.

Shells	$A = 2$	$A = 6$	$A = 12$	$A = 20$
3	0.52690277	4.4357396	17.272337	0
4	0.52690277	4.0197867	15.320991	43.30327
5	0.52566619	3.9631485	14.098239	38.031297
6	0.52566619	3.8706166	10.537292	32.681662
7	0.52563535	3.8631345	8.2391371	22.924841
8	0.52563535	3.8528799	3.9106977	10.445496
9	0.52563475	3.8525909	2.2137941	3.1205042
10	0.52563475	3.8523927	1.2779387	0.32567241
11	0	0	0	0

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

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

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

$$
\Phi = C\Psi \tag{23}
$$

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

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

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

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

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.

$$\langle \psi_p | \psi_q \rangle = \int \left(\sum_\lambda C^*_{p\lambda} \phi_\lambda \right) \left(\sum_\eta C_{q\eta} \phi_\eta \right) d\mathbf{r}_i$$

$$= \sum_{\lambda,\eta} C^*_{p\lambda} C_{q\eta} \int \phi_\lambda \phi_\eta d\mathbf{r}_i$$

$$= \sum_{\lambda,\eta} C^*_{p\lambda} C_{q\eta} \delta_{\lambda\eta}$$

$$= \sum_\lambda C^*_{p\lambda} C_{q\lambda}$$

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