Project 1 in FYS4411: Computational Physics 2

March 11, 2017

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. For our project, 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*, $N = 2, 6, 12, 20, 30$ and so on.

In order to present my results, I will begin repeating the physics involved in this project, and finally go through the Hartree-Fock algorithm.

2 Theory

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

$$\begin{aligned} H &= H_0 + H_I \\ &= \sum_{i=0}^{N} \left(-\frac{1}{2}\nabla_i^2 + \frac{1}{2}\omega^2 r_i^2 \right) + \sum_{i<j}^{N} \frac{1}{r_{ij}}, \end{aligned} \tag{1}$$

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 N.

An unperturbed two dimensional harmonic oscillator have energies given as

$$\varepsilon_{n_x,n_y} = \omega(n_x + n_y + 1) \tag{2}$$

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

$$\begin{aligned} \phi_{n_x,n_y}(x,y) = AH_{n_x}(\sqrt{\omega}x)H_{n_y}(\sqrt{\omega}y)\times \\ \exp(-\omega(x^2+y^2)/2) \end{aligned} \tag{3}$$

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

$$\varepsilon_{n,m} = \omega(2n + |m| + 1) \tag{4}$$

2.1 Hartree-Fock

In order to derive the Hartree-Fock equations, we begin by setting up the functional for the ground

state energy which we are to minimize,

$$E_0 \leq E[\Phi] = \int \Phi^* \hat{H} \Phi d\tau. \tag{5}$$

with $d\tau = d\mathbf{r}_1 d\mathbf{r}_2 \dots d\mathbf{r}_N$ and Φ as a wave function function we wish to use to minimize the energy for. Inserting for the Hamiltonian we set up earlier (1), we get

$$E[\Phi] = \int \Phi^* H_0 \Phi d\tau + \int \Phi^* H_I \Phi d\tau \tag{6}$$

We start by looking at the first term.

Considering a basis transformation of $\phi_\lambda(x)$ to $\psi_p(x)$ through

$$\psi_p(x) = \sum_\lambda C_{p\lambda} \phi_\lambda(x), \tag{7}$$

where the $C_{p\lambda}$ is an unitary matrix.

2.1.1 Hartree-Fock algorithm

3 Results

3.1 Unperturbed results

3.2 Unit tests

4 Conclusions and discussions

5 Appendix A: mathematical formulas

5.1 Slater determinants

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

$$\Phi(x_1, x_2, \dots, x_N; \alpha, \dots, \sigma) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_\alpha(x_1) & \dots & \psi_\alpha(x_N) \\ \dots & \dots & \dots \\ \psi_\sigma(x_1) & \dots & \psi_\sigma(x_N) \end{vmatrix} \tag{8}$$

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

$$\hat{A} = \frac{1}{N!} \sum_P (-1)^P \hat{P} \tag{9}$$

Combining the Slater determinant (8) with $\hat{A}$, we get

$$\begin{aligned} &\Phi(x_1, \dots, x_N; \alpha, \dots, \nu) \\ &= \frac{1}{\sqrt{N!}} \sum_P (-1)^P \hat{P} \psi_\alpha(x_1) \dots \psi_\nu(x_N) \\ &= \frac{1}{\sqrt{N!}} \sum_P (-1)^P \hat{P} \prod_s \psi_s(x_s) \\ &= \sqrt{N!} \hat{A} \Phi_H, \end{aligned} \tag{10}$$

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

The 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 $\alpha, \beta, \dots, \nu$. We have that ϕ_λ is an orthogonal basis, and we can show from this that ψ_p also must be an orthogonal basis.

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