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. 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.

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,

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

2.1 Hartree-Fock

2.1.1 Hartree-Fock algorithm

3 Results

3.1 Unperturbed results

4 Conclusions and discussions