Project 2 in FYS4411: Computational Physics 2

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Abstract

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1 Introduction

The goal of this project is to study closed shell systems of electrons confined in a harmonic oscillator potential - a quantum dot. Within this scope we are investigating the ground state energies, exception values kinetic and potential energies, single particle densities and one-body densities . The system we are interested in is a two dimensional system of N electrons, and since we have closed shell systems we will look at $N = 2, 6$ and 12 electrons.

2 Theory

As tradition demands we begin by looking at the Hamiltonian of the system we are to solve,

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

In order to accommodate a modern notational benefits and simplifications, we use natural units($\hbar = c = e = m_e = 1$). We can also observe that N is the number of particles we are using, and the ω is the oscillator frequency for the harmonic oscillator part. The first part, we recognize as the unperturbed part of the Hamiltonian,

$$\hat{H}_0 = \sum_{i=1}^{N} \left(-\frac{1}{2}\nabla_i^2 + \frac{1}{2}\omega^2 r_i^2 \right), \tag{2}$$

and the last part is the perturbation to our system,

$$\hat{H}_1 = \sum_{i<j}^{N} \frac{1}{r_{ij}} \tag{3}$$

such that $\hat{H} = \hat{H}_0 + \hat{H}_1$. The distance between two electrons is defined as following,

$$r_{ij} = |\mathbf{r}_i - \mathbf{r}_j| = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2} \tag{4}$$

2.1 Variational Monte Carlo

In order to make any progress with variational Monte Carlo, we need to get ourselves a wave function.

2.2 Electron wave function

Our wave function will consist of two parts: one that comes from the harmonic oscillator potential and is built up based on the fermionic nature of the system, and one that proved a correlation between two particles - the so-called Jastrow factor. The wave function we construct, will be called our *trial wave function*.

$$\psi_T(\mathbf{r}) = \psi_C(\mathbf{r})\psi_{OB}(\mathbf{r}) \tag{5}$$

2.2.1 Slater determinants

The wave function for an electron in a two dimensional harmonic oscillator potential can be written as a Hermite polynomial,

$$\phi_{n_x,n_y}(x,y) = AH_{n_x}(\sqrt{\omega\alpha}x)H_{n_y}(\sqrt{\omega\alpha}y)\exp\left(-\frac{\omega\alpha}{2}\left(x^2+y^2\right)\right) \tag{6}$$

The details surrounding the mysterious variational parameter α will be explained further on. For now, we will place these ϕ's into a Slater determinant. The Slater determinant is a creature that describes the wave function of a fermionic system, while also enforcing anti-symmetrization and thus the Pauli principle. Our Slater determinant will take the following form, when we describe the specific state of a system by n_x, n_y and a specific particle $\mathbf{r}_i = x_i\mathbf{i} + y_i\mathbf{j}$,

$$Det(\Phi(\mathbf{r})) \equiv \frac{1}{\sqrt{N!}}\begin{vmatrix} \phi_1(\mathbf{r}_1) & \phi_2(\mathbf{r}_1) & \dots & \phi_N(\mathbf{r}_1) \\ \phi_1(\mathbf{r}_2) & \phi_2(\mathbf{r}_2) & \dots & \phi_N(\mathbf{r}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\mathbf{r}_N) & \phi_2(\mathbf{r}_N) & \dots & \phi_N(\mathbf{r}_N) \end{vmatrix} \tag{7}$$

Note that we have defined $\mathbf{r} \equiv (\mathbf{r_1}, \mathbf{r_2}, \dots, \mathbf{r_N})$. To pull this definition back to our trial wave function (5), we get

$$\psi_{OB}(\mathbf{r}) = Det(\Phi(\mathbf{r})) \tag{8}$$

Where the OB stands for one body, as in one body wave function. We now need to look into the part that accounts for many body effects, the Jastrow factor.

2.2.2 The Jastrow factor

The correlation term is called a *Jastrow factor* is as mentioned here to take into account many-body effects of our system. The general shape of it is

$$\psi_C(\mathbf{r}) = \prod_{i<j}^{N} \exp\left(\frac{ar_{ij}}{1+\beta r_{ij}}\right) \tag{9}$$

where the C stands for correlation. The a is a parameter that is 1 for parallel spin, and 1/3 for anti-parallel spin. The β is another variational parameter and the r_{ij} is defined by the equation (4) as the distance between two electrons. For now, we shall begin by looking closer at the two-electron case.

2.3 Two electron case

For the two electron case the Hamiltonian takes on familiar form,

$$\hat{H} = -\frac{1}{2}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial y_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial y_2^2}\right) + \frac{1}{2}\omega^2(x_1^2 + y_1^2 + x_2^2 + y_2^2) + \frac{1}{r_{12}} \tag{10}$$

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