FYS4150 Project 3:
Numerical integration

Marie Foss, Maria Hammerstrøm

Abstract

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Github: *https://github.com/mariahammerstrom/Project3*

1 Introduction

In this project we will determine the ground state correlation energy between two electrons in an helium atom by calculating a six-dimensional integral that appears in many quantum mechanical applications. The methods we will use are Gauss-Legendre and Gauss-Laguerre quadrature and Monte-Carlo integration.

We assume that the wave function of each electron can be modeled like the single-particle wave function of an electron in the hydrogen atom. The single-particle wave function for an electron i in the $1s$ state is given in terms of a dimensionless variable (the wave function is not properly normalized)

$$\mathbf{r}_i = x_i\mathbf{e}_x + y_i\mathbf{e}_y + z_i\mathbf{e}_z, \tag{1}$$

as

$$\psi_{1s}(\mathbf{r}_i) = e^{-\alpha r_i}, \tag{2}$$

where α is a parameter and

$$r_i = \sqrt{x_i^2 + y_i^2 + z_i^2}. \tag{3}$$

We will fix $\alpha = 2$, which should correspond to the charge of the helium atom $Z = 2$.

The ansatz for the wave function for two electrons is then given by the product of two so-called $1s$ wave functions as

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = e^{-\alpha(r_1+r_2)}. \tag{4}$$

The integral we need to solve is the quantum mechanical expectation value of the correlation energy between two electrons which repel each other via the classical Coulomb interaction, namely

$$\langle \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \rangle = \int_{-\infty}^{\infty} d\mathbf{r}_1 d\mathbf{r}_2 e^{-2\alpha(r_1+r_2)} \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}. \tag{5}$$

This integral can be solved in closed form, which gives an answer of $5\pi^2/16^2$.

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2 Methods

2.1 Gauss-Legendre

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2.2 Gauss-Laguerre

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2.3 Monte-Carlo

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3 Results

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4 Conclusions

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5 List of codes

The codes developed for this project are:
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