

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)

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

as

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

where α is a parameter and

$$r_i = \sqrt{x_i^2 + y_i^2 + z_i^2}. \quad (3)$$

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

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

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

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

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 and Gauss-Laguerre

Gaussian quadrature (hereafter GQ) is a method that solves integrals with excellent results, giving high precision for few integration points, compared to simpler integration methods such as Newton-Cotes quadrature.

The basic idea behind all integration methods is to approximate the integral

$$I = \int_a^b f(x) dx \approx \sum_{i=1}^N \omega_i f(x_i), \quad (6)$$

where ω are the weights and x are the chosen mesh points. The theory behind GQ is to obtain an arbitrary weight ω , which will not be equally spaced, through the use of orthogonal polynomials, namely Legendre and Laguerre polynomials in this case. For GQ we thus make the approximation

$$f(x) \approx P_{2N-1}(x), \quad (7)$$

where $P_{2N-1}(x)$ is a polynomial of degree $2N - 1$ with N mesh points. The mesh points are the zeros of the chosen orthogonal polynomial of order N , and the weights are determined from the inverse of a matrix defined by the orthogonal polynomials. Thus, GQ says that

$$\int f(x) dx \approx \int P_{2N-1}(x) dx \approx \sum_{i=1}^{N-1} P_{2N-1}(x_i) \omega_i. \quad (8)$$

The **Legendre polynomials** are solutions to a differential equation arising in for example the solution of the *angular dependence* of Schrödinger's equation with spherically symmetric potentials such as the Coulomb potential. The Legendre polynomials are defined as

$$L_k(x) = \frac{1}{2^k k!} \frac{d^k}{dx^k} (x^2 - 1)^k, k = 0, 1, 2, \dots \quad (9)$$

Similarly, the **Laguerre polynomials** are solutions to the differential equation arising in for example the solution of the *radial* Schrödinger's equation as described above. The Laguerre polynomials are defined as

$$L_n(x) = e^x \frac{d^n}{dx^n} (x^n e^{-x}), n = 0, 1, 2, \dots \quad (10)$$

2.2 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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