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 and Gauss-Laguerre quadrature

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

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

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 Legende and Laguerre polynomials in this case. For GQ we thus make the approximation

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

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

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

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

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

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

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

2.2 Monte-Carlo

The Monte-Carlo method is a statistical simulation method which can be used for systems that are described by their probability distribution functions (PDFs). The Monte-Carlo method proceeds by random samplings from the PDF. The final result is taken as an average over the number of simulations.

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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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