FYS4150 Project 3:
Numerical integration

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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)

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

as

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

where α is a parameter and

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

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

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = e^{-\alpha(r_1+r_2)}. \tag{1}$$

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

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

This integral can be solved in closed form, which gives an answer of $5\pi^2/16^2 \approx 0.192765710958777$.

2 Methods

2.1 Gaussian 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 the method is to approximate the given function by a polynomial of degree $2N - 1$ so that we can calculate our integral in the following way:

$$I = \int_a^b f(x)dx = \int_a^b W(x)g(x)dx \approx \sum_{i=0}^{N-1} \omega_i f(x),$$

(3)

where ω are the weights given by the weight function $W(x)$ 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, such as Legende and Laguerre polynomials.

2.1.1 Gauss-Legendre quadrature

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

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

(4)

Using **Gauss-Legendre quadrature** means solving an integral from $-\infty$ to $+\infty$. This can however not be achieved numerically. To find out how we can substitute the infinite limits with finite limits, we plot the single-particle wave function shown in Fig. 1, which shows that the function $e^{-\alpha r_i}$ reaches zero at approximately $r_i \approx 3$. We therefore used the limits [-3,3].
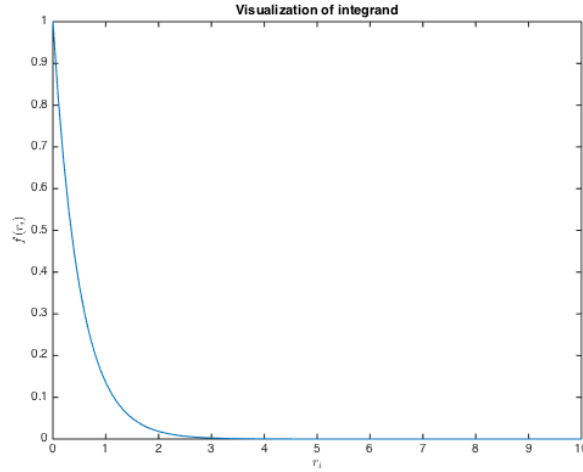
Figure 1: The single-particle wave function $e^{-\alpha r_i}$.

2.1.2 Gauss-Laguerre quadrature

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

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

(5)

Our integral in Eq. (2) can be rewritten with spherical coordinates to better deal with the infinite limits. Then the integral in Eq. (2) becomes:

$$I = \int \int \int \int \int \int r_1^2 r_2^2 \frac{e^{-2\alpha(r_1+r_2)}}{r_{12}} sin\theta_1 sin\theta_2 dr_1 dr_2 d\theta_1 d\theta_2 d\phi_1 d\phi_2$$

(6)

with

$$\frac{1}{r_{12}} = \frac{1}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 cos(\beta)}},$$

where

$$cos(\beta) = cos(\theta_1)cos(\theta_2) + sin(\theta_1)sin(\theta_2)cos(\phi_1 - \phi_2)).$$

The radial part of the integral has limits $[0,\infty)$ and we can use Laguerre polynomials with a weight function $W(x) = r^\alpha e^{-r}$. But first we need to do a variable change where we substitute $r_1 = u_1/2\alpha$ and $r_2 = u_2/2\alpha$, and $dr_1 = du_1/2\alpha$ and $dr_2 = du_2/2\alpha$. In our case $\alpha = 2$. Thus the integral becomes:

$$I = \frac{1}{1024} \int_0^\pi sin\theta_1 sin\theta_2 d\theta_1 d\theta_2 \int_0^{2\pi} d\phi_1 d\phi_2 \int_0^\infty du_1 du_2 u_1^2 u_2^2 \frac{e^{-(u_1+u_2)}}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 cos(\beta)}} \tag{7}$$

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.

We also want to run the Monte Carlo method by using importance sampling. In the regular Monte Carlo method we use uniformly distributed random numbers, but when considering importance sampling we will instead use exponentially distributed random numbers. We will also switch to spherical coordinates. ...

3   Results

The results for the various methods are collected here:

Method	N	I	σ	t (s)
Gauss-Legendre	25	0.1958	-	51
Gauss-Laguerre	25	0.1917	-	38
Monte Carlo	$5 \cdot 10^7$	0.1972	$7.00147 \cdot 10^{-3}$	23
Monte Carlo (with importance sampling)	$1 \cdot 10^5$	0.1959	$1.45335 \cdot 10^{-2}$	0

COMMENTS.

4   Conclusions

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5   List of codes

The codes developed for this project are:
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