Project 3

Anna Stray Rongve
Knut Magnus Aasrud
Amund Midtgard Raniseth

October 18, 2019

Abstract

This paper adresses different methods for solving a sixdimensional integral in a brute force way. The integral of interest is of the wave function for a helium atom in order to determine the ground energy between its two electrons. We will assume that the wave function for each elektron can be modelled like the single - particle wace function of an electron in the hydrogen atom. The function appears in several quantum mechanical applications and the methodes used to solve it are widley used when computing numericaly.

1 Introduction

Development in methods for solving integrals has been important in order to solve problems with a increasing degree of complexety. Guassian quadrature is a good example which is a method first developed by Jacobi in 1676. The first version would produce exact results for algebraic polynomials of negree n-1 or less. The "new" Guassian version has a significant increase in accuaracy with exact results for polynomials of degree 2n-1 or less due to free choise of weights.

KILDE: https://www.jstor.org/stable/24898684?seq=2metadata$_i nf o_t ab_c ontents$

Gauss-Legendre and Gauss-Laguerre are two Guassian quadrature which, togheter with the well known Monte Carlo method, will be compared in accuaracy and speed for a multidimensional integral for a Helium atom.

The main idea of Gaussian quadrature is to integrate over a set of points x_i not equally spaced with weights w_i. A part of the job is to find these points and weights(Program:Gauleg and Gauss Legendre). The weights are found throug ortogonal polynomials a set interval. The points x_i are chosen in a optimal sense and lie in the interval.

Some theory is first presented with a following discussion of the three methodes mentioned above.

Figure 1: Plot of function

2 Theory

2.1 The Quantum Mechanical Problem

. The single-particle wave function of an electron i in the $1s$ state is given in terms of a dimensionless variable (the wave function is not normalized)

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

as

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

Where α is a parameter set to 2, due to the two electrons, and the length r_i is defined by

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

For our system with two electrons, we have the product of the two $1s$ wave functions defined as

$$\Psi(\vec{r}_1, \vec{r}_2) = e^{-\alpha(r_1+r_2)}$$

This leads to the integral, see below, which will be solved nummericaly with the three different methods mentioned earlier. The value of the integral corresponds to the energy between the two electrons repelling each other due to Columb interactions.

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

The analytical result $5\pi/16^2$.

2.2 Gauss-Legendre Quadrature

Using Gauss-Legendre quadrature will make it possible to utilize the integral numerically. The first step is to change the integration limits from $-\infty$ and ∞ to $-\lambda$ and λ. The λ's are found by inserting it for r_i in the expression $e^{-\alpha r_i}$ because $r_i \approx \lambda$ when $e^{-\alpha r_i} \approx 0$. By plotting the expression as a function of r one can simply read of the function where it is approximatly zero.

2.3 Improved Gauss-Quadrature

While the Gauss-Legendre quadrature gets the job done, its not a pretty sight. What can be improved is to replace the Legendre polynomials with the Laguerre polynomials. These polynomials are defined for $x \in [0, \infty)$.

We will change our original integral from cartesian coordinates to spherical, thus the following relations:

$$d\vec{r}_1 d\vec{r}_2 = r_1^2 dr_1 r_2^2 dr_2 dcos(\theta_1) dcos(\theta_2) d\phi_1 d\phi_2$$

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

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

As previousley described, our integral is:

$$\int_{\infty}^{\infty} d\vec{r}_1 d\vec{r}_2 e^{-2\alpha(r_1+r_2)} \frac{1}{\vec{r_1} - \vec{r_2}}$$

For numerical integration, the deployment of the following relation is nessecary:

$$\int_0^{\infty} e^{-x} f(x) dx \approx \sum_{i=1}^{n} w_i f(x_i)$$

where x_i is the i-th root of the Laguerre polynomial $L_n(x)$ and the weight w_i is given by

$$w_i = \frac{x_i}{(n+1)^2 [L_{n+1}(x_i)]^2}$$

The Laguerre polynomials are defined by Rodrigues formula:

$$L_n(x) = \frac{e^x}{n!} \frac{d^n}{dx^n} \left(e^{-x} x^n\right) = \frac{1}{n!} \left(\frac{d}{dx} - 1\right)^n x^n$$

or recursively relations:

$$\begin{aligned} L_0(x) &= 1 \\ L_1(x) &= 1 - x \\ L_{n+1}(x) &= \frac{(2n + 1 - x)L_n(x) - nL_{n-1}(x)}{n+1} \end{aligned}$$

??

3 Results

3.1 Laguerre/Legendre

$$N \in [-5, 5]$$

Legandre		
N	Value	Error
11	0.297447	0.104681
15	0.315863	0.123098
21	0.268075	0.075310
25	0.240135	0.047370
27	0.229623	0.036858

Laguerre		
N	Value	Error
11	0.183021	0.009743
15	0.193285	0.000520
21	0.194807	0.002050
25	0.194804	0.002030
27	0.194795	0.002029

4 Discussion

5 Conclusion

this is a reference to intro: 1