Project 3

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October 10, 2019

Abstract

Ever done numerical integration? Well we will do it test

1 Introduction

this is intro

2 Theory

2.1 The Quantum Mechanical Problem

The problem in question is a quantum mechanical one with two electrons in a system.

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 and the length r_i is defined by

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

In this paper we will fix $\alpha = 2$, which corresponds to the helium atom Z = 2.

Four 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 us to the integral that needs solving, namely the quantum mechanical expectation value of the energy between two electrons which repel each other via the classical Coulomb interaction.

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

2.2 Gauss-Legendre Quadrature

To compute this integral we will first be utilizing the Gauss-Legendre quadrature. The first step is to change the integration limits to something a little more suitable for a computer. We will therefore change the limits $-\infty$ and ∞ to $-\lambda$ and λ. We can find these since the single-particle wavefunction $e^{-\alpha r_i}$ is approximately zero when $r_i \approx \lambda$ and we have found the correct limit for λ. We will also check that this approximation is satisfactory by plotting the function.

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:

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

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3 Discussion

4 Conclusion

this is a reference to intro: 1