

# Project 3

Anna Stray Rongve  
Knut Magnus Aasrud  
Amund Midtgard Raniseth

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  $\alpha$  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. Step one is to change the integration limits to something a little more suitable for a computer. We will therefore change the limits  $-\infty$  and  $\infty$  to  $-\lambda$  and  $\lambda$ . The values of  $\lambda$  can be found by inserting it for  $r_i$  in the formula  $e^{-\alpha r_i}$  and getting it sufficiently close to zero. 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:

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

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

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

As previously 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 necessary:

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

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:

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

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 Discussion

### 4 Conclusion

this is a reference to intro: 1