Nummerical Integration Using Gaussian Quadrature and Monte Carlo Method

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Abstract

This article set forth to integrate a six-dimensional integral which is used to determine the ground state correlation energy between two electrons in a helium atom. The integral appears in many quantum mechanical applications. We will first solve the integral true a brute force manner and employ both Gauss-Legendre and Gauss-Laguerre quadrature and Monte-Carlo integration.

I. Introduction

II. Theory

We assume that the wave function of each electron can be modelled 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

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

Note that it is not possible to find a closed-form or analytical solution to Schrödinger's equation for two interacting electrons in the helium atom.

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

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

Note that our wave function is not normalized. There is a normalization factor missing, but for this project we don't need to worry about that.

This integral can be solved in closed form and the answer is $5\pi^2/16^2$. Can you derive this value?

III. Methods

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*https://github.com/AndreasFagerheim/Fys4150

Table 1: *Example table*

Name		
First name	Last Name	Grade
John	Doe	7.5
Richard	Miles	2

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Text requiring further explanation[1].

IV. Results

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$$e = mc^2 \tag{2}$$

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V. Discussion

i. Subsection One

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[1] Example footnote

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ii. Subsection Two

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References

[Figueredo and Wolf, 2009] Figueredo, A. J. and Wolf, P. S. A. (2009). Assortative pairing and life history strategy - a cross-cultural study. *Human Nature*, 20:317–330.