Numerical integration methods

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Abstract

Key results, why is this work worthwhile? Credibility for my claims.

1 Introduction

The ground state corrolation energy between two electrons in a helium atom can be determined by solving a 6-dimensional integral. This integral is derived by modelling the wave function of each electron as an single-particle wave function of the electron in the hydrogen atom. For an electron i in the 1s state, the dimensionless and unnormalized single-particle wave function can be expressed as

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

where α is a parameter, and

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

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

The parameter $\alpha = 2$ gives the charge of the helium atom ($Z = 2$). Further, the wave function of the two 1s electrons are given by

$$\Psi(r_1 + r_2) = e^{-\alpha(r_2+r_2)}$$

The integral to solve in this report is the expectation value for the corrolation energy between the two electrons in the helium atom. The corrolation energy depends on the classical Coluomb interactions of the two electrons, and is given by

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

This (unnormalized) integral can be solved on closed form to be $5\pi^2/16^2 \approx 0.19276571$. This can be showed to be correct by ####

2 Methods

2.1 Gauss Quadrature

Gauss Quadrature is a method that uses orthogonal polynomials with weight functions to estimate integrals and are referenced in [@gaussQuad]. However, the topic is quite extensively to cover for this report and is therefore just explaned in short and otherwise sited.

2.2.1 Gauss-Legendre Quadrature First off is using the Gaussian Quadrature with Legendre polinomials. These polinomials are defined at the interval $x \in [-1, 1]$ with the weight function $W(x) = 1$. The integral in Eq. (1) can be rewritten in terms of dx_i, dy_i and dz_i as

$$\langle \frac{1}{|\mathbf{r}_1 - \mathbf{r_2}|} \rangle =$$

$$\int\int\int\int\int\int_{-\infty}^{\infty} \frac{dx_1 dx_2 dy_1 dy_2 dz_1 dz_2 e^{-2\alpha(\sqrt{(x_1+x_2)^2+(y_1+y_2)^2+(z_1+z_2)^2})}}{\sqrt{(x_1-x_2)^2+(y_1-y_2)^2+(z_1-z_2)^2}} \tag{2}$$

Now, every variable is defined on the interval $[-\infty, \infty]$, but since infinity cannot be represented exactly from a numerical point of view, it is here necessery to define infinity as a number. This is done to get small enough mesh points, so that the integral becomes more "continous". In this report, the interval $[-2, 2]$ should suffice based on Figure 1 underneath

Figure 1: Plot of the wavefunction ψ when ...

Figure here

The integral to solve with Gauss-Legendre Quadrature is then the integral

$$\int\int\int\int\int\int_{-2}^{2} \frac{dx_1 dx_2 dy_1 dy_2 dz_1 dz_2 e^{-2\alpha(\sqrt{(x_1+x_2)^2+(y_1+y_2)^2+(z_1+z_2)^2})}}{\sqrt{(x_1-x_2)^2+(y_1-y_2)^2+(z_1-z_2)^2}} \tag{3}$$

This is solved by the program ###

2.2.2 Gauss-Laguerre Quadrature (Improved Gauss Quadrature) The Gaussian Quadrature with Laguerre polinomials is defined at the interval $x \in [0, \infty]$ and has the corresponding weight function $W(x) = x^{\alpha}e^{-x}$. By changing to spherical coordinates

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

with

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

and

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

it is possible to rewrite the integral with different integration limits ($\theta \in [0, \pi]$ and $\phi \in [0, 2\pi]$). This reads

$$\langle \frac{1}{|\mathbf{r}_1 - \mathbf{r_2}|} \rangle =$$
$$\int_0^{\infty} r_1^2 dr_1 \int_0^{\infty} r_2^2 dr_2 \int_0^{\pi} dcos(\theta_1) \int_0^{\pi} dcos(\theta_2) \int_0^{2\pi} d\phi_1 \int_0^{2\pi} d\phi_2 \frac{e^{-2\alpha(r_1+r_2)}}{r_{12}}$$

where

$$dcos(\theta_1) = -\sin(\theta_1) d\theta$$

such that

$$\langle \frac{1}{|\mathbf{r}_1 - \mathbf{r_2}|} \rangle =$$
$$\int_0^{\infty} r_1^2 dr_1 \int_0^{\infty} r_2^2 dr_2 \int_0^{\pi} sin(\theta_1) d\theta \int_0^{\pi} sin(\theta_2) d\theta \int_0^{2\pi} d\phi_1 \int_0^{2\pi} d\phi_2 \frac{e^{-2\alpha(r_1+r_2)}}{r_{12}} \tag{4}$$

Among these integrals, it is easiest to map ϕ_1, ϕ_2, θ_1 and θ_2 using Lagendre polynomials and r_1 and r_2 using Laguerre polynomials. This is because $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi]$ is easily transformed to $\theta \in [-1, 1]$ and r is already defined at the interval $[0, \infty]$.

This integral is solved by the program ###

2.2 Monte Carlo Integration

When using Monte Carlo integration, the integration points are defined using a probability distribution. As long as a sufficient number of psudo-random integration points are chosen; this is supposed to make the numerical approximation of the integral have less error. It is the choice of the probability distribution function (PDF) that determines the presicion of the Monte Carlo integration. A thorough explanation of the Monte Carlo methods can found in the lecture notes [@monteCarlo] of FYS3150.

2.2.1 Brute force Monte Carlo Integration The brute force Monte Carlo integration uses the uniform PDF given by

$$p(x) = \frac{1}{b-a}\Theta(x-a)\Theta(b-x)$$

In the case of Eq. (4)

2.2.2 Improved Monte Carlo Integration

2.2.3 Improved Monte Carlo Integration with Parallization

3 Resulsts

4 Discusson

5 Conclusion

6 Appendix

Rererences