Project 3, FYS4150

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Abstract

About the problem

The task of this project is to compute, with increasing degree of cleverness, the six dimensional integral used to determine the ground state correlation energy between two electrons in a helium atom. We will start off with "brute force" Gauss Legendre quadrature, proceed to Gauss Laguerre quadrature, and finish off with Monte Carlo integration. 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 (we ommit normalization of the wave functions)

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

as

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

where α is a parameter and

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

In this project we will fix $\alpha = 2$ which should correspond to the charge of the Helium atom $Z = 2$. The ansatz for the two-electron wave function is then given by the product of two one-electron wave funtions.

$$\psi_{l,s}(\mathbf{r}_1, \mathbf{r_2}) = \psi_{l,s}(\mathbf{r}_1)\psi_{l,s}(\mathbf{r_2}) = e^{-2\alpha(r_1+r_2)}$$

The algorithm

Source code

Analytic solution

Results

N	ϵ_r LU decomposition	CPU time LU decomposition	ϵ_r	CPU time tridiagonal decomposition
5	-12.5	-	-0.7	-
10	?	-	-1.2	-
100	-1.3	-	-3.0	-
500	-1.9	-	-4.4	-
1000	-2.2	30	-4.8	-
10000	-3.2	3160	-5.0	-
10^5	x	out of memory	-5.1	-
10^6	x	out of memory	-5.07	20
10^7	x	out of memory	x	250
10^8	x	out of memory	x	2380
$1.5 * 10^8$	x	out of memory	x	3480

Stability and precision

Final comments