Numerical integration methods

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21.10.2019

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 ($Z = 2$).

2 Methods

2.1 Gauss Quadrature

2.2.1 Gauss-Legendre Quadrature

2.2.2 Gauss-Laguerre Quadrature (Improved Gauss Quadrature)