Two electron integrals - Particle in a cube

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March 11, 2017

Abstract

Analytical expressions for two-electron repulsion integrals in particle in a cube basis

1 Introduction

Two-electron integrals for particle in a cube:

Each integral is of the form:

$$(ab|cd) = \int \frac{\phi_a(r_1)\phi_b(r_1)\phi_c(r_2)\phi_d(r_2)}{|r_1 - r_2|} dr_1 dr_2 \tag{1}$$

where $\phi_a(r_1) = \left(\frac{2}{\pi}\right)^{3/2} \sin(a_x x_1)\sin(a_y y_1)\sin(a_z z_1)$.

Using the trigonometric identity

$$2\sin(a_x x_1)\sin(b_x x_1) = \cos((a_x - b_x)x_1) - \cos((a_x + b_x)x_1) \tag{2}$$

leads to the realization that the two electron integrals $(ab|cd)$ can be expanded as linear combinations of integrals of the form

$$(p|q) = \frac{1}{\pi^6} \int \frac{\cos(p_x x_1)\cos(p_y y_1)\cos(p_z z_1)\cos(q_x x_2)\cos(q_y y_2)\cos(q_z z_2)}{|r_1 - r_2|} dr_1 dr_2. \tag{3}$$

$$\cos(\mathrm{pxx1})\cos(\mathrm{rxx2})\cos(\mathrm{pyy1})\cos(\mathrm{ryy2})\cos(\mathrm{pzz1})\cos(\mathrm{rzz2}) - \cos(\mathrm{qxx1})\cos(\mathrm{rxx2})\cos(\mathrm{pyy1})\cos(\mathrm{ryy2}) \tag{4}$$