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Cuboidal basis functions

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Summary. An evaluation of the coulomb integral for a cuboid with uniform density is presented in analytic form, leading to the development of non-overlapping cube basis functions. The coulomb energy of the hydrogen molecule is determined with these functions fitted to the molecular orbital, and this result is compared with the *ab initio* coulomb energy.

Key words: Coulomb integrals – Basis functions – Numerical grids

1 Introduction

It may be argued that the introduction of newer basis sets for atomic and molecular systems have generally resulted from a simplification of the form of hydrogenic wavefunctions. Slater's function dispensed with the radial nodes of the hydrogenic functions. Subsequently, the use gaussian functions, introduced by Boys [1], further simplified the evaluation of the one- and two-electron integrals, despite the need for a larger number of Gaussians to describe adequately the Slater or hydrogenic functions. In addition, the use of gaussian functions has facilitated the development of analytic derivative methods.

Hall described the use of a discontinuous function [2], representing the radial part of the hydrogen atom solution as a single step function; by variationally optimising the radius at which the step occurred he managed to obtain approximately 60% of the energy of the hydrogen atom. This paper examines the suitability of a particular class of discontinuous functions as a basis set for use in quantum mechanical calculations of molecular systems. These functions have the form

$$\phi = f(x,y,z)\cdot\Delta \begin{cases} \Delta = 1 \text{ in range } x_{\min} < x < x_{\max}, y_{\min} < y < y_{\max}, z_{\min} < z < z_{\max}, \\ \Delta = 0 \text{ otherwise,} \end{cases} \tag{1}$$

and, while the dimensions (or sides) of the cuboid may differ, we choose to develop functions with identical dimensions (on account of the form of the multipole expansion of a uniformly dense cube) and so we call them cube functions. In this paper, we consider only the case where $f(x,y,z)$ is a non-zero constant.

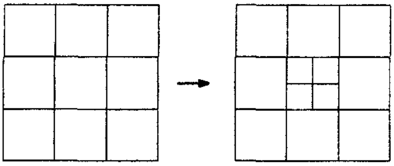

Fig. 1. Fragmentation of the middle square into four subsquares – the same fragmentation scheme may be extended to three dimensions

Space may be filled with these cubes such that they may share faces but do not overlap with one another; this cellular net can comprise a numerical basis set where functions over the whole space can be described within this basis as a linear combination of the cube functions. As the cube sizes are reduced the basis set approaches completeness. This reduction in the size of the cubes may be achieved by fragmenting a particular cube into 8 component cubes; a 2-dimensional example is shown in Fig. 1. There has recently been a tendency to move away from continuous basis sets towards methods involving quadrature [3–6] and comparisons may be made with finite element approaches to SCF calculations [7].

In the next section some useful properties of these cube functions are discussed and in the subsequent sections the one- and two-electron integrals are evaluated. Finally, results are presented for the hydrogen molecule which compare the coulomb energy calculated analytically with an STO-3G basis [8] with that calculated using an array of cube functions with coefficients derived from the STO-3G wavefunction. Recognising that, due to the discontinuity of a cube function, the regular manner of calculation of the kinetic energy is not possible, we present results for the kinetic energy of the hydrogen molecule using a numerical method.

2 Cube functions

Consider the two electron integral

$$\int \phi_i^*(1)\phi_j(1)r_{12}^{-1}\phi_k^*(2)\phi_l(2)\,\mathrm{d}\tau_1\,\mathrm{d}\tau_2 = (ij\,|\,kl). \tag{2}$$

If the functions ϕ_a, $a = \{i, j, k, l\}$, are cube functions then

$$(ij\,|\,kl) = (ii\,|\,kk)\delta_{ij}\delta_{kl}. \tag{3}$$

This reduces the two-electron integral evaluation from scaling as N^4 to N^2 in a manner similar to the NDO approximation of semi-empirical methods [9]. For the two-electron integral this corresponds to the repulsion of the density in cubes i and k. If $i \neq k$ and the distance between the cubes is large the repulsion can be treated as the interaction of two point charges. As the cubes approach one another the multipoles of the charge distribution begin to become important. A uniform cube density has the advantage of only containing multipoles of even rank greater than 2 and, in practice, one can often neglect contributions of multipoles of rank greater than 6; thus, it is possible, for moderately close cubes, to express the interaction of the uniform cube densities in terms of multipole moments [10, 11]. However, for co-incident or proximate cubes the multipole expansion does not converge rapidly. Therefore, we develop analytic expressions for the integral $(ii\,|\,ii)$, the co-incident case in the next section, and also expressions for the nuclear attraction integrals. We can use these expressions to determine the interaction between proximate cubes.

It is worthwhile to note that the cube size need not be uniform throughout the grid and that expressions for the coulomb interaction between cubes of different sizes can be calculated exactly.

3 Analytic expressions for the two-electron cube integrals

3.1 *The first three dimensions*

The intention in this section is to integrate over three dimensions of the six-dimensional integral $(ii \mid ii)$, for a cuboid of side $J \times K \times L$, where the edge of length J is aligned with the x axis, length K with the y axis, and L with the z axis.

The integral with limits is given by

$$I = \int_0^J \mathrm{d}x_1 \int_0^J \mathrm{d}x_2 \int_0^K \mathrm{d}y_1 \int_0^K \mathrm{d}y_2 \int_0^L \mathrm{d}z_1 \int_0^L \mathrm{d}z_2 \times \frac{1}{\sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2}}. \tag{4}$$

The first consideration is to decide upon the coordinate system to be used. The following change of coordinates is useful:

$$\begin{aligned} \alpha &= \tfrac{1}{2}(x_1 + x_2), \\ \beta &= \tfrac{1}{2}(x_1 - x_2), \\ \mu &= \tfrac{1}{2}(y_1 + y_2), \\ \nu &= \tfrac{1}{2}(y_1 - y_2), \\ \rho &= \tfrac{1}{2}(z_1 + z_2), \\ \sigma &= \tfrac{1}{2}(z_1 - z_2), \end{aligned} \tag{5}$$

An elementary jacobian transformation from x_1 and x_2 to α and β yields

$$\mathrm{d}x_1\,\mathrm{d}x_2 = 2d\alpha\,d\beta, \tag{6}$$

with a change in limits of either

- the limits with respect to β involve α.

$$\int_0^J \mathrm{d}x_1 \int_0^J \mathrm{d}x_2\, F(x_1,x_2) = \int_0^{J/2} \mathrm{d}\alpha \int_{-\alpha}^{\alpha} \mathrm{d}\beta\, 2F(\alpha,\beta) + \int_{J/2}^{J} \mathrm{d}\alpha \int_{\alpha-J}^{J-\alpha} \mathrm{d}\beta\, 2F(\alpha,\beta) \tag{7}$$

or

- the limits with respect to α involve β

$$\int_0^J \mathrm{d}x_1 \int_0^J \mathrm{d}x_2\, F(x_1,x_2) = \int_{-J/2}^{J/2} \mathrm{d}\beta \int_{|\beta|}^{J-|\beta|} \mathrm{d}\alpha\, 2F(\alpha,\beta). \tag{8}$$

Using Eq. (8), Eq. (4) can be rewritten as

$$I = \int_{-J/2}^{J/2} \mathrm{d}\beta \int_{|\beta|}^{J-|\beta|} \mathrm{d}\alpha \int_{-K/2}^{K/2} \mathrm{d}\nu \int_{|\nu|}^{K-|\nu|} \mathrm{d}\mu \int_{-L/2}^{L/2} \mathrm{d}\sigma \int_{|\sigma|}^{L-|\sigma|} \mathrm{d}\rho\, \frac{4}{\sqrt{\beta^2 + \nu^2 + \sigma^2}}. \tag{9}$$

Firstly carrying out the integration in Eq. (9) over α, μ and ρ yields the integral over the other three coordinates as

$$I = \int_{-J/2}^{J/2} \mathrm{d}\beta \int_{-K/2}^{K/2} \mathrm{d}\nu \int_{-L/2}^{L/2} \mathrm{d}\sigma \frac{4}{\sqrt{\beta^2 + \nu^2 + \sigma^2}} \begin{pmatrix} JKL - 2|\beta|KL - 2J|\nu|L - 2JK|\sigma| \\ + 4J|\nu||\sigma| + 4|\beta|K|\sigma| + 4|\beta||\nu|L - 8|\beta||\nu||\sigma| \end{pmatrix}. \tag{10}$$

As the integrand is symmetric with respect to each of the remaining coordinates the integral in Eq. (10), it may be expressed (with moduli signs no longer necessary) as

$$I = \int_{0}^{J/2} \mathrm{d}\beta \int_{0}^{K/2} \mathrm{d}\nu \int_{0}^{L/2} \mathrm{d}\sigma \frac{32}{\sqrt{\beta^2 + \nu^2 + \sigma^2}} \begin{pmatrix} JKL - 2\beta KL - 2J\nu L - 2JK\sigma \\ + 4J\nu\sigma + 4\beta K\sigma + 4\beta\nu L - 8\beta\nu\sigma \end{pmatrix}. \tag{11}$$

This may be expressed in spherical polar coordinates using the substitutions

$$\begin{aligned} \beta &= r\cos\vartheta, \\ \nu &= r\sin\vartheta\sin\varphi, \\ \sigma &= r\sin\vartheta\cos\varphi, \end{aligned} \tag{12}$$

where $r = \sqrt{\beta^2 + \nu^2 + \sigma^2}$, ϑ is the polar angle and φ is the azimuthal angle.

The integral may be partitioned into eight parts as

$$I = I_{JKL} + I_{\beta KL} + I_{J\nu L} + I_{JK\sigma} + I_{J\nu\sigma} + I_{\beta K\sigma} + I_{\beta\nu L} + I_{\beta\nu\sigma}, \tag{13}$$

where each of the definite integrals of the type I_{ijk} is defined by

$$\begin{aligned} I_{JKL} &= 32JKL \int \mathrm{d}\varphi \int \mathrm{d}\vartheta \int \mathrm{d}r\, r\sin\vartheta, \\ I_{\beta KL} &= -64KL \int \mathrm{d}\varphi \int \mathrm{d}\vartheta \int \mathrm{d}r\, r^2 \cos\vartheta \sin\vartheta, \\ I_{J\nu L} &= -64JL \int \mathrm{d}\varphi \int \mathrm{d}\vartheta \int \mathrm{d}r\, r^2 \sin^2\vartheta \sin\varphi, \\ I_{JK\sigma} &= -64JK \int \mathrm{d}\varphi \int \mathrm{d}\vartheta \int \mathrm{d}r\, r^2 \sin^2\vartheta \cos\varphi, \\ I_{J\nu\sigma} &= 128J \int \mathrm{d}\varphi \int \mathrm{d}\vartheta \int \mathrm{d}r\, r^3 \sin^3\vartheta \sin\varphi \cos\varphi, \\ I_{\beta K\sigma} &= 128K \int \mathrm{d}\varphi \int \mathrm{d}\vartheta \int \mathrm{d}r\, r^3 \cos\vartheta \sin^2\vartheta \cos\varphi, \\ I_{\beta\nu L} &= 128L \int \mathrm{d}\varphi \int \mathrm{d}\vartheta \int \mathrm{d}r\, r^3 \cos\vartheta \sin^2\vartheta \sin\varphi, \\ I_{\beta\nu\sigma} &= -256K \int \mathrm{d}\varphi \int \mathrm{d}\vartheta \int \mathrm{d}r\, r^4 \cos\vartheta \sin^3\vartheta \sin\varphi \cos\varphi. \end{aligned} \tag{14}$$

Here the limits of the integrals are complicated and so are not explicitly shown; the next section discusses these limits in some detail.

3.2 The last three dimensions

Each integration is carried out in one octant of the original cuboid so the limits for integration are for $0 \leqslant \vartheta \leqslant \pi/2$ and $0 \leqslant \varphi \leqslant \pi/2$. The octant may be divided into four regions as is demonstrated with the example for the integrand F_{ex}

$$\begin{aligned} I_{ex} = \int_0^{\tan^{-1}(K/L)} \mathrm{d}\varphi \Bigg(\int_0^{\tan^{-1}(L/J\cos\varphi)} \mathrm{d}\vartheta \int_0^{J/2\cos\vartheta} \mathrm{d}\boldsymbol{r}\, F_{ex}(\boldsymbol{r}, \vartheta, \varphi) \\ + \int_{\tan^{-1}(L/J\cos\varphi)}^{\pi/2} \mathrm{d}\vartheta \int_0^{L/2\sin\vartheta\cos\varphi} \mathrm{d}\vartheta\, F_{ex}(\boldsymbol{r}, \vartheta, \varphi) \Bigg) \\ + \int_{\tan^{-1}(K/L)}^{\pi/2} \mathrm{d}\varphi \Bigg(\int_0^{\tan^{-1}(K/J\sin\varphi)} \mathrm{d}\vartheta \int_0^{J/2\cos\vartheta} \mathrm{d}\boldsymbol{r}\, F_{ex}(\boldsymbol{r}, \vartheta, \varphi) \\ + \int_{\tan^{-1}(K/J\sin\varphi)}^{\pi/2} \mathrm{d}\vartheta \int_0^{K/2\sin\vartheta\sin\varphi} \mathrm{d}\boldsymbol{r}\, F_{ex}(\boldsymbol{r}, \vartheta, \varphi) \Bigg). \end{aligned} \tag{15}$$

These regions are labelled TS, TE, MS, and ME, where T (top) describes the part of the integral $0 \leqslant \vartheta \leqslant \xi$, M (middle) describes the part of the integral $\xi \leqslant \vartheta \leqslant \pi/2$, S (south) describes the part of the integral for $0 \leqslant \varphi \leqslant \tan^{-1}(K/L)$ and E (east) the part for $\tan^{-1}(K/L) \leqslant \varphi < \pi/2$, and ξ is the value of intermediate limit of the integral over ϑ.

The set of integrals to be evaluated are shown in Table 1. On integration with respect to $\boldsymbol{r}$ the resulting integrals in the top regions, TS and TE, have identical integrands. These integrals over ϑ and φ, and the corresponding integrals for the MS and ME regions, are presented in Table 2. The reference to Gradshteyn and Ryzhik is given by Ref. [12].

There are only five distinct types of integral with respect to ϑ in Table 2; the limit ϑ_{inter} depends on φ but is of the form $\tan^{-1}(1/p\,\mathrm{trig}\,\varphi)$ where $p = J/M$, with $(M, \mathrm{trig}) = (L, \cos)$ for $\varphi < \tan^{-1}(K/L)$ (this region being labelled S) and $(M, \mathrm{trig}) = (K, \sin)$ for $\varphi > \tan^{-1}(K/L)$ (this region being labelled E). We have the following result.

1. Gradshteyn and Ryzhik [12, §2.526.21, p. 137]:

$$\int_0^{\vartheta_{\text{inter}}} \frac{\sin\vartheta\,\mathrm{d}\vartheta}{\cos^2\vartheta} = \frac{\sqrt{1 + p^2\,\mathrm{trig}^2\,\varphi}}{p\,\mathrm{trig}\,\varphi} - 1. \tag{16}$$

2. Gradshteyn and Ryzhik [12, §2.526.26, p. 137]:

$$\int_0^{\vartheta_{\text{inter}}} \frac{\sin^2\vartheta\,\mathrm{d}\vartheta}{\cos^3\vartheta} = \frac{\sqrt{1 + p^2\,\mathrm{trig}^2\,\varphi}}{2p^2\,\mathrm{trig}^2\,\varphi} - \frac{1}{4}\log\left(\frac{\sqrt{1 + p^2\,\mathrm{trig}^2\,\varphi} + 1}{\sqrt{1 + p^2\,\mathrm{trig}^2\,\varphi} - 1}\right). \tag{17}$$

3. Gradshteyn and Ryzhik [12, §2.526.31, p. 137]:

$$\int_0^{\vartheta_{\text{inter}}} \frac{\sin^3\vartheta\,\mathrm{d}\vartheta}{\cos^4\vartheta} = \frac{\sqrt{1 + p^2\,\mathrm{trig}^2\,\varphi}}{p\,\mathrm{trig}\,\varphi} + \frac{(1 + p^2\,\mathrm{trig}^2\,\varphi)^{3/2}}{3p^3\,\mathrm{trig}^3\,\varphi} + \frac{2}{3} \tag{18}$$

Table 1. Table of integrals over r, ϑ and φ

#	Label	Cartesian integrand	Integral in spherical polar coordinates
1.	JKL	$\frac{1}{r}$	$\int r \sin\vartheta \, \mathrm{d}r \, \mathrm{d}\vartheta \, \mathrm{d}\varphi$
2.	βKL	$\frac{\beta}{r}$	$\int r^2 \cos\vartheta \sin\vartheta \, \mathrm{d}r \, \mathrm{d}\vartheta \, \mathrm{d}\varphi$
3.	$J\nu L$	$\frac{\nu}{r}$	$\int r^2 \sin^2\vartheta \sin\varphi \, \mathrm{d}r \, \mathrm{d}\vartheta \, \mathrm{d}\varphi$
4.	$JK\sigma$	$\frac{\sigma}{r}$	$\int r^2 \sin^2\vartheta \cos\varphi \, \mathrm{d}r \, \mathrm{d}\vartheta \, \mathrm{d}\varphi$
5.	$J\nu\sigma$	$\frac{\nu\sigma}{r}$	$\int r^3 \sin^3\vartheta \sin\varphi \cos\varphi \, \mathrm{d}r \, \mathrm{d}\vartheta \, \mathrm{d}\varphi$
6.	$\beta K\sigma$	$\frac{\beta\sigma}{r}$	$\int r^3 \cos\vartheta \sin^2\vartheta \cos\varphi \, \mathrm{d}r \, \mathrm{d}\vartheta \, \mathrm{d}\varphi$
7.	$\beta\nu L$	$\frac{\sigma\nu}{r}$	$\int r^3 \cos\vartheta \sin^2\vartheta \sin\varphi \, \mathrm{d}r \, \mathrm{d}\vartheta \, \mathrm{d}\varphi$
8.	$\beta\nu\sigma$	$\frac{\beta\nu\sigma}{r}$	$\int r^4 \cos\vartheta \sin^3\vartheta \sin\varphi \cos\varphi \, \mathrm{d}r \, \mathrm{d}\vartheta \, \mathrm{d}\varphi$

4. Gradshteyn and Ryzhik [12, §2.526.1, p. 136]:

$$\int_{\vartheta_{\mathrm{inter}}}^{\pi/2} \frac{\mathrm{d}\vartheta}{\sin\vartheta} = \frac{1}{2} \log\left(\frac{\sqrt{1 + p^2 \operatorname{trig}^2 \varphi} + p \operatorname{trig} \varphi}{\sqrt{1 + p^2 \operatorname{trig}^2 \varphi} - p \operatorname{trig} \varphi}\right) \tag{19}$$

5. Gradshteyn and Ryzhik [12, §2.526.37, p. 138]:

$$\int_{\vartheta_{\mathrm{inter}}}^{\pi/2} \frac{\cos\vartheta \, \mathrm{d}\vartheta}{\sin^2\vartheta} = \sqrt{1 + p^2 \operatorname{trig}^2 \varphi} - 1. \tag{20}$$

The integrals with respect to ϑ and φ in Table 2 then result in integrals over φ for each of the regions TS, TE, MS and ME, and these are presented in Tables 3–6.

Tables 3–6 contain eight general types of integral which may be further subclassified. To describe these integral types it is useful to introduce three new functions,

$$u = \sqrt{1 + p^2 \operatorname{trig}^2 \varphi}, \tag{21}$$

$$g = \operatorname{trig} \varphi, \tag{22}$$

$$h = \sqrt{1 - \operatorname{trig}^2 \varphi}, \tag{23}$$

The functions g and h have the same relationship to each other as $\sin\varphi$ and $\cos\varphi$. Initially, let us assume that trig is sin. For the cases where trig is cos the identity $\sin(\varphi) = \cos(\pi/2 - \varphi)$ becomes useful. The necessary integrals are

Table 2. Table of integrals over ϑ and φ. The heading of each of the columns contains the label for the region of the integral and the upper limit of r used in each region used to obtain these integrals

#	Label	$\frac{J}{2\cos\vartheta}$ TS, TE	$\frac{K}{2\sin\vartheta\sin\varphi}$ ME	$\frac{L}{2\sin\vartheta\cos\varphi}$ MS
1.	JKL	$\int\frac{J^2}{8}\frac{\sin\vartheta\,\mathrm{d}\vartheta}{\cos^2\vartheta}\,\mathrm{d}\varphi$	$\int\frac{K^2}{8}\frac{\mathrm{d}\vartheta}{\sin\vartheta}\frac{\mathrm{d}\varphi}{\sin^2\varphi}$	$\int\frac{L^2}{8}\frac{\mathrm{d}\vartheta}{\sin\vartheta}\frac{\mathrm{d}\varphi}{\cos^2\varphi}$
2.	βKL	$\int\frac{J^3}{24}\frac{\sin\vartheta\,\mathrm{d}\vartheta}{\cos^2\vartheta}\,\mathrm{d}\varphi$	$\int\frac{K^3}{24}\frac{\cos\vartheta\,\mathrm{d}\vartheta}{\sin^2\vartheta}\frac{\mathrm{d}\varphi}{\sin^3\varphi}$	$\int\frac{L^3}{24}\frac{\cos\vartheta\,\mathrm{d}\vartheta}{\sin^2\vartheta}\frac{\mathrm{d}\varphi}{\cos^3\varphi}$
3.	$J\nu L$	$\int\frac{J^3}{24}\frac{\sin^2\vartheta\,\mathrm{d}\vartheta}{\cos^3\vartheta}\sin\varphi\,\mathrm{d}\varphi$	$\int\frac{K^3}{24}\frac{\mathrm{d}\vartheta}{\sin\vartheta}\frac{\mathrm{d}\varphi}{\sin^2\varphi}$	$\int\frac{L^3}{24}\frac{\mathrm{d}\vartheta}{\sin\vartheta}\frac{\sin\varphi\,\mathrm{d}\varphi}{\cos^3\varphi}$
4.	$JK\sigma$	$\int\frac{J^3}{24}\frac{\sin^2\vartheta\,\mathrm{d}\vartheta}{\cos^3\vartheta}\cos\varphi\,\mathrm{d}\varphi$	$\int\frac{K^3}{24}\frac{\mathrm{d}\vartheta}{\sin\vartheta}\frac{\cos\varphi\,\mathrm{d}\varphi}{\sin^3\varphi}$	$\int\frac{L^3}{24}\frac{\mathrm{d}\vartheta}{\sin\vartheta}\frac{\mathrm{d}\varphi}{\cos^2\varphi}$
5.	$J\nu\sigma$	$\int\frac{J^4}{64}\frac{\sin^3\vartheta\,\mathrm{d}\vartheta}{\cos^4\vartheta}\sin\varphi\cos\varphi\,\mathrm{d}\varphi$	$\int\frac{K^4}{64}\frac{\mathrm{d}\vartheta}{\sin\vartheta}\frac{\cos\varphi\,\mathrm{d}\varphi}{\sin^3\varphi}$	$\int\frac{L^4}{64}\frac{\mathrm{d}\vartheta}{\sin\vartheta}\frac{\sin\varphi\,\mathrm{d}\varphi}{\cos^3\varphi}$
6.	$\beta K\sigma$	$\int\frac{J^4}{64}\frac{\sin^2\vartheta\,\mathrm{d}\vartheta}{\cos^3\vartheta}\cos\varphi\,\mathrm{d}\varphi$	$\int\frac{K^4}{64}\frac{\cos\varphi\,\mathrm{d}\vartheta}{\sin^2\vartheta}\frac{\cos\varphi\,\mathrm{d}\varphi}{\sin^4\varphi}$	$\int\frac{L^4}{64}\frac{\cos\vartheta\,\mathrm{d}\vartheta}{\sin^2\vartheta}\frac{\mathrm{d}\varphi}{\cos^3\varphi}$
7.	$\beta\nu L$	$\int\frac{J^4}{64}\frac{\sin^2\vartheta\,\mathrm{d}\vartheta}{\cos^3\vartheta}\sin\varphi\,\mathrm{d}\varphi$	$\int\frac{K^4}{64}\frac{\cos\vartheta\,\mathrm{d}\vartheta}{\sin^2\vartheta}\frac{\mathrm{d}\varphi}{\sin^3\varphi}$	$\int\frac{L^4}{64}\frac{\cos\vartheta\,\mathrm{d}\vartheta}{\sin^2\vartheta}\frac{\sin\varphi\,\mathrm{d}\varphi}{\cos^4\varphi}$
8.	$\beta\nu\sigma$	$\int\frac{J^5}{160}\frac{\sin^3\vartheta\,\mathrm{d}\vartheta}{\cos^4\vartheta}\sin\varphi\cos\varphi\,\mathrm{d}\varphi$	$\int\frac{K^5}{160}\frac{\cos\vartheta\,\mathrm{d}\vartheta}{\sin^2\vartheta}\frac{\cos\varphi\,\mathrm{d}\varphi}{\sin^4\varphi}$	$\int\frac{L^5}{160}\frac{\cos\vartheta\,\mathrm{d}\vartheta}{\sin^2\vartheta}\frac{\sin\varphi\,\mathrm{d}\varphi}{\cos^4\varphi}$

Table 3. Table of integrals over φ in TS region of cuboid

#	Label	Limits $0 < \varphi < \tan^{-1}(K/L)$ with $(p, \mathrm{trig}) = (J/L, \cos)$
1.	JKL	$\int \frac{J^2}{8}\left(\frac{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}}{p\,\mathrm{trig}\,\varphi}-1\right)\mathrm{d}\varphi$
2.	βKL	$\int \frac{J^3}{24}\left(\frac{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}}{p\,\mathrm{trig}\,\varphi}-1\right)\mathrm{d}\varphi$
3.	$J\nu L$	$\int \frac{J^3}{24}\left(\frac{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}}{2p^2\,\mathrm{trig}^2\,\varphi}-\frac{1}{4}\log\left(\frac{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}+1}{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}-1}\right)\right)\sin\varphi\,\mathrm{d}\varphi$
4.	$JK\sigma$	$\int \frac{J^3}{24}\left(\frac{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}}{2p^2\,\mathrm{trig}^2\,\varphi}-\frac{1}{4}\log\left(\frac{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}+1}{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}-1}\right)\right)\cos\varphi\,\mathrm{d}\varphi$
5.	$J\nu\sigma$	$\int \frac{J^4}{64}\left(-\frac{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}}{p\,\mathrm{trig}\,\varphi}+\frac{(1+p^2\,\mathrm{trig}^2\,\varphi)^{3/2}}{3p^3\,\mathrm{trig}^3\,\varphi}+\frac{2}{3}\right)\sin\varphi\cos\varphi\,\mathrm{d}\varphi$
6.	$\beta K\sigma$	$\int \frac{J^4}{64}\left(\frac{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}}{2p^2\,\mathrm{trig}^2\,\varphi}-\frac{1}{4}\log\left(\frac{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}+1}{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}-1}\right)\right)\cos\varphi\,\mathrm{d}\varphi$
7.	$\beta\nu L$	$\int \frac{J^4}{64}\left(\frac{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}}{2p^2\,\mathrm{trig}^2\,\varphi}-\frac{1}{4}\log\left(\frac{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}+1}{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}-1}\right)\right)\sin\varphi\,\mathrm{d}\varphi$
8.	$\beta\nu\sigma$	$\int \frac{J^5}{160}\left(-\frac{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}}{p\,\mathrm{trig}\,\varphi}+\frac{(1+p^2\,\mathrm{trig}^2\,\varphi)^{3/2}}{3p^3\,\mathrm{trig}^3\,\varphi}+\frac{2}{3}\right)\sin\varphi\cos\varphi\,\mathrm{d}\varphi$

Table 4. Table of integrals over φ in TE region of cuboid

#	Label	Limits $\tan^{-1}(K/L) < \varphi < \pi/2$ with $(p, \mathrm{trig}) = (J/K, \sin)$
1.	JKL	$\int \frac{J^2}{8}\left(\frac{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}}{p\,\mathrm{trig}\,\varphi}-1\right)\mathrm{d}\varphi$
2.	βKL	$\int \frac{J^3}{24}\left(\frac{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}}{p\,\mathrm{trig}\,\varphi}-1\right)\mathrm{d}\varphi$
3.	$J\nu L$	$\int \frac{J^3}{24}\left(\frac{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}}{2p^2\,\mathrm{trig}^2\,\varphi}-\frac{1}{4}\log\left(\frac{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}+1}{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}-1}\right)\right)\sin\varphi\,\mathrm{d}\varphi$
4.	$JK\sigma$	$\int \frac{J^3}{24}\left(\frac{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}}{2p^2\,\mathrm{trig}^2\,\varphi}-\frac{1}{4}\log\left(\frac{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}+1}{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}-1}\right)\right)\cos\varphi\,\mathrm{d}\varphi$
5.	$J\nu\sigma$	$\int \frac{J^4}{64}\left(-\frac{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}}{p\,\mathrm{trig}\,\varphi}+\frac{(1+p^2\,\mathrm{trig}^2\,\varphi)^{3/2}}{3p^3\,\mathrm{trig}^3\,\varphi}+\frac{2}{3}\right)\sin\varphi\cos\varphi\,\mathrm{d}\varphi$
6.	$\beta K\sigma$	$\int \frac{J^4}{64}\left(\frac{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}}{2p^2\,\mathrm{trig}^2\,\varphi}-\frac{1}{4}\log\left(\frac{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}+1}{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}-1}\right)\right)\cos\varphi\,\mathrm{d}\varphi$
7.	$\beta\nu L$	$\int \frac{J^4}{64}\left(\frac{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}}{2p^2\,\mathrm{trig}^2\,\varphi}-\frac{1}{4}\log\left(\frac{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}+1}{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}-1}\right)\right)\sin\varphi\,\mathrm{d}\varphi$
8.	$\beta\nu\sigma$	$\int \frac{J^5}{160}\left(-\frac{\sqrt{1+p^2\,\mathrm{trig}^2\,\varphi}}{p\,\mathrm{trig}\,\varphi}+\frac{(1+p^2\,\mathrm{trig}^2\,\varphi)^{3/2}}{3p^3\,\mathrm{trig}^3\,\varphi}+\frac{2}{3}\right)\sin\varphi\cos\varphi\,\mathrm{d}\varphi$

Table 5. Table of integrals over φ in ME region of cuboid

#	Label	Limits $\tan^{-1}(K/L) < \varphi < \pi/2$ with $(p, \text{trig}) = (J/K, \sin)$
1.	JKL	$\int \frac{K^2}{8}\left(\frac{1}{2}\log\left(\frac{\sqrt{1+p^2\,\text{trig}^2\,\varphi}+p\,\text{trig}\,\varphi}{\sqrt{1+p^2\,\text{trig}^2\,\varphi}-p\,\text{trig}\,\varphi}\right)\right)\frac{\mathrm{d}\varphi}{\sin^2\varphi}$
2.	βKL	$\int \frac{K^3}{24}\left(\sqrt{1+p^2\,\text{trig}^2\,\varphi}-1\right)\frac{\mathrm{d}\varphi}{\sin^3\varphi}$
3.	$J\nu L$	$\int \frac{K^3}{24}\left(\frac{1}{2}\log\left(\frac{\sqrt{1+p^2\,\text{trig}^2\,\varphi}+p\,\text{trig}\,\varphi}{\sqrt{1+p^2\,\text{trig}^2\,\varphi}-p\,\text{trig}^2\,\varphi}\right)\right)\frac{\mathrm{d}\varphi}{\sin^2\varphi}$
4.	$JK\sigma$	$\int \frac{K^3}{24}\left(\frac{1}{2}\log\left(\frac{\sqrt{1+p^2\,\text{trig}^2\,\varphi}+p\,\text{trig}\,\varphi}{\sqrt{1+p^2\,\text{trig}^2\,\varphi}-p\,\text{trig}\,\varphi}\right)\right)\frac{\cos\varphi\,\mathrm{d}\varphi}{\sin^3\varphi}$
5.	$J\nu\sigma$	$\int \frac{K^4}{64}\left(\frac{1}{2}\log\left(\frac{\sqrt{1+p^2\,\text{trig}^2\,\varphi}+p\,\text{trig}\,\varphi}{\sqrt{1+p^2\,\text{trig}^2\,\varphi}-p\,\text{trig}\,\varphi}\right)\right)\frac{\cos\varphi\,\mathrm{d}\varphi}{\sin^3\varphi}$
6.	$\beta K\sigma$	$\int \frac{K^3}{64}(\sqrt{1+p^2\,\text{trig}^2\,\varphi}-1)\frac{\cos\varphi\,\mathrm{d}\varphi}{\sin^4\varphi}$
7.	$\beta\nu L$	$\int \frac{K^4}{64}(\sqrt{1+p^2\,\text{trig}^2\,\varphi}-1)\frac{\mathrm{d}\varphi}{\sin^3\varphi}$
8.	$\beta\nu\sigma$	$\int \frac{K^5}{160}(\sqrt{1+p^2\,\text{trig}^2\,\varphi}-1)\frac{\cos\varphi\,\mathrm{d}\varphi}{\sin^4\varphi}$

Table 6. Table of integrals over φ in MS region of cuboid

#	Label	Limits $0 < \varphi < \tan^{-1}(K/L)$ with $(p, \text{trig}) = (J/L, \cos)$
1.	JKL	$\int \frac{L^2}{8}\left(\frac{1}{2}\log\left(\frac{\sqrt{1+p^2\,\text{trig}^2\,\varphi}+p\,\text{trig}\,\varphi}{\sqrt{1+p^2\,\text{trig}^2\,\varphi}-p\,\text{trig}\,\varphi}\right)\right)\frac{\mathrm{d}\varphi}{\cos^2\varphi}$
2.	βKL	$\int \frac{L^3}{24}\left(\sqrt{1+p^2\,\text{trig}^2\,\varphi}-1\right)\frac{\mathrm{d}\varphi}{\cos^3\varphi}$
3.	$J\nu L$	$\int \frac{L^3}{24}\left(\frac{1}{2}\log\left(\frac{\sqrt{1+p^2\,\text{trig}^2\,\varphi}+p\,\text{trig}\,\varphi}{\sqrt{1+p^2\,\text{trig}^2\,\varphi}-p\,\text{trig}\,\varphi}\right)\right)\frac{\sin\varphi\,\mathrm{d}\varphi}{\cos^3\varphi}$
4.	$JK\sigma$	$\int \frac{L^3}{24}\left(\frac{1}{2}\log\left(\frac{\sqrt{1+p^2\,\text{trig}^2\,\varphi}+p\,\text{trig}\,\varphi}{\sqrt{1+p^2\,\text{trig}^2\,\varphi}-p\,\text{trig}\,\varphi}\right)\right)\frac{\mathrm{d}\varphi}{\cos^2\varphi}$
5.	$J\nu\sigma$	$\int \frac{L^4}{64}\left(\frac{1}{2}\log\left(\frac{\sqrt{1+p^2\,\text{trig}^2\,\varphi}+p\,\text{trig}\,\varphi}{\sqrt{1+p^2\,\text{trig}^2\,\varphi}-p\,\text{trig}\,\varphi}\right)\right)\frac{\sin\varphi\,\mathrm{d}\varphi}{\cos^3\varphi}$
6.	$\beta K\sigma$	$\int \frac{L^4}{64}(\sqrt{1+p^2\,\text{trig}^2\,\varphi}-1)\frac{\mathrm{d}\varphi}{\cos^3\varphi}$
7.	$\beta\nu L$	$\int \frac{L^4}{64}(\sqrt{1+p^2\,\text{trig}^2\,\varphi}-1)\frac{\sin\varphi\,\mathrm{d}\varphi}{\cos^4\varphi}$
8.	$\beta\nu\sigma$	$\int \frac{L^5}{160}(\sqrt{1+p^2\,\text{trig}^2\,\varphi}-1)\frac{\sin\varphi\,\mathrm{d}\varphi}{\cos^4\varphi}$

evaluated in the tables of Gradshteyn and Ryzhik and Appendix A. Thus, the integral types are

1. Solution for *JKL*-TS, *JKL*-TE, *βKL*-TS, *βKL*-TE is found in Gradshteyn and Ryzhik [12, §2.583.32, p. 160 and §2.598, p. 174]:

$$\int_{\varphi_{\min}}^{\varphi_{\max}} \left(\frac{u}{pg} - 1\right) \mathrm{d}\varphi = \left[-\frac{1}{2p}\log\left(\frac{u+h}{u-h}\right) - \sin^{-1}\left(\frac{ph}{\sqrt{1+p^2}}\right) - \varphi \right]_{\varphi_{\min}}^{\varphi_{\max}}, \tag{24}$$

2. Solutions for *JvL*-TE, *βvL*-TE, *βKσ*-TS, *JKσ*-TS are found in Gradshteyn and Ryzhik [12, §2.583.32, p. 160, §2.597.4, p. 174, §2.597.6, p. 174] and in Eq. 53 in Appendix A:

$$\int_{\varphi_{\min}}^{\varphi_{\max}} \left(\frac{u}{2p^2 g} - \frac{g}{4}\log\left(\frac{u+1}{u-1}\right)\right) \mathrm{d}\varphi = \left[-\frac{(1+p^2)}{4p^2}\log\left(\frac{u+h}{u-h}\right) + \frac{h}{4}\log\left(\frac{u+1}{u-1}\right) \right]_{\varphi_{\min}}^{\varphi_{\max}}. \tag{25}$$

3. Solutions for *JKσ*-TE, *βKσ*-TE, *JvL*-TS, *βvL*-TS are found in Gradshteyn and Ryzhik [12, §2.583.44, p. 161, §2.598, p. 174, §2.271.4, p. 86] and in Eq (54) in Appendix A:

$$\int_{\varphi_{\min}}^{\varphi_{\max}} \left(\frac{u}{2p^2 g^2} - \frac{1}{4}\log\left(\frac{u+1}{u-1}\right)\right) h\,\mathrm{d}\varphi = \left[-\frac{u}{2p^2 g} - \frac{g}{4}\log\left(\frac{u+1}{u-1}\right) \right]_{\varphi_{\min}}^{\varphi_{\max}} \tag{26}$$

4. Solutions for *Jvσ*-TE, *βvσ*-TE, *Jvσ*-TS, *βvσ*-TS are found in Gradshteyn and Ryzhik [12, §2.583.3, p. 158, §2.275.7, p. 88, §2.598, p. 174]:

$$\int_{\varphi_{\min}}^{\varphi_{\max}} \left(-\frac{u}{p} + \frac{u^3}{3p^3 g^2} + \frac{2g}{3}\right) h\,\mathrm{d}\varphi = \left[-\frac{u^3}{3p^2 g} + \frac{g^2}{3} \right]_{\varphi_{\min}}^{\varphi_{\max}}. \tag{27}$$

5. Solutions for *βKL*-MS, *βKL*-ME, *βKσ*-MS, *βvL*-ME are found in Gradshteyn and Ryzhik [12, §2.583.39 (p. 161: note the typographical sign error in the second term) and §2.526.3, p. 136]

$$\int_{\varphi_{\min}}^{\varphi_{\max}} \left(\frac{u-1}{g^3}\right) \mathrm{d}\varphi = \left[-\frac{(1+p^2)}{4}\log\left(\frac{u+h}{u-h}\right) + \frac{(1-u)h}{2g^2} + \frac{1}{4}\log\left(\frac{1+h}{1-h}\right) \right]_{\varphi_{\min}}^{\varphi_{\max}}. \tag{28}$$

6. Solutions for *JKL*-ME, *JvL*-ME, *JKL*-MS, *JKσ*-MS are found in Gradshteyn and Ryzhik [12, §2.584.82 (but there is believed to be a sign error in this formula so consider the formulae §2.597.4 and §2.597.6, p. 173 instead)] and in Eq. (55) in Appendix A:

$$\int_{\varphi_{\min}}^{\varphi_{\max}} \left(\frac{1}{2g^2}\log\left(\frac{u+pg}{u-pg}\right)\right) \mathrm{d}\varphi = \left[-\frac{h}{2g}\log\left(\frac{u+pg}{u-pg}\right) - \frac{p}{2}\log\left(\frac{u+h}{u-h}\right) + \sin^{-1}\left(\frac{ph}{\sqrt{1+p^2}}\right) \right]_{\varphi_{\min}}^{\varphi_{\max}}. \tag{29}$$

7. Solutions for *JKσ*-ME, *Jvσ*-ME, *JvL*-MS, *Jvσ*-MS are found in Gradshteyn and Ryzhik [12, §2.584.80, p. 166] and in Eq. (56) in Appendix A:

$$\int_{\varphi_{\min}}^{\varphi_{\max}} \left(\frac{1}{2g^3}\log\left(\frac{u+pg}{u-pg}\right)\right) h\,\mathrm{d}\varphi = \left[-\frac{1}{4g^2}\log\left(\frac{u+pg}{u-pg}\right) - \frac{pu}{2g} \right]_{\varphi_{\min}}^{\varphi_{\max}}. \tag{30}$$

8. Solutions for $\beta\nu L$-MS, $\beta K\sigma$-ME, $\beta\nu\sigma$-MS, $\beta\nu\sigma$-ME are found in Gradshteyn and Ryzhik [12, §2.583.65, p. 162 and §2.526.45, p. 138]:

$$\int_{\varphi_{\min}}^{\varphi_{\max}} \left(\frac{u-1}{g^4}\right) h \,\mathrm{d}\varphi = \left[\frac{(1-u^3)}{3g^3}\right]_{\varphi_{\min}}^{\varphi_{\max}}. \tag{31}$$

Using the results of Eqs (24)–(31) in the integrals in Tables 3–6 and introducing the appropriate limits and the variable $R = \sqrt{L^2 + K^2 + J^2}$, the evaluated integrals of the I_{ijk} in Eq. (13) become

$$\begin{aligned} I_{JKL} = 4JKL\Bigg\{ & JK \log\left(\frac{R+L}{R-L}\right) + JL \log\left(\frac{R+K}{R-K}\right) + KL \log\left(\frac{R+J}{R-J}\right) \\ & - \frac{J^2\pi}{2} + (J^2 - K^2)\sin^{-1}\left(\frac{JL}{\sqrt{K^2+J^2}\sqrt{L^2+K^2}}\right) \\ & + (J^2 - L^2)\sin^{-1}\left(\frac{JK}{\sqrt{L^2+J^2}\sqrt{L^2+K^2}}\right)\Bigg\}, \end{aligned} \tag{32}$$

$$\begin{aligned} I_{\beta KL} = \frac{2KL}{3}\Bigg\{ & K^3 \log\left(\frac{\sqrt{L^2+K^2}+L}{\sqrt{L^2+K^2}-L}\right) + L^3 \log\left(\frac{\sqrt{L^2+K^2}+K}{\sqrt{L^2+K^2}-K}\right) \\ & - (K^3 + 3J^2K)\log\left(\frac{R+L}{R-L}\right) - (L^3 + 3J^2L)\log\left(\frac{R+K}{R-K}\right) \\ & - 4J^3\Bigg[\sin^{-1}\left(\frac{JL}{\sqrt{K^2+J^2}\sqrt{L^2+K^2}}\right) \\ & + \sin^{-1}\left(\frac{JK}{\sqrt{L^2+J^2}\sqrt{L^2+K^2}}\right)\Bigg] \\ & - 4KLR + 4KL\sqrt{L^2+K^2} + 2J^3\pi\Bigg\}, \end{aligned} \tag{33}$$

$$\begin{aligned} I_{J\nu L} = \frac{2JL}{3}\Bigg\{ & J^3 \log\left(\frac{\sqrt{L^2+J^2}+L}{\sqrt{L^2+J^2}-L}\right) + L^3 \log\left(\frac{\sqrt{L^2+J^2}+J}{\sqrt{L^2+J^2}-J}\right) \\ & - (3JK^2 + J^3)\log\left(\frac{R+L}{R-L}\right) - (L^3 + 3K^2L)\log\left(\frac{R+J}{R-J}\right) \\ & + 4K^3\sin^{-1}\left(\frac{JL}{\sqrt{K^2+J^2}\sqrt{L^2+K^2}}\right) \\ & - 4JLR + 4JL\sqrt{L^2+J^2}\Bigg\}. \end{aligned} \tag{34}$$

$$
\begin{aligned}
I_{JK\sigma} = \frac{2JK}{3}\Bigg\{ & J^3 \log\left(\frac{\sqrt{K^2+J^2}+K}{\sqrt{K^2+J^2}-K}\right) + K^3 \log\left(\frac{\sqrt{K^2+J^2}+J}{\sqrt{K^2+J^2}-J}\right) \\
& - (3JL^2 + J^3)\log\left(\frac{R+K}{R-K}\right) - (3KL^2 + K^3)\log\left(\frac{R+J}{R-J}\right) \\
& + 4L^3 \sin^{-1}\left(\frac{JK}{\sqrt{L^2+J^2}\sqrt{L^2+K^2}}\right) \\
& - 4JKR + 4JK\sqrt{K^2+J^2}\Bigg\}. \qquad (35)
\end{aligned}
$$

$$
\begin{aligned}
I_{J\nu\sigma} = \frac{J}{6}\Bigg\{ & -3K^4 \log\left(\frac{\sqrt{K^2+J^2}+J}{\sqrt{K^2+J^2}-J}\right) - 3L^4 \log\left(\frac{\sqrt{L^2+J^2}+J}{\sqrt{L^2+J^2}-J}\right) \\
& + (3L^4 + 6K^2L^2 + 3K^4)\log\left(\frac{R+J}{R-J}\right) \\
& + (10JL^2 + 10JK^2 + 4J^3)R + 4J^4 \\
& - (10JL^2 + 4J^3)\sqrt{L^2+J^2} - (10JK^2 + 4J^3)\sqrt{K^2+J^2}\Bigg\}, \qquad (36)
\end{aligned}
$$

$$
\begin{aligned}
I_{\beta K\sigma} = \frac{K}{6}\Bigg\{ & -3J^4 \log\left(\frac{\sqrt{K^2+J^2}+K}{\sqrt{K^2+J^2}-K}\right) - 3L^4 \log\left(\frac{\sqrt{L^2+K^2}+K}{\sqrt{L^2+K^2}-K}\right) \\
& + 3(L^4 + 2J^2L^2 + J^4)\log\left(\frac{R+K}{R-K}\right) \\
& - (10KL^2 + 4K^3)\sqrt{L^2+K^2} + (10KL^2 + 4K^3 + 10J^2K)R \\
& - (4K^3 + 10J^2K)\sqrt{K^2+J^2} + 4K^4\Bigg\}, \qquad (37)
\end{aligned}
$$

$$
\begin{aligned}
I_{\beta\nu L} = \frac{L}{6}\Bigg\{ & -3J^4 \log\left(\frac{\sqrt{L^2+J^2}+L}{\sqrt{L^2+J^2}-L}\right) - 3K^4 \log\left(\frac{\sqrt{L^2+K^2}+L}{\sqrt{L^2+K^2}-L}\right) \\
& + 3(K^4 + 2J^2K^2 + J^4)\log\left(\frac{R+L}{R-L}\right) \\
& - (4L^3 + 10K^2L)\sqrt{L^2+K^2} + (4L^3 + 10K^2L + 10J^2L)R \\
& - (4L^3 + 10J^2L)\sqrt{L^2+J^2} + 4L^4\Bigg\}, \qquad (38)
\end{aligned}
$$

$$
\begin{aligned}
I_{\beta\nu\sigma} = \tfrac{8}{15}\{ & -(L^4 + 2(K^2+J^2)L^2 + K^4 + 2J^2K^2 + J^4)R - L^5 - K^5 - J^5 \\
& + (L^4 + 2K^2L^2 + K^4)\sqrt{L^2+K^2} + (L^4 + 2J^2L^2 + J^4)\sqrt{L^2+J^2} \\
& + (K^4 + 2J^2K^2 + J^4)\sqrt{K^2+J^2}\}. \qquad (39)
\end{aligned}
$$

Thus, the I_{ijk} terms are summed to obtain I, the elegant and simple form of the coulomb integral for the cuboid of side $J \times K \times L$, and I is given in Eq. (40):

$$
\begin{aligned}
I = \frac{1}{30}\Bigg\{ & 5J^4K \log\left(\frac{\sqrt{K^2+J^2}+K}{\sqrt{K^2+J^2}-K}\right) + 5KL^4 \log\left(\frac{\sqrt{L^2+K^2}+K}{\sqrt{L^2+K^2}-K}\right) \\
& + 5JK^4 \log\left(\frac{\sqrt{K^2+J^2}+J}{\sqrt{K^2+J^2}-J}\right) + 5J^4L \log\left(\frac{\sqrt{L^2+J^2}+L}{\sqrt{L^2+J^2}-L}\right) \\
& + 5JL^4 \log\left(\frac{\sqrt{L^2+J^2}+J}{\sqrt{L^2+J^2}-J}\right) + 5K^4L \log\left(\frac{\sqrt{L^2+K^2}+L}{\sqrt{L^2+K^2}-L}\right) \\
& - 5L(K^4 - 6J^2K^2 + J^4)\log\left(\frac{R+L}{R-L}\right) \\
& - 5K(L^4 - 6J^2L^2 + J^4)\log\left(\frac{R+K}{R-K}\right) \\
& - 5J(L^4 - 6K^2L^2 + K^4)\log\left(\frac{R+J}{R-J}\right) \\
& + 40JKL(J^2 - K^2)\sin^{-1}\left(\frac{JL}{\sqrt{K^2+J^2}\sqrt{L^2+K^2}}\right) \\
& + 40JKL(J^2 - L^2)\sin^{-1}\left(\frac{JK}{\sqrt{L^2+J^2}\sqrt{L^2+K^2}}\right) \\
& + 4(L^4 - 3(K^2+J^2)L^2 + K^4 - 3J^2K^2 + J^4)R + 4L^5 + 4K^5 + 4J^5 \\
& - 4(L^4 - 3K^2L^2 + K^4)\sqrt{L^2+K^2} - 4(L^4 - 3J^2L^2 + J^4)\sqrt{L^2+J^2} \\
& - 4(K^4 - 3J^2K^2 + J^4)\sqrt{K^2+J^2} - 20J^3KL\pi \Bigg\}.
\end{aligned}
\tag{40}
$$

For a unit cube with unit charge density this leads to a coulomb energy of 1.88231264. This result was checked by use of Euler–Maclaurin quadrature with the jacobian of the form $dx = At^2(1-t)^2\,dt$ for x being the coordinates β, ν and σ in Eq. (11). One can see that the pole in the integrand is avoided in the numerical integration; consider a cube of side L and the elements are $N \times N \times N$ along each side and so the interval δ is $\delta = L/N$. The element nearest the pole is centred on $(\delta/2, \delta/2, \delta/2)$ and so the contribution to the integral, Δ, for the function $1/\sqrt{\beta^2 + \nu^2 + \sigma^2}$ is

$$
\Delta = \frac{\delta^3}{\delta\sqrt{3/4}},
\tag{41}
$$

so that $\Delta \to 0$ as $\delta \to 0$ and the pole is avoided. The numerical results for the unit cube agreed with the analytic results to 8 significant figures when $N = 200$. The analytic results are shown in Table 7.

In addition to the numerical checking, integrals were also tested by differentiation using the numerical algebra package 'Axiom' [13]. The package was used to ensure the correct summation and simplification of component expressions of the two-electron integral I.

Table 7. Table of evaluated cuboid integrals. The first four rows contain the contributions to the unit cube with unit density of the integrals I_{ijk}, as given in Eq. (13). The final three rows show the coulomb energy for the cubes of unit density with their size (dimensions) shown as a subscript

Integral	Coulomb energy
I_{JKL}	9.52030946
$I_{\beta KL}$, $I_{J\nu L}$, $I_{JK\sigma}$	−4.12474847
$I_{J\nu\sigma}$, $I_{\beta K\sigma}$, $I_{\beta\nu L}$	1.86637523
$I_{\beta\nu\sigma}$	−0.86287708
$I_{1\times1\times1}$	1.88231264
$I_{2\times1\times1}$	5.72639566
$I_{2\times2\times1}$	18.21031255
$I_{2\times2\times2}$	60.23400462

4 Proximate cube integrals

To obtain the two-electron integrals for proximate cubes consider the case of the interaction between two cubes which share a face. The total cuboid has sides $1\times1\times2$ and is comprised of two cubes of sides $1\times1\times1$, the latter we label A and B. We use the notation $\{A|B\}$ to denote the energy of the coulomb interaction of the density in cuboid A with the density in cuboid B. The self-interaction energy in the cuboid is known from Eq. (40) but is also made up of the self-interaction energies of A and B, and of the interaction between A and B and this may be expressed by

$$\{A+B|A+B\} = \{A|A\} + \{B|B\} + 2\{A|B\}. \tag{42}$$

As the left-hand side and the first two terms of the right-hand side of Eq. (42) are known, the interaction between the cubes is easily found.

A similar process can be followed for three unit cubes in a row, labelled sequentially as A, B and C, comprising a $1\times1\times3$ cuboid to give the expression

$$\begin{aligned}\{A+B+C|A+B+C\} = {} & \{A|A\} + \{B|B\} + \{C|C\} + 2\{A|B\} \\ & + 2\{B|C\} + 2\{A|C\}.\end{aligned} \tag{43}$$

All expressions except $\{A|C\}$ are known from Eqs. (40) and (42), and so the next-nearest neighbour interaction, $\{A|C\}$, is thus determined. This procedure can be continued until all desired interactions are calculated. Table 8 shows the results for the coulomb energy between two cubes of unit edge and unit charge density for different separations given by a vector in units of the cube edge. It can be seen that the cube derived energy differs markedly from the multipole energy when the cubes are close enough to touch each other, but as the separation increases so does the agreement.

Table 8. Coulomb energy calculated using cube integrals between two cubes of unit edge and unit charge density for different separations given by a vector in units of the cube edge. Also shown is the corresponding multipole energy which contain charge-charge, charge-hexadecapole and charge-64 pole interactions [10, 11], and then the simple point charge interaction $1/R$ is tabulated. The final column shows the difference between the cube coulomb energies and the multipole energies

Vector	Cube coulomb energy	Multipole energy	$1/R$ energy	Energy difference
0 0 0	1.88231264			
1 0 0	0.98088518	0.973810	1.000000	7.076e-03
1 1 0	0.70849513	0.707968	0.707107	5.268e-04
1 1 1	0.57879700	0.578711	0.577350	8.623e-04
2 0 0	0.49913985	0.499112	0.500000	2.805e-05
2 1 0	0.44710040	0.447102	0.447214	−1.610e-06
2 1 1	0.40833127	0.408334	0.408248	−2.597e-06
2 2 0	0.35359118	0.353590	0.353553	8.515e-07
2 2 1	0.33339189	0.333392	0.333333	1.892e-07
2 2 2	0.28871509	0.288715	0.288675	8.855e-08
3 0 0	0.33321548	0.333215	0.333333	8.143e-07
3 1 0	0.31617706	0.316177	0.316228	−3.049e-08
3 1 1	0.30149561	0.301511	0.301511	−2.091e-07
3 2 0	0.27735277	0.277353	0.277350	2.317e-08
3 2 1	0.26727114	0.267271	0.267261	−1.704e-08
3 2 2	0.24254859	0.242549	0.242536	1.400e-09
3 3 0	0.23570739	0.235707	0.235702	2.182e-08
3 3 1	0.22942257	0.229423	0.229416	9.798e-09
3 3 2	0.21320825	0.213208	0.213201	3.700e-09
3 3 3	0.19245528	0.192455	0.192450	2.042e-09
4 0 0	0.24997176	0.249972	0.250000	6.319e-08
4 1 0	0.24251800	0.242518	0.242536	1.049e-08
4 1 1	0.23569187	0.235692	0.235702	−1.158e-08
4 2 0	0.22360348	0.223603	0.223607	−4.572e-09
4 2 1	0.21821718	0.218217	0.218218	−8.387e-09
4 2 2	0.20412675	0.204127	0.204124	−4.430e-09
4 3 0	0.20000137	0.200001	0.200000	2.740e-09
4 3 1	0.19611823	0.196118	0.196116	9.529e-10
4 3 2	0.18569826	0.185698	0.185695	7.165e-11
4 3 3	0.17150118	0.171501	0.171499	3.975e-10
4 4 0	0.17677793	0.176778	0.176777	1.633e-09
4 4 1	0.17407915	0.174079	0.174078	1.033e-09
4 4 2	0.16666848	0.166668	0.166667	3.950e-10
4 4 3	0.15617545	0.156175	0.156174	2.177e-10
4 4 4	0.14433879	0.144339	0.144338	1.873e-10

5 Nuclear electronic integral

The nuclear electronic integral for the interaction between nucleus A and the electron labelled 1 is

$$I_{\mathrm{N}} = \int \frac{\phi_i^*(1)\phi_j(1)}{r_{A1}}\,\mathrm{d}\tau_1 \qquad (44)$$

and I_{N} is zero unless $i = j$ for non-overlapping cuboidal functions. Suppose that nucleus A lies within the cuboid of side $J \times K \times L$ at an arbitrary position; the cuboid divides naturally into eight sub-cuboids of $J_{\pm} \times K_{\pm} \times L_{\pm}$, where the subscript $\pm$ denotes perpendicular distance to the face of the cuboid from the nucleus in either the positive (+) or negative (−) direction. Thus, for example $J_{+} + J_{-} = J$ and it is apparent that $J_{\pm}$ is a function of A. The evaluation of the integral over one of these sub-cuboids, $I_{\mathrm{N}}(J_{\pm}, K_{\pm}, L_{\pm})$, proceeds in the same manner as the integral I_{JKL} (equations 14 and 32) save that the upper limits for $\boldsymbol{r}$ in each of the eight cuboids now contain $\mathrm{J}_{\pm}$ instead of $J/2$, $K_{\pm}$ instead of $K/2$, and $L_{\pm}$ instead of $L/2$. The sub-integral is evaluated as

$$
\begin{aligned}
I_{\mathrm{N}}(J_{\pm}, K_{\pm}, L_{\pm}) = \Bigg\{ & \frac{J_{\pm}K_{\pm}}{2} \log\left(\frac{R + L_{\pm}}{R - L_{\pm}}\right) + \frac{J_{\pm}\ L_{\pm}}{2} \log\left(\frac{R + K_{\pm}}{R - K_{\pm}}\right) \\
& + \frac{K_{\pm}L_{\pm}}{2} \log\left(\frac{R + J_{\pm}}{R - J_{\pm}}\right) - \frac{J_{\pm}^{2}\pi}{4} \\
& + \left(\frac{J_{\pm}^{2} - K_{\pm}^{2}}{2}\right) \sin^{-1}\left(\frac{J_{\pm}L_{\pm}}{\sqrt{K_{\pm}^{2} + J_{\pm}^{2}}\sqrt{L_{\pm}^{2} + K_{\pm}^{2}}}\right) \\
& + \left(\frac{J_{\pm}^{2} - L_{\pm}^{2}}{2}\right) \sin^{-1}\left(\frac{J_{\pm}K_{\pm}}{\sqrt{L_{\pm}^{2} + J_{\pm}^{2}}\sqrt{L_{\pm}^{2} + K_{\pm}^{2}}}\right)\Bigg\}, \qquad (45)
\end{aligned}
$$

where

$$R = \sqrt{L_{\pm}^{2} + K_{\pm}^{2} + J_{\pm}^{2}}. \qquad (46)$$

The whole integral for the nucleus in the cuboid is the sum of the results for each of the sub-cuboids.

To calculate the value for proximate cubes, consider two face-sharing cubes B and C. When the nucleus lies in cube B, and $I_{\mathrm{N}}(B)$ and $I_{\mathrm{N}}(B + C)$ are known, the interaction between the nucleus and the cube C, $I_{\mathrm{N}}(C)$, is obtained by subtraction from

$$I_{\mathrm{N}}(B + C) = I_{\mathrm{N}}(B) + I_{\mathrm{N}}(C). \qquad (47)$$

Because the nucleus is considered to be a point charge, the interaction between the nucleus and non-proximate cubes can be expressed as a set of charge–multipole interactions and these effectively become a charge–charge interaction at longer distances. This is demonstrated in Table 9.

6 Coulomb energy of the hydrogen molecule

In order to test the efficacy of the cube functions for the calculation of molecular energies, a basis set of cube functions are fitted to an STO-3G [8] wave function for the hydrogen molecule (H–H = 1.4 a.u.) and the coulomb energy is calculated with this basis. In all subsequent calculations the hydrogen molecule axis is rectilinear with the orientation of the cubes and lies in the centre of the region covered by the cubes. A number of factors need to be determined and these include:

- the method for determining the density within a cube;
- the size of the cubes;
- the size of the region covered by the cube functions.

Table 9. Nuclear electronic energy calculated between a cubes of unit edge and unit charge density for different separations between a nucleus of unit charge and the centre of a unit cube with unit charge density given by a vector in units of the cube edge. Also shown is the corresponding multipole energy which contain charge-charge, charge-hexadecapole and charge-64 pole interactions [10, 11], and then the simple point charge interaction $1/R$. The final column shows the difference between the Nuclear electronic energy calculated by the method described in this paper and the multipole energies

Vector			Cube–Nucleus interaction energy	Multiple energy	$1/R$ energy	Energy difference
0	0	0	2.38007736			
1	0	0	0.98759240	0.986905	1.000000	6.876e-04
1	1	0	0.70756582	0.707538	0.707107	2.827e-05
1	1	1	0.57803433	0.578031	0.577350	3.815e-06
2	0	0	0.49955780	0.499556	0.500000	1.905e-06
2	1	0	0.44715769	0.447158	0.447214	−1.133e-07
2	1	1	0.40829093	0.408291	0.408248	−1.518e-07
2	2	0	0.35357191	0.353572	0.353553	5.248e-08
2	2	1	0.33336253	0.333363	0.333333	1.207e-08
2	2	2	0.28869507	0.288695	0.288675	5.146e-09
3	0	0	0.33327405	0.333274	0.333333	5.237e-08
3	1	0	0.31620243	0.316202	0.316228	−2.316e-09
3	1	1	0.30150357	0.301504	0.301511	−1.301e-08
3	2	0	0.27735142	0.277351	0.277350	1.377e-09
3	2	1	0.26726620	0.267266	0.267261	−1.004e-09
3	2	2	0.24254211	0.242542	0.242536	8.161e-11
3	3	0	0.23570482	0.235705	0.235702	1.359e-09
3	3	1	0.22941915	0.229419	0.229416	6.207e-10
3	3	2	0.21320448	0.213204	0.213201	2.267e-10
3	3	3	0.19245268	0.192453	0.192453	2.235e-10
4	0	0	0.24998585	0.249986	0.250000	4.005e-09
4	1	0	0.24252681	0.242527	0.242536	6.476e-10
4	1	1	0.23569707	0.235697	0.235702	−7.697e-10
4	2	0	0.22360514	0.223605	0.223607	−2.975e-10
4	2	1	0.21821754	0.218218	0.218218	−5.220e-10
4	2	2	0.20412545	0.204125	0.204124	−2.726e-10
4	3	0	0.20000068	0.200001	0.200000	1.726e-10
4	3	1	0.19611718	0.196117	0.196116	6.075e-11
4	3	2	0.18569680	0.185697	0.185695	4.927e-12
4	3	3	0.17149988	0.171500	0.171499	2.360e-11
4	4	0	0.17677731	0.176777	0.176777	1.020e-10
4	4	1	0.17407840	0.174078	0.174078	6.478e-11
4	4	2	0.16666757	0.166668	0.166667	2.445e-11
4	4	3	0.15617460	0.156175	0.156174	1.498e-11
4	4	4	0.14433818	0.144338	0.144338	8.947e-12

The quadrature schemes used for determining the density within a cube were comprised of (a) simple quadrature, SQ (the value for the MO at the centre of the cube was taken to be the value throughout the cube) and (b) contracted simple quadrature, CSQ(n). In the latter case the density in the cube was calculated by using simple quadrature for a number of sub-cubes fitting precisely in the cube; the number of sub-cubes, n^3, in a cube could be varied and typically n was 2, 4, 6 or 8.

As the total electronic charge in the system is 2 electrons, we initially consider a large region for coverage, small cube size and a good quadrature scheme within individual cubes to reproduce the total electronic charge in the system. It was found that cubes of 0.125 a.u. in a region of 20 × 20 × 20 a.u. with simple quadrature gave an integrated density of 2.000000000025. Table 10 shows the integrated density using simple quadrature, and contracted simple quadrature using 4^3 sub-cubes, for the hydrogen molecule with different cube dimensions over a region of 20 × 20 × 20 a.u.; it can be seen that the simple quadrature at cube side of 1.000 a.u. is identical to the contracted simple quadrature at cube side of 4.000 a.u., and similarly the simple quadrature at cube side of 0.125 is identical to the contracted simple quadrature at cube side of 1.000; the cost of calculation is essentially equivalent for each particular pair of identical integrated densities.

The coulomb energy is 1.34468 a.u. when calculated using CSQ(8) over the region $(20\text{ a.u.})^3$ with cubes of side 0.5 a.u., which is appreciably lower than the STO-3G value of 1.34683 a.u. The difference is supposed to come mainly from the regions nearest the atoms and, thus, a scheme may be devised to improve quadrature and the coulomb energy nearer the molecular centre. The couple (A, s) denotes the coulomb energy of a region A filled with cubes of side s. If region B lies within region A then $(A, s) - (B, s) + (B, s/2)$ will improve the description of the self-interaction in the region B and so improve the coulomb energy for the region A.

Using CSQ(4), the scheme $(20, 0.5) - (10, 0.5) + (10, 0.25) - (5, 0.25) + (5, 0.125) - (2.5, 0.125) + (2.5, 0.0625)$, the coulomb energy was 1.34610 a.u. and this compares well with the STO-3G result of 1.34683 a.u.

Finally, we calculate the kinetic energy of the molecular orbital. Approximate methods must be used because the cuboidal basis functions are discontinuous and thus not differentiable. One way forward is to use a three-dimensional central difference second derivative formula [14] for the kinetic energy, KE,

$$\mathrm{KE} = -h \sum_{i}^{\text{all cubes}} c_{io}(-6c_{io} + c_{ix+} + c_{ix-} + c_{iy+} + c_{iy-} + c_{iz+} + c_{iz-}), \quad (48)$$

Table 10. Results for quadrature of density of the hydrogen molecule over a region of 20 × 20 × 20 a.u. using simple quadrature (1) and contracted simple quadrature of 4^3 and 8^3 subcubes

Quadrature in cube	Cube size a.u.	Integrated density
4^3	4.000	1.920334963917
1	1.000	1.920334963917
1	0.800	2.043538605089
1	0.600	1.996207588699
4^3	2.000	1.999729670509
1	0.500	1.999729670509
1	0.400	1.999984981706
1	0.300	2.000000010316
8^3	2.000	2.000000000016
4^3	2.000	2.000000000016
1	0.250	2.000000000016
1	0.200	2.000000000030
1	0.125	2.000000000025

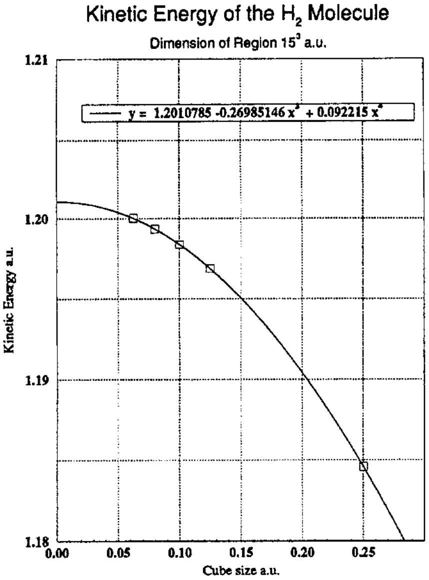

Fig. 2. The kinetic energy is shown as a function of cube side and fitted to an even polynomial of fourth degree in cube side

where h is the size of the cube side, c_{i0} is the coefficient of the ith cube function in the molecular orbital and $c_{i\nu\pm}$, ($\nu = \{x, y, z\}$), is the coefficient of the neighbouring cube or zero if this cube would lie beyond the boundary of the region described by the cube functions; a region of 15 × 15 × 15 a.u. was partitioned into cubes of side 0.25, 0.125, 0.100, 0.080 and 0.0625 a.u. and the kinetic energy calculated for each respective cube size; the kinetic energy may be considered to be a function of the cube side and was thus fitted to an even polynomial of fourth degree in cube side. This is shown in Fig. 2. Extrapolated to a cube side of zero, the kinetic energy is 1.2010785 a.u. and this compares very well with the STO-3G result of 1.2010795 a.u. Clearly, Richardson extrapolation [15] is of value for cube function calculations.

We recognise that the use of Eq. (48) may be considered unsatisfactory because it is an expression for the kinetic energy of a different approximation for the molecular orbital. However, in the limit of an infinite number of infinitesimal cubes the result is the one required. As a practical procedure we believe that the combination of Eq. (48) for the kinetic energy and the analytic expressions for the nuclear attraction and two-electron integrals derived in this paper is justified.

7 Summary

In this paper the analytic forms of the coulomb and nuclear electronic energies are presented for a cuboid of uniform density ($f = 1$ in Eq. (1)) and arbitrary dimensions. These results are used to obtain coulomb and nuclear attraction energies for a cellular network of cube functions (Tables 9 and 8). A program has been written to test the suitability of these cuboidal functions to form a basis set by calculating the coulomb and kinetic energy of the STO-3G hydrogen molecule. The fundamental approximation that the density in a cube may be represented by a constant may be a large one but, nonetheless, the results for the hydrogen molecule show that a reasonable value for the coulomb energy may be obtained. A new class of basis functions for which all the integrals are evaluated has been demonstrated as being appropriate for regular quantum mechanical calculations.

Of course, this is only a preliminary investigation using cuboidal functions. We have simply obtained the coefficients of each cube from a given molecular orbital of the STO-3G hydrogen molecule, and then evaluated kinetic and coulomb energies. But the principal idea is that the cuboids should be basis functions for molecular orbitals to be used in an iterative SCF approach. In principle, we have given all the necessary machinery, but in practice presumably a very large number of cuboids will have to be used, leading to a large Fock matrix which would be impractical to manipulate with conventional techniques. However, the correspondence between the cuboidal basis functions and numerical techniques (i.e. finite element, partitioning schemes) is considerable and may allow, for example, the use of dynamic optimisation over traditional diagonalisation techniques and multi-grid methods to solve Poisson's equation to obtain the coulomb energy more rapidly. One of the particularly attractive features of the use of cube functions is that the partitioning of space is controlled by only one parameter, namely the cube size; this allows one to extrapolate to the infinitesimal cube limit and obtain benchmark results. All this, however, lies beyond the scope of this paper, the purpose of which is to introduce the cuboidal functions.

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Log integrals

To evaluate integrals of the form

$$\int f(x)\log(g(x))\,\mathrm{d}x, \tag{49}$$

proceed by partial integration with $F(x) = \int f(x)\,\mathrm{d}x$ to get

$$\int f(x)\log(g(x))\,\mathrm{d}x = F(x)\log(g(x)) - \int F(x)\frac{g'(x)}{g(x)}\,\mathrm{d}x, \tag{50}$$

where prime indicates the derivative with respect to x. In the case of

$$\int f(x)\log\left(\frac{a(x)}{b(x)}\right)\mathrm{d}x, \tag{51}$$

we find

$$\int f(x)\log\left(\frac{a(x)}{b(x)}\right)\mathrm{d}x = F(x)\log\left(\frac{a(x)}{b(x)}\right) - \int F(x)\left(\frac{ba' - ab'}{b^2}\right)\frac{b}{a}\,\mathrm{d}x. \tag{52}$$

There are four cases to be considered in this work and they are:

$$\int g\log\left(\frac{u+1}{u-1}\right)\mathrm{d}\varphi, \quad \int h\log\left(\frac{u+1}{u-1}\right)\mathrm{d}\varphi, \quad \int \frac{1}{g^2}\log\left(\frac{u+pg}{u-pg}\right)\mathrm{d}\varphi,$$

$$\int \frac{h}{g^3}\log\left(\frac{u+pg}{u-pg}\right)\mathrm{d}\varphi,$$

where u, g and h are as defined before in Eqs. (21), (22) and (23), respectively. In these examples it is assumed that $g = \sin\varphi$.

The results are

$$\int g \log\left(\frac{u+1}{u-1}\right) d\varphi = -h \log\left(\frac{u+1}{u-1}\right) + \log\left(\frac{u+h}{u-h}\right) - \frac{2}{p}\sin^{-1}\left(\frac{ph}{\sqrt{1+p^2}}\right), \tag{53}$$

$$\int h \log\left(\frac{u+1}{u-1}\right) d\varphi = g \log\left(\frac{u+1}{u-1}\right) + \frac{2}{p}\log(u + pg), \tag{54}$$

$$\int \frac{1}{g^2} \log\left(\frac{u+pg}{u-pg}\right) d\varphi = -\frac{h}{g}\log\left(\frac{u+pg}{u-pg}\right) - p\log\left(\frac{u+h}{u-h}\right) + 2\sin^{-1}\left(\frac{ph}{\sqrt{1+p^2}}\right), \tag{55}$$

$$\int \frac{h}{g^3} \log\left(\frac{u+pg}{u-pg}\right) d\varphi = -\frac{1}{2g^2}\log\left(\frac{u+pg}{u-pg}\right) - \frac{pu}{g}. \tag{56}$$

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