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An extremely efficient approach for accurate and rapid evaluation of three-centre two-electron Coulomb and hybrid integrals over B functions

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Abstract

Analytic expressions of three-centre two-electron Coulomb and hybrid integrals over B functions are obtained using the Fourier transform method thoroughly explored by Steinborn's group. These analytic expressions involve semi-infinite integrals which are slowly convergent due to the presence of hypergeometric and spherical Bessel functions in the integrands. We have proven that these hypergeometric functions can be expressed as finite expansions and the integrands involving these series satisfy all the conditions required to apply the $H\bar{D}$ approach which greatly simplifies the application of the nonlinear $\bar{D}$-transformation. This work presents a rapid and accurate evaluation of these integrals, obtained by using a new approach, which we called $S\bar{D}$. This new method is based on the $H\bar{D}$ and $\bar{D}$ methods and some practical properties of spherical Bessel, reduced Bessel and sine functions. The $S\bar{D}$ method has greatly simplified the calculations, avoiding the long and difficult implementation of the successive zeros of the spherical Bessel function and a method for solving linear systems, which are required by $H\bar{D}$ and $\bar{D}$.

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1. Introduction

This paper continues a series of previous studies [1, 2], concerning the rapid and accurate evaluation of molecular multicentre integrals to a high pre-determined accuracy for the development of molecular electronic structure calculations over Slater-type orbitals (STOs) [3, 4].

STOs constitute an important basis set for all calculations of physical properties of molecules and solids, which use the linear combination of atomic orbitals (LCAO) approach [5]. However, the systematic use of STOs has been prevented by the fact that their multicentre integrals turned out to be extremely complicated. Gaussian-type orbitals (GTOs) were introduced by Boys [6] and successfully used in the LCAO calculations [6–8]. This is due to the fact that GTOs can readily be translated. Unfortunately, these functions failed to satisfy two pragmatic requirements for analytic solutions of the appropriate Schrödinger equation, namely the cusp condition [9] and exponential decay at long distances [10]. As is well known, STOs fulfil the cusp condition and decline exponentially for large distances like exact solutions of the Schrödinger equation. This is why the use of STOs instead of GTOs reduces considerably the number of molecular integrals that occur in an LCAO calculation (short expansions of atomic orbitals are needed if STOs are used as basis functions).

In this paper, we use the so-called B functions [11–13]. Although these functions have a more complicated mathematical structure than STOs, they have much more suitable properties in multicentre integral problems [12, 14–17], among them being the exceptional simplicity of their Fourier transforms [15, 18]. Note that STOs can be expressed as finite linear combinations of B functions [13, 14].

The basis set of B functions is well adapted to the Fourier transform method [19–21]. This method allowed analytic expressions to be developed for multicentre bielectronic integrals [20, 21]. These analytic expressions involve semi-infinite very oscillatory integrals.

In the case of three-centre two-electron Coulomb and hybrid integrals over B functions, the integrands involve hypergeometric series and spherical Bessel functions. We have shown [22, 23] that these hypergeometric series can be expressed as finite expansions and that the integrands of interest satisfy fourth-order linear differential equations of the form required to apply the nonlinear D- [24] and $\bar{D}$-transformations [25, 26]. We also shown the superiority of these transformations over the alternatives using Gauss–Laguerre quadrature, the ϵ-algorithm of Wynn [27] or Levin's u transform [28], in evaluating these kinds of integrals. Unfortunately, the calculations required by these nonlinear transformations present severe numerical and computation difficulties. In previous work [23, 29, 30], we showed that the order of the linear differential equation satisfied by a function $f(x)$ of the form $f(x) = g(x) j_l(x)$, where $j_l(x)$ denotes the spherical Bessel function of order l and $g(x) = h(x)\,\mathrm{e}^{\phi(x)}$, where $h(x)$ and $\phi(x)$ have asymptotic expansions in inverse powers of x as $x \to +\infty$, can be reduced to two by keeping all the conditions required to apply D and $\bar{D}$ fulfilled. This led to the HD and $H\bar{D}$ methods which greatly simplified the calculations.

The aim of this work is to further simplify the application of the above methods as well as to reduce the calculation times while maintaining the same high accuracy.

As is well known the numerical integration of oscillatory integrands is very difficult when the oscillatory part is a (spherical) Bessel function [31, 32]. The main idea of this work is to replace the spherical Bessel function by a simple trigonometric function ($\sin(x)$) using practical properties of reduced Bessel functions, involved in the analytic expressions of the integrals of interest, and some properties of spherical Bessel and sine functions. This led to the $S\bar{D}$ method where the long and difficult implementation of the successive positive zeros of $j_l(x)$ and a method for solving linear systems, which are very time consuming and are required by $H\bar{D}$ and $\bar{D}$, are avoided. In the $S\bar{D}$ approach, the use of Cramer's rule to calculate the approximations of semi-infinite highly oscillatory integrands was made possible by the fact that the zeros of the sine function are equidistant.

The numerical results given in the appendix show the efficiency of the new approach in the evaluation of the integrals of interest. The numerical evaluation of the semi-infinite integrals are obtained for $s = 0.001$ and 0.999. In the regions where s is closer to 0 or 1, the oscillations of the integrands become very rapid. Indeed, when we make the substitutions $s = 0$ or 1, the rapid oscillations of the spherical Bessel function cannot be damped and suppressed by the exponentially decreasing function $\hat{k}_\nu$ involved in the integrand. This is due to the fact that when $s = 0$ or 1, the argument of the reduced Bessel function $\hat{k}_\nu$ becomes a constant. It should also be mentioned that the regions where s is close to 0 or 1 carry a very small weight due to the factors $s^{i_2}(1-s)^{i_1}$ in the integrands [33–36].

2. General definitions and properties

The three-centre two-electron Coulomb integral over B functions is

$$\mathcal{K}^{n_2 l_2 m_2, n_4 l_4 m_4}_{n_1 l_1 m_1, n_3 l_3 m_3} = \int_{\vec{R},\vec{R}'} \left[B^{m_1}_{n_1,l_1}\left(\zeta_1, \vec{R} - \overrightarrow{OA}\right)\right]^* \left[B^{m_3}_{n_3,l_3}\left(\zeta_3, \vec{R}' - \overrightarrow{OB}\right)\right]^*$$
$$\times \frac{1}{|\vec{R} - \vec{R}'|} B^{m_2}_{n_2,l_2}\left(\zeta_2, \vec{R} - \overrightarrow{OA}\right) B^{m_4}_{n_4,l_4}\left(\zeta_4, \vec{R}' - \overrightarrow{OC}\right) \mathrm{d}\vec{R}\, \mathrm{d}\vec{R}' \tag{1}$$

where A, B and C are three arbitrary points of the Euclidean space $\mathcal{E}_3$, while O is the origin of the fixed coordinate system.

The hybrid integral over B functions is

$$\mathcal{H}^{n_2 l_2 m_2, n_4 l_4 m_4}_{n_1 l_1 m_1, n_3 l_3 m_3} = \int_{\vec{R},\vec{R}'} \left[B^{m_1}_{n_1,l_1}\left(\zeta_1, \vec{R} - \overrightarrow{OA}\right)\right]^* \left[B^{m_3}_{n_3,l_3}\left(\zeta_3, \vec{R}' - \overrightarrow{OA}\right)\right]^*$$
$$\times \frac{1}{|\vec{R} - \vec{R}'|} B^{m_2}_{n_2,l_2}\left(\zeta_2, \vec{R} - \overrightarrow{OA}\right) B^{m_4}_{n_4,l_4}\left(\zeta_4, \vec{R}' - \overrightarrow{OB}\right) \mathrm{d}\vec{R}\, \mathrm{d}\vec{R}' \tag{2}$$

where A and B are two arbitrary points of the Euclidean space $\mathcal{E}_3$, while O is the origin of the fixed coordinate system.

The B function is defined as follows [12, 13]:

$$B^m_{n,l}(\zeta, \vec{r}) = \frac{(\zeta r)^l}{2^{n+l}(n+l)!} \hat{k}_{n-1/2}(\zeta r) Y^m_l(\theta_{\vec{r}}, \varphi_{\vec{r}}). \tag{3}$$

The B function can only be used as an LCAO basis functions if $n \in \mathbb{N}$ holds. For $-l \leqslant n \leqslant 0$, a B function is singular at the origin, and if $n = -l - \nu$ with $\nu \in \mathbb{N}$ holds, then a B function is no longer a function in the sense of classical analysis but a derivation of the three-dimensional Dirac delta function [37].

$Y^m_l(\theta, \varphi)$ denotes the surface spherical harmonic and is defined by [38]

$$Y^m_l(\theta, \varphi) = \mathrm{i}^{m+|m|} \left[\frac{(2l+1)(l-|m|)!)}{4\pi(l+|m|)!)} \right]^{1/2} P^{|m|}_l(\cos\theta)\, \mathrm{e}^{\mathrm{i}m\varphi} \tag{4}$$

where $P^m_l(x)$ is the associated Legendre polynomial of lth degree and mth order.

The reduced Bessel function $\hat{k}_{n+1/2}(z)$ is defined by [11, 12]

$$\hat{k}_{n+1/2}(z) = \sqrt{\frac{2}{\pi}} (z)^{n+1/2} K_{n+1/2}(z) \tag{5}$$

$$= z^n \mathrm{e}^{-z} \sum_{j=0}^{n} \frac{(n+j)!}{j!\,(n-j)!} \frac{1}{(2\,z)^j} \tag{6}$$

where $K_{n+1/2}$ denotes the modified Bessel function of the second kind [39].

Reduced Bessel functions satisfy the recurrence relation [11]

$$\hat{k}_{n+1/2}(z) = (2n-1)\, \hat{k}_{n-1/2}(z) + z^2 \hat{k}_{(n-1)-1/2}(z). \tag{7}$$

A useful property satisfied by $\hat{k}_{n+1/2}(z)$ is given by [39]

$$\left(\frac{\mathrm{d}}{z\,\mathrm{d}z}\right)^m \left[\frac{\hat{k}_{n+1/2}(z)}{z^{2n+1}}\right] = \left(\frac{\mathrm{d}}{z\,\mathrm{d}z}\right)^m \left[\sqrt{\frac{\pi}{2}}\,\frac{K_{n+1/2}(z)}{z^{n+1/2}}\right]$$
$$= (-1)^m \,\frac{\hat{k}_{n+m+1/2}(z)}{z^{2(n+m)+1}}. \tag{8}$$

Slater-type orbitals are defined in normalized form according to the following relationship [3, 4]:

$$\chi^m_{n,l}(\zeta, \vec{r}) = N(n, \zeta)\, r^{n-1}\, \mathrm{e}^{-\zeta r}\, Y^m_l(\theta_{\vec{r}}, \varphi_{\vec{r}}) \tag{9}$$

where $n = 1, 2, \ldots, l = 0, 1, \ldots, n-1$ and $m = -l, -l+1, \ldots, l-1, l$ and where $N(n, \zeta) = \zeta^{-n+1}\,[(2\zeta)^{2n+1}/(2n)!]^{1/2}$ denotes the normalization factor.

Slater-type orbitals can be expressed as finite linear combination of B functions [13]:

$$\chi^m_{n,l}(\zeta, \vec{r}) = \sum_{p=\tilde{p}}^{n-l} \frac{(-1)^{n-l-p}(n-l)!2^{l+p}(l+p)!}{(2p-n-l)!(2n-2l-2p)!!}\, B^m_{p,l}(\zeta, \vec{r}) \tag{10}$$

where

$$\tilde{p} = \begin{cases} (n-l)/2 & \text{if} \quad n-l \text{ is even} \\ (n-l+1)/2 & \text{if} \quad n-l \text{ is odd} \end{cases} \tag{11}$$

and where the double factorial is defined by

$$\begin{aligned} &(2k)!! = 2 \times 4 \times 6 \times \cdots \times (2k) = 2^k k! \\ &(2k+1)!! = 1 \times 3 \times 5 \times \cdots \times (2k+1) = \frac{(2k+1)!}{2^k k!} \\ &0!! = 1. \end{aligned} \tag{12}$$

The Fourier transform $\overline{B}^m_{n,l}(\zeta, \vec{p})$ of $B^m_{n,l}(\zeta, \vec{r})$ is given by [15, 18]

$$\overline{B}^m_{n,l}(\zeta, \vec{p}) = \frac{1}{(2\pi)^{3/2}} \int_{\vec{r}} \mathrm{e}^{-\mathrm{i}\vec{p}\cdot\vec{r}}\, B^m_{n,l}(\zeta, \vec{r})\, \mathrm{d}\vec{r} \tag{13}$$

$$= \sqrt{\frac{2}{\pi}}\,\zeta^{2n+l-1} \frac{(-\mathrm{i}|p|)^l}{(\zeta^2 + |p|^2)^{n+l+1}}\, Y^m_l(\theta_{\vec{p}}, \varphi_{\vec{p}}). \tag{14}$$

The Rayleigh expansion of the plane wavefunctions is given by [40]

$$\mathrm{e}^{\pm \mathrm{i}\vec{p}\cdot\vec{r}} = \sum_{l=0}^{+\infty} \sum_{m=-l}^{l} 4\pi\, (\pm\mathrm{i})^l\, j_l(|\vec{p}||\vec{r}|)\, Y^m_l(\theta_{\vec{r}}, \varphi_{\vec{r}})\, [Y^m_l(\theta_{\vec{p}}, \varphi_{\vec{p}})]^*. \tag{15}$$

The spherical Bessel function $j_l(x)$ of order $l \in \mathbb{N}_0$ is given by [39]

$$j_l(x) = [\pi/(2x)]^{1/2}\, J_{l+1/2}(x) \tag{16}$$

where $J_{l+1/2}(x)$ denotes the Bessel function of the first kind [39].

The spherical Bessel function is also defined by [39, 41]

$$j_l(x) = (-1)^l\, x^l \left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^l \left(\frac{\sin(x)}{x}\right). \tag{17}$$

$j_l(x)$ and its first derivative $j_l'(x)$ satisfy the recurrence relations [39]

$$\begin{aligned} x j_{l-1}(x) + x j_{l+1}(x) &= (2l+1) j_l(x) \\ l j_{l-1}(x) - (l+1) j_{l+1}(x) &= (2l+1) j_l'(x). \end{aligned} \tag{18}$$

For the following, we set $j_{l+1/2}^n$ for $n = 1, 2, \ldots$ the successive positive zeros of $j_l(x)$. $j_{l+1/2}^0$ is assumed to be 0.

Gaunt coefficients are defined as [42–48]

$$\langle l_1 m_1 | l_2 m_2 | l_3 m_3 \rangle = \int_{\theta=0}^{\pi} \int_{\varphi=0}^{2\pi} [Y_{l_1}^{m_1}(\theta,\varphi)]^* Y_{l_2}^{m_2}(\theta,\varphi) Y_{l_3}^{m_3}(\theta,\varphi) \sin\theta \, \mathrm{d}\theta \, \mathrm{d}\varphi. \tag{19}$$

These coefficients linearize the product of two spherical harmonics:

$$[Y_{l_1}^{m_1}(\theta,\varphi)]^* Y_{l_2}^{m_2}(\theta,\varphi) = \sum_{l=l_{\min,2}}^{l_1+l_2} \langle l_2 m_2 | l_1 m_1 | l m_2 - m_1 \rangle Y_l^{m_2-m_1}(\theta,\varphi) \tag{20}$$

where the subscript $l = l_{\min,2}$ in the summation symbol implies that the summation index l runs in steps of 2 from $l_{\min}$ to $l_1 + l_2$ and the constant $l_{\min}$ is given by [45]

$$l_{\min} = \begin{cases} \max(|l_1 - l_2|, |m_2 - m_1|) & \text{if} \quad l_1 + l_2 + \max(|l_1 - l_2|, |m_2 - m_1|) \text{ is even} \\ \max(|l_1 - l_2|, |m_2 - m_1|) + 1 & \text{if} \quad l_1 + l_2 + \max(|l_1 - l_2|, |m_2 - m_1|) \text{ is odd.} \end{cases} \tag{21}$$

The Fourier integral representation of the Coulomb operator $1/|\vec{r} - \vec{R}_1|$ is given by [49]

$$\frac{1}{|\vec{r} - \vec{R}_1|} = \frac{1}{2\pi^2} \int_{\vec{k}} \frac{\mathrm{e}^{-\mathrm{i}\vec{k}\cdot(\vec{r}-\vec{R}_1)}}{k^2} \, \mathrm{d}\vec{k}. \tag{22}$$

The hypergeometric function is given by [39]

$${}_2F_1(\alpha, \beta; \gamma; x) = \sum_{r=0}^{+\infty} \frac{(\alpha)_r (\beta)_r x^r}{(\gamma)_r r!} \tag{23}$$

where $(\alpha)_n$ represents the Pochhammer symbol, which is defined by [39]

$$\begin{aligned} (\alpha)_0 &= 1 \\ (\alpha)_n &= \alpha(\alpha+1)(\alpha+2)\cdots(\alpha+n-1) \qquad \text{for} \quad n \neq 0 \end{aligned} \tag{24}$$

where Γ denotes the Gamma function [39]. For $n \in \mathbb{N}_0$:

$$\Gamma(n+1) = n! \qquad \text{and} \qquad \Gamma\left(n + \tfrac{1}{2}\right) = \frac{(2n)!}{2^{2n}\, n!} \sqrt{\pi}. \tag{25}$$

The infinite series (23) converge only for $|x| < 1$, and they converge quite slowly if $|x|$ is slightly less than one. The corresponding functions nevertheless are defined in a much larger subset of the complex plane, including the case $|x| > 1$. Convergence problems of this kind can often be overcome by using nonlinear sequence transformations [50].

Let α be a negative integer. For $n \in \mathbb{N}_0$:

$$(\alpha)_n = \begin{cases} (\alpha)_n = 1 & n = 0 \\ (\alpha)_n = \alpha(\alpha+1)(\alpha+2)\cdots(\alpha+n-1) & n \leqslant -\alpha \\ (\alpha)_n = 0 & n \geqslant -\alpha + 1. \end{cases} \tag{26}$$

Now if α or β in the infinite series (23) is a negative integer, then by using the above relations we can show that the infinite series (23) will be reduced to a finite sum.

For the following, we define $A^{(\gamma)}$ for a certain γ, as the set of infinitely differentiable functions $p(x)$, which have asymptotic expansions in inverse powers of x as $x \to +\infty$, of the form

$$p(x) \sim x^{\gamma} \left(a_0 + \frac{a_1}{x} + \frac{a_2}{x^2} + \cdots \right) \tag{27}$$

and their derivatives of any order have asymptotic expansions, which can be obtained by differentiating that in (27) term by term.

From (27) it follows that $A^{(\gamma)} \supset A^{(\gamma-1)} \supset \cdots$.

We denote by $\tilde{A}^{(\gamma)}$ for $\gamma \in \mathbb{R}$, the set of functions $p(x)$ such that $p(x) \in A^{(\gamma)}$ and $\lim_{x\to+\infty} x^{-\gamma} p(x) \neq 0$. From this definition, it follows that if $p \in \tilde{A}^{(\gamma)}$ then $p(x)$ has an asymptotic expansion in inverse powers of x as $x \to +\infty$ of the form given by (27) with $a_0 \neq 0$.

We defined the functional $\alpha_0(p)$ by $\alpha_0(p) = a_o = \lim_{x\to+\infty} x^{-\gamma} p(x)$.

We defined $\mathrm{e}^{\tilde{A}^{(k)}}$ for some k as the set of $g(x) = \mathrm{e}^{\phi(x)}$, where $\phi(x) \in \tilde{A}^{(k)}$.

Lemma 1. *Let $p(x)$ be in $\tilde{A}^{(\gamma)}$ for a certain γ. Then*

(a) If $\gamma \neq 0$ then $p'(x) \in \tilde{A}^{(\gamma-1)}$, otherwise $p'(x) \in A^{(-2)}$.
(b) If $q(x) \in \tilde{A}^{(\delta)}$ then $p(x)\,q(x) \in \tilde{A}^{(\gamma+\delta)}$ and $\alpha_0(p\,q) = \alpha_0(p)\,\alpha_0(q)$.
(c) $\forall k \in \mathbb{R}$, $x^k p(x) \in \tilde{A}^{(k+\gamma)}$ and $\alpha_0(x^k p) = \alpha_0(p)$.
(d) The function $c\,p(x) \in \tilde{A}^{(\gamma)}$ and $\alpha_0(c\,p) = c\,\alpha_0(p)$ for all $c \neq 0$.
(e) If $q(x) \in A^{(\delta)}$ and $\gamma - \delta > 0$ then the function $p(x)+q(x) \in \tilde{A}^{(\gamma)}$ and $\alpha_0(p+q) = \alpha_0(p)$. If $\gamma = \delta$ and $\alpha_0(p) \neq -\alpha_0(q)$ then the function $p(x)+q(x) \in \tilde{A}^{(\gamma)}$ and $\alpha_0(p+q) = \alpha_0(p) + \alpha_0(q)$.
(f) For $m > 0$ an integer, $p^m(x) \in \tilde{A}^{(m\gamma)}$ and $\alpha_0(p^m) = \alpha_0(p)^m$.
(g) The function $1/p(x) \in \tilde{A}^{(-\gamma)}$ and $\alpha_0(1/p) = 1/\alpha_0(p)$.

Proofs of the above properties can easily be obtained by using the properties of Poincaré series [51].

Lemma 2. *Let $\phi(x)$ be in $\tilde{A}^{(\gamma)}$ for a certain γ.*

The function $\hat{k}_{n+1/2}(\phi(x))$ is in $\tilde{A}^{(n\gamma)}\mathrm{e}^{\tilde{A}^{(\gamma)}}$ and can be written in the following form:

$$\hat{k}_{n+1/2}(\phi(x)) = \phi_1(x)\,\mathrm{e}^{-\phi(x)}$$

where

$$\phi_1 \in \tilde{A}^{(n\gamma)} \qquad \text{and} \qquad \alpha_0(\phi_1) = (\alpha_0(\phi))^n \neq 0.$$

By using the analytic expression of the reduced Bessel function which is given by equation (6) and using the properties of Poincaré series, one can easily prove lemma 2.

3. Three-centre two-electron Coulomb and hybrid integrals over B functions

By substituting the integral representation of the Coulomb operator (22) in the expression of the three-centre two-electron Coulomb integral (1), we obtain

$$\mathcal{K}^{n_2l_2m_2,n_4l_4m_4}_{n_1l_1m_1,n_3l_3m_3} = \frac{1}{2\pi^2} \int_{\vec{x}} \mathrm{e}^{\mathrm{i}\vec{x}\cdot\vec{R}_4} \big\langle B^{m_1}_{n_1,l_1}(\zeta_1,\vec{r}) \big| \mathrm{e}^{-\mathrm{i}\vec{x}\cdot\vec{r}} \big| B^{m_2}_{n_2,l_2}(\zeta_2,\vec{r}) \big\rangle_{\vec{r}}$$
$$\times \big\langle B^{m_4}_{n_4,l_4}(\zeta_4,\vec{r}'') \big| \mathrm{e}^{-\mathrm{i}\vec{x}\cdot\vec{r}''} \big| B^{m_3}_{n_3,l_3}\big(\zeta_3,\vec{r}'' - (\vec{R}_3 - \vec{R}_4)\big) \big\rangle^*_{\vec{r}''} \frac{\mathrm{d}\vec{x}}{x^2} \tag{28}$$

where

$$\vec{r} = \vec{R} - \overrightarrow{OA} \qquad \vec{r}'' = -\vec{R}' + \overrightarrow{OA} \qquad \vec{R}_3 = \overrightarrow{AB} \qquad \vec{R}_4 = \overrightarrow{AC}.$$

For the hybrid integral we obtain

$$\mathcal{H}^{n_2l_2m_2,n_4l_4m_4}_{n_1l_1m_1,n_3l_3m_3} = \frac{1}{2\pi^2}\int_{\vec{x}} \mathrm{e}^{-\mathrm{i}\vec{x}\cdot\vec{R}_1} \left\langle B^{m_1}_{n_1,l_1}(\zeta_1,\vec{r})\middle|\mathrm{e}^{-\mathrm{i}\vec{x}\cdot\vec{r}}\middle|B^{m_2}_{n_2,l_2}(\zeta_2,\vec{r})\right\rangle_{\vec{r}}$$
$$\times\left\langle B^{m_4}_{n_4,l_4}(\zeta_4,\vec{r}'')\middle|\mathrm{e}^{-\mathrm{i}\vec{x}\cdot\vec{r}''}\middle|B^{m_3}_{n_3,l_3}\big(\zeta_3,\vec{r}''-\vec{R}_1\big)\right\rangle^*_{\vec{r}''}\frac{\mathrm{d}\vec{x}}{x^2} \tag{29}$$

where

$$\vec{r} = \vec{R} - \overrightarrow{OA} \qquad \vec{r}'' = \vec{R}' - \overrightarrow{OB} \qquad \vec{R}_1 = -\overrightarrow{AB}.$$

The following arguments can also be applied to the hybrid integral.

In [22, 29], we showed that the term $\left\langle B^{m_1}_{n_1,l_1}(\zeta_1,\vec{r})\middle|\mathrm{e}^{-\mathrm{i}\vec{x}\cdot\vec{r}}\middle|B^{m_2}_{n_2,l_2}(\zeta_2,\vec{r})\right\rangle_{\vec{r}}$ in the above equations, has an analytic expression involving a hypergeometric function which is given by

$${}_2F_1\left(\frac{l-k-l_1-l_2+1}{2}, \frac{l-k-l_1-l_2}{2}+1; l+\frac{3}{2}; -\frac{x^2}{\zeta_s^2}\right) \tag{30}$$

where k and l are positive integers.

One of the first two arguments $(l-k-l_1-l_2+1)/2$, $(l-k-l_1-l_2)/2+1$ of the hypergeometric function is a negative integer. Thus, the above infinite series is reduced to a finite expansion. The analytic expression of the term in $\vec{r}$, involving in equations (28) and (29), is given by [22, 29]

$$\left\langle B^{m_1}_{n_1,l_1}(\zeta_1,\vec{r})\middle|\mathrm{e}^{-\mathrm{i}\vec{x}\cdot\vec{r}}\middle|B^{m_2}_{n_2,l_2}(\zeta_2,\vec{r})\right\rangle_{\vec{r}} = \frac{(4\pi)\sqrt{\pi}\,\zeta_1^{l_1}\zeta_2^{l_2}}{2^{n_1+l_1+n_2+l_2}(n_1+l_1)!(n_2+l_2)!}$$
$$\times\sum_{l=l_{\min},2}^{l_{\max}}(-\mathrm{i})^l\langle l_2m_2|l_1m_1|lm_2-m_1\rangle Y_l^{m_1-m_2}(\theta_{\vec{x}},\varphi_{\vec{x}})$$
$$\times\sum_{k=2}^{n_1+n_2}\sum_{i=k_1}^{k_2}\left[\frac{(2n_1-i-1)!\,(2n_2-i-1)!\,\zeta_1^{i-1}\,\zeta_2^{k-i-1}}{(i-1)!\,(n_1-i)!\,(k-i-1)!\,(n_2-k+i)!\,2^{n_1+n_2-k}}\right]$$
$$\times\frac{\Gamma(k+l_1+l_2+l+1)\zeta_s^{n_k-l-1}}{2^{l+1}\Gamma\left(l+\frac{3}{2}\right)\left[\zeta_s^2+x^2\right]^{k+l_1+l_2}}\sum_{r=0}^{\eta'}(-1)^r\frac{(\eta/2)_r\,((\eta+1)/2)_r}{\left(l+\frac{3}{2}\right)_r r!\zeta_s^{2r}}x^{2r+l} \tag{31}$$

where

$$k_1 = \max(1, k-n_2),\ k_2 = \min(n_1, k-1),\ \zeta_s = \zeta_1+\zeta_2$$
$$\begin{cases} \eta' = -\dfrac{\eta}{2} & \text{if } \quad \eta \text{ is even} \\[2mm] \eta' = -\dfrac{\eta+1}{2} & \text{otherwise.}\end{cases}$$

The Fourier transform method allowed analytic expression to be developed for the second term in the integrand [20, 21]:

$$\left\langle B^{m_4}_{n_4,l_4}(\zeta_4,\vec{r}'')\middle|\mathrm{e}^{-\mathrm{i}\vec{x}\cdot\vec{r}''}\middle|B^{m_3}_{n_3,l_3}\big(\zeta_3,\vec{r}''-(\vec{R}_3-\vec{R}_4)\big)\right\rangle^*_{\vec{r}''}.$$

The above results led to an analytic expression for the three-centre two-electron Coulomb integral over B functions, which is given by

$$
\begin{aligned}
n_x &= l_3 - l_3' + l_4 - l_4' + 2r + l \qquad n_k = k + l_1 + l_2 \\
n_\gamma &= 2(n_3 + l_3 + n_4 + l_4) - (l_3' + l_4') - l' + 1 \\
\mu &= (m_2 - m_1) - (m_3 - m_3') + (m_4 - m_4') \\
[\gamma(s,x)]^2 &= (1-s)\zeta_4^2 + s\zeta_3^2 + s(1-s)x^2 \\
\eta &= l - k - l_1 - l_2 + 1 \qquad \Delta l = \frac{l_3 + l_4 - l'}{2} \\
\vec{v} &= (1-s)(\vec{R}_3 - \vec{R}_4) - \vec{R}_4 \\
\nu &= n_3 + n_4 + l_3 + l_4 - l' - j + \tfrac{1}{2} \\
m_{34} &= (m_3 - m_3') - (m_4 - m_4')
\end{aligned}
$$

$$
\begin{aligned}
\mathcal{K}_{n_1 l_1 m_1, n_3 l_3 m_3}^{n_2 l_2 m_2, n_4 l_4 m_4} &= 8(4\pi)^3 \sqrt{\pi}\, \zeta_1^{l_1}\, \zeta_2^{l_2}\, \zeta_3^{2n_3+l_3-1}\, \zeta_4^{2n_4+l_4-1} \\
&\times \frac{(2l_3+1)!!\,(2l_4+1)!!\,(n_3+l_3+n_4+l_4+1)!}{2^{l_1+l_2+1}\,(n_1+l_1)!\,(n_2+l_2)!\,(n_3+l_3)!\,(n_4+l_4)!} \\
&\times \sum_{l=l_{\min},2}^{l_1+l_2} \frac{(-\mathrm{i})^l}{2^{2n_1+2n_2+l}} \langle l_1 m_1 | l_2 m_2 | l m_1 - m_2 \rangle \\
&\times \sum_{k=2}^{n_1+n_2} \sum_{i=k_1}^{k_2} \left[\frac{2^k\,(2n_1-i-1)!\,(2n_2-i-1)!\,\zeta_1^{i-1}\,\zeta_2^{k-i-1}}{(i-1)!\,(n_1-i)!\,(k-i-1)!\,(n_2-k+i)!} \right] \\
&\times \sum_{l_4'=0}^{l_4} \sum_{m_4'=-l_4'}^{l_4'} i^{l_4} (-1)^{l_4'} \frac{\langle l_4 m_4 | l_4 - l_4' m_4 - m_4' | l_4' m_4' \rangle}{(2l_4'+1)!![2(l_4-l_4')+1]!!} \\
&\times \sum_{l_3'=0}^{l_3} \sum_{m_2'=-l_3'}^{l_3'} i^{l_3} \frac{\langle l_3 m_3 | l_3 - l_3' m_3 - m_3' | l_3' m_3' \rangle}{(2l_3'+1)!![2(l_3-l_3')+1]!!} \\
&\times \sum_{l'=l'_{min,2}}^{l_3'+l_4'} \langle l_3' m_3' | l_4' m_4' | l' m_3' - m_4' \rangle R_{34}^{l'}\, Y_{l'}^{m_3'-m_4'}(\theta_{\vec{R}_{34}}, \varphi_{\vec{R}_{34}}) \\
&\times \sum_{l_{34}=l''_{min,2}}^{l_3-l_3'+l_4-l_4'} \langle l_3 - l_3' m_3 - m_3' | l_4 - l_4' m_4 - m_4' | l_{34} m_{34} \rangle \\
&\times \sum_{\lambda=\lambda_{min,2}}^{l+l_{34}} \mathrm{i}^{\lambda} \langle l m_2 - m_1 | l_{34} (m_3 - m_3') - (m_4 - m_4') | \lambda \mu \rangle \\
&\times \sum_{j=0}^{\Delta l} \binom{\Delta l}{j} \frac{(-1)^{(l_4'+l_3'+l')/2}\,(-1)^j}{2^{n_3+n_4+l_3+l_4-j+1}(n_3+n_4+l_3+l_4-j+1)!} \\
&\times \frac{\zeta_s^{n_k-l-1}\,\Gamma(k+l_1+l_2+l+1)}{\Gamma(l+3/2)} \sum_{r=0}^{\eta'} (-1)^r \frac{(\eta/2)_r\,((\eta+1)/2)_r}{(l+3/2)_r\, r!\, \zeta_s^{2r}}
\end{aligned}
$$

$$\times \int_{s=0}^{1} s^{n_3+l_3+l_4-l'_4}\,(1-s)^{n_4+l_4+l_3-l'_3}\,Y_\lambda^\mu(\theta_{\vec{v}},\varphi_{\vec{v}})$$

$$\times \int_{x=0}^{+\infty} \left[\zeta_s^2+x^2\right]^{-n_k} x^{n_x}\,\frac{\hat{k}_\nu[R_{34}\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}\,j_\lambda(vx)\,\mathrm{d}x\,\mathrm{d}s. \tag{32}$$

The numerical evaluation of the above analytic expression turned out to be very difficult. This is due to the presence of semi-infinite integrals, which will be referred to as $\tilde{\mathcal{K}}(s)$, whose integrands oscillate rapidly, due to the spherical Bessel functions $j_\lambda(vx)$, in particular for large values of λ and v since the zeros of the function become closer.

The semi-infinite integral $\tilde{\mathcal{K}}(s)$ involved in equation (32) is given by

$$\tilde{\mathcal{K}}(s) = \int_{x=0}^{+\infty} \left[\zeta_s^2+x^2\right]^{-n_k} x^{n_x}\,\frac{\hat{k}_\nu[R_{34}\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}\,j_\lambda(vx)\,\mathrm{d}x. \tag{33}$$

The above semi-infinite oscillatory integral can be transformed into an infinite series of integrals of alternating sign. This infinite series is given by

$$\tilde{\mathcal{K}}(s) = \sum_{n=0}^{+\infty} \int_{j_{\lambda,v}^{n}}^{j_{\lambda,v}^{n+1}} \left[\zeta_s^2+x^2\right]^{-n_k} x^{n_x}\,\frac{\hat{k}_\nu[R_{34}\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}\,j_\lambda(vx)\,\mathrm{d}x \tag{34}$$

where $j_{\lambda,v}^n = j_{\lambda+1/2}^n/v,\ n = 1, 2, \ldots$ which are the successive positive zeros of $j_\lambda(vx)$. $j_{\lambda,v}^0$ is assumed to be 0.

The above infinite series is convergent and alternating, therefore the sum of N first terms, for N sufficiently large, gives a good approximation of the semi-infinite integral. Unfortunately, the use of this approach is very time consuming.

In previous work [22], we showed that the integrand of $\tilde{\mathcal{K}}(s)$, which will be referred to as $\mathcal{F}_{\tilde{\mathcal{K}}}(x)$, satisfies a fourth-order linear differential equation of the form required to apply the nonlinear $\bar{D}$-transformation. The results obtained were satisfactory compared with the others obtained using the quadrature of Gauss–Laguerre, the ϵ-algorithm of Wynn [27] and Levin's u transform [28].

The approximation $\bar{D}_n^{(4)}$ of $\tilde{\mathcal{K}}(s)$ is given by [22]

$$\bar{D}_n^{(4)} = \int_0^{x_l} \mathcal{F}_{\tilde{\mathcal{K}}}(t)\,\mathrm{d}t + \sum_{k=1}^{3} \mathcal{F}_{\tilde{\mathcal{K}}}^{(k)}(x_l)x_l^{k+1} \sum_{i=0}^{n-1} \frac{\bar{\beta}_{k,i}}{x_l^i} \qquad l = 0, 1, \ldots, 3n \tag{35}$$

where $x_l = j_{\lambda,v}^{l+1}$ for $l = 0, 1, \ldots, 3n$. $D_n^{(4)}$ and the $\bar{\beta}_{k,i}$ for $k = 1, 2, 3$ and $i = 0, 1, \ldots, n-1$ are the $(3n+1)$ unknowns of the linear system.

As can be seen from the above equation, the computation of the three successive derivatives of $\mathcal{F}_{\tilde{\mathcal{K}}}(x)$ is required for the calculations.

The calculation of $3n$ successive zeros of the spherical Bessel function is also necessary. This presents severe numerical and computation difficulties. Added to this is the fact that the order of the linear system increases as n becomes large.

In [23, 29, 30], we showed by using some practical properties of spherical Bessel, reduced Bessel functions and Poincaré series that we can obtain a second-order linear differential equation satisfied by $f(x) = g(x)j_\lambda(x)$, where $g(x) = h(x)\,\mathrm{e}^{\phi(x)}$ and where $h(x) \in \tilde{A}^{(\gamma)}$ and $\phi(x) \in \tilde{A}^{(k)}$ for some γ and k. We also showed that if $k > 0$ and $\alpha_0(\phi) < 0$ then $f(x)$ satisfies all the conditions required to apply the nonlinear $\bar{D}$-transformation using the second-order differential equation. This result led to the $H\bar{D}$ approach.

The integrand $\mathcal{F}_{\tilde{\mathcal{K}}}(x)$ can be written as

$$\mathcal{F}_{\tilde{\mathcal{K}}}(x) = g(x)\,j_\lambda(x)$$

where

$$g(x) = \left[\zeta_s^2 + x^2\right]^{-n_k} \; x^{n_x} \; \frac{\hat{k}_\nu[R_{34}\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}.$$

It is shown that $g(x)$ is of the form $h(x)\,\mathrm{e}^{\phi(x)}$, where $h(x)$ and $\phi(x)$ satisfy all of the above conditions. The approximation of $\tilde{\mathcal{K}}(s)$ using the $H\bar{D}$ method is given by [23, 29, 30]

$$H\bar{D}_n^{(2)} = \int_0^{x_l} \mathcal{F}_{\tilde{\mathcal{K}}}(t)\,\mathrm{d}t + g(x_l)\,j_\lambda'(vx)x_l^2 \sum_{i=0}^{n-1} \frac{\bar{\beta}_{1,i}}{x_l^i} \qquad l = 0, 1, \ldots, n \tag{36}$$

where $x_l = j_{\lambda,v}^{l+1}$, $l = 0, 1, \ldots, n$. $H\bar{D}_n^{(2)}$ and $\bar{\beta}_{1,i}$ for $i = 0, 1, \ldots, n-1$ are the $(n+1)$ unknowns of the linear system.

It is clear from equation (36) that the reduction of the order of the linear differential equation has greatly simplified the application of the nonlinear $\bar{D}$-transformation. The calculation of the successive derivatives of the integrand is avoided, the order of the linear system to solve is reduced to $(n+1)$. However, we still have to calculate n successive zeros of the spherical Bessel function. In [23, 29, 30], we showed that the $H\bar{D}$ approach led to a high accuracy and a substantial gain in the calculation times. The convergence properties of this approach were analysed [23, 30] and they showed that from a numerical point of view the $H\bar{D}$ method corresponds to the most ideal situation.

The aim of this paper is to further simplify the calculations as well as to reduce the calculation times while maintaining the same high accuracy.

4. The $S\bar{D}$ method for improving convergence of semi-infinite oscillatory integrals

Theorem. *Let $f(x)$ be a function of the form $f(x) = g(x)\,j_\lambda(x)$, where $g(x) \in \mathcal{C}^2\big([0, +\infty[\big)$, which is the set of twice continuously differentiable functions, and of the form $g(x) = h(x)\,\mathrm{e}^{\phi(x)}$, where $h(x) \in \tilde{A}^{(\gamma)}$ for a certain γ and $\phi(x) \in \tilde{A}^{(k)}$ for a certain k.*

If $k > 0$, $\alpha_0(\phi) < 0$ and for all $l = 0, 1, \ldots, \lambda - 1$:

$$\lim_{x \to 0} x^{l-\lambda+1} \left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^l \left(x^{\lambda-1} g(x)\right) j_{\lambda-1-l}(x) = 0$$

then $f(x)$ is integrable on $[0, +\infty[$ and an approximation of $\int_0^{+\infty} f(x)\,\mathrm{d}x$ is given by

$$S\bar{D}_n^{(2,j)} = \frac{\sum_{i=0}^{n+1} \binom{n+1}{i} (x_0/\alpha + i + j)^n \; F(x_{i+j}) \big/ \left[x_{i+j}^2 G(x_{i+j})\right]}{\sum_{i=0}^{n+1} \binom{n+1}{i} (x_0/\alpha + i + j)^n \; \big/ \left[x_{i+j}^2 G(x_{i+j})\right]} \tag{37}$$

where $\alpha = \pi$, $x_l = (l+1)\alpha$ for $l = 0, 1, \ldots$, $G(x) = \left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^\lambda \left(x^{\lambda-1} g(x)\right)$ and where $F(x) = \int_0^x G(t)\,\sin(t)\,\mathrm{d}t$.

Proof. Let us consider $\int_0^{+\infty} f(x)\,\mathrm{d}x = \int_0^{+\infty} g(x)\,j_\lambda(x)$.

By replacing the spherical Bessel function $j_\lambda(x)$ by its analytic expression given by (17), one can obtain

$$\int_0^{+\infty} f(x)\,\mathrm{d}x = (-1)^\lambda \int_0^{+\infty} x^\lambda\, g(x) \left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^\lambda j_0(x)\,\mathrm{d}x. \tag{38}$$

By integrating by parts until all the derivatives of $j_0(x)$, with respect to $x\,\mathrm{d}x$, disappear in the last term on the right-hand side of (38), we obtain

$$\int_0^{+\infty} f(x)\,\mathrm{d}x = \left[\sum_{l=0}^{\lambda-1}(-1)^{\lambda+l}\left(\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{l}\left(x^{\lambda-1}g(x)\right)\right)\left(\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{\lambda-1-l} j_0(x)\right)\right]_0^{+\infty} + \int_0^{+\infty}\left(\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{\lambda}\left(x^{\lambda-1}\,g(x)\right)\right) j_0(x)\,x\,\mathrm{d}x. \tag{39}$$

Using equation (17) and replacing $j_0(x)$ by $\sin(x)/x$, the above equation can be rewritten as follows:

$$\int_0^{+\infty} f(x)\,\mathrm{d}x = -\left[\sum_{l=0}^{\lambda-1} x^{l-\lambda+1}\left(\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{l}\left(x^{\lambda-1}g(x)\right)\right) j_{\lambda-1-l}(x)\right]_0^{+\infty} + \int_0^{+\infty}\left(\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{\lambda}\left(x^{\lambda-1}\,g(x)\right)\right)\sin(x)\,\mathrm{d}x \tag{40}$$

where $g(x)$ is exponentially decreasing as $x \to +\infty$. From this it follows that $\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{l}\left(x^{\lambda-1}g(x)\right)$ is also exponentially decreasing as $x \to +\infty$ and consequently for all $l \geqslant 0$:

$$\lim_{x\to+\infty} x^{l-\lambda+1}\left(\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{l}\left(x^{\lambda-1}g(x)\right)\right) j_{\lambda-1-l}(x) = 0$$

As $\lim_{x\to 0} x^{l-\lambda+1}\left(\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{l}\left(x^{\lambda-1}g(x)\right)\right) j_{\lambda-1-l}(x) = 0$, for $l = 0, \ldots, \lambda-1$ then the above equation can be rewritten as

$$\int_0^{+\infty} f(x)\,\mathrm{d}x = \int_0^{+\infty}\left[\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{\lambda}\left(x^{\lambda-1}\,g(x)\right)\right]\sin(x)\,\mathrm{d}x. \tag{41}$$

Let us consider the function $G(x) = \left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{\lambda}\left(x^{\lambda-1}\,g(x)\right)$. By using the Leibnitz formulae and the fact that $g(x) = h(x)\,\mathrm{e}^{\phi(x)}$, we can obtain

$$G(x) = \sum_{i=0}^{\lambda}\frac{\lambda!!}{(\lambda-2i)!!}x^{\lambda-2i}\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{\lambda-i} g(x) = \sum_{i=0}^{\lambda}\sum_{m=0}^{\lambda-i}\frac{\lambda!!}{(\lambda-2i)!!}\binom{\lambda-i}{m}x^{\lambda-2i} \times\left(\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{m} h(x)\right)\left(\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{\lambda-i-m}\mathrm{e}^{\phi(x)}\right). \tag{42}$$

Using the properties of asymptotic expansions given by lemma 1, we can show that

$$\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{m} h(x) \in A^{(\gamma-2m)}$$

$$\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{\alpha}\mathrm{e}^{\phi(x)} = \varphi(x)\,\mathrm{e}^{\phi(x)} \qquad \text{where} \quad \varphi \in A^{(\alpha(k-2))}$$

and consequently

$$x^{\lambda-2i}\left(\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{m} h(x)\right)\left(\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{\lambda-i-m}\mathrm{e}^{\phi(x)}\right) = H_{i,m}(x)\,\mathrm{e}^{\phi(x)}$$

where the function $H_{i,m}(x) \in A^{(\gamma+(\lambda-i-m)k-\lambda)}$.

By using lemma 1, we can show that $G(x)$ can be rewritten as

$$G(x) = H(x)\,\mathrm{e}^{\phi(x)} \qquad \text{where} \quad H(x) \in \tilde{A}^{(\gamma+\lambda k-\lambda)} \tag{43}$$

$\sin(x)$ satisfies a second-order linear differential equation given by

$$\sin(x) = -\sin''(x). \tag{44}$$

Let the function $\mathcal{F}(x)$ be defined by

$$\mathcal{F}(x) = G(x)\ \sin(x)$$

then

$$\sin(x) = \mathcal{F}(x)/G(x).$$

By substituting this in the linear differential equation satisfied by $\sin(x)$ we can obtain, after replacing $G(x)$ by $H(x)\,\mathrm{e}^{\phi(x)}$, a second-order linear differential equation satisfied by $\mathcal{F}(x)$, which is given by

$$\mathcal{F}(x) = q_1(x)\mathcal{F}'(x) + q_2(x)\mathcal{F}''(x) \tag{45}$$

where the coefficients $q_1(x)$ and $q_2(x)$ are defined by

$$\begin{aligned} q_1(x) &= \frac{2\left(\phi'(x) + H'(x)/H(x)\right)}{1 + (\phi'(x) + H'(x)/H(x))^2 - (\phi'(x) + H'(x)/H(x))'} \\ q_2(x) &= \frac{-1}{1 + (\phi'(x) + H'(x)/H(x))^2 - (\phi'(x) + H'(x)/H(x))'}. \end{aligned} \tag{46}$$

Using lemma 1, we can show that if $k = 0$ then $q_1(x) \in A^{(-1)}$ and $q_2(x) \in A^{(0)}$, otherwise $q_1(x) \in A^{(-k+1)}$ and $q_2(x) \in A^{(-k+1)}$.

Since $k > 0$ and $\alpha_0(\phi) < 0$, then the function $\mathcal{F}(x)$ is exponentially decreasing as $x \to +\infty$ and consequently is integrable on $[0, +\infty[$ and for all $l = i, 2;\ i = 1, 2$:

$$\lim_{x\to+\infty} q_l^{(i-1)}(x)\,\mathcal{F}^{(l-i)}(x) = 0.$$

It is easy to show that $q_{i,0} = \lim_{x\to+\infty} x^{-i} q_i(x) = 0$ for $i = 1, 2$. From this it follows that for every integer $l \geqslant -1$:

$$\sum_{i=1}^{2} l(l-1)\ldots(l-i+1)q_{i,0} = 0 \neq 1.$$

All the conditions required to apply the $\bar{D}$-transformation are now shown to be satisfied by $\mathcal{F}(x)$.

The approximation of $\int_0^{+\infty} \mathcal{F}(x)\,\mathrm{d}x = \int_0^{+\infty} f(x)\,\mathrm{d}x$ is given by

$$S\bar{D}_n^{(2)} = \int_0^{x_l} \mathcal{F}(x)\,\mathrm{d}x + (-1)^{l+1}\,G(x_l)\,x_l^2 \sum_{i=0}^{n-1} \frac{\bar{\beta}_{1,i}}{x_l^i} \qquad l = 0, 1, \ldots, n \tag{47}$$

where $x_l = (l+1)\pi$ for $l = 0, 1, \ldots$ which are the successive zeros of $\sin(x)$.

Following Levin in [28], we can use Cramer's rule, since the zeros of $\sin(x)$ are equidistant, to obtain the simple solution which is given by equation (37) for the unknown $S\bar{D}_n^{(2)}$. $\square$

5. Evaluation of three-centre two-electron Coulomb and hybrid integrals

The integrand of $\tilde{\mathcal{K}}(s)$ is given by $\mathcal{F}_{\tilde{\mathcal{K}}}(x) = g(x)\, j_\lambda(vx)$, where $g(x)$ is defined by

$$g(x) = \left[\zeta_s^2 + x^2\right]^{-n_k} x^{n_x} \frac{\hat{k}_\nu[R_{34}\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}.$$

It is clear that the function $g(x)$ belongs to $\mathcal{C}^2\big([0,+\infty[\big)$.

Let the function $\phi(x)$ be defined by

$$\begin{aligned}\phi(x) &= R_{34}\gamma(s,x)\\ &= R_{34}\sqrt{(1-s)\zeta_4^2 + s\zeta_3^2 + s(1-s)x^2}.\end{aligned}$$

From lemma 1, it follows that $\phi(x) \in \tilde{A}^{(1)}$ and $1/[\gamma(s,x)]^{n_\gamma} \in \tilde{A}^{(-n_\gamma)}$.

The function $\left[\zeta_s^2 + x^2\right]^{-n_k} = x^{-2n_k}\left[1 + \zeta_s^2/x^2\right]^{-n_k} \in \tilde{A}^{(-2n_k)}$.

Using lemmas 1 and 2, we can obtain an expression for $g(x)$, which is given by

$$g(x) = h(x)\,\mathrm{e}^{-\phi(x)} \quad \begin{cases} h(x) \in \tilde{A}^{(\nu+n_x-2n_k-n_\gamma)} \\ \phi \in \tilde{A}^{(1)} \qquad \text{with} \quad \alpha_0(\phi) > 0. \end{cases}$$

With the help of equation (8) and the fact that $\frac{\mathrm{d}}{\mathrm{d}x} = \frac{\mathrm{d}z}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}z}$, one can easily show that if $n_\gamma = 2\nu$ then for $j \in \mathbb{N}$:

$$\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^j \left[\frac{\hat{k}_\nu[R_{34}\gamma(s,x)]}{[\gamma(s,x)]^{2\nu}}\right] = (-1)^j\, s^j\,(1-s)^j\,\frac{\hat{k}_{\nu+j}\,[R_{34}\gamma(s,x)]}{[\gamma(s,x)]^{2(\nu+j)}} \tag{48}$$

and for $n_\gamma < 2\nu$, we obtain

$$\begin{aligned}\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^j \left[\frac{\hat{k}_\nu[R_{34}\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}\right] &= \sum_{i=0}^{j}\binom{j}{i}(-1)^{j-i}\,\frac{(2\nu-n_\gamma)!!}{(2\nu-n_\gamma-2i)!!}\\ &\quad \times s^i(1-s)^i\,\frac{\hat{k}_{\nu+j-i}\,[R_{34}\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma+2i}}.\end{aligned} \tag{49}$$

For $l \in \mathbb{N}$, we obtain after some algebraic operations

$$\begin{aligned}\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^l \left(x^{\lambda-1}g(x)\right) &= \sum_{i=0}^{l}\sum_{j=0}^{i}\binom{l}{i}\binom{i}{j}\frac{(n_x+\lambda-1)!!}{(n_x+\lambda-1-2i)!!}x^{n_x+\lambda-1-2i}\\ &\quad \times M(n_k, i-j)\left[\zeta_s^2+x^2\right]^{-n_k-i+j}\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{l-i}\left[\frac{\hat{k}_\nu[R_{34}\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}\right]\end{aligned} \tag{50}$$

where

$$M(n_k, i-j) = (-2)^{i-j} n_k(n_k+1)\ldots(n_k+i-j-1).$$

As can be seen from equation (32), $\lambda \leqslant l + l_3 - l_3' + l_4 - l_4' \leqslant n_x$. From this it follows that if $l \leqslant \lambda - 1$ then $l \leqslant n_x - 1$. Using this, we can show that $n_x + l - 2i > 0$ for all $i \leqslant l$.

Now by using this argument and with the help of equations (48)–(50), we can show that

$$\lim_{x\to 0} x^{l-\lambda+1}\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{l}\left(x^{\lambda-1}g(x)\right) j_{\lambda-1-l}(vx) = 0.$$

Now it is shown that the integrand $\mathcal{F}_{\tilde{\mathcal{K}}}(x)$ of $\tilde{\mathcal{K}}(s)$ satisfies all the conditions of the theorem. Consequently, $\tilde{\mathcal{K}}(s)$ can be rewritten as

$$\tilde{\mathcal{K}}(s) = \frac{1}{v^{\lambda+1}}\int_{x=0}^{+\infty}\left(\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{\lambda}\left[\frac{x^{n_x+\lambda-1}}{\left[\zeta_s^2+x^2\right]^{n_k}}\,\frac{\hat{k}_\nu[R_{34}\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}\right]\right)\sin(vx)\,\mathrm{d}x \tag{51}$$

$$= \frac{1}{v^{\lambda+1}}\sum_{n=0}^{+\infty}\int_{n\pi/v}^{(n+1)\pi/v}\left(\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{\lambda}\left[\frac{x^{n_x+\lambda-1}}{\left[\zeta_s^2+x^2\right]^{n_k}}\,\frac{\hat{k}_\nu[R_{34}\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}\right]\right)\sin(vx)\,\mathrm{d}x. \tag{52}$$

The approximation of $\tilde{\mathcal{K}}(s)$ is given by

$$S\bar{D}_n^{(2,j)} = \frac{1}{v^{\lambda+1}}\,\frac{\sum_{i=0}^{n+1}\binom{n+1}{i}(1+i+j)^n F(x_{i+j})\big/\left[x_{i+j}^2 G(x_{i+j})\right]}{\sum_{i=0}^{n+1}\binom{n+1}{i}(1+i+j)^n\big/\left[x_{i+j}^2 G(x_{i+j})\right]} \tag{53}$$

where $x_l = (l+1)\frac{\pi}{v}$ for $l = 0, 1, \ldots$, $G(x) = \left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{\lambda}\left(x^{\lambda-1}g(x)\right)$ and where $F(x) = \int_0^x G(t)\,\sin(vt)\,\mathrm{d}t$.

As can be seen from equations (48)–(50), the calculation of $G(x)$ does not present any computation difficulties.

In the case of the hybrid integral $\mathcal{H}_{n_1l_1m_1,n_3l_3m_3}^{n_2l_2m_2,n_4l_4m_4}$, the semi-infinite integral is given by

$$\tilde{\mathcal{H}}(s) = \int_{x=0}^{+\infty}\left[\zeta_s^2+x^2\right]^{-n_k} x^{n_x}\,\frac{\hat{k}_\nu[R_1\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}\, j_\lambda(vx)\,\mathrm{d}x \tag{54}$$

$$= \sum_{n=0}^{+\infty}\int_{j_{\lambda,v}^{n}}^{j_{\lambda,v}^{n+1}}\left[\zeta_s^2+x^2\right]^{-n_k} x^{n_x}\,\frac{\hat{k}_\nu[R_1\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}\, j_\lambda(vx)\,\mathrm{d}x \tag{55}$$

where $\vec{v} = (2-s)\vec{R}_1$. $\zeta_s, n_k, n_x, \nu, n_\gamma, \gamma(s,x)$ and λ are defined according to equation (32).

As can be seen from the above equation, the integrand of $\tilde{\mathcal{H}}(s)$ is similar to $\mathcal{F}_{\tilde{\mathcal{K}}}(x)$. From this it follows that

$$\tilde{\mathcal{H}}(s) = \frac{1}{v^{\lambda+1}}\int_{x=0}^{+\infty}\left(\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{\lambda}\left[\frac{x^{n_x+\lambda-1}}{\left[\zeta_s^2+x^2\right]^{n_k}}\,\frac{\hat{k}_\nu[R_1\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}\right]\right)\sin(vx)\,\mathrm{d}x \tag{56}$$

$$= \frac{1}{v^{\lambda+1}}\sum_{n=0}^{+\infty}\int_{n\pi/v}^{(n+1)\pi/v}\left(\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{\lambda}\left[\frac{x^{n_x+\lambda-1}}{\left[\zeta_s^2+x^2\right]^{n_k}}\,\frac{\hat{k}_\nu[R_1\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}\right]\right)\sin(vx)\,\mathrm{d}x. \tag{57}$$

An approximation of $\tilde{\mathcal{H}}(s)$ can be obtained using the $S\bar{D}$ approach (53).

The use of equation (53) for calculating the approximations of $\tilde{\mathcal{K}}(s)$ and $\tilde{\mathcal{H}}(s)$ is more advantageous than the use of the linear systems given by (35) or (36) where the computation of the successive zeros of spherical Bessel function is necessary and where it is required to compute a method for solving linear systems, which in the case of the integrals of interest, is much more time consuming than using Cramer's rule.

6. Conclusion

Three-centre two-electron Coulomb and hybrid integrals appear in molecular calculations. An atomic orbitals basis of Slater-type functions can be expressed as B functions in order to apply the Fourier transform method that allowed analytic expressions to be developed for molecular integrals of interest. The numerical evaluation of these analytic expressions presents severe computation difficulties due to the presence of semi-infinite very oscillatory integrals, whose integrands involve a product of hypergeometric series, spherical Bessel and reduced Bessel functions. We have proven that these hypergeometric series are reduced to finite sums and the integrands satisfy all the conditions required to apply the $H\bar{D}$ method which greatly simplified the application of the nonlinear $\bar{D}$-transformation.

This work presents an extremely efficient evaluation of the integrals of question using the new approach which we called $S\bar{D}$. This approach relies on some practical properties of Bessel and sine functions, which allowed the use of Cramer's rule to calculate the approximations $S\bar{D}_n^{(2,j)}$ of semi-infinite integrals. This led to a substantial simplification in the calculations since the computation of the successive zeros of the spherical Bessel function and a method to solve linear systems is avoided. For a given high accuracy, the $S\bar{D}$ method is faster than the $H\bar{D}$.

The progress obtained by the new approach is another useful step in developing software for evaluating molecular integrals over Slater-type orbitals.

Appendix. Numerical results and discussion

The finite integrals involved in equation (53) are evaluated using Gauss–Legendre quadrature of order 16. The finite integrals involved in equations (52) and (57) are transformed into finite sums:

$$\int_0^{x_n} f(x)\,\mathrm{d}x = \sum_{l=0}^{n-1} \int_{x_l}^{x_{l+1}} f(x)\,\mathrm{d}x.$$

The terms of the above finite sum are evaluated using Gauss–Legendre quadrature of order 16.

The values with 15 correct decimal places are obtained for the integrals by using the infinite series (52), (34), (57) and (55) which we sum until $N = \max$ (see tables A1, A2, A5, A6, A9, A10, A13 and A14). Note that by using the infinite series involving the sine function (52) and (57) instead of the infinite series involving the spherical Bessel function (34) and (55), we need fewer terms in evaluating the integrals with 15 exact decimal places.

Table A1. Exact values of the semi-infinite integral $\tilde{\mathcal{K}}(s)$ obtained to 15 correct decimal places using the infinite series given by equation (52). ($s = 0.001$, $n_x = \lambda$, $\nu = n_3 + n_4 + \frac{1}{2}$, $n_\gamma = 2(n_3 + n_4) + 1$ and $\zeta_s = \zeta_1 + \zeta_2$.)

n_3	n_4	n_k	λ	R_3	R_4	ζ_1	ζ_2	ζ_3	ζ_4	max	$\tilde{\mathcal{K}}(s)$
1	1	2	0	7.5	1.5	1.5	1.0	1.0	1.0	125	0.126 414 190 755 008D−02
2	1	2	1	3.5	7.0	1.0	1.0	1.5	1.0	361	0.492 082 994 200 939D−02
2	2	3	2	4.5	4.0	1.0	1.0	1.0	1.0	106	0.146 157 629 412 064D+00
3	2	2	3	3.5	3.0	0.5	0.5	1.5	1.5	135	0.861 150 036 617 796D+00
3	3	4	4	8.5	2.0	1.5	1.0	1.5	1.0	77	0.100 445 620 385 459D+00
4	3	3	4	3.5	3.0	1.0	1.0	1.0	1.5	81	0.204 664 014 657 073D+01
4	4	4	5	5.5	4.5	1.0	1.0	2.0	1.5	71	0.169 055 658 807 174D+01

Table A2. Exact values of the semi-infinite integral $\tilde{\mathcal{K}}(s)$ obtained to 15 correct decimal places using the infinite series given by equation (34). ($s = 0.001$, $n_x = \lambda$, $\nu = n_3 + n_4 + \frac{1}{2}$, $n_\gamma = 2(n_3 + n_4) + 1$ and $\zeta_s = \zeta_1 + \zeta_2$.)

n_3	n_4	n_k	λ	R_3	R_4	ζ_1	ζ_2	ζ_3	ζ_4	max	$\tilde{\mathcal{K}}(s)$
1	1	2	0	7.5	1.5	1.5	1.0	1.0	1.0	124	0.126 414 190 755 008D−02
2	1	2	1	3.5	7.0	1.0	1.0	1.5	1.0	442	0.492 082 994 200 938D−02
2	2	3	2	4.5	4.0	1.0	1.0	1.0	1.0	166	0.146 157 629 412 064D+00
3	2	2	3	3.5	3.0	0.5	0.5	1.5	1.5	300	0.861 150 036 617 796D+00
3	3	4	4	8.5	2.0	1.5	1.0	1.5	1.0	116	0.100 445 620 385 459D+00
4	3	3	4	3.5	3.0	1.0	1.0	1.0	1.5	157	0.204 664 014 657 074D+01
4	4	4	5	5.5	4.5	1.0	1.0	2.0	1.5	158	0.169 055 658 807 174D+01

Table A3. Evaluation of the semi-infinite integral $\tilde{\mathcal{K}}(s)$ using the $S\bar{D}$ method (53) of order 5 ($S\bar{D}_5^{(2,5)}$). ($s = 0.001$, $n_x = \lambda$, $\nu = n_3 + n_4 + \frac{1}{2}$, $n_\gamma = 2(n_3 + n_4) + 1$ and $\zeta_s = \zeta_1 + \zeta_2$.)

n_3	n_4	n_k	λ	R_3	R_4	ζ_1	ζ_2	ζ_3	ζ_4	$S\bar{D}_5^{(2,5)}$	Error
1	1	2	0	7.5	1.5	1.5	1.0	1.0	1.0	0.126 414 1908D−02	0.26D−13
2	1	2	1	3.5	7.0	1.0	1.0	1.5	1.0	0.492 082 9973D−02	0.31D−10
2	2	3	2	4.5	4.0	1.0	1.0	1.0	1.0	0.146 157 6294D+00	0.46D−12
3	2	2	3	3.5	3.0	0.5	0.5	1.5	1.5	0.861 150 0366D+00	0.33D−12
3	3	4	4	8.5	2.0	1.5	1.0	1.5	1.0	0.100 445 6204D+00	0.39D−10
4	3	3	4	3.5	3.0	1.0	1.0	1.0	1.5	0.204 664 0147D+01	0.89D−13
4	4	4	5	5.5	4.5	1.0	1.0	2.0	1.5	0.169 055 6588D+01	0.16D−11

Table A4. Evaluation of the semi-infinite integral $\tilde{\mathcal{K}}(s)$ using the $H\bar{D}$ method (36) of order 7 ($H\bar{D}_7^{(2)}$). ($s = 0.001$, $n_x = \lambda$, $\nu = n_3 + n_4 + \frac{1}{2}$, $n_\gamma = 2(n_3 + n_4) + 1$ and $\zeta_s = \zeta_1 + \zeta_2$.)

n_3	n_4	n_k	λ	R_3	R_4	ζ_1	ζ_2	ζ_3	ζ_4	$H\bar{D}_7^{(2)}$	Error
1	1	2	0	7.5	1.5	1.5	1.0	1.0	1.0	0.126 414 1908D−02	0.17D−12
2	1	2	1	3.5	7.0	1.0	1.0	1.5	1.0	0.492 082 9639D−02	0.30D−09
2	2	3	2	4.5	4.0	1.0	1.0	1.0	1.0	0.146 157 6294D+00	0.19D−10
3	2	2	3	3.5	3.0	0.5	0.5	1.5	1.5	0.861 150 0366D+00	0.12D−10
3	3	4	4	8.5	2.0	1.5	1.0	1.5	1.0	0.100 445 6206D+00	0.17D−09
4	3	3	4	3.5	3.0	1.0	1.0	1.0	1.5	0.204 664 0147D+01	0.29D−10
4	4	4	5	5.5	4.5	1.0	1.0	2.0	1.5	0.169 055 6588D+01	0.71D−10

Table A5. Exact values of the semi-infinite integral $\tilde{\mathcal{K}}(s)$ obtained to 15 correct decimal places using the infinite series given by equation (52). ($s = 0.999$, $n_x = \lambda$, $\nu = n_3 + n_4 + \frac{1}{2}$, $n_\gamma = 2(n_3 + n_4) + 1$ and $\zeta_s = \zeta_1 + \zeta_2$.)

n_3	n_4	n_k	λ	R_3	R_4	ζ_1	ζ_2	ζ_3	ζ_4	max	$\tilde{\mathcal{K}}(s)$
1	1	2	0	2.5	2.0	1.5	1.5	1.0	1.0	155	0.276 599 387 190 865D−01
2	1	2	1	4.0	3.0	1.5	0.5	1.0	2.5	162	0.136 665 163 437 581D+00
2	2	3	2	5.5	4.0	1.0	1.0	1.0	1.5	113	0.924 821 866 479 653D−01
3	2	2	3	6.0	3.5	1.0	1.0	1.5	1.5	166	0.443 353 247 114 632D−01
3	3	3	4	3.0	2.5	1.0	1.0	2.0	1.5	103	0.826 191 642 949 067D−02
4	3	3	4	4.5	3.5	1.0	0.5	2.0	2.5	120	0.288 150 089 225 324D−01
4	4	4	5	6.0	5.5	1.5	1.5	1.5	1.0	125	0.163 254 589 286 851D−01

Table A6. Exact values of the semi-infinite integral $\tilde{\mathcal{K}}(s)$ obtained to 15 correct decimal places using the infinite series given by equation (34). ($s = 0.999$, $n_x = \lambda$, $\nu = n_3 + n_4 + \frac{1}{2}$, $n_\gamma = 2(n_3 + n_4) + 1$ and $\zeta_s = \zeta_1 + \zeta_2$.)

n_3	n_4	n_k	λ	R_3	R_4	ζ_1	ζ_2	ζ_3	ζ_4	max	$\tilde{\mathcal{K}}(s)$
1	1	2	0	2.5	2.0	1.5	1.5	1.0	1.0	155	0.276 599 387 190 864D−01
2	1	2	1	4.0	3.0	1.5	0.5	1.0	2.5	206	0.136 665 163 437 580D+00
2	2	3	2	5.5	4.0	1.0	1.0	1.0	1.5	170	0.924 821 866 479 653D−01
3	2	2	3	6.0	3.5	1.0	1.0	1.5	1.5	255	0.443 353 247 114 634D−01
3	3	3	4	3.0	2.5	1.0	1.0	2.0	1.5	233	0.826 191 642 949 064D−02
4	3	3	4	4.5	3.5	1.0	0.5	2.0	2.5	256	0.288 150 089 225 324D−01
4	4	4	5	6.0	5.5	1.5	1.5	1.5	1.0	302	0.163 254 589 286 853D−01

Table A7. Evaluation of the semi-infinite integral $\tilde{\mathcal{K}}(s)$ using the $S\bar{D}$ method (53) of order 5 ($S\bar{D}_5^{(2,5)}$). ($s = 0.999$, $n_x = \lambda$, $\nu = n_3 + n_4 + \frac{1}{2}$, $n_\gamma = 2(n_3 + n_4) + 1$ and $\zeta_s = \zeta_1 + \zeta_2$.)

n_3	n_4	n_k	λ	R_3	R_4	ζ_1	ζ_2	ζ_3	ζ_4	$S\bar{D}_5^{(2,5)}$	Error
1	1	2	0	2.5	2.0	1.5	1.5	1.0	1.0	0.276 599 3872D−01	0.29D−13
2	1	2	1	4.0	3.0	1.5	0.5	1.0	2.5	0.136 665 1634D+00	0.74D−12
2	2	3	2	5.5	4.0	1.0	1.0	1.0	1.5	0.924 821 8665D−01	0.20D−11
3	2	2	3	6.0	3.5	1.0	1.0	1.5	1.5	0.443 353 2471D−01	0.94D−12
3	3	3	4	3.0	2.5	1.0	1.0	2.0	1.5	0.826 191 6429D−02	0.47D−14
4	3	3	4	4.5	3.5	1.0	0.5	2.0	2.5	0.288 150 0892D−01	0.30D−13
4	4	4	5	6.0	5.5	1.5	1.5	1.5	1.0	0.163 254 5890D−01	0.32D−10

Table A8. Evaluation of the semi-infinite integral $\tilde{\mathcal{K}}(s)$ using the $H\bar{D}$ method (36) of order 7 ($H\bar{D}_7^{(2)}$). ($s = 0.999$, $n_x = \lambda$, $\nu = n_3 + n_4 + \frac{1}{2}$, $n_\gamma = 2(n_3 + n_4) + 1$ and $\zeta_s = \zeta_1 + \zeta_2$.)

n_3	n_4	n_k	λ	R_3	R_4	ζ_1	ζ_2	ζ_3	ζ_4	$H\bar{D}_7^{(2)}$	Error
1	1	2	0	2.5	2.0	1.5	1.5	1.0	1.0	0.276 599 3872D−01	0.11D−11
2	1	2	1	4.0	3.0	1.5	0.5	1.0	2.5	0.136 665 1635D+00	0.20D−10
2	2	3	2	5.5	4.0	1.0	1.0	1.0	1.5	0.924 821 8668D−01	0.28D−10
3	2	2	3	6.0	3.5	1.0	1.0	1.5	1.5	0.443 353 2473D−01	0.15D−10
3	3	3	4	3.0	2.5	1.0	1.0	2.0	1.5	0.826 191 6429D−02	0.59D−12
4	3	3	4	4.5	3.5	1.0	0.5	2.0	2.5	0.288 150 0892D−01	0.19D−11
4	4	4	5	6.0	5.5	1.5	1.5	1.5	1.0	0.163 254 5981D−01	0.88D−09

Table A9. Exact values of the semi-infinite integral $\tilde{\mathcal{H}}(s)$ obtained to 15 correct decimal places using the infinite series given by equation (57). ($s = 0.001$, $n_x = \lambda$, $\nu = n_3 + n_4 + \frac{1}{2}$, $n_\gamma = 2(n_3 + n_4) + 1$ and $\zeta_s = \zeta_1 + \zeta_2$.)

n_3	n_4	n_k	λ	R_1	ζ_1	ζ_2	ζ_3	ζ_4	max	$\tilde{\mathcal{K}}(s)$
1	1	2	0	5.0	1.0	1.0	1.0	1.0	281	0.284 585 738 157 463D−02
2	1	2	1	5.0	1.0	1.0	1.0	1.0	306	0.241 687 700 195 433D−02
2	2	2	2	5.0	2.0	1.0	1.0	1.0	328	0.142 508 881 938 776D−02
3	2	3	2	2.0	1.0	0.5	1.0	1.0	91	0.351 424 918 755 458D+01
3	3	3	3	5.0	1.0	0.5	1.0	1.5	231	0.131 384 356 685 596D−02
4	3	4	3	3.5	0.5	0.5	0.5	2.0	101	0.426 258 207 725 837D−02
4	4	4	4	2.0	1.5	1.5	1.0	1.5	90	0.344 688 004 983 810D−01

Table A10. Exact values of the semi-infinite integral $\tilde{\mathcal{H}}(s)$ obtained to 15 correct decimal places using the infinite series given by equation (55). ($s = 0.001$, $n_x = \lambda$, $\nu = n_3 + n_4 + \frac{1}{2}$, $n_\gamma = 2(n_3 + n_4) + 1$ and $\zeta_s = \zeta_1 + \zeta_2$.)

n_3	n_4	n_k	λ	R_1	ζ_1	ζ_2	ζ_3	ζ_4	max	$\tilde{\mathcal{K}}(s)$
1	1	2	0	5.0	1.0	1.0	1.0	1.0	278	0.284 585 738 157 462D−02
2	1	2	1	5.0	1.0	1.0	1.0	1.0	352	0.241 687 700 195 433D−02
2	2	2	2	5.0	2.0	1.0	1.0	1.0	438	0.142 508 881 938 776D−02
3	2	3	2	2.0	1.0	0.5	1.0	1.0	129	0.351 424 918 755 458D+01
3	3	3	3	5.0	1.0	0.5	1.0	1.5	368	0.131 384 356 685 597D−02
4	3	4	3	3.5	0.5	0.5	0.5	2.0	188	0.426 258 207 725 837D−02
4	4	4	4	2.0	1.5	1.5	1.0	1.5	156	0.344 688 004 983 809D−01

Table A11. Evaluation of the semi-infinite integral $\tilde{\mathcal{H}}(s)$ using the $S\bar{D}$ method (53) of order 5 ($S\bar{D}_5^{(2,5)}$). ($s = 0.001$, $n_x = \lambda$, $\nu = n_3 + n_4 + \frac{1}{2}$, $n_\gamma = 2(n_3 + n_4) + 1$ and $\zeta_s = \zeta_1 + \zeta_2$.)

n_3	n_4	n_k	λ	R_1	ζ_1	ζ_2	ζ_3	ζ_4	$S\bar{D}_5^{(2,5)}$	Error
1	1	2	0	5.0	1.0	1.0	1.0	1.0	0.284 585 7381D−02	0.45D−12
2	1	2	1	5.0	1.0	1.0	1.0	1.0	0.241 687 7012D−02	0.98D−11
2	2	2	2	5.0	2.0	1.0	1.0	1.0	0.142 508 8829D−02	0.94D−11
3	2	3	2	2.0	1.0	0.5	1.0	1.0	0.351 424 9188D+01	0.93D−13
3	3	3	3	5.0	1.0	0.5	1.0	1.5	0.131 384 3563D−02	0.41D−11
4	3	4	3	3.5	0.5	0.5	0.5	2.0	0.426 258 2077D−02	0.84D−13
4	4	4	4	2.0	1.5	1.5	1.0	1.5	0.344 688 0050D−01	0.15D−11

Table A12. Evaluation of the semi-infinite integral $\tilde{\mathcal{H}}(s)$ using the $H\bar{D}$ method (36) of order 7 ($H\bar{D}_7^{(2)}$). ($s = 0.001$, $n_x = \lambda$, $\nu = n_3 + n_4 + \frac{1}{2}$, $n_\gamma = 2(n_3 + n_4) + 1$ and $\zeta_s = \zeta_1 + \zeta_2$.)

n_3	n_4	n_k	λ	R_1	ζ_1	ζ_2	ζ_3	ζ_4	$H\bar{D}_7^{(2)}$	Error
1	1	2	0	5.0	1.0	1.0	1.0	1.0	0.284 585 7365D−02	0.16D−10
2	1	2	1	5.0	1.0	1.0	1.0	1.0	0.241 687 6874D−02	0.13D−09
2	2	2	2	5.0	2.0	1.0	1.0	1.0	0.142 508 8662D−02	0.16D−09
3	2	3	2	2.0	1.0	0.5	1.0	1.0	0.351 424 9188D+01	0.12D−09
3	3	3	3	5.0	1.0	0.5	1.0	1.5	0.131 384 3597D−02	0.30D−10
4	3	4	3	3.5	0.5	0.5	0.5	2.0	0.426 258 2077D−02	0.14D−12
4	4	4	4	2.0	1.5	1.5	1.0	1.5	0.344 688 0062D−01	0.13D−09

Table A13. Exact values of the semi-infinite integral $\tilde{\mathcal{H}}(s)$ obtained to 15 correct decimal places using the infinite series given by equation (57). ($s = 0.999$, $n_x = \lambda$, $\nu = n_3 + n_4 + \frac{1}{2}$, $n_\gamma = 2(n_3 + n_4) + 1$ and $\zeta_s = \zeta_1 + \zeta_2$.)

n_3	n_4	n_k	λ	R_1	ζ_1	ζ_2	ζ_3	ζ_4	max	$\tilde{\mathcal{K}}(s)$
1	1	2	0	3.0	1.0	1.0	1.0	1.0	111	0.338 401 188 224 347D−01
2	1	2	1	4.0	1.5	1.5	0.5	1.0	117	0.159 408 922 374 825D+01
2	2	2	2	6.5	2.0	1.5	1.0	1.0	198	0.123 752 317 696 277D−02
3	2	3	2	3.0	2.0	2.0	1.0	1.0	87	0.248 683 747 889 112D−01
3	3	3	3	5.0	1.5	1.0	1.5	0.5	136	0.965 754 433 724 946D−03
4	3	3	3	5.0	2.0	1.0	1.5	1.0	138	0.242 694 501 548 593D−02
4	4	4	4	4.0	1.5	1.0	1.5	1.0	83	0.556 025 856 060 273D−01

Table A14. Exact values of the semi-infinite integral $\tilde{\mathcal{H}}(s)$ obtained to 15 correct decimal places using the infinite series given by equation (55). ($s = 0.999$, $n_x = \lambda$, $\nu = n_3 + n_4 + \frac{1}{2}$, $n_\gamma = 2(n_3 + n_4) + 1$ and $\zeta_s = \zeta_1 + \zeta_2$.)

n_3	n_4	n_k	λ	R_1	ζ_1	ζ_2	ζ_3	ζ_4	max	$\tilde{\mathcal{K}}(s)$
1	1	2	0	3.0	1.0	1.0	1.0	1.0	109	0.338 401 188 224 347D−01
2	1	2	1	4.0	1.5	1.5	0.5	1.0	135	0.159 408 922 374 824D+01
2	2	2	2	6.5	2.0	1.5	1.0	1.0	246	0.123 752 317 696 278D−02
3	2	3	2	3.0	2.0	2.0	1.0	1.0	113	0.248 683 747 889 112D−01
3	3	3	3	5.0	1.5	1.0	1.5	0.5	197	0.965 754 433 724 948D−03
4	3	3	3	5.0	2.0	1.0	1.5	1.0	191	0.242 694 501 548 593D−02
4	4	4	4	4.0	1.5	1.0	1.5	1.0	132	0.556 025 856 060 273D−01

Table A15. Evaluation of the semi-infinite integral $\tilde{\mathcal{H}}(s)$ using the $S\bar{D}$ method (53) of order 5 ($S\bar{D}_5^{(2,5)}$). ($s = 0.999$, $n_x = \lambda$, $\nu = n_3 + n_4 + \frac{1}{2}$, $n_\gamma = 2(n_3 + n_4) + 1$ and $\zeta_s = \zeta_1 + \zeta_2$.)

n_3	n_4	n_k	λ	R_1	ζ_1	ζ_2	ζ_3	ζ_4	$S\bar{D}_5^{(2,5)}$	Error
1	1	2	0	3.0	1.0	1.0	1.0	1.0	0.338 401 1882D−01	0.38D−13
2	1	2	1	4.0	1.5	1.5	0.5	1.0	0.159 408 9224D+01	0.92D−10
2	2	2	2	6.5	2.0	1.5	1.0	1.0	0.123 752 3131D−02	0.46D−10
3	2	3	2	3.0	2.0	2.0	1.0	1.0	0.248 683 7479D−01	0.94D−12
3	3	3	3	5.0	1.5	1.0	1.5	0.5	0.965 754 4370D−03	0.33D−11
4	3	3	3	5.0	2.0	1.0	1.5	1.0	0.242 694 5011D−02	0.47D−11
4	4	4	4	4.0	1.5	1.0	1.5	1.0	0.556 025 8560D−01	0.17D−11

Table A16. Evaluation of the semi-infinite integral $\tilde{\mathcal{H}}(s)$ using the $H\bar{D}$ method (36) of order 7 ($H\bar{D}_7^{(2)}$). ($s = 0.999$, $n_x = \lambda$, $\nu = n_3 + n_4 + \frac{1}{2}$, $n_\gamma = 2(n_3 + n_4) + 1$ and $\zeta_s = \zeta_1 + \zeta_2$.)

n_3	n_4	n_k	λ	R_1	ζ_1	ζ_2	ζ_3	ζ_4	$H\bar{D}_7^{(2)}$	Error
1	1	2	0	3.0	1.0	1.0	1.0	1.0	0.338 401 1882D−01	0.82D−12
2	1	2	1	4.0	1.5	1.5	0.5	1.0	0.159 408 9232D+01	0.86D−08
2	2	2	2	6.5	2.0	1.5	1.0	1.0	0.123 752 2853D−02	0.32D−09
3	2	3	2	3.0	2.0	2.0	1.0	1.0	0.248 683 7488D−01	0.95D−10
3	3	3	3	5.0	1.5	1.0	1.5	0.5	0.965 754 4452D−03	0.12D−10
4	3	3	3	5.0	2.0	1.0	1.5	1.0	0.242 694 5060D−02	0.44D−10
4	4	4	4	4.0	1.5	1.0	1.5	1.0	0.556 025 8564D−01	0.36D−10

Table A17. Values of $\mathcal{K}_{n_1 00, n_3 00}^{n_2 00, n_4 00}$ with 15 exact decimal places obtained using the infinite series with the sine function (52) for evaluating the semi-infinite integrals. ($\vec{R}_i = (R_i, 0, 0)$, $i = 3, 4$.)

n_1	n_2	n_3	n_4	n_γ	R_3	R_4	ζ_1	ζ_2	ζ_3	ζ_4	$\mathcal{K}_{n_1 00, n_2 00}^{n_3 00, n_4 00}$
1	1	1	1	5	5.0	3.5	2.0	1.0	2.0	1.0	0.284 363 465 672 292D+00
2	1	2	1	7	8.5	5.0	2.0	2.5	2.0	2.5	0.110 336 129 722 211D+00
2	2	2	2	9	7.5	5.0	1.0	0.5	4.5	5.0	0.191 523 537 406 420D−01
2	2	3	2	11	7.5	5.5	1.0	0.5	4.0	4.5	0.339 147 631 001 087D+00
2	2	3	3	13	8.5	6.0	1.0	0.5	4.0	5.0	0.368 375 307 409 424D−02
2	2	4	3	15	8.0	4.5	1.0	1.0	4.0	5.0	0.417 362 637 051 378D−02
2	2	4	4	17	7.0	4.5	1.0	0.5	4.0	3.5	0.165 335 595 051 352D−01

Table A18. Evaluation of $\mathcal{K}_{n_1 00, n_3 00}^{n_2 00, n_4 00}$ using $S\bar{D}_5^{(2,5)}$ for evaluating the semi-infinite integrals. ($\vec{R}_i = (R_i, 0, 0)$, $i = 3, 4$.)

n_1	n_2	n_3	n_4	n_γ	R_3	R_4	ζ_1	ζ_2	ζ_3	ζ_4	$\mathcal{K}_{n_1 00, n_2 00}^{n_3 00, n_4 00}$	Error
1	1	1	1	5	5.0	3.5	2.0	1.0	2.0	1.0	0.284 363 4657D+00	0.19D−15
2	1	2	1	7	8.5	5.0	2.0	2.5	2.0	2.5	0.110 336 1297D+00	0.32D−12
2	2	2	2	9	7.5	5.0	1.0	0.5	4.5	5.0	0.191 523 5374D−01	0.18D−14
2	2	3	2	11	7.5	5.5	1.0	0.5	4.0	4.5	0.339 147 6310D+00	0.13D−12
2	2	3	3	13	8.5	6.0	1.0	0.5	4.0	5.0	0.368 375 3074D−02	0.15D−14
2	2	4	3	15	8.0	4.5	1.0	1.0	4.0	5.0	0.417 362 6371D−02	0.19D−15
2	2	4	4	17	7.0	4.5	1.0	0.5	4.0	3.5	0.165 335 5951D−01	0.11D−16

Table A19. Evaluation of $\mathcal{K}_{n_1 00, n_3 00}^{n_2 00, n_4 00}$ using $H\bar{D}_7^{(2)}$ for evaluating the semi-infinite integrals. ($\vec{R}_i = (R_i, 0, 0)$, $i = 3, 4$.)

n_1	n_2	n_3	n_4	n_γ	R_3	R_4	ζ_1	ζ_2	ζ_3	ζ_4	$\mathcal{K}_{n_1 00, n_2 00}^{n_3 00, n_4 00}$	Error
1	1	1	1	5	5.0	3.5	2.0	1.0	2.0	1.0	0.284 363 4657D+00	0.53D−13
2	1	2	1	7	8.5	5.0	2.0	2.5	2.0	2.5	0.110 336 1297D+00	0.54D−11
2	2	2	2	9	7.5	5.0	1.0	0.5	4.5	5.0	0.191 523 5374D−01	0.27D−12
2	2	3	2	11	7.5	5.5	1.0	0.5	4.0	4.5	0.339 147 6310D+00	0.18D−10
2	2	3	3	13	8.5	6.0	1.0	0.5	4.0	5.0	0.368 375 3074D−02	0.21D−12
2	2	4	3	15	8.0	4.5	1.0	1.0	4.0	5.0	0.417 362 6371D−02	0.39D−13
2	2	4	4	17	7.0	4.5	1.0	0.5	4.0	3.5	0.165 335 5951D−01	0.44D−14

Table A20. Values of $\mathcal{H}_{n_1 00, n_3 00}^{n_2 00, n_4 00}$ with 15 exact decimal places obtained using the infinite series involving the sine function (57) for evaluating the semi-infinite integrals. ($\vec{R}_1 = (R_1, 0, 0)$.)

n_1	n_2	n_3	n_4	n_γ	R_1	ζ_1	ζ_2	ζ_3	ζ_4	$\mathcal{H}_{n_1 00, n_2 00}^{n_3 00, n_4 00}$
1	1	1	1	5	4.0	3.0	1.5	2.0	1.5	0.858 504 667 474 839 674D−03
2	1	2	1	7	3.0	2.0	1.0	2.5	2.5	0.130 454 565 516 659 766D+00
2	2	2	2	9	8.0	2.5	2.0	3.0	4.0	0.100 293 050 393 527 849D−03
2	2	3	2	11	6.0	1.0	0.5	2.0	3.5	0.276 854 998 374 092 832D−01
2	2	3	3	13	7.5	1.0	1.5	3.0	3.5	0.579 455 660 776 437 258D−04
2	2	4	3	15	6.5	1.0	1.0	3.0	3.5	0.426 260 750 526 356 967D−03
2	2	4	4	17	6.5	1.0	0.5	2.5	2.5	0.290 068 840 927 043 548D−02

Table A21. Evaluation of $\mathcal{H}_{n_1 00, n_3 00}^{n_2 00, n_4 00}$ using $S\bar{D}_5^{(2,5)}$ for evaluating the semi-infinite integrals. ($\vec{R}_1 = (R_1, 0, 0)$.)

n_1	n_2	n_3	n_4	n_γ	R_1	ζ_1	ζ_2	ζ_3	ζ_4	$\mathcal{H}_{n_1 00, n_2 00}^{n_3 00, n_4 00}$	Error
1	1	1	1	5	4.0	3.0	1.5	2.0	1.5	0.858 504 6675D−03	0.71D−14
2	1	2	1	7	3.0	2.0	1.0	2.5	2.5	0.130 454 5655D+00	0.80D−12
2	2	2	2	9	8.0	2.5	2.0	3.0	4.0	0.100 293 0481D−03	0.16D−12
2	2	3	2	11	6.0	1.0	0.5	2.0	3.5	0.276 854 9984D−01	0.21D−13
2	2	3	3	13	7.5	1.0	1.5	3.0	3.5	0.579 455 6606D−04	0.18D−13
2	2	4	3	15	6.5	1.0	1.0	3.0	3.5	0.426 260 7505D−03	0.16D−13
2	2	4	4	17	6.5	1.0	0.5	2.5	2.5	0.290 068 8409D−02	0.18D−13

Table A22. Evaluation of $\mathcal{H}^{n_2 00, n_4 00}_{n_1 00, n_3 00}$ using $H\bar{D}^{(2)}_7$ for evaluating the semi-infinite integrals. ($\vec{R}_1 = (R_1, 0, 0)$.)

n_1	n_2	n_3	n_4	n_γ	R_1	ζ_1	ζ_2	ζ_3	ζ_4	$\mathcal{H}^{n_3 00, n_4 00}_{n_1 00, n_2 00}$	Error
1	1	1	1	5	4.0	3.0	1.5	2.0	1.5	0.858 504 6687D−03	0.13D−11
2	1	2	1	7	3.0	2.0	1.0	2.5	2.5	0.130 454 5655D+00	0.20D−11
2	2	2	2	9	8.0	2.5	2.0	3.0	4.0	0.100 293 0473D−03	0.31D−11
2	2	3	2	11	6.0	1.0	0.5	2.0	3.5	0.276 854 9984D−01	0.33D−11
2	2	3	3	13	7.5	1.0	1.5	3.0	3.5	0.579 455 6599D−04	0.86D−13
2	2	4	3	15	6.5	1.0	1.0	3.0	3.5	0.426 260 7504D−03	0.13D−12
2	2	4	4	17	6.5	1.0	0.5	2.5	2.5	0.290 068 8410D−02	0.44D−12

The numerical values of the semi-infinite integrals $\tilde{\mathcal{K}}(s)$ and $\tilde{\mathcal{H}}(s)$ are obtained for $s = 0.001$ and 0.999. In these regions, the integrand oscillates rapidly. If we let $s = 0$ or 1, the integrand will be reduced to the term $[\zeta_s^2 + x^2]^{-n_k} x^{n_x} j_\lambda(vx)$, because the terms $\hat{k}_\nu[R\gamma(s,x)]/[\gamma(s,x)]^{n_\gamma}$ becomes constant and hence the asymptotic behaviour of the integrand cannot be represented by a function of the form $e^{-\alpha x}\, j_\lambda(x)$. Consequently, the rapid oscillations of the spherical Bessel functions cannot be damped and suppressed by the exponential decreasing functions $\hat{k}_\nu$.

In the numerical evaluation of $\mathcal{K}^{n_2 00, n_4 00}_{n_1 00, n_3 00}$ and $\mathcal{H}^{n_2 00, n_4 00}_{n_1 00, n_3 00}$ we let λ and n_x vary to show the efficiency of the new approach in evaluating the integrals of interest in the case where the oscillations of the integrand are very rapid.

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