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The properties of sine, spherical Bessel and reduced Bessel functions for improving convergence of semi-infinite very oscillatory integrals: the evaluation of three-centre nuclear attraction integrals over B functions

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Abstract

This paper focuses on the use of useful properties of sine, spherical Bessel and reduced Bessel functions to simplify the application of the nonlinear D- and $\bar{D}$-transformations for accelerating the convergence of semi-infinite very oscillatory integrals and to reduce the calculation times keeping a high predetermined accuracy.

Three-centre nuclear attraction integrals, which are one of the most difficult type involved in density functional theory methods when using a basis set of B functions, are evaluated using the new approach.

The numerical results show the efficiency of the new method compared with other alternatives.

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1. Introduction

In applied mathematics and in the numerical treatment of scientific problems, slowly convergent or divergent sequences and series and oscillatory integrals occur abundantly. Therefore, convergence accelerators and nonlinear transformation methods for accelerating the convergence of infinite series and integrals have been invented and applied to various situations. They are based on the idea of extrapolation. Their utility for enhancing and even inducing convergence has been amply demonstrated by Shanks [1]. Via sequence transformations slowly convergent and divergent sequences and series can be transformed into sequences and series with hopefully numerical properties. Thus, they are useful for accelerating convergence. In the case of nonlinear transformations the improvement of convergence can be remarkable. These

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methods form the basis of new methods for solving various problems which were unsolvable otherwise and have many applications as well [2, 3].

In previous work [4–7], we have demonstrated the efficiency of the nonlinear transformations D due to Levin and Sidi [8] and $\bar{D}$ due to Sidi [9–11], in evaluating one- and two-electron multicentre integrals over B functions via integral representations in terms of non-physical variables. The application of these transformations depends strongly on the order of the differential equation that the integrand satisfies. The approximations $D_n^{(m)}$ and $\bar{D}_n^{(m)}$, which converge very quickly to the exact value of the integral as n becomes large and where m is the order of the differential equation satisfied by the integrand, are obtained by solving sets of equations of the order of $nm + 1$ and $n(m - 1) + 1$, respectively, where the computation of the $m - 1$ successive derivatives of the integrand and its $nm + 1$ or $n(m - 1) + 1$ successive zeros is necessary. This presents severe numerical and computation difficulties when dealing with one- and two-electron multicentre integrals especially when values of quantum numbers are large.

We have shown [7, 12–15], that we can reduce the order of the linear differential equation satisfied by the integrand $f(x) = g(x) j_\lambda(x)$, where $j_\lambda(x)$ is a spherical Bessel function, to two keeping all the conditions to apply the D- and $\bar{D}$-transformations satisfied. This led to the HD and $H\bar{D}$ methods, where the calculation of the successive derivatives of the integrand is avoided and the orders of the linear sets of equations to solve are reduced to $2n + 1$ and $n + 1$, respectively. This led to a substantial gain in the calculation times, but it is still necessary for the calculations to compute the $2n + 1$ or $n + 1$ successive zeros of spherical Bessel function.

In this paper, we showed how we can use some useful properties of sine, spherical Bessel and reduced Bessel functions to simplify the application of these above nonlinear transformations and to further reduce the calculation times keeping the same high predetermined accuracy. The calculation of the successive zeros and the computation of a method for solving a linear set of equations are avoided.

Three-centre nuclear attraction integrals are evaluated using the new approach. These integrals are the rate determining step of *ab initio* and density functional theory (DFT) molecular structure calculations and they contribute to the total energy of the molecule. The *ab initio* calculations using the LCAO-MO approach, where molecular orbitals are built from a linear combination of atomic orbitals, are strongly dependent on the choice of the basis functions for the reliability of the electronic distributions they provide. A good atomic orbital basis should satisfy two pragmatic conditions for analytical solutions of the appropriate Schrödinger equation, namely the cusp at the origin [16] and exponential decay at infinity [17, 18].

Ab initio calculations are carried out mostly by using the so-called Gaussian-type functions (GTFs) [19]. This is due to the fact that with GTFs the numerous molecular integrals can be evaluated rather easily. Unfortunately, these Gaussian functions fail to satisfy the above mathematical conditions for atomic electronic distributions.

The Schrödinger equation can be exactly solved for one-electron atoms such as hydrogen. In this case we obtain hydrogen-like wavefunctions. It is convenient mathematically to use linear combinations of these functions containing a single power of r. The obtained functions which are called Slater-type functions (STFs) [20,21] satisfy the aforementioned requirements, but the use of these functions as a basis set of atomic orbitals has been prevented by the fact that their multicentre integrals are extremely difficult to evaluate for polyatomic molecules.

Various studies have focused on the use of B functions that have been proposed by Shavitt [22] and introduced by Filter and Steinborn [23,24]. These functions can be expressed as linear combinations of STFs [24, 25]. Although B functions are more complicated than STFs, they have some remarkable mathematical properties applicable to multicentre integral problems.

It was shown that B functions possess a relatively simple addition theorem [23, 25–27], extremely compact convolution integrals [25,28] and their Fourier transform is of exceptional simplicity [26, 29]. The B functions are well adapted to the Fourier transformation method introduced by Bonham *et al* [30] and generalized by Steinborn *et al* [31, 32].

The Fourier transformation method, which is one of the most successful approaches for the evaluation of multicentre integrals, allowed analytical expressions for the three-centre nuclear attraction integrals over B functions to be developed. These analytical expressions involve semi-infinite integrals, which oscillate quite strongly due to the presence of the spherical Bessel function $j_\lambda(vx)$, in particular for large values of λ and v.

The molecular integrals under consideration are to be evaluated via a numerical quadrature of integral representations in terms of *non-physical* integration variables. These integral representations were derived with the help of the Fourier transformation method.

Numerical integration of oscillatory integrands is difficult, especially when the oscillatory part is a spherical Bessel function and not a simple trigonometric function [33,34]. It is possible to break up semi-infinite oscillatory integrals into infinite series of integrals of alternating sign. These series are slowly convergent, that is why their use has been prevented. By using the epsilon algorithm of Wynn [48] or Levin's u transform [49], we can accelerate the convergence of such infinite series but in the case of the semi-infinite integrals involved in the analytical expressions of molecular integrals, the calculation times are prohibitively long for a sufficient accuracy especially for large values of λ and v since the zeros of $j_\lambda(vx)$ become closer.

2. General definitions and properties

The spherical Bessel function $j_l(x)$ of the order of $l \in \mathbb{N}$ is defined by [35, 36]

$$j_l(x) = (-1)^l x^l \left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^l j_0(x) = (-1)^l x^l \left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^l \left(\frac{\sin(x)}{x}\right). \tag{1}$$

$j_l(x)$ and its first derivative $j_l'(x)$ satisfy the recurrence relations [35, 36]:

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

For the following, we write $j^n_{l+\frac{1}{2}}$ with $n = 1, 2, \ldots$ for the successive positive zeros of $j_l(x)$. $j^0_{l+\frac{1}{2}}$ are assumed to be 0.

The reduced Bessel function $\hat{k}_{n+\frac{1}{2}}(z)$ is defined by [22,23]

$$\hat{k}_{n+\frac{1}{2}}(z) = \sqrt{\frac{2}{\pi}}(z)^{n+\frac{1}{2}} K_{n+\frac{1}{2}}(z) = z^n\, \mathrm{e}^{-z} \sum_{j=0}^{n} \frac{(n+j)!}{j!\,(n-j)!} \frac{1}{(2\,z)^j} \tag{3}$$

where $K_{n+\frac{1}{2}}$ denotes the modified Bessel function of the second kind [37].

The reduced Bessel functions satisfy the recurrence relation [22]

$$\hat{k}_{n+\frac{1}{2}}(z) = (2n-1)\,\hat{k}_{n-\frac{1}{2}}(z) + z^2 \hat{k}_{(n-1)-\frac{1}{2}}(z). \tag{4}$$

A useful property satisfied by $\hat{k}_{n+\frac{1}{2}}(z)$ is given by [37]

$$\left(\frac{\mathrm{d}}{z\,\mathrm{d}z}\right)^m \frac{\hat{k}_{n+\frac{1}{2}}(z)}{z^{2n+1}} = \left(\frac{\mathrm{d}}{z\,\mathrm{d}z}\right)^m \left[\sqrt{\frac{\pi}{2}}\, \frac{K_{n+\frac{1}{2}}(z)}{z^{n+\frac{1}{2}}}\right] = (-1)^m \frac{\hat{k}_{n+m+\frac{1}{2}}(z)}{z^{2(n+m)+1}}. \tag{5}$$

The B functions are defined as follows [23,24]:

$$B_{n,l}^{m}(\zeta,\vec{r}) = \frac{(\zeta r)^{l}}{2^{n+l}(n+l)!}\,\hat{k}_{n-\frac{1}{2}}(\zeta r)\;Y_{l}^{m}(\theta_{\vec{r}},\varphi_{\vec{r}}) \tag{6}$$

where n, l, m are the quantum numbers and they are such that $n = 1, 2, \ldots, l = 0, 1, \ldots, n-1$ and $m = -l, -l+1, \ldots, l-1, l$, and where $Y_l^m(\theta,\varphi)$ denotes the surface spherical harmonic and is defined explicitly using the Condon–Shortley phase convention as follows [38]:

$$Y_{l}^{m}(\theta,\varphi) = \mathrm{i}^{m+|m|}\left[\frac{(2l+1)(l-|m|)!)}{4\pi(l+|m|)!)}\right]^{1/2} P_{l}^{|m|}(\cos\theta)\,\mathrm{e}^{\mathrm{i}m\varphi}. \tag{7}$$

$P_l^m(x)$ is the associated Legendre polynomial of lth degree and mth order:

$$P_{l}^{m}(x) = \left(1-x^{2}\right)^{m/2}\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^{l+m}\left[\frac{\left(x^{2}-1\right)^{l}}{2^{l}l!}\right]. \tag{8}$$

The Rayleigh expansion of the plane wavefunctions is defined by [39]

$$\mathrm{e}^{\pm\mathrm{i}\vec{p}\cdot\vec{r}} = \sum_{l=0}^{+\infty}\sum_{m=-l}^{l} 4\pi\,(\pm\mathrm{i})^{\lambda}\,j_{l}(|\vec{p}||\vec{r}|)\,Y_{l}^{m}(\theta_{\vec{r}},\varphi_{\vec{r}})\,[Y_{l}^{m}(\theta_{\vec{p}},\varphi_{\vec{p}})]^{*}. \tag{9}$$

The Fourier transform $\overline{B}_{n,l}^{m}(\zeta,\vec{p})$ of $B_{n,l}^{m}(\zeta,\vec{r})$ is given by [26,29]

$$\overline{B}_{n,l}^{m}(\zeta,\vec{p}) = \frac{1}{(2\pi)^{3/2}}\int_{\vec{r}}\mathrm{e}^{-\mathrm{i}\vec{p}\cdot\vec{r}}\,B_{n,l}^{m}(\zeta,\vec{r})\,\mathrm{d}\vec{r} \tag{10}$$

$$= \sqrt{\frac{2}{\pi}}\,\zeta^{2n+l-1}\,\frac{(-\mathrm{i}|p|)^{l}}{(\zeta^{2}+|p|^{2})^{n+l+1}}\,Y_{l}^{m}(\theta_{\vec{p}},\varphi_{\vec{p}}) \tag{11}$$

the analytical expression of $\overline{B}_{n,l}^{m}(\zeta,\vec{p})$ is obtained by inserting the Rayleigh expansion of the plane wavefunctions in (10).

The Slater-type orbitals are defined in normalized form according to the following relationship [20,21]:

$$\chi_{n,l}^{m}(\zeta,\vec{r}) = N(n,\zeta)\,r^{n-1}\,\mathrm{e}^{-\zeta r}\,Y_{l}^{m}(\theta_{\vec{r}},\varphi_{\vec{r}}) \tag{12}$$

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

The Slater-type orbitals can be expressed as finite linear combinations of B functions [24]:

$$\chi_{n,l}^{m}(\zeta,\vec{r}) = \sum_{p=\tilde{p}}^{n-l}\frac{(-1)^{n-l-p}(n-l)!2^{l+p}(l+p)!}{(2p-n-l)!(2n-2l-2p)!!}\,B_{p,l}^{m}(\zeta,\vec{r}) \tag{13}$$

where

$$\tilde{p} = \begin{cases}(n-l)/2 & \text{if} \quad n-l \quad \text{even}\\ (n-l+1)/2 & \text{if} \quad n-l \quad \text{odd}\end{cases} \tag{14}$$

and where the double factorial is defined by

$$\begin{aligned}&(2k)!! = 2\times4\times6\times\cdots\times(2k) = 2^{k}k!\\ &(2k+1)!! = 1\times3\times5\times\cdots\times(2k+1) = \frac{(2k+1)!}{2^{k}k!}\\ &0!! = 1.\end{aligned} \tag{15}$$

The Fourier integral representation of the Coulomb operator $\frac{1}{|\vec{r}-\vec{R}_1|}$ is given by [40]

$$\frac{1}{|\vec{r}-\vec{R}_1|} = \frac{1}{2\pi^2}\int_{\vec{k}} \frac{\mathrm{e}^{-\mathrm{i}\vec{k}\cdot(\vec{r}-\vec{R}_1)}}{k^2}\,\mathrm{d}\vec{k}. \tag{16}$$

The Gaunt coefficients are defined as [41–47]

$$\langle l_1 m_1 | l_2 m_2 | l_3 m_3\rangle = \int_{\theta=0}^{\pi}\int_{\varphi=0}^{2\pi} [Y_{l_1}^{m_1}(\theta,\varphi)]^* Y_{l_2}^{m_2}(\theta,\varphi) Y_{l_3}^{m_3}(\theta,\varphi)\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\varphi. \tag{17}$$

These coefficients linearize the product of two spherical harmonics:

$$[Y_{l_1}^{m_1}(\theta,\varphi)]^* Y_{l_2}^{m_2}(\theta,\varphi) = \sum_{l=l_{\min,2}}^{l_1+l_2} \langle l_2 m_2 | l_1 m_1 | l m_2 - m_1\rangle Y_l^{m_2-m_1}(\theta,\varphi) \tag{18}$$

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 [44]:

$$l_{\min} = \begin{cases} \max(|l_1 - l_2|, |m_2 - m_1|) & \text{if} \quad l_1 + l_2 + \max(|l_1 - l_2|, |m_2 - m_1|) \text{ is even} \\ \max(|l_1 - l_2|, |m_2 - m_1|) + 1 & \text{if} \quad l_1 + l_2 + \max(|l_1 - l_2|, |m_2 - m_1|) \text{ is odd.} \end{cases} \tag{19}$$

The three-centre nuclear attraction integrals over B functions are given by

$$\mathcal{I}_{n_1,l_1,m_1}^{n_2,l_2,m_2} = \int_{\vec{R}} \left[B_{n_1,l_1}^{m_1}\left(\zeta_1, \vec{R} - \overrightarrow{OA}\right)\right]^* \frac{1}{|\vec{R} - \overrightarrow{OC}|} B_{n_2,l_2}^{m_2}\left(\zeta_2, \vec{R} - \overrightarrow{OB}\right)\mathrm{d}\vec{R} \tag{20}$$

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.

By performing a translation of vector $\overrightarrow{OA}$ and substituting the integral representation of the Coulomb operator (16) in the above equation, we can rewrite the above integral as

$$\mathcal{I}_{n_1,l_1,m_1}^{n_2,l_2,m_2} = \frac{1}{2\pi^2}\int \frac{\mathrm{e}^{\mathrm{i}\vec{x}\cdot\vec{R}_1}}{x^2} \left\langle B_{n_1,l_1}^{m_1}\left(\zeta_1,\vec{r}\right)\middle|\mathrm{e}^{-\mathrm{i}\vec{x}\cdot\vec{r}}\middle| B_{n_2,l_2}^{m_2}\left(\zeta_2,\vec{r}-\vec{R}_2\right)\right\rangle_{\vec{r}}\,\mathrm{d}\vec{x} \tag{21}$$

where

$$\left\langle B_{n_1,l_1}^{m_1}\left(\zeta_1,\vec{r}\right)\middle|\mathrm{e}^{-\mathrm{i}\vec{x}\cdot\vec{r}}\middle| B_{n_2,l_2}^{m_2}\left(\zeta_2,\vec{r}-\vec{R}_2\right)\right\rangle_{\vec{r}} = \int \left[B_{n_1,l_1}^{m_1}\left(\zeta_1,\vec{r}\right)\right]^* \mathrm{e}^{-\mathrm{i}\vec{x}\cdot\vec{r}}\, B_{n_2,l_2}^{m_2}\left(\zeta_2,\vec{r}-\vec{R}_2\right)\mathrm{d}\vec{r}$$

and where $\vec{r} = \vec{R} - \overrightarrow{OA}$, $\vec{R}_1 = \overrightarrow{OC}$ and $\vec{R}_2 = \overrightarrow{AB}$.

3. Nonlinear transformations for improving convergence of semi-infinite integrals

For the following, we define $A^{(\gamma)}$ for 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

$$p(x) \sim x^{\gamma}\left(a_0 + \frac{a_1}{x} + \frac{a_2}{x^2} + \cdots\right) \tag{22}$$

and their derivatives of any order have asymptotic expansions, which can be obtained by differentiating that in (22) term by term.

From (22) it follows that $A^{(\gamma)} \supset A^{(\gamma-1)} \supset \ldots.$

We denote $\tilde{A}^{(\gamma)}$ for some γ, the set of functions $p(x)$ such that $p(x) \in A^{(\gamma)}$ and $\lim_{x\to+\infty} x^{-\gamma} p(x) \neq 0$. Thus, $p \in \tilde{A}^{(\gamma)}$ has an asymptotic expansion in inverse powers of x as $x \to +\infty$ of the form given by (22) with $a_0 \neq 0$. We define the functional $\alpha_0(p)$ by $\alpha_0(p) = a_o = \lim_{x\to+\infty} x^{-\gamma} p(x)$.

We define $\mathrm{e}^{\tilde{A}^{(k)}}$ 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 some 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 functional $\alpha_0(cp) = c\,\alpha_0(p)$ for all constant c.
(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 $\alpha_0(1/p) = 1/\alpha_0(p)$.

The proof of lemma 1 follows from the properties of Poincaré series.

Lemma 2. *Let $\phi \in \tilde{A}^{(k)}$ where k is a positive integer and $k \neq 0$. The function $\hat{k}_{n+\frac{1}{2}}(\phi(x)) \in \tilde{A}^{(n\,k)}\mathrm{e}^{\tilde{A}^{(k)}}$ and can be written in the following form*

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

where $\phi_1 \in \tilde{A}^{(n\,k)}$ and $\alpha_0(\phi_1) = (\alpha_0(\phi))^n \neq 0$.

By using the analytical expression of the reduced Bessel function which is given by equation (3) and using the properties of Poincaré series, one can easily prove lemma 2.

Theorem 1 (see [8,9]). *Let $f(x)$ be integrable on $[0, +\infty[$ (i.e. $\int_0^{+\infty} f(t)\,\mathrm{d}t$ exists) and satisfies a linear differential equation of the order of m of the form:*

$$f(x) = \sum_{k=1}^{m} p_k(x) f^{(k)}(x) \quad p_k \in A^{(i_k)} \quad i_k \leqslant k. \tag{23}$$

Also let $\lim_{x\to+\infty} p_k^{(i-1)}(x)\, f^{(k-i)}(x) = 0$, $i \leqslant k \leqslant m$, $1 \leqslant i \leqslant m$.

If for every integer $l \geqslant -1$, $\sum_{k=1}^{m} l(l-1)\ldots(l-k+1)p_{k,0} \neq 1$, where

$$p_{k,0} = \lim_{x\to+\infty} x^{-k} p_k(x) \qquad 1 \leqslant k \leqslant m$$

then as $x \to +\infty$:

$$\int_x^{+\infty} f(t)\,\mathrm{d}t \sim \sum_{k=0}^{m-1} f^{(k)}(x) x^{j_k} \left(\beta_{0,k} + \frac{\beta_{1,k}}{x} + \frac{\beta_{2,k}}{x^2} + \cdots\right) \tag{24}$$

where

$$j_k \leqslant \max(i_{k+1}, i_{k+2} - 1, \ldots, i_m - m + k + 1),\ k = 0, 1, \ldots, m-1.$$

The approximation $D_n^{(m)}$ of $\int_0^{\infty} f(t)\,\mathrm{d}t$, using the nonlinear D-transformation, satisfies the $(nm+1)$ equations given by [8]

$$D_n^{(m)} = \int_0^{x_l} f(t)\,\mathrm{d}t + \sum_{k=0}^{m-1} f^{(k)}(x_l) x_l^{\sigma_k} \sum_{i=0}^{n-1} \frac{\bar{\beta}_{k,i}}{x_l^i} \qquad l = 0, 1, \ldots, nm. \tag{25}$$

σ_k for $k = 0, 1, \ldots, m-1$, are the minima of $k+1$ and s_k where s_k is the largest of the integers s for which $\lim_{x\to+\infty} x^s f^{(k)}(x) = 0$.

$D_n^{(m)}$ and $\bar{\beta}_{k,i}$ for $k = 0, 1, \ldots, m-1$, $i = 0, 1, \ldots, n-1$ are the $(nm+1)$ unknowns. The x_l, $l = 0, 1, \ldots$ are chosen to satisfy $0 < x_0 < x_1 < \cdots$ and $\lim_{l\to+\infty} x_l = +\infty$.

The order of the above set of equations can be reduced to $n(m-1)+1$ by choosing x_l, $l = 0, 1, \ldots$ to be the leading positive zeros of $f(x)$. In this case (25) can be rewritten as [9]

$$\bar{D}_n^{(m)} = \int_0^{x_l} f(t)\,\mathrm{d}t + \sum_{k=1}^{m-1} f^{(k)}(x_l) x_l^{\sigma_k} \sum_{i=0}^{n-1} \frac{\bar{\beta}_{k,i}}{x_l^i} \qquad l = 0, 1, \ldots, n(m-1). \tag{26}$$

In previous work [4–7], we have shown the efficiency of the nonlinear D- and $\bar{D}$-transformations in accelerating the convergence of semi-infinite highly oscillatory integrals occurring in the analytical expressions of multicentre bielectronic integrals, in particular the three-centre nuclear attraction integral over B functions, compared with other alternatives, namely the Gauss–Laguerre quadrature, the epsilon algorithm of Wynn [48] and Levin's u-transform [49], which accelerate the convergence of the semi-infinite integrals after transforming them into infinite series (see equation (45)).

As can be seen from (25) and (26), the calculation of the $(m-1)$ successive derivatives of the integrand and its nm or $n(m-1)$ successive zeros is necessary to apply the D- and $\bar{D}$-transformations. This presents severe numerical and computational difficulties when we evaluate multicentre bielectronic integrals, in particular when the values of the quantum numbers n_i, l_i and m_i are large. The order of the linear set of equations to solve for calculating the approximation $\bar{D}_n^{(m)}$ of the semi-infinite integral is equal to $n(m-1)+1$, thus when the values of m and n are large, the calculations become very difficult. In the case of multicentre integrals m is equal to 4 when dealing with three-centre one- and two-electron integrals and 6 for four-centre two-electron integrals.

Now, let us consider a function $f(x)$ of the form $f(x) = g(x)\, j_\lambda(x)$.

Now, we shall state a theorem which is proven in [7, 12, 14].

Theorem 2 (see [7, 12, 14]). *Let* $g(x) = h(x)\,\mathrm{e}^{\phi(x)}$ *be in* $\mathcal{C}^2([0,+\infty[)$*, which is the set of functions that are twice continuously differentiable on* $[0,+\infty[$*, where* $h(x) \in \tilde{A}^{(\gamma)}$ *for some* γ *and* $\phi(x) \in \tilde{A}^{(k)}$ *for some* k.

The function $f(x) = g(x)\, j_\lambda(x)$ *satisfies a second-order linear differential equation given by*

$$f(x) = p_1(x) f'(x) + p_2(x) f''(x) \tag{27}$$

where

$$p_1(x) \in A^{(-1)} \quad \text{and} \quad p_2(x) \in A^{(0)} \qquad \text{if} \quad k = 0$$
$$p_1(x) \in A^{(-k+1)} \quad \text{and} \quad p_2(x) \in A^{(-2k+2)} \qquad \text{if} \quad k \neq 0.$$

Furthermore, if $k > 0$ *and* $\alpha_0(\phi) < 0$*, then* $f(x)$ *is integrable on* $[0,+\infty[$ *and satisfies all the conditions to apply the* D*- and* $\bar{D}$*-transformations.*

The approximation $HD_n^{(2)}$ *of* $\int_0^{+\infty} f(t)\,\mathrm{d}t$ *using the D-transformation is given by*

$$HD_n^{(2)} = \int_0^{x_l} f(t)\,\mathrm{d}t + \sum_{k=0}^{1} f^{(k)}(x_l)\,x_l^{k+1} \sum_{i=0}^{n-1} \frac{\bar{\beta}_{k,i}}{x_l^i} \qquad l = 0, 1, \ldots, 2n \quad (28)$$

$HD_n^{(2)}$ *and* $\bar{\beta}_{k,i}$, $i = 0, 1, \ldots, n-1$ *and* $k = 0, 1$ *are the* $(2n+1)$ *unknowns of the above linear system.*

By choosing $x_l = j_{\lambda+\frac{1}{2}}^{l+1}$ *for* $l = 0, 1, \ldots$ *and using the fact that for all* $l = 1, 2, \ldots,$ $f'(x_l) = g(x_l)\,j'_\lambda(x_l)$, *the above set of equations can be re-expressed as*

$$H\bar{D}_n^{(2)} = \int_0^{x_l} f(t)\,\mathrm{d}t + g(x_l)\,j'_\lambda(x_l)x_l^2 \sum_{i=0}^{n-1} \frac{\bar{\beta}_{1,i}}{x_l^i} \qquad l = 0, 1, \ldots, n \qquad (29)$$

$H\bar{D}_n^{(2)}$ *and* $\bar{\beta}_{1,i}$, $i = 0, 1, \ldots, n-1$ *are the* $(n+1)$ *unknowns of the above linear system.*

In [14, 15], we showed that all the integrands of semi-infinite integrals involved in the analytical expressions of multicentre bielectronic integrals over B functions satisfy the conditions of theorem 2, and consequently they satisfy second-order linear differential equations of the form required to apply the D- and $\bar{D}$-transformations. The HD and $H\bar{D}$ methods led to great simplification, the calculation of the successive derivatives is avoided, we only need to calculate the first derivative of the spherical Bessel function $j_\lambda(x)$, which is very simple as can be seen from (2). The orders of the linear systems to solve using the $H\bar{D}$ method are reduced to $n+1$. This led to a substantial reduction in the calculation times for high predetermined accuracy, but it is still necessary to compute the n successive zeros of $j_\lambda(x)$ and a method to solve the linear system (29).

In this paper, we focused on the use of some properties of sine, reduced Bessel and spherical Bessel functions, to simplify the application of these nonlinear transformations and to further reduce the calculation times keeping the same high predetermined accuracy.

Theorem 3. *Let* $f(x)$ *be a function of the form*

$$f(x) = g(x)\,j_\lambda(x)$$

where $g(x)$ *is in* $\mathcal{C}^2([0, +\infty[)$ *and of the form* $g(x) = h(x)\,\mathrm{e}^{\phi(x)}$ *and where* $h(x) \in \tilde{A}^{(\gamma)}$ *and* $\phi(x) \in \tilde{A}^{(k)}$ *for some* γ *and* k. *If* $k > 0$, $\alpha_0(\varphi) < 0$ *and for all* $l = 0, \ldots, \lambda - 1$, $\lim_{x\to 0} x^{l-\lambda+1} \left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^l \left(x^{\lambda-1} g(x)\right) j_{\lambda-1-l}(x) = 0$ *then* $f(x)$ *is integrable on* $[0, +\infty[$ *and an approximation of* $\int_0^{+\infty} f(x)\,\mathrm{d}x$ *is given by*

$$S\bar{D}_n^{(2,j)} = \frac{\sum_{i=0}^{n+1} \binom{n+1}{i} (1+i+j)^n F(x_{i+j}) \big/ \left[x_{i+j}^2 G(x_{i+j})\right]}{\sum_{i=0}^{n+1} \binom{n+1}{i} (1+i+j)^n \big/ \left[x_{i+j}^2 G(x_{i+j})\right]} \qquad (30)$$

where $x_l = (l+1)\pi$ *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 analytical expression given by (1), we obtain

$$\int_0^{+\infty} f(x)\,\mathrm{d}x = (-1)^\lambda \int_0^{+\infty} x^\lambda\,g(x) \left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^\lambda j_0(x)\,\mathrm{d}x. \qquad (31)$$

Integrating by parts the right-hand side of (31), we obtain

$$\int_0^{+\infty} f(x)\,\mathrm{d}x = (-1)^\lambda \left[x^{\lambda-1}\, g(x) \left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{\lambda-1} j_0(x)\right]_0^{+\infty} + (-1)^{\lambda-1} \int_0^{+\infty} \left[\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right) \left(x^{\lambda-1}\, g(x)\right)\right] \left[\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{\lambda-1} j_0(x)\right] x\,\mathrm{d}x. \tag{32}$$

By integrating by parts until all the derivatives of $j_0(x)$ disappear in the last term on the right-hand side of (32), one can obtain

$$\int_0^{+\infty} f(x)\,\mathrm{d}x = \left[\sum_{l=0}^{\lambda-1} (-1)^{\lambda+l} \left(\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^l \left(x^{\lambda-1} g(x)\right)\right) \left(\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{\lambda-1-l} j_0(x)\right)\right]_0^{+\infty} + \int_0^{+\infty} \left[\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^\lambda \left(x^{\lambda-1}\, g(x)\right)\right] j_0(x)\, x\,\mathrm{d}x. \tag{33}$$

Using equation (1) and replacing $j_0(x)$ by $\frac{\sin(x)}{x}$, the above equation can be rewritten as follows:

$$\int_0^{+\infty} f(x)\,\mathrm{d}x = -\left[\sum_{l=0}^{\lambda-1} x^{l-\lambda+1} \left(\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^l \left(x^{\lambda-1} g(x)\right)\right) j_{\lambda-1-l}(x)\right]_0^{+\infty} + \int_0^{+\infty} \left[\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^\lambda \left(x^{\lambda-1}\, g(x)\right)\right] \sin(x)\,\mathrm{d}x. \tag{34}$$

The function $g(x)$ is exponentially decreasing as $x \to +\infty$, thus the function $\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^l \left(x^{\lambda-1} g(x)\right)$ is also exponentially decreasing as $x \to +\infty$. From this it follows that $\forall\, l \geqslant 0$, $\lim_{x\to+\infty} x^{l-\lambda+1} \left[\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^l \left(x^{\lambda-1} g(x)\right)\right] j_{\lambda-1-l}(x) = 0$.

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 first term on the right-hand side of (34) vanishes and therefore (34) can be rewritten as

$$\int_0^{+\infty} f(x)\,\mathrm{d}x = \int_0^{+\infty} \left[\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^\lambda \left(x^{\lambda-1}\, g(x)\right)\right] \sin(x)\,\mathrm{d}x. \tag{35}$$

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, we can obtain

$$\begin{aligned} G(x) &= \sum_{i=0}^{\lambda} \frac{\lambda!!}{(\lambda-2i)!!} x^{\lambda-2i} \left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{\lambda-i} g(x) \\ &= \sum_{i=0}^{\lambda} \sum_{m=0}^{\lambda-i} \frac{\lambda!!}{(\lambda-2i)!!} \binom{\lambda-i}{m} x^{\lambda-2i} \left[\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^m h(x)\right] \left[\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{\lambda-i-m} \mathrm{e}^{\phi(x)}\right]. \end{aligned} \tag{36}$$

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

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

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

Now, by using lemma 1, we can easily show that the function $G(x)$ can be rewritten as

$$G(x) = H(x)\,\mathrm{e}^{\phi(x)} \qquad \text{where} \quad H(x) \in \tilde{A}^{(\gamma+\lambda k-\lambda)}. \tag{37}$$

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

$$\sin(x) = -\sin''(x). \tag{38}$$

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

$$\mathcal{F}(x) = q_1(x)\mathcal{F}'(x) + q_2(x)\mathcal{F}''(x) \tag{39}$$

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

$$\begin{aligned} q_1(x) &= \frac{2\left(\phi'(x) + H'(x)/H(x)\right)}{1 + (\phi'(x) + H'(x)/H(x))^2 - (\phi'(x) + H'(x)/H(x))'} \\ q_2(x) &= \frac{-1}{1 + (\phi'(x) + H'(x)/H(x))^2 - (\phi'(x) + H'(x)/H(x))'}. \end{aligned} \tag{40}$$

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 $q_2(x) \in A^{(-k+1)}$.

If $k > 0$ 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 $i = 1, 2$, thus for every integer $l \geqslant -1$, $\sum_{i=1}^{m} l(l-1)\ldots(l-i+1)q_{i,0} = 0 \neq 1$.

All the conditions of the applicability of the D- and $\bar{D}$-transformations are now shown to be satisfied by $\mathcal{F}(x)$.

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

$$S\bar{D}_n^{(2)} = \int_0^{x_l} G(x)\sin(x)\,\mathrm{d}x + (-1)^{l+1}\,G(x_l)\,x_l^2 \sum_{i=0}^{n-1} \frac{\bar{\beta}_{1,i}}{x_l^i} \qquad l = 0, 1, \ldots, n \tag{41}$$

where $x_l = (l+1)\pi$ for $l = 0, 1, \ldots$.

Now, following Levin in [49], we can use Cramer's rule, since the zeros of $\sin(x)$ are equidistant, to obtain a simple solution for the unknown $S\bar{D}_n^{(2)}$, which is an approximation of $\int_0^{+\infty} f(x)\,\mathrm{d}x$ and which is given by (30). □

4. Three-centre nuclear attraction integrals over B functions

These integrals are defined by (21) and can be re-expressed as [31, 32]:

$$\mathcal{I}_{n_1,l_1,m_1}^{n_2,l_2,m_2} = \frac{1}{2\pi^2}\int \frac{\mathrm{e}^{\mathrm{i}\vec{x}\cdot(\vec{R}_1-\vec{R}_2)}}{x^2}\left\langle \overline{B}_{n_1,l_1}^{m_1}(\zeta_1, \vec{q})\,\middle|\,\mathrm{e}^{-\mathrm{i}\vec{q}\cdot\vec{R}_2}\,\middle|\,\overline{B}_{n_2,l_2}^{m_2}(\zeta_2, \vec{q}+\vec{x})\right\rangle_{\vec{q}}\,\mathrm{d}\vec{x}. \tag{42}$$

The analytic expression involving the semi-infinite highly oscillatory integral was obtained for the above integral by applying the Fourier-transform method after substituting the analytical expression of the Fourier transform of the B function (11) into the above equation and using the Rayleigh expansion of the plane wavefunctions (9) and the Feynman's identity, which is given by

$$(ab)^{-1} = \int_0^1 [a + (b - a)s]^{-2}\,\mathrm{d}s.$$

The expression of $\mathcal{I}_{n_1,l_1,m_1}^{n_2,l_2,m_2}$ is given by [31, 32]

$$\begin{aligned}
\mathcal{I}_{n_1,l_1,m_1}^{n_2,l_2,m_2} &= 8(4\pi)^2(2l_1+1)!!(2l_2+1)!!\frac{(n_1+l_1+n_2+l_2+1)!}{(n_1+l_1)!(n_2+l_2)!}\zeta_1^{2n_1+l_1-1}\zeta_2^{2n_2+l_2-1} \\
&\quad\times \sum_{l_1'=0}^{l_1}\sum_{m_1'=-l_1'}^{l_1'} (\mathrm{i})^{l_1+l_1'}(-1)^{l_1'}\frac{\langle l_1m_1|l_1'm_1'|l_1-l_1'm_1-m_1'\rangle}{(2l_1'+1)!![2(l_1-l_1')+1]!!} \\
&\quad\times \sum_{l_2'=0}^{l_2}\sum_{m_2'=-l_2'}^{l_2'} (\mathrm{i})^{l_2+l_2'}(-1)^{l_2'}\frac{\langle l_2m_2|l_2'm_2'|l_2-l_2'm_2-m_2'\rangle}{(2l_2'+1)!![2(l_2-l_2')+1]!!} \\
&\quad\times \sum_{l=l_{\min}',2}^{l_2'+l_1'} \langle l_2'm_2'|l_1'm_1'|lm_2'-m_1'\rangle\, R_2^l\, Y_l^{m_2'-m_1'}(\theta_{\vec{R}_2},\varphi_{\vec{R}_2}) \\
&\quad\times \sum_{\lambda=l_{\min}'',2}^{l_2-l_2'+l_1-l_1'} (-\mathrm{i})^{\lambda}\langle l_2-l_2'm_2-m_2'|l_1-l_1'm_1-m_1'|\lambda\mu\rangle \\
&\quad\times \sum_{j=0}^{\Delta l}\binom{\Delta l}{j}\frac{(-1)^j}{2^{n_1+n_2+l_1+l_2-j+1}(n_1+n_2+l_1+l_2-j+1)!} \\
&\quad\times \int_{s=0}^{1} s^{n_2+l_1+l_2-l_1'}(1-s)^{n_1+l_1+l_2-l_2'}\,Y_\lambda^\mu(\theta_{\vec{v}},\varphi_{\vec{v}}) \\
&\quad\times \left[\int_{x=0}^{+\infty} x^{n_x}\frac{\hat{k}_\nu[R_2\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}\,j_\lambda(vx)\,\mathrm{d}x\right]\mathrm{d}s
\end{aligned} \tag{43}$$

where

$$[\gamma(s,x)]^2 = (1-s)\zeta_1^2 + s\zeta_2^2 + s(1-s)x^2$$

$$\vec{v} = (1-s)\vec{R}_2 - \vec{R}_1 \qquad v = \|\vec{v}\| \qquad \text{and} \qquad R_2 = \|\vec{R}_2\|$$

$$n_x = l_1 - l_1' + l_2 - l_2' \qquad \text{and} \qquad \Delta l = [(l_1' + l_2' - l)/2]$$

$$n_\gamma = 2(n_1 + l_1 + n_2 + l_2) - (l_1' + l_2') - l + 1$$

$$\nu = n_1 + n_2 + l_1 + l_2 - l - j + \tfrac{1}{2}$$

$$\mu = (m_2 - m_2') - (m_1 - m_1').$$

The constant $l_{\min}$ is given by (19).

The semi-infinite x integral involved in the above equation, which will be referred to as $\tilde{\mathcal{I}}(s)$, is defined by

$$\tilde{\mathcal{I}}(s) = \int_0^{+\infty} x^{n_x} \frac{\hat{k}_\nu[R_2\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}} j_\lambda(vx)\,\mathrm{d}x \tag{44}$$

$$= \sum_{n=0}^{+\infty} \int_{j^n_{\lambda,v}}^{j^{n+1}_{\lambda,v}/v} x^{n_x} \frac{\hat{k}_\nu[R_2\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}} j_\lambda(vx)\,\mathrm{d}x \tag{45}$$

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

The numerical difficulties in the evaluation of the analytical expression (43) arise mainly from the presence of the semi-infinite integral $\tilde{\mathcal{I}}(s)$, whose integrand oscillates rapidly due to the presence of the spherical Bessel function especially for large values of λ and v.

In previous work [12, 14], we demonstrated the superiority of $H\bar{D}$ in the evaluation of these kind of semi-infinite integrals compared with $\bar{D}$. The approximation $H\bar{D}^{(2)}_n$ of $\tilde{\mathcal{I}}(s)$ is given by

$$H\bar{D}^{(2)}_n = \int_0^{x_l} f(t)\,\mathrm{d}t + g(x_l)\, j'_\lambda(vx)x_l^2 \sum_{i=0}^{n-1} \frac{\bar{\beta}_{1,i}}{x_l^i} \qquad l = 0, 1, 2, \ldots, n \tag{46}$$

where $f(x)$ is the integrand of $\tilde{\mathcal{I}}(s)$ and

$$g(x) = x^{n_x} \frac{\hat{k}_\nu\,[R_2\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}$$

and where $x_l = j^l_{\lambda,v}$ for $l = 0, 1, \ldots.$

Now, let us consider the integrand $f(x)$ of $\tilde{\mathcal{I}}(s)$, which is given by

$$f(x) = g(x)\, j_\lambda(vx) \qquad \text{where} \quad g(x) = x^{n_x} \frac{\hat{k}_\nu\,[R_2\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}} \in \mathcal{C}^2([0,+\infty[).$$

Let the function $\phi(x) = R_2\gamma(s,x)$. It can be rewritten as

$$\phi(x) = R_2\sqrt{(1-s)\zeta_1^2 + s\zeta_2^2 + s(1-s)x^2} \in \tilde{A}^{(1)} \qquad \left(\text{lemma 1 for } m = \tfrac{1}{2}\right).$$

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

By using the lemmas 1 and 2, $g(x)$ can be re-expressed as follows:

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

Let the function

$$\Phi(x) = \frac{\hat{k}_\nu\,[R_2\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}$$

then $g(x) = x^{n_x}\Phi(x)$ where n_x is given by equation (43). For all l in $\{0, 1, \ldots, \lambda-1\}$:

$$x^{l-\lambda+1}\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^l \left(x^{\lambda-1}g(x)\right) = x^{l-\lambda+1}\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^l \left(x^{n_x+\lambda-1}\Phi(x)\right)$$

$$= \sum_{i=0}^{l} \binom{l}{i} \frac{(n_x+\lambda-1)!!}{(n_x+\lambda-1-2i)!!} x^{n_x+l-2i} \left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{l-i} \Phi(x). \tag{47}$$

The function $\Phi(x)$ is defined for $x = 0$. From equation (5), we can easily show that for all positive integers i, $\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^i \Phi(x)$ is also defined for $x = 0$.

According to equation (43), $n_x = l_2 - l_2' + l_1 - l_1'$. The integer λ varies from $l_{\min}$ which is given by equation (19) to $l_2 - l_2' + l_1 - l_1' = n_x$, thus for all $l = 0, 1, \ldots, \lambda - 1$, $l < n_x$. Consequently, for all $i = 0, 1, \ldots, l$, the integer $n_x + l - 2i \geqslant 1$.

From the above arguments it follows that for all $l = 0, \ldots, \lambda - 1$:

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

All the conditions of theorem 3, are now shown to be satisfied by the integrand $f(x)$. The semi-infinite integral $\tilde{\mathcal{I}}(s)$ can be rewritten as

$$\tilde{\mathcal{I}}(s) = \frac{1}{v^{\lambda+1}} \int_0^{+\infty} \left[\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^\lambda \left(x^{n_x+\lambda-1} \frac{\hat{k}_\nu[R_2\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}\right)\right] \sin(vx)\,\mathrm{d}x \tag{48}$$

$$= \frac{1}{v^{\lambda+1}} \sum_{n=0}^{+\infty} \int_{n\pi/v}^{(n+1)\pi/v} \left[\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^\lambda \left(x^{n_x+\lambda-1} \frac{\hat{k}_\nu[R_2\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}\right)\right] \sin(vx)\,\mathrm{d}x. \tag{49}$$

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

$$S\bar{D}_n^{(2,j)} = \frac{1}{v^{\lambda+1}} \frac{\sum_{i=0}^{n+1} \binom{n+1}{i} (1+i+j)^n F(x_{i+j}) \big/ \left[x_{i+j}^2 G(x_{i+j})\right]}{\sum_{i=0}^{n+1} \binom{n+1}{i} (1+i+j)^n \big/ \left[x_{i+j}^2 G(x_{i+j})\right]} \tag{50}$$

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 $F(x) = \int_0^x G(t)\sin(vt)\,\mathrm{d}t$.

Let us consider $G(x)$. Using equation (5) and the fact that $\frac{\mathrm{d}}{\mathrm{d}x} = \frac{\mathrm{d}z}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}z}$, we obtain for $\alpha, j \in \mathbb{N}$ in the case where $n_\gamma < 2\nu$:

$$\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^j \left(x^\alpha \frac{\hat{k}_\nu[R_2\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}\right) = \sum_{l=0}^{j} \binom{j}{l} \frac{\alpha!!}{(\alpha-2l))!!} x^{\alpha-2l} \sum_{i=0}^{j-l} \binom{j-l}{i}$$
$$\times(-1)^{j-l-i} \frac{(2\nu-n_\gamma)!!}{(2\nu-n_\gamma-2i)!!} s^i(1-s)^i \frac{\hat{k}_{\nu+j-l-i}[R_2\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma+2i}} \tag{51}$$

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

$$\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^j \left(x^\alpha \frac{\hat{k}_\nu[R_2\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}\right) = \sum_{l=0}^{j} (-1)^{j-l} \binom{j}{l} \frac{\alpha!!}{(\alpha-2l))!!} x^{\alpha-2l}$$
$$\times s^{j-l}(1-s)^{j-l} \frac{\hat{k}_{\nu+j-l}[R_2\gamma(s,x)]}{[\gamma(s,x)]^{2(\nu+j-l)}}. \tag{52}$$

As can be seen from the above equations, the calculation of $G(x)$ does not present any computational difficulties. The use of equation (50) for calculating the approximation of $\tilde{\mathcal{I}}(s)$ is more advantageous than the use of the linear systems (26) or (29) where the computational of the $(n+1)$ successive zeros of spherical Bessel function is necessary and where it is required to compute a method for solving linear systems which is much more time consuming than the use of Cramer's rule.

5. Numerical results and discussion

The finite integrals involved in equations (45) and (49) are evaluated using Gauss–Legendre quadrature of the order of 16. The finite integrals involved in equations (46) and (50) are transformed to 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 the order of 16.

The values with 15 correct decimal places are obtained for the integrals by using the infinite series (45) and (49) which we sum until max (see tables 1, 2, 5 and 6).

Table 1. Values of $\tilde{\mathcal{I}}(s)$ obtained with 15 correct decimal places by using the infinite series (45).

s	ν	n_γ	n_x	λ	R_1	ζ_1	R_2	ζ_2	Max	$\tilde{\mathcal{I}}(s)$
0.01	$\frac{5}{2}$	5	0	0	6.31	1.0	2.0	1.0	156	0.638 243 453 884 445D+00
0.99	$\frac{5}{2}$	5	0	0	4.50	2.0	1.5	1.0	202	0.701 581 269 512 310D+00
0.99	$\frac{9}{2}$	9	1	1	6.00	2.0	3.5	1.0	145	0.183 138 910 224 196D+01
0.99	$\frac{9}{2}$	9	2	1	6.00	2.0	3.0	1.0	195	0.476 698 176 142 361D+00
0.01	$\frac{9}{2}$	9	2	1	8.50	2.0	3.5	2.0	156	0.248 336 723 989 967D−03
0.01	$\frac{9}{2}$	9	2	2	9.00	2.0	3.5	1.0	206	0.183 269 571 025 289D−02
0.99	$\frac{13}{2}$	11	3	3	6.50	2.5	3.5	2.0	239	0.993 192 009 882 242D−02
0.01	$\frac{13}{2}$	13	3	3	7.50	2.0	3.5	1.0	134	0.181 139 626 222 753D−01

Table 2. Values of $\tilde{\mathcal{I}}(s)$ obtained with 15 correct decimal places by using the infinite series (49).

s	ν	n_γ	n_x	λ	R_1	ζ_1	R_2	ζ_2	Max	$\tilde{\mathcal{I}}(s)$
0.01	$\frac{5}{2}$	5	0	0	6.31	1.0	2.0	1.0	156	0.638 243 453 884 445D+00
0.99	$\frac{5}{2}$	5	0	0	4.50	2.0	1.5	1.0	202	0.701 581 269 512 310D+00
0.99	$\frac{9}{2}$	9	1	1	6.00	2.0	3.5	1.0	145	0.183 138 910 224 197D+01
0.99	$\frac{9}{2}$	9	2	1	6.00	2.0	3.0	1.0	195	0.476 698 176 142 352D+00
0.01	$\frac{9}{2}$	9	2	1	8.50	2.0	3.5	2.0	156	0.248 336 723 989 985D−03
0.01	$\frac{9}{2}$	9	2	2	9.00	2.0	3.5	1.0	206	0.183 269 571 025 634D−02
0.99	$\frac{13}{2}$	11	3	3	6.50	2.5	3.5	2.0	239	0.993 192 007 213 570D−02
0.01	$\frac{13}{2}$	13	3	3	7.50	2.0	3.5	1.0	134	0.181 139 626 222 771D−01

The linear set of equations (46) is solved using the LU decomposition method.

In the evaluation of $\mathcal{I}_{n_1 00}^{n_2 00}$ which is given by equation (43) we let n_x and λ vary to compare the efficiency of the new method in the evaluation of semi-infinite integrals whose integrands are very oscillating.

The numerical values of the semi-infinite integral $\tilde{\mathcal{I}}(s)$, are obtained for $s = 0.01$ or 0.99. In this region, the integrand oscillates rapidly. If we let $s = 0$ or 1, the integrand will be reduced to the term $x^{n_x} j_\lambda(vx)$, because the terms

$$\frac{\hat{k}_\nu[R_2\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}$$

Table 3. Evaluation of $\tilde{\mathcal{I}}(s)$ using $H\bar{D}_n^{(2)}$ (29).

s	ν	n_γ	n_x	λ	R_1	ζ_1	R_2	ζ_2	n	$\tilde{\mathcal{I}}(s)$	Error
0.01	$\frac{5}{2}$	5	0	0	6.31	1.0	2.0	1.00	9	0.638 243 4540D+00	0.73D−10
0.99	$\frac{5}{2}$	5	0	0	4.50	2.0	1.5	1.00	6	0.701 581 2749D+00	0.54D−08
0.99	$\frac{9}{2}$	9	1	1	6.00	2.0	3.5	1.00	6	0.183 138 9173D+01	0.71D−07
0.99	$\frac{9}{2}$	9	2	1	6.00	2.0	3.0	1.00	8	0.476 698 1567D+00	0.19D−07
0.01	$\frac{9}{2}$	9	2	1	8.50	2.0	3.5	2.00	7	0.248 336 7950D−03	0.71D−10
0.01	$\frac{9}{2}$	7	2	2	9.00	2.0	3.5	1.00	6	0.183 269 5268D−02	0.44D−09
0.99	$\frac{13}{2}$	11	3	3	6.50	2.5	3.5	2.00	9	0.993 191 9510D−02	0.59D−09
0.01	$\frac{13}{2}$	13	3	3	7.50	2.0	3.5	1.00	7	0.181 139 5757D−01	0.50D−08

Table 4. Evaluation of $\tilde{\mathcal{I}}(s)$ using $S\bar{D}_n^{(2,5)}$ (50).

s	ν	n_γ	n_x	λ	R_1	ζ_1	R_2	ζ_2	n	$\tilde{\mathcal{I}}(s)$	Error
0.01	$\frac{5}{2}$	5	0	0	6.31	1.0	2.0	1.00	9	0.638 243 4538D+00	0.74D−10
0.99	$\frac{5}{2}$	5	0	0	4.50	2.0	1.5	1.00	6	0.701 581 2695D+00	0.13D−10
0.99	$\frac{9}{2}$	9	1	1	6.00	2.0	3.5	1.00	6	0.183 138 9102D+01	0.25D−10
0.99	$\frac{9}{2}$	9	2	1	6.00	2.0	3.0	1.00	8	0.476 698 1761D+00	0.31D−10
0.01	$\frac{9}{2}$	9	2	1	8.50	2.0	3.5	2.00	7	0.248 336 7149D−03	0.91D−11
0.01	$\frac{9}{2}$	7	2	2	9.00	2.0	3.5	1.00	6	0.183 269 5716D−02	0.57D−11
0.99	$\frac{13}{2}$	11	3	3	6.50	2.5	3.5	2.00	9	0.993 192 0012D−02	0.87D−10
0.01	$\frac{13}{2}$	13	3	3	7.50	2.0	3.5	1.00	7	0.181 139 6261D−01	0.81D−11

Table 5. Values of $\mathcal{I}_{n_1 00}^{n_2 00}$ with 15 correct decimal places obtained by using the semi-infinite series (45) for evaluating the semi-infinite integrals.

n_1	n_2	n_γ	n_x	λ	R_1	ζ_1	R_2	ζ_2	$\mathcal{I}_{n_1 00}^{n_2 00}$
1	1	5	0	0	6.00	2.50	2.50	1.50	0.985 707 949 076 0591D−01
2	1	7	1	1	4.50	1.50	2.50	1.00	0.876 172 059 571 9185D+00
2	1	7	2	1	5.50	2.50	1.50	1.50	0.302 146 653 451 6112D−01
2	2	9	2	2	9.00	1.00	1.50	0.50	0.445 961 267 998 7873D+00
2	2	9	3	2	7.00	2.00	3.50	1.00	0.152 962 414 830 2400D−01
3	2	11	3	3	3.50	1.00	2.00	1.00	0.291 429 448 234 6616D+01
3	3	13	3	3	8.50	2.00	2.50	1.50	0.175 035 053 459 4521D−01
4	3	15	4	4	4.00	1.50	1.50	1.00	0.167 986 460 269 3797D+01
4	4	17	4	4	4.50	0.50	1.00	1.00	0.472 323 260 481 3232D+00

becomes a constant and hence the exponential decreasing part $\hat{k}_\nu$ of the integrands becomes a constant and thus the rapid oscillations of $j_\lambda(vx)$ cannot be damped and suppressed. The asymptotic behaviour of the integrand cannot be represented by a function of the form $\mathrm{e}^{-\alpha x}\, j_\lambda(x)$.

We also note that the region close to $s = 0$ or 1 carry a very small weight because of their expressions $s^{i_2}(1-s)^{i_1}$ in the integrals (43) [50–53].

Table 6. Values of $\mathcal{I}_{n_1 00}^{n_2 00}$ with 15 correct decimal places obtained by using the semi-infinite series (49) for evaluating the semi-infinite integrals.

n_1	n_2	n_γ	n_x	λ	R_1	ζ_1	R_2	ζ_2	$\mathcal{I}_{n_1 00}^{n_2 00}$
1	1	5	0	0	6.00	2.50	2.50	1.50	0.985 707 949 076 0592D−01
2	1	7	1	1	4.50	1.50	2.50	1.00	0.876 172 059 571 9185D+00
2	1	7	2	1	5.50	2.50	1.50	1.50	0.302 146 653 451 6114D−01
2	2	9	2	2	9.00	1.00	1.50	0.50	0.445 961 267 998 7876D+00
2	2	9	3	2	7.00	2.00	3.50	1.00	0.152 962 414 830 2401D−01
3	2	11	3	3	3.50	1.00	2.00	1.00	0.291 429 448 235 4614D+01
3	3	13	3	3	8.50	2.00	2.50	1.50	0.175 035 053 459 4524D−01
4	3	15	4	4	4.00	1.50	1.50	1.00	0.167 986 460 269 3796D+01
4	4	17	4	4	4.50	0.50	1.00	1.00	0.472 323 260 481 3232D+00

Table 7. Evaluation of $\mathcal{I}_{n_1 00}^{n_2 00}$ using $H\bar{D}_n^{(2)}$ for evaluating the semi-infinite integrals.

n_1	n_2	n_γ	n_x	λ	R_1	ζ_1	R_2	ζ_2	n	$\mathcal{I}_{n_1 00}^{n_2 00}$	Error
1	1	5	0	0	6.00	2.50	2.50	1.50	8	0.985 707 949 061D−01	0.15D−11
2	1	7	1	1	4.50	1.50	2.50	1.00	6	0.876 172 059 815D+00	0.24D−09
2	1	7	2	1	5.50	2.50	1.50	1.50	9	0.302 146 652 701D−01	0.75D−10
2	2	9	2	2	9.00	1.00	1.50	0.50	7	0.445 961 265 550D+00	0.24D−08
2	2	9	3	2	7.00	2.00	3.50	1.00	7	0.152 962 409 896D−01	0.49D−09
3	2	11	3	3	3.50	1.00	2.00	1.00	7	0.291 429 448 221D+01	0.13D−09
3	3	13	3	3	8.50	2.00	2.50	1.50	7	0.175 035 042 045D−01	0.11D−08
4	3	15	4	4	4.00	1.50	1.50	1.00	7	0.167 986 460 265D+01	0.48D−10
4	4	17	4	4	4.50	0.50	1.00	1.00	6	0.472 323 260 506D+00	0.24D−10

Table 8. Evaluation of $\mathcal{I}_{n_1 00}^{n_2 00}$ using $S\bar{D}_n^{(2,5)}$ for evaluating the semi-infinite integrals.

n_1	n_2	n_γ	n_x	λ	R_1	ζ_1	R_2	ζ_2	n	$\mathcal{I}_{n_1 00}^{n_2 00}$	Error
1	1	5	0	0	6.00	2.50	2.50	1.50	5	0.985 707 949 076D−01	0.38D−13
2	1	7	1	1	4.50	1.50	2.50	1.00	6	0.876 172 059 631D+00	0.59D−10
2	1	7	2	1	5.50	2.50	1.50	1.50	7	0.302 146 653 118D−01	0.33D−10
2	2	9	2	2	9.00	1.00	1.50	0.50	6	0.445 961 268 947D+00	0.95D−09
2	2	9	3	2	7.00	2.00	3.50	1.00	6	0.152 962 414 961D−01	0.13D−10
3	2	11	3	3	3.50	1.00	2.00	1.00	6	0.291 429 448 236D+01	0.85D−11
3	3	13	3	3	8.50	2.00	2.50	1.50	7	0.175 035 059 369D−01	0.59D−09
4	3	15	4	4	4.00	1.50	1.50	1.00	6	0.167 986 460 270D+01	0.57D−11
4	4	17	4	4	4.50	0.50	1.00	1.00	6	0.472 323 260 531D+00	0.50D−10

6. Conclusion

This work presents a new approach for improving convergence of semi-infinite oscillatory integrals whose integrands are of the form $f(x) = g(x)\, j_\lambda(x)$ and where $g(x) = h(x)\, \mathrm{e}^{\phi(x)}$.

The properties of the spherical Bessel and sine functions allowed the use of Cramer's rule for calculating the approximations $S\bar{D}_n^{(2,j)}$ of the semi-infinite integrals. This led to a great simplification in the calculations since the computation of the successive zeros of the spherical Bessel function and a method to solve the linear systems are avoided.

The numerical results show the high accuracy obtained by applying the $S\bar{D}$ method. The three-centre nuclear attraction integrals which contribute to total molecular energies can be obtained to a precision of 10^{-10} au which is quite sufficient for energies of chemical processes. In the molecular context, many millions of such integrals are required for close-range terms (long-range terms being treated by asymptotic expansions or multipole approaches), therefore rapidity is the primordial criterion when the precision has been reached.

The $S\bar{D}$ method is also able to reach a precision of 10^{-15} au and certainly some applications of this extremely high accuracy will be developed in future work.

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