Journal of Mathematical Chemistry Vol. 29, No. 3, 2001

Numerical evaluation of three-center two-electron Coulomb and hybrid integrals over B functions using the HD and $H\overline{D}$ methods and convergence properties

Hassan Safouhi

Département de Mathématiques, Université du Québec à Montréal, C.P. 8888, Succursale Centre-Ville, Montréal, Québec, Canada H3C 3P8
E-mail: safouhi@math.uqam.ca

Received 9 February 2000

The difficulties of the numerical evaluation of three-center two-electron Coulomb and hybrid integrals over B functions, arise mainly from the presence of the hypergeometric series and semi-infinite very oscillatory integrals in their analytical expressions, which are obtained using the Fourier transform method.

This work presents a general approach for accelerating the convergence of these integrals by first demonstrating that the hypergeometric function, involved in the analytical expressions of the integrals of interest, can be expressed as a finite sum and by applying nonlinear transformations for accelerating the convergence of the semi-infinite oscillatory integrals after reducing the order of the differential equation satisfied by the integrand.

The convergence properties of the new approach are analysed to show that from the numerical point of view the $H\overline{D}$ method corresponds to the most ideal situation.

The numerical results section illustrates the accuracy and unprecedented efficiency of evaluation of these integrals.

KEY WORDS: Nonlinear transformations for accelerating the convergence of semi-infinite integrals, three-center two-electron Coulomb integrals, hybrid integrals

1. Introduction

Three-center two-electron Coulomb and hybrid integrals occur in the molecular context and are numerous and difficult to evaluate to high accuracy. The B functions [1–3] are chosen as the basis set of atomic orbitals. These functions are linear combinations of Slater type orbitals [3,4] and they are well adapted to the Fourier transform method [5,6] which allowed analytical expressions for molecular multicenter integrals to be developed [7–22].

The principal source of difficulties regarding accuracy and speed up of the numerical evaluation of the analytical expressions obtained for three-center two-electron Coulomb and hybrid integrals arises from the presence of the hypergeometric series and the spherical Bessel function in the integrands. Bessel functions lead to rapid oscillations

0259-9791/01/0400-0213$19.50/0

of the integrands, whereas the hypergeometric series ${}_{p+1}F_p$ with $p = 0, 1, \ldots$ converges as long as its argument z satisfies $|z| < 1$. If $|z|$ is sufficiently small, convergence is usually good and the series can be used for the evaluation of the hypergeometric function. If, however, $|z|$ is slightly smaller than 1, convergence can become so slow that the infinite series is computationally useless. Finally, for $|z| > 1$, the hypergeometric series diverges. However, it is often possible to find an analytic continuation – for instance with the help of sequence transformations – which makes it possible to associate a finite value to a divergent hypergeometric series even outside its circle of convergence [23]. These properties can cause difficulty in the evaluation of the integrals. It is in fact not obvious that the nonlinear transformations can be applied to such integrals.

After a re-arrangement of the combined indices appearing as arguments in the hypergeometric functions, it is shown that they can be expressed in the form of a finite sum.

In previous work [24,25], we showed that the integrands of the semi-infinite integrals, involved in the analytical expressions of three-center two-electron Coulomb and hybrid integrals, satisfy all the condition of application of the nonlinear D- and $\overline{D}$-transformations [26,27]. It is shown that these transformations are very efficient in the evaluation of semi-infinite oscillatory integrals, unfortunately, their application depends strongly on the order of the differential equation required to be satisfied by the integrand.

In [25,28], we showed that this order can be reduced for a function of the form $f(x) = g(x) j_\lambda(x)$ where $g(x) \sim h(x)\mathrm{e}^{\phi(x)}$ as $x \to +\infty$ such that $h(x)$ has an asymptotic expansion in inverse powers of x and $\phi(x)$ is real polynomial of degree k in x as $x \to +\infty$. This method led to substantial simplifications in the application of D and $\overline{D}$ [28]. Unfortunately, it cannot be applied to a large set of oscillatory functions since we need $g(x)$ to satisfy the above conditions.

This work presents a general method, based on the use of practical properties of the reduced and spherical Bessel functions and Poincaré series, for reducing the orders of differential equations, required to apply D and $\overline{D}$, to two keeping all the other conditions satisfied. Great simplifications are obtained using the new approach leading to new method which we called HD and $H\overline{D}$.

The convergence properties showed that from the numerical point of view, the $H\overline{D}$ correponds to the most ideal situation.

The numerical results section illustrates clearly the substantial gain in the calculation times for a high predetermined accuracy.

2. Definitions and properties

The B functions are defined as follows [2,3]:

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

where the reduced Bessel function $\widehat{k}_{n-1/2}(\zeta r)$ is defined by [1,2]

$$\widehat{k}_{n-1/2}(\zeta r) = \frac{\mathrm{e}^{-\zeta r}}{\zeta r} \sum_{j=1}^{n} \frac{(2n-j-1)!}{(j-1)!(n-j)!} 2^{j-n} (\zeta r)^j \tag{2}$$

and the surface spherical harmonic $Y_l^m(\theta, \varphi)$ is defined as follows [29]:

$$Y_l^m(\theta, \varphi) = \mathrm{i}^{m+|m|} \left[\frac{(2l+1)(l-|m|)!)}{4\pi(l+|m|)!)} \right]^{1/2} P_l^{|m|}(\cos\theta) \mathrm{e}^{im\varphi}, \tag{3}$$

$P_l^m(x)$ stands for the associated Legendre function of lth degree and mth order [30]:

$$P_l^m(x) = \left(1-x^2\right)^{m/2} \left(\frac{\mathrm{d}}{\mathrm{d}x} \right)^{l+m} \left[\frac{\left(x^2-1\right)^l}{2^l l!} \right]. \tag{4}$$

The Slater type orbitals (STOs) are defined in normalized form according to the following relationship [31,32]:

$$\chi_{n,l}^m\left(\zeta\vec{r}\right) = N(n,\zeta) r^{n-1} \mathrm{e}^{-\zeta r} Y_l^m(\theta_{\vec{r}}, \varphi_{\vec{r}}),$$

where $n = 1, 2, \ldots, 0 \leqslant l \leqslant n-1$ and $-l \leqslant m \leqslant l$. $N(n,\zeta)$ stands for the normalisation factor defined by

$$N(n,\zeta) = \zeta^{-n+1} \left[\frac{(2\zeta)^{2n+1}}{(2n)!} \right]^{1/2}. \tag{5}$$

The Slater type orbitals can be expressed as finite linear combinations of B functions [2]:

$$\chi_{n,l}^m\left(\zeta\vec{r}\right) = \sum_{p=\widetilde{p}}^{n-l} \frac{(-1)^{n-l-p}(n-l)!2^{l+p}(l+p)!}{(2p-n-l)!(2n-2l-2p)!!} B_{p,l}^m\left(\zeta\vec{r}\right), \tag{6}$$

where

$$\widetilde{p} = \begin{cases} (n-l)/2 & \text{if } n-l \text{ even}, \\ (n-l+1)/2 & \text{if } n-l \text{ odd} \end{cases} \tag{7}$$

and where the double factorial is defined by:

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

The Fourier transform $\overline{B}_{n,l}^m(\zeta, \vec{p})$ of $B_{n,l}^m(\zeta\vec{r})$ is given by [5,6]

$$\overline{B}_{n,l}^m\left(\zeta, \vec{p}\right) = \frac{1}{(2\pi)^{3/2}} \int_{\vec{r}} \mathrm{e}^{-\mathrm{i}\vec{p}\,\vec{r}} B_{n,l}^m\left(\zeta\vec{r}\right) \mathrm{d}\vec{r} \tag{8}$$

$$= \sqrt{\frac{2}{\pi}} \zeta^{2n+l-1} \frac{(-\mathrm{i}|p|)^l}{(\zeta^2+|p|^2)^{n+l+1}} Y_l^m(\theta_{\vec{p}}, \varphi_{\vec{p}}). \tag{9}$$

The analytical expression of the Fourier transform $\overline{B}^{m}_{n,l}(\zeta, \vec{p})$ of $B^{m}_{n,l}(\zeta\vec{r})$ is obtained by using the Rayleigh expansion of the plane wave function [33]:

$$e^{\pm i\vec{p}\,\vec{r}} = \sum_{\lambda=0}^{+\infty} \sum_{m=-\lambda}^{\lambda} 4\pi(\pm i)^{\lambda} j_{\lambda}\big(|\vec{p}||\vec{r}|\big) Y_{\lambda}^{m}(\theta_{\vec{r}}, \varphi_{\vec{r}}) \big[Y_{\lambda}^{m}(\theta_{\vec{p}}, \varphi_{\vec{p}})\big]^{*}, \tag{10}$$

where $j_{\lambda}(x)$ stands for the spherical Bessel function of order $\lambda \in \mathbb{N}$, which is defined by [30]

$$j_{\lambda}(x) = (-1)^{\lambda} x^{\lambda} \left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^{\lambda} \left(\frac{\sin(x)}{x}\right). \tag{11}$$

Function $j_{\lambda}(x)$ satisfies the recurrence relations [30]

$$\begin{aligned} x j_{\lambda-1}(x) + x j_{\lambda+1}(x) &= 2\lambda j_{\lambda}(x), \\ j_{\lambda-1}(x) - j_{\lambda+1}(x) &= 2 j'_{\lambda}(x), \end{aligned} \tag{12}$$

where

$$j_0(x) = \frac{\sin x}{x} \quad \text{and} \quad j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}. \tag{13}$$

Also $j_{\lambda}(x)$ satisfies a 2nd order differential equation given by

$$j_{\lambda}(x) = -\frac{2x}{x^2 - \lambda^2 - \lambda} j'_{\lambda}(x) - \frac{x^2}{x^2 - \lambda^2 - \lambda} j''_{\lambda}(x). \tag{14}$$

The zeros of $j_{\lambda}(x)$ will be referred to as $j^{n}_{\lambda+1/2}$, $n = 1, 2, \ldots$; $j^{0}_{\lambda+1/2}$ is assumed to be zero. For $v \in \mathbb{R}$, $j^{n}_{\lambda,v} = j^{n}_{\lambda+1/2}/v$, $n = 1, 2, \ldots$, are the successive zeros of $j_{\lambda}(vx)$ and $j^{0}_{\lambda,v} = 0$.

We define the product EF, where E and F are sets of functions, as the set of functions $f(x)$ such that $f(x) = g(x)h(x)$ where $g \in E$ and $h \in F$.

We define $A^{(\gamma)}$ to be the set of infinitely differentiable functions $p(x)$, which have asymptotic expansions in inverse powers of x as $x \to +\infty$, of the form:

$$p(x) \sim x^{\gamma} \left(a_0 + \frac{a_1}{x} + \frac{a_2}{x^2} + \cdots\right) \tag{15}$$

and their derivatives of any order have asymptotic expansions, which can be obtained by differentiating that in equation (15) formally term by term.

We let $\overline{A}^{(\gamma)}$, for $\gamma \in \mathbb{R}$, be the set of functions $p(x)$ such that $p \in A^{(\gamma)}$ and $\lim_{x\to+\infty} x^{-\gamma} p(x) \neq 0$. Thus, $p \in \overline{A}^{(\gamma)}$ has an asymptotic expansion in inverse powers of x as $x \to +\infty$ of the form given by equation (15) with $a_0 \neq 0$.

We define the function $\alpha_0(p)$ by $\alpha_0(p) = a_0$; $\alpha_0(p) \neq 0$ if $p \in \overline{A}^{(\gamma)}$. $e^{\overline{A}^{(\gamma)}}$ is defined as the set of functions $g(x)$:

$$g(x) = e^{p(x)}, \quad \text{where } p \in \overline{A}^{(\gamma)}.$$

The Fourier integral representation of the Coulomb operator $1/|\vec{r}-\vec{R}_1|$ is given by [34]

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

The Gaunt coefficients are defined as [35–41]

$$\langle l_1m_1|l_2m_2|l_3m_3\rangle=\int_{\theta=0}^{\pi}\int_{\varphi=0}^{2\pi}\left[Y_{l_1}^{m_1}(\theta,\varphi)\right]^*Y_{l_2}^{m_2}(\theta,\varphi)Y_{l_3}^{m_3}(\theta,\varphi)\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\varphi.$$

The hypergeometric function is given by [30]

$${}_2F_1(\alpha,\beta;\gamma;x)=\sum_{r=0}^{+\infty}\frac{(\alpha)_r(\beta)_rx^r}{(\gamma)_r r!}, \tag{17}$$

where $(\alpha)_n$ represents the Pochhammer symbol, which is defined by [30]

$$\begin{cases}(\alpha)_0=1,\\ (\alpha)_n=\alpha(\alpha+1)(\alpha+2)\cdots(\alpha+n-1)=\dfrac{\Gamma(\alpha+n)}{\Gamma(\alpha)}\quad(n\neq 0),\end{cases} \tag{18}$$

where Γ stands for the Gamma function [30]. For $n\in\mathbb{N}$

$$\begin{cases}\Gamma(n+1)=n!=1\cdot2\cdot3\cdots n,\\ \Gamma\left(n+\frac{1}{2}\right)=\dfrac{(2n)!}{2^{2n}\,n!}\sqrt{\pi}.\end{cases} \tag{19}$$

The infinite series equation (17) 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 [23].

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

$$(\alpha)_n=\begin{cases}(\alpha)_n=1 & \text{if } n=0,\\ (\alpha)_n=\alpha(\alpha+1)(\alpha+2)\cdots(\alpha+n-1) & \text{if } n\leqslant-\alpha,\\ (\alpha)_n=0 & \text{if } n\geqslant-\alpha+1.\end{cases} \tag{20}$$

3. The HD and $H\overline{D}$ methods for accelerating the convergence of semi-infinite oscillatory integrals

Theorem 1 [26]. Let $f(x)$ be integrable on $[0,+\infty[$ and satisfies a linear differential equation of order m of the form

$$f(x)=\sum_{k=1}^{m}p_k(x)f^{(k)}(x). \tag{21}$$

If p_k for $k = 1, 2, \ldots, m$ satisfy the following conditions:

(1) p_k are in $A^{(i_k)}$, where $i_k \leqslant k$ for $k = 1, 2, \ldots, m$,

(2) $\lim_{x\to+\infty} p_k^{(i-1)}(x) f^{(k-i)}(x) = 0$ for $k = i, i+1, \ldots, m$; $i = 1, \ldots, m$,

(3) $\forall l \geqslant -1$, $\sum_{k=1}^{m} l(l-1)\cdots(l-k+1)p_{k,0} \neq 1$; $p_{k,0} = \lim_{x\to+\infty} x^{-k} p_k(x)$,

then, by using the nonlinear D-transformation, the approximation $D_n^{(m)}$ to $S = \int_0^\infty f(t)\,\mathrm{d}t$ is given by [26]:

$$D_n^{(m)} = \int_0^{x_l} f(t)\,\mathrm{d}t + \sum_{k=0}^{m-1} f^{(k)}(x_l) x_l^{\sigma_k} \sum_{i=0}^{n-1} \frac{\overline{\beta}_{i,k}}{x_l^i}, \quad l = 0, 1, \ldots, mn, \tag{22}$$

where $D_n^{(m)}$ and $\overline{\beta}_{i,k}$, for $k = 0, 1, \ldots, m-1$, $i = 0, 1, \ldots, n-1$, are the $(mn+1)$ unknowns, x_l, $l = 0, 1, \ldots$, are chosen to satisfy $0 < x_0 < x_1 < \cdots$, $\lim_{l\to+\infty} x_l = +\infty$ and $\sigma_k = \min\{k+1, s_k\}$, where $s_k = \max\{s \in \mathbb{Z}, \lim_{x\to+\infty} x^s f^{(k)}(x) = 0\}$, for $k = 0, 1, \ldots, m-1$.

The order of the above set of equations can be reduced by choosing x_l, $l = 0, 1, \ldots$, to be the successive positive zeros of $f(x)$. In this case the equation (22) can be re-written as [27]

$$\overline{D}_n^{(m)} = \int_0^{x_l} f(t)\,\mathrm{d}t + \sum_{k=1}^{m-1} f^{(k)}(x_l) x_l^{\sigma_k} \sum_{i=0}^{n-1} \frac{\overline{\beta}_{i,k}}{x_l^i}, \quad l = 0, 1, \ldots, (m-1)n. \tag{23}$$

It is shown that D and $\overline{D}$ are efficient in accelerating the convergence of semi-infinite very oscillatory integrals. Unfortunately, these transformations require the calculation of the $(m-1)$ successive derivatives of the integrand, where m is the order of the differential equation. This presents severe computational difficulties especially for large values of quantum numbers when dealling with the semi-infinite integrals involved in the analytical expressions of molecular multicenter integrals. The order of the linear set to resolve for calculating the approximation of the semi-infinite integral is equal to $(mn+1)$ or $((m-1)n+1)$ and can be very large if m and n increase.

We demonstrated that we can reduce the order of the differential equation satisfied by a function $f(x)$, which is of the form $f(x) = g(x) j_\lambda(x)$, where $g(x) \sim h(x)\mathrm{e}^{\phi(x)}$ as $x \to +\infty$ and where $h(x) \in \overline{A}^{(\gamma)}$ for some γ and $\phi(x)$ is a real polynomial of degree k in x as $x \to +\infty$.

This approach is now generalized and can be applicable to a large set of functions keeping all the other conditions required to apply D and $\overline{D}$ satisfied.

Theorem 2. Let $g(x)$ be a function in $C^2[0, +\infty[$ of the form

$$g(x) = h(x)\mathrm{e}^{\phi(x)}, \quad \text{where } h \in \overline{A}^{(\gamma)}, \phi \in \overline{A}^{(k)}, \quad \text{for some } \gamma \text{ and } k.$$

The function $f(x) = g(x) j_\lambda(x)$ satisfies the 2nd order linear differential equation

$$f(x) = p_1(x) f'(x) + p_2(x) f''(x), \tag{24}$$

where

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

Proof. By replacing in equation (14) $j_\lambda(x)$ by $f(x)/g(x)$, one can obtain the 2nd order linear differential equation (24) satisfied by $f(x)$, where

$$p_1(x) = \frac{2x^2(h'(x)/h(x) + \phi') - 2x}{w(x)}, \qquad p_2(x) = \frac{-x^2}{w(x)} \tag{25}$$

and

$$\begin{aligned} w(x) = -x^2\left[\left(\frac{h'(x)}{h(x)} + \phi'\right)' - \left(\frac{h'(x)}{h(x)} + \phi'\right)^2\right] \\ - 2x\left(\frac{h'(x)}{h(x)} + \phi'\right) + x^2 - \lambda^2 - \lambda. \end{aligned} \tag{26}$$

If $k = 0$ then $p_1(x) \in A^{(-1)}$ and $p_2(x) \in A^{(0)}$.
If $k \neq 0$ then $p_1(x) \in A^{(-k+1)}$ and $p_2(x) \in A^{(-2k+2)}$. □

The symbolic programming language Axiom [42] is used to develop analytically the expressions of $\alpha_0(p_1)$ and $\alpha_0(p_2)$:

$$\alpha_0(p_1) = \frac{\alpha_0(\phi)}{1 + \alpha_0(\phi)^2} \quad \text{and} \quad \alpha_0(p_2) = -\frac{1}{1 + \alpha_0(\phi)^2}.$$

$\alpha_0(p_1)$ and $\alpha_0(p_2)$ are not equal to zero, thus the coefficients $p_1(x)$ and $p_2(x)$ are in $\overline{A}^{(i)}$ and $\overline{A}^{(j)}$ where i and j are given in theorem 1.

Lemma 1. Let $f(x)$ be in $\overline{A}^{(\gamma)}$ for some γ. Then:

(1) If $g \in \overline{A}^{(\delta)}$ then $fg \in \overline{A}^{(\gamma+\delta)}$ and $\alpha_0(fg) = \alpha_0(f)\alpha_0(g)$.

(2) $\forall k \in \mathbb{R}$, $x^k f \in \overline{A}^{(k+\gamma)}$ and $\alpha_0(x^k f) = \alpha_0(f)$.

(3) For all $c \neq 0$, the function $cf \in \overline{A}^{(\gamma)}$ and $\alpha_0(cf) = c\alpha_0(f)$.

(4) If $g \in \overline{A}^{(\delta)}$ and $\gamma - \delta > 0$ then $f + g \in \overline{A}^{(\gamma)}$ and $\alpha_0(f + g) = \alpha_0(f)$. If $\gamma = \delta$ and $\alpha_0(f) \neq -\alpha_0(g)$ then $f + g \in \overline{A}^{(\gamma)}$ and $\alpha_0(f + g) = \alpha_0(f) + \alpha_0(g)$.

(5) Let $m > 0$ be an integer. If $\alpha_0(f) > 0$ then $f^m \in \overline{A}^{(m\gamma)}$ and $\alpha_0(f^m) = \alpha_0(f)^m$.

(6) Function $1/f \in \overline{A}^{(-\gamma)}$ and $\alpha_0(1/f) = 1/\alpha_0(f)$.

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

Lemma 2. Let $f \in \overline{A}^{(\gamma)}$ where $\gamma \in \mathbb{R}$ and $\gamma \neq 0$. Function $\widehat{k}_{n+1/2}(f(x))$ can be expressed by

$$\widehat{k}_{n+1/2}\big(f(x)\big) = f_1(x)\mathrm{e}^{-f(x)} \in \overline{A}^{(n\gamma)}\mathrm{e}^{\overline{A}^{(\gamma)}}, \quad \alpha_0(f_1) = \big(\alpha_0(f)\big)^n \neq 0.$$

By using the analytical expression of the reduced Bessel function which is given by equation (2), one can easily demonstrate lemma 2.

Theorem 3. If $g(x)$ is a function in $C^2[0, +\infty[$ of the form

$$g(x) = h(x)\mathrm{e}^{\phi(x)}$$

such that $h \in \overline{A}^{(\gamma)}$, $\phi \in \overline{A}^{(k)}$ with $k > 0$ and $\alpha_0(\phi) < 0$, then the function $f(x) = g(x)j_\lambda(x)$ is integrable on $[0, +\infty[$ and satisfies all the conditions of applicability of the nonlinear D- and $\overline{D}$-transformations.

Proof. The integrability of $f(x) = g(x)j_\lambda(x)$ on $[0, +\infty[$ follows from the fact that $g(x) \in C^2[0, +\infty[$ and $\lim_{x\to+\infty}\phi(x) = -\infty$ ($k > 0$ and $\alpha_0(\phi) < 0$).

By using theorem 2, we can show that $f(x)$ satisfies the 2nd order linear differential equation with coefficients $p_1(x) \in A^{(-k+1)}$ and $p_2(x) \in A^{(-2k+2)}$.

Function $f(x)$ is exponentially decreasing, then

$$\lim_{x\to+\infty} p_k^{(i-1)}(x)f^{(k-i)}(x) = 0, \quad k = 1, 2;\ i = 1, 2.$$

Since $p_1(x) \in A^{(-k+1)}$ and $p_2(x) \in A^{(-2k+2)}$, then

$$p_{1,0} = \lim_{x\to+\infty}\frac{1}{x}p_1(x) = 0 \quad \text{and} \quad p_{2,0} = \lim_{x\to+\infty}\frac{1}{x^2}p_2(x) = 0,$$

thus

$$\forall l \geqslant -1, \quad \sum_{k=1}^{2} l(l-1)\cdots(l-k+1)p_{k,0} = 0 \neq 1.$$

From theorem 1 it follows that $f(x)$ satisfies all the conditions of applicability of D and $\overline{D}$ for accelerating the convergence of $\int_0^{+\infty} f(t)\,\mathrm{d}t$.

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

$$HD_n^{(2)} = \int_0^{x_l} f(t)\,\mathrm{d}t + \sum_{k=0}^{1} f^{(k)}(x_l)x_l^{\sigma_k}\sum_{i=0}^{n-1}\frac{\overline{\beta}_{i,k}}{x_l^i}, \quad l = 0, 1, \ldots, 2n. \tag{27}$$

$HD_n^{(2)}$ and $\overline{\beta}_{i,k}$, $i = 0, 1, \ldots, n-1$, $k = 0, 1$, are the $(2n+1)$ unknowns of linear system (27).

By choosing $x_l = j_{\lambda+1/2}^{l+1}$ for $l = 0, 1, \ldots, n$, linear system of equations (27) can be rewritten as

$$H\overline{D}_n^{(2)} = \int_0^{x_l} f(t)\,\mathrm{d}t + g(x_l)\,j_\lambda'(x_l)x_l^{\sigma_1}\sum_{i=0}^{n-1}\frac{\overline{\beta}_{i,1}}{x_l^i}, \quad l = 0, 1, \ldots, n. \tag{28}$$

with the $(n+1)$ unknowns $H\overline{D}_n^{(2)}$ and $\overline{\beta}_{i,1}$, $i = 0, 1, \ldots, n-1$. □

4. Three-center two-electron Coulomb and hybrid integrals over B functions

The three-center two-electron Coulomb integrals:

$$\begin{aligned}\mathcal{K}_{n_1l_1m_1,n_3l_3m_3}^{n_2l_2m_2,n_4l_4m_4} &= \int_{\vec{R},\vec{R}'}\big[B_{n_1,l_1}^{m_1}\big[\zeta_1\big(\vec{R}-\overrightarrow{OA}\big)\big]\big]^*\big[B_{n_3,l_3}^{m_3}\big[\zeta_3\big(\vec{R}'-\overrightarrow{OB}\big)\big]\big]^*\\ &\quad\times\frac{1}{|\vec{R}-\vec{R}'|}B_{n_2,l_2}^{m_2}\big[\zeta_2\big(\vec{R}-\overrightarrow{OA}\big)\big]B_{n_4,l_4}^{m_4}\big[\zeta_4\big(\vec{R}'-\overrightarrow{OC}\big)\big]\,\mathrm{d}\vec{R}\,\mathrm{d}\vec{R}'\\ &= \int_{\vec{r},\vec{r}'}\big[B_{n_1,l_1}^{m_1}\big(\zeta_1\vec{r}\big)\big]^*\big[B_{n_3,l_3}^{m_3}\big[\zeta_3\big(\vec{r}'-\vec{R}_3\big)\big]\big]^*\frac{1}{|\vec{r}-\vec{r}'|}\\ &\quad\times B_{n_2,l_2}^{m_2}\big(\zeta_2\vec{r}\big)B_{n_4,l_4}^{m_4}\big[\zeta_4\big(\vec{r}'-\vec{R}_4\big)\big]\,\mathrm{d}\vec{r}\,\mathrm{d}\vec{r}',\end{aligned} \tag{29}$$

where $\vec{r} = \vec{R} - \overrightarrow{OA}$, $\vec{r}' = \vec{R}' - \overrightarrow{OA}$, $\vec{R}_3 = \overrightarrow{AB}$ and $\vec{R}_4 = \overrightarrow{AC}$.

The hybrid integrals:

$$\begin{aligned}\mathcal{H}_{n_1l_1m_1,n_3l_3m_3}^{n_2l_2m_2,n_4l_4m_4} &= \int_{\vec{R},\vec{R}'}\big[B_{n_1,l_1}^{m_1}\big[\zeta_1\big(\vec{R}-\overrightarrow{OA}\big)\big]\big]^*\big[B_{n_3,l_3}^{m_3}\big[\zeta_3\big(\vec{R}'-\overrightarrow{OA}\big)\big]\big]^*\frac{1}{|\vec{R}-\vec{R}'|}\\ &\quad\times B_{n_2,l_2}^{m_2}\big[\zeta_2\big(\vec{R}-\overrightarrow{OA}\big)\big]B_{n_4,l_4}^{m_4}\big[\zeta_4\big(\vec{R}'-\overrightarrow{OB}\big)\big]\,\mathrm{d}\vec{R}\,\mathrm{d}\vec{R}'\\ &= \int_{\vec{r},\vec{r}'}\big[B_{n_1,l_1}^{m_1}\big(\zeta_1\vec{r}\big)\big]^*\big[B_{n_3,l_3}^{m_3}\big(\zeta_3\vec{r}'\big)\big]^*\frac{1}{|\vec{r}-\vec{r}'|}B_{n_2,l_2}^{m_2}\big(\zeta_2\vec{r}\big)\\ &\quad\times B_{n_4,l_4}^{m_4}\big[\zeta_4\big(\vec{r}'-\vec{R}\big)\big]\,\mathrm{d}\vec{r}\,\mathrm{d}\vec{r}',\end{aligned} \tag{30}$$

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

The following arguments can also be applied to hybrid integrals.

Let us consider $\mathcal{K}_{n_1l_1m_1,n_3l_3m_3}^{n_2l_2m_2,n_4l_4m_4}$. By inserting the Fourier integral representation of the Coulomb operator (16) into (29), one can obtain

$$\begin{aligned}\mathcal{K}_{n_1l_1m_1,n_3l_3m_3}^{n_2l_2m_2,n_4l_4m_4} &= \frac{1}{2\pi^2}\int_{\vec{x}}\mathrm{e}^{\mathrm{i}\vec{x}\cdot\vec{R}_4}\big\langle B_{n_1l_1}^{m_1}\big(\zeta_1\vec{r}\big)\big|\mathrm{e}^{-\mathrm{i}\vec{x}\cdot\vec{r}}\big|B_{n_2l_2}^{m_2}\big(\zeta_2\vec{r}\big)\big\rangle_{\vec{r}}\\ &\quad\times\big\langle B_{n_4l_4}^{m_4}\big(\zeta_4\vec{r''}\big)\big|\mathrm{e}^{-\mathrm{i}\vec{x}\cdot\vec{r''}}\big|B_{n_3l_3}^{m_3}\big[\zeta_3\big(\vec{r''}-\big(\vec{R}_3-\vec{R}_4\big)\big)\big]\big\rangle_{\vec{r''}}^*\frac{\mathrm{d}\vec{x}}{x^2}.\end{aligned} \tag{31}$$

In the term $T_1 = \langle B_{n_1l_1}^{m_1}(\zeta_1\vec{r})|\mathrm{e}^{-\mathrm{i}\vec{x}\cdot\vec{r}}|B_{n_2l_2}^{m_2}(\zeta_2\vec{r})\rangle_{\vec{r}}$ involved in the above expression, the two B functions are centered on the same point and therefore the radial part of their

product has an analytical expression which can easily be obtained using equations (1) and (2). Consequently, T_1 has an analytical expression which is given by

$$\begin{aligned}
T_1 = {} & \left[2^{n_1+l_1+n_2+l_2}(n_1+l_1)!(n_2+l_2)!\right]^{-1}\zeta_1^{l_1}\zeta_2^{l_2}\sqrt{\frac{\pi}{2x}} \\
& \times \sum_{l=l_{\min},2}^{l_{\max}} (-\mathrm{i})^l \langle l_1 m_1 | l m_1 - m_2 | l_2 m_2\rangle \left[Y_l^{m_1-m_2}(\theta_{\vec{x}}, \varphi_{\vec{x}})\right]^* \\
& \times \sum_{k=2}^{n_1+n_2} \sum_{i=k_1}^{k_2} \left[\frac{(2n_1-i-1)!(2n_2-k+i-1)!\zeta_1^{i-1}\zeta_2^{k-i-1}}{(i-1)!(n_1-i)!(k-i-1)!(n_2-k+i)!2^{n_1+n_2-k}}\right] \\
& \times \frac{[x/2\zeta_s]^{l+1/2}\Gamma(k+l_1+l_2+l+1)}{\zeta_s^{k+l_1+l_2+1/2}\Gamma(l+3/2)}\left[1+\frac{x^2}{\zeta_s^2}\right]^{-k-l_1-l_2} \\
& \times {}_2F_1\left(\frac{l-k-l_1-l_2+1}{2}, \frac{l-k-l_1-l_2}{2}+1; l+\frac{3}{2}; -\frac{x^2}{\zeta_s^2}\right), \qquad (32)
\end{aligned}$$

where

$$k_1 = \max(1, k-n_2), \qquad k_2 = \min(n_1, k-1), \qquad \zeta_s = \zeta_1+\zeta_2$$

and where [38]

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

The subscript $l = l_{\min}, 2$ in the first summation symbol in equation (32) implies that the summation index l runs in steps of 2 from $l_{\min}$ to $l_{\max}$.

One of the arguments of the hypergeometric function $\eta/2 = (l-k-l_1-l_2+1)/2$ or $(l-k-l_1-l_2)/2+1 = (\eta+1)/2$ is a negative integer. By using equation (20), one can easily show that the hypergeometric series involved in equation (32) is reduced to a finite expansion:

$${}_2F_1\left(\frac{\eta}{2}, \frac{\eta+1}{2}; l+\frac{3}{2}; -\frac{x^2}{\zeta_s^2}\right) = \sum_{r=0}^{\eta'} (-1)^r \frac{(\eta/2)_r((\eta+1)/2)_r x^{2r}}{(l+3/2)_r r!\zeta_s^{2r}}, \qquad (33)$$

where $\eta' = -\eta/2$ if η is even, otherwise $\eta' = -(\eta+1)/2$.

By applying the Fourier transform method to the term in $\vec{r}''$ from equation (31) after substituting the Rayleigh expansion equation (10) of a plane wave, we obtain an expression for $\mathcal{K}_{n_1 l_1 m_1, n_3 l_3 m_3}^{n_2 l_2 m_2, n_4 l_4 m_4}$, involving a semi infinite very oscillatory integral, which is

given by [13,22,25]:

$$
\begin{aligned}
\mathcal{K}_{n_1l_1m_1,n_3l_3m_3}^{n_2l_2m_2,n_4l_4m_4} &= 8(4\pi)^3(2l_3+1)!!(2l_4+1)!!\zeta_1^{l_1}\zeta_2^{l_2}\zeta_3^{2n_3+l_3-1}\zeta_4^{2n_4+l_4-1}\\
&\times\frac{(n_3+l_3+n_4+l_4+1)!}{(n_3+l_3)!(n_4+l_4)!}\sum_{l=l_{\min,2}}^{l_{\max}}(-\mathrm{i})^l\langle l_1m_1|l_2m_2|lm_1-m_2\rangle\\
&\times\sum_{k=2}^{n_1+n_2}\sum_{i=k_1}^{k_2}\left[\frac{(2n_1-i-1)!(2n_2-i-1)!\zeta_1^{i-1}\zeta_2^{k-i-1}}{(i-1)!(n_1-i)!(k-i-1)!(n_2-k+i)!2^{n_1+n_2-k}}\right]\\
&\times\sum_{l_4'=0}^{l_4}\sum_{m_4'=-l_4'}^{l_4'}(\mathrm{i})^{l_4+l_4'}(-1)^{l_4'}\frac{\langle l_4m_4|l_4-l_4'm_4-m_4'|l_4'm_4'\rangle}{(2l_4'+1)!![2(l_4-l_4')+1]!!}\\
&\times\sum_{l_3'=0}^{l_3}\sum_{m_2'=-l_3'}^{l_3'}(\mathrm{i})^{l_3+l_3'}\frac{\langle l_3m_3|l_3-l_3'm_3-m_3'|l_3'm_3'\rangle}{(2l_3'+1)!![2(l_3-l_3')+1]!!}\\
&\times\sum_{l'=|l_3'-l_4'|}^{l_3'+l_4'}\left\langle l_4'm_4'\middle|l_3'm_3'\middle|l'm_4'-m_3'\right\rangle R_{34}^{l'}Y_{l'}^{m_4'-m_3'}(\theta_{\vec{R}_{34}},\varphi_{\vec{R}_{34}})\\
&\times\sum_{l_{34}}\left\langle l_3-l_3'm_3-m_3'\middle|l_4-l_4'm_4-m_4'\middle|l_{34}m_{34}\right\rangle\\
&\times\sum_{\lambda=|l-l_{34}|}^{l+l_{34}}\mathrm{i}^{\lambda}\left\langle lm_1-m_2\middle|l_{34}\middle(m_4-m_4'\middle)-\middle(m_3-m_3'\middle)\middle|\lambda\mu\right\rangle\\
&\times\sum_{j=0}^{\Delta l}\binom{\Delta l}{j}\frac{(-1)^j\Gamma(k+l_1+l_2+l+1)}{2^{n_3+n_4+l_3+l_4-j+1+l+1/2}(n_3+n_4+l_3+l_4-j+1)!}\\
&\times\frac{\zeta_s^{n_k-l-1}}{\Gamma(l+3/2)}\sum_{r=0}^{\eta'}(-1)^r\frac{(\eta/2)_r((\eta+1)/2)_r}{(l+3/2)_r r!\zeta_s^{2r}}\\
&\times\int_{s=0}^{1}s^{n_{33}}(1-s)^{n_{44}}Y_{\lambda}^{-\mu}(\theta_{\vec{v}},\varphi_{\vec{v}})\\
&\times\int_{x=0}^{+\infty}\left[\zeta_s^2+x^2\right]^{-n_k}x^{n_x+1/2}j_{\lambda}(vx)\frac{\widehat{k}_v[R_{34}\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}\,\mathrm{d}x\,\mathrm{d}s, \qquad (34)
\end{aligned}
$$

where

$$
\begin{aligned}
&k_1=\max(1,k-n_2),\quad k_2=\min(n_1,k-1),\quad \zeta_s=\zeta_1+\zeta_2,\\
&\left|\left(l_3-l_3'\right)-\left(l_4-l_4'\right)\right|\leqslant l_{34}\leqslant\left(l_3-l_3'\right)+\left(l_4-l_4'\right),\\
&n_x=l_3-l_3'+l_4-l_4'+2r+l,\quad n_k=k+l_1+l_2,\\
&n_{33}=n_3+l_3+l_4-l_4',\quad n_{44}=n_4+l_4+l_3-l_3',
\end{aligned}
$$

$$
\begin{aligned}
&n_\gamma = 2(n_3 + l_3 + n_4 + l_4) - \left(l_3' + l_4'\right) - l' + 1,\\
&\mu = (m_1 - m_2) - \left(m_4 - m_4'\right) + \left(m_3 - m_3'\right),\\
&\left[\gamma(s,x)\right]^2 = (1-s)\zeta_4^2 + s\zeta_3^2 + s(1-s)x^2,\\
&\eta' = -\eta/2 \text{ if } \eta \text{ is even, otherwise } \eta' = -(\eta+1)/2,\\
&\eta = l - k - l_1 - l_2 + 1, \quad \Delta l = (l_3 + l_4 - l')/2,\\
&\vec{v} = s\left(\vec{R}_3 - \vec{R}_4\right) - \vec{R}_3 = s\vec{R}_{34} - \vec{R}_3,\\
&\nu = n_3 + n_4 + l_3 + l_4 - l' - j + 1/2,\\
&m_{34} = \left(m_3 - m_3'\right) - \left(m_4 - m_4'\right).
\end{aligned}
$$

The numerical evaluation of the above analytical expression presents severe numerical and computational difficulties. This is due to the presence of the semi-infinite integrals, which will be referred to as $\widetilde{\mathcal{K}}(s)$, whose integrands oscillate rapidly, due to the presence of 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 use of Gauss–Laguerre quadrature even to high order gives inaccurate results in particular when s is close to 0 or 1. This region carry a very small weight because of the expression $s^{n_{33}}(1-s)^{n_{44}}$ [19–21,43–45].

The epsilon algorithm of Wynn [46] and Levin's u-transform [47] were also used [48] to accelerate the convergence of the semi-infinite integral after transforming it into infinite series

$$
\widetilde{\mathcal{K}}(s) = \sum_{n=0}^{+\infty} \int_{j_{\lambda,v}^n}^{j_{\lambda,v}^{n+1}} \left[\zeta_s^2 + x^2\right]^{-n_k} x^{n_x+1/2} j_\lambda(vx) \frac{\widehat{k}_\nu[R_{34}\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}\,\mathrm{d}x. \tag{35}
$$

Unfortunately, as it has been shown [24,25], the use of these methods is prohibitively long for sufficient accuracy.

Now, let us consider the integrand of $\widetilde{\mathcal{K}}(s)$ given by

$$
f_{k,s}(x) = g_k(x) j_\lambda(vx),
$$

where

$$
g_k(x) = x^{n_x - 2n_k + 1/2}\left[1 + \frac{\zeta_s^2}{x^2}\right]^{-n_k} \frac{\widehat{k}_\nu[R_{34}\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}.
$$

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

$$
\phi(x) = R_{34}\gamma(s,x) = R_2\sqrt{(1-s)\zeta_4^2 + s\zeta_3^2 + s(1-s)x^2}.
$$

From lemma 1, it follows that $\phi(x) \in \overline{A}^{(1)}$ and $1/[\gamma(s,x)]^{n_\gamma} \in \overline{A}^{(-n_\gamma)}$. Using lemmas 1 and 2, we can obtain an expression for $g_k(x)$, which is given by

$$
g_k(x) = g_1(x)\mathrm{e}^{-\phi(x)} \quad \text{where} \quad \begin{cases} g_1 \in \overline{A}^{(n+n_x-2n_k-n_\gamma-1/2)}, \\ \phi \in \overline{A}^{(1)} \text{ with } \alpha_0(\phi) > 0. \end{cases}
$$

By using theorem 2, we can show that $f_{k,s}(x)$ satisfies 2nd order linear differential equation of the form given by equation (24). From theorem 3, it follows that $f_{k,s}(x)$ is integrable on $[0, +\infty[$ and satisfies all the conditions of applicability of D- and $\overline{D}$-transformations. Since $f_{k,s}(x)$ is exponentially decreasing, $\sigma_k = k + 1$.

The approximations $H\overline{D}_n{}^{(2)}$ of $\widetilde{\mathcal{K}}(s)$ can be obtained by solving the following set of linear equations:

$$H\overline{D}_n^{(2)} = \int_0^{x_l} f(t)\,\mathrm{d}t + g(x_l) j'_\lambda(vx) x_l^2 \sum_{i=0}^{n-1} \frac{\overline{\beta}_{i,1}}{x_l^i}, \quad l = 0, 1, \ldots, n, \tag{36}$$

where $x_l = j_{\lambda,v}^{l+1}$, $n = 0, 1, 2, \ldots$, which are the successive zeros of $j_l(vx)$. $H\overline{D}_n^{(2)}$ and $\overline{\beta}_{i,1}$ for $i = 0, 1, \ldots, n-1$ are the $(n+1)$ unknowns of linear system (36).

For the hybrid integral, the integrand $f_{h,s}(x)$ of the semi-infinite integral which will be referred to as $\widetilde{\mathcal{H}}(s)$ is given by

$$f_{h,s}(x) = \left[\zeta_s^2 + x^2\right]^{-n_k} x^{n_x+1/2} j_\lambda(vx) \frac{\widehat{k}_v[R_1\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}},$$

where $\vec{v} = s\vec{R}_1$ and all the other arguments are defined according to the equation (34).

Using the same arguments, one can show that $f_{h,s}(x)$ satisfies a 2nd order differential equation of the form required to apply the D- and $\overline{D}$-transformations. The approximation $H\overline{D}_n^{(2)}$ of $\widetilde{\mathcal{H}}(s)$ can be obtained by solving equation (36).

5. Convergence properties

Let us consider the linear system equation (22). We let

$$S = \int_0^{+\infty} f(t)\,\mathrm{d}t, \qquad F(x) = \int_0^x f(t)\,\mathrm{d}t$$

and $\Phi_k(x) = x^{\sigma_k} f^{(k)}(x)$ for $k = 0, 1, \ldots, m-1$. Let vector $(\gamma_0, \gamma_1, \ldots, \gamma_{mn})$ be the first row of the inverse of the matrix of the system equation (22).

Using the fact that the first column of the matrix of the linear system equation (22) is the vector $(1, 1, \ldots, 1)^{\mathrm{T}}$ ($^{\mathrm{T}}$ denotes transpose), we can easily show that $\sum_{l=0}^{mn} \gamma_l = 1$ and therefore $\sum_{l=0}^{mn} |\gamma_l| \geqslant 1$.

Corollary 1 [49].

$$\left|S - D_n^{(m)}\right| \leqslant \left(\sum_{l=0}^{mn} |\gamma_l|\right) \mathrm{o}\left(n^{-j}\right), \quad \forall j > 0 \text{ as } n \to +\infty.$$

Corollary 2 [49]. If $\sum_{l=0}^{mn} |\gamma_l| \leqslant L < \infty$, then

$$\left|S - D_n^{(m)}\right| = \mathrm{o}\left(n^{-j}\right), \quad \forall j > 0 \text{ as } n \to +\infty. \tag{37}$$

Now, let us consider the linear system given by equation (28). We define the matrix M_2 by

$$M_2 = \begin{pmatrix} \frac{F(x_0)}{\Phi_1(x_0)} & \frac{F(x_1)}{\Phi_1(x_1)} & \cdots & \frac{F(x_n)}{\Phi_1(x_n)} \\ 1 & 1 & \cdots & 1 \\ x_0^{-1} & x_1^{-1} & \cdots & x_n^{-1} \\ \vdots & \vdots & & \vdots \\ x_0^{-n+1} & x_1^{-n+1} & \cdots & x_n^{-n+1} \end{pmatrix} \tag{38}$$

and let K_2 be the matrix obtained after replacing the first row of M_2 by the vector

$$\left(\frac{1}{\Phi_1(x_0)}, \frac{1}{\Phi_1(x_1)}, \ldots, \frac{1}{\Phi_1(x_n)}\right).$$

Let V_l be the minor of $F(x_l)/\Phi_1(x_l)$ in M_2 or of $1/\Phi_1(x_l)$ in K_2. Using the Cramer's rule, one can express $H\overline{D}_n^{(2)}$ as

$$H\overline{D}_n^{(2)} = \frac{\det(M_2)}{\det(K_2)} = \frac{\sum_{l=0}^{n}(-1)^l[V_l/\Phi_1(x_l)]F(x_l)}{\sum_{l=0}^{n}(-1)^l[V_l/\Phi_1(x_l)]}. \tag{39}$$

The minors V_l, $l = 0, 1, \ldots, n$, are given by

$$V_0 = V\left(x_1^{-1}, \ldots, x_n^{-1}\right), \qquad V_n = V\left(x_0^{-1}, \ldots, x_{n-1}^{-1}\right),$$
$$V_l = V\left(x_0^{-1}, \ldots, x_{l-1}^{-1}, x_{l+1}^{-1}, \ldots, x_{n-1}^{-1}\right), \quad l = 1, \ldots, n-1,$$

where $V(x_0, x_1, \ldots, x_{n-1})$ is the Vandermonde determinant which can be expressed by

$$V(x_0, x_1, \ldots, x_{n-1}) = \prod_{0 \leqslant i < j \leqslant n-1} (x_j - x_i). \tag{40}$$

Since $x_0 < x_1 < \cdots < x_{n-1}$, it follows that $V(x_0, x_1, \ldots, x_{n-1}) > 0$, and therefore all V_l, for $l = 0, 1, \ldots, n$ have the same sign.

Using the fact that $H\overline{D}_n^{(2)} = \sum_{l=0}^{n} \gamma_l F(x_l)$, we can obtain

$$\gamma_l = \frac{(-1)^l[V_l/\Phi_1(x_l)]}{\sum_{i=0}^{n}(-1)^i[V_i/\Phi_1(x_i)]}, \quad 0 \leqslant l \leqslant n. \tag{41}$$

Using the fact that $x_l = j_{\lambda+1/2}^l$, for $l = 0, 1, \ldots$, which are the successive zeros of $j_\lambda(x)$, one can easily show that the function $\Phi_1(x) = x^{\sigma_1} g(x) j_\lambda'(x)$ satisfies

$$\Phi_1(x_l)\Phi_1(x_{l+1}) < 0, \quad l = 0, 1, 2, \ldots. \tag{42}$$

It is easy to show that all $(-1)^l[V_l/\Phi_1(x_l)]$, for $l = 0, 1, \ldots, n$, have the same sign. Therefore, $\forall l$, $\gamma_l > 0$ holds and, consequently,

$$\sum_{l=0}^{n} |\gamma_l| = \sum_{l=0}^{n} \gamma_l = 1.$$

Now corollary 2 becomes:

Corollary 3. $|S - H\overline{D}_n^{(2)}| = o(n^{-j}), \forall j > 0$ as $n \to +\infty$.

The convergence properties of the nonlinear $H\overline{D}$-transformation are without any constraint. From the numerical point of view, the situation in which $\gamma_l > 0$, $\forall l$, corresponds to the most ideal one.

6. Conclusion

This work presents a general approach for reducing the order of the differential equation required to apply the nonlinear D- and $\overline{D}$-transformations, keeping all the other conditions satisfied. The integrand should be of the form $f(x) = g(x)j_\lambda(x)$, where $g(x) = h(x)e^{\phi(x)}$ and where $h \in \overline{A}^{(\gamma)}$, $\phi \in \overline{A}^{(k)}$ with $k > 0$ and $\alpha_0(\phi) < 0$.

These conditions are now shown to be satisfied by the integrands of the semi-infinite integrals involved in the analytical expressions of molecular bielectronic integrals over B functions, which occur in molecular context and are numerous and difficult to evaluate. Therefore rapidity is the primordial criterion when the precision has been reached.

The present work illustrates the substantial optimisation regarding calculation times obtained using the $H\overline{D}$ method over the nonlinear D- and $\overline{D}$-transformations, which as we showed [24,28] are more rapid than Levin's u-transform and the ε-algorithm of Wynn.

7. Numerical results

The symbolic programming language Axiom was used to provide the exact values of $\widetilde{\mathcal{K}}(s)$ and $\widetilde{\mathcal{H}}(s)$ to 20 exact decimals using the infinite series (35) which we sum until $N = \max$ (see tables 1 and 4).

Table 1
Exact values of $\widetilde{\mathcal{K}}(s)$ obtained with 20 correct decimals ($n_x = \lambda$, $\nu = n_3 + n_4 + 1/2$, $n_\gamma = 2(n_3 + n_4) + 1$, $\zeta_3 = \zeta_1$ and $\zeta_4 = \zeta_2$).

s	n_3	n_4	n_k	λ	R_3	ζ_1	R_4	ζ_2	max	$\widetilde{\mathcal{K}}(s)$
0.005	1	1	2	0	2.5	1.5	1.5	0.5	81	0.1711045428280131D+01
0.005	2	1	3	1	4.5	2.5	4.0	1.5	225	0.8773983854881832D−05
0.999	2	2	3	2	3.0	2.0	2.5	2.5	292	0.6582270306670542D−05
0.999	3	2	2	3	3.5	1.5	2.5	0.5	304	0.2602612259522619D+00
0.999	3	3	3	4	2.0	2.0	1.5	1.5	186	0.7482795301329374D−02
0.010	4	3	3	4	3.5	2.0	3.0	1.5	116	0.4784629408043506D−01
0.999	4	3	5	5	6.5	1.0	5.5	0.5	145	0.3900383649993194D+02
0.005	4	4	5	5	4.5	1.5	3.0	1.0	67	0.2412209767998331D+02

Table 2
Evaluation of $\widetilde{\mathcal{K}}(s)$ using $H\overline{D}$ of order n. Time T is in msecs ($n_x = \lambda$, $\nu = n_3 + n_4 + 1/2$, $n_\gamma = 2(n_3 + n_4) + 1$, $\zeta_3 = \zeta_1$ and $\zeta_4 = \zeta_2$).

s	n_3	n_4	n_k	λ	R_3	ζ_3	R_4	ζ_4	n	$\widetilde{\mathcal{K}}(s)$	Error	T
0.005	1	1	2	0	2.5	1.5	1.5	0.5	5	0.1711045428D+01	0.82D−10	0.02
0.005	2	1	3	1	4.5	2.5	4.0	1.5	5	0.8773983369D−05	0.49D−12	0.03
0.999	2	2	3	2	3.0	2.0	2.5	2.5	5	0.6582262522D−05	0.78D−11	0.03
0.999	3	2	2	3	3.5	1.5	2.5	0.5	8	0.2602612260D+00	0.12D−12	0.06
0.999	3	3	3	4	2.0	2.0	1.5	1.5	5	0.7482795317D−02	0.15D−10	0.02
0.010	4	3	3	4	3.5	2.0	3.0	1.5	9	0.4784629403D−01	0.49D−10	0.07
0.999	4	3	5	5	6.5	1.0	5.5	0.5	8	0.3900383650D+02	0.12D−10	0.05
0.005	4	4	5	5	4.5	1.5	3.0	1.0	9	0.2412209768D+02	0.20D−09	0.07

Table 3
Evaluation of $\widetilde{\mathcal{K}}(s)$ using $\overline{D}$ of order n. Time T is in msecs ($n_x = \lambda$, $\nu = n_3+n_4+1/2$, $n_\gamma = 2(n_3+n_4)+1$, $\zeta_3 = \zeta_1$ and $\zeta_4 = \zeta_2$).

s	n_3	n_4	n_k	λ	R_3	ζ_3	R_4	ζ_4	n	$\widetilde{\mathcal{K}}(s)$	Error	T
0.005	1	1	2	0	2.5	1.5	1.5	0.5	3	0.1711045428D+01	0.14D−10	0.05
0.005	2	1	3	1	4.5	2.5	4.0	1.5	3	0.8773984785D−05	0.93D−12	0.05
0.999	2	2	3	2	3.0	2.0	2.5	2.5	3	0.6582271450D−05	0.11D−11	0.05
0.999	3	2	2	3	3.5	1.5	2.5	0.5	4	0.2602612260D+00	0.41D−11	0.10
0.999	3	3	3	4	2.0	2.0	1.5	1.5	3	0.7482795284D−02	0.17D−10	0.05
0.010	4	3	3	4	3.5	2.0	3.0	1.5	4	0.4784629410D−01	0.18D−10	0.11
0.999	4	3	5	5	6.5	1.0	5.5	0.5	4	0.3900383650D+02	0.10D−09	0.10
0.005	4	4	5	5	4.5	1.5	3.0	1.0	4	0.2412209768D+02	0.19D−09	0.10

Table 4
Exact values of $\widetilde{\mathcal{H}}(s)$ obtained with 20 correct decimals ($n_x = \lambda$, $\nu = n_3 + n_4 + 1/2$, $n_\gamma = 2(n_3 + n_4) + 1$ and $\zeta_1 = \zeta_2 = 0.50$).

s	n_3	n_4	n_k	λ	R_1	ζ_3	ζ_4	max	$\widetilde{\mathcal{H}}(s)$
0.999	1	1	2	0	2.0	1.5	1.0	106	0.4389694792638539D−01
0.999	2	1	2	1	2.5	1.0	1.0	128	0.8381930319971030D+00
0.999	2	2	2	2	4.5	1.5	0.5	225	0.6591267598109963D−02
0.999	2	2	3	2	3.0	1.5	0.5	123	0.2511838981888497D−01
0.999	3	2	3	2	5.0	2.0	1.0	177	0.1464115160117386D−03
0.999	3	3	3	3	4.5	1.5	0.5	168	0.1444960390423629D+00
0.999	4	3	3	3	2.0	2.0	1.0	109	0.7352140095334253D−01
0.999	4	4	4	4	4.0	2.0	1.0	139	0.2113558106217673D−01

All the finite integrals are evaluated using the Gauss–Legendre quadrature of order 16. The linear systems (28) and (36) are solved using the LU decomposition method.

In the numerical evaluation of $\mathcal{K}_{n_1 00, n_3 00}^{n_2 00, n_4 00}$, we let n_x and λ vary to show the efficiency of the new methods in the evaluation of the semi-infinite integrals whose integrands are very oscillating (see tables 7–9).

The calculation times are computed using an IBM RS6000 340 to illustrate the rapidity of the new method for a high predetermined accuracy.

Table 5
Evaluation of $\widetilde{\mathcal{H}}(s)$ using $H\overline{D}$ of order n. Time T is in msecs ($n_x = \lambda$, $\nu = n_3 + n_4 + 1/2$, $n_\gamma = 2(n_3 + n_4) + 1$ and $\zeta_1 = \zeta_2 = 0.50$).

s	n_3	n_4	n_k	λ	R_1	ζ_3	ζ_4	n	$\widetilde{\mathcal{H}}(s)$	Error	T
0.999	1	1	2	0	2.0	1.5	1.0	6	0.4389694793D−01	0.52D−12	0.03
0.999	2	1	2	1	2.5	1.0	1.0	5	0.8381930327D+00	0.70D−09	0.02
0.999	2	2	2	2	4.5	1.5	0.5	6	0.6591267592D−02	0.66D−11	0.03
0.999	2	2	3	2	3.0	1.5	0.5	6	0.2511838982D−01	0.66D−12	0.03
0.999	3	2	3	2	5.0	2.0	1.0	6	0.1464115159D−03	0.76D−13	0.03
0.999	3	3	3	3	4.5	1.5	0.5	5	0.1444960396D+00	0.57D−09	0.03
0.999	4	3	3	3	2.0	2.0	1.0	6	0.7352140096D−01	0.52D−11	0.03
0.999	4	4	4	4	4.0	2.0	1.0	6	0.2113558106D−01	0.35D−12	0.03

Table 6
Evaluation of $\widetilde{\mathcal{H}}(s)$ using $\overline{D}$ of order n. Time T is in msecs ($n_x = \lambda$, $\nu = n_3+n_4+1/2$, $n_\gamma = 2(n_3+n_4)+1$ and $\zeta_1 = \zeta_2 = 0.50$).

s	n_3	n_4	n_k	λ	R_1	ζ_3	ζ_4	n	$\widetilde{\mathcal{H}}(s)$	Error	T
0.999	1	1	2	0	2.0	1.5	1.0	3	0.4389694793D−01	0.37D−12	0.06
0.999	2	1	2	1	2.5	1.0	1.0	3	0.8381930323D+00	0.34D−09	0.05
0.999	2	2	2	2	4.5	1.5	0.5	3	0.6591267633D−02	0.34D−10	0.06
0.999	2	2	3	3	3.0	1.5	0.5	3	0.2511838982D−01	0.41D−12	0.05
0.999	3	2	3	3	5.0	2.0	1.0	3	0.1464115161D−03	0.96D−13	0.05
0.999	3	3	3	3	4.5	1.5	0.5	3	0.1444960392D+00	0.15D−09	0.05
0.999	4	3	3	4	2.0	2.0	1.0	3	0.7352140096D−01	0.53D−11	0.06
0.999	4	4	4	4	4.0	2.0	1.0	3	0.2113558106D−01	0.16D−11	0.05

Table 7
Exact values of $\mathcal{K}_{n_100,n_300}^{n_200,n_400}$ obtained with 20 correct decimals ($\zeta_1 = \zeta_3$ and $\zeta_2 = \zeta_4$).

n_1	n_2	n_3	n_4	n_γ	R_3	ζ_3	R_4	ζ_4	$\mathcal{K}_{n_100,n_200}^{n_300,n_400}$
1	1	1	1	5	6.50	2.50	2.00	1.00	0.1499696884201018D−01
2	1	2	1	7	6.50	4.00	4.00	3.00	0.1131392221111710D+00
2	2	2	2	9	8.00	3.50	2.00	3.00	0.4605249321948066D+01
2	2	3	2	11	9.50	3.50	3.00	3.00	0.1849981520442438D+01
2	2	3	3	13	7.00	2.50	3.00	3.00	0.1069300805307034D+04
2	2	4	3	15	9.50	3.50	4.00	3.00	0.1097122311454484D+02
2	2	4	4	17	8.00	3.00	3.50	3.50	0.1356218523398202D+02

Acknowledgements

Special thanks from the author to Professor André Joyal from Département de Mathématiques, Université du Québec à Montréal, and Professor Cherif Hamzaoui from Département de Physique, Université du Québec à Montréal, for their helpful assistance.

Table 8
Evaluation of $\mathcal{K}_{n_100,n_300}^{n_200,n_400}$ using $H\overline{D}$ of order n. Time T is in msecs ($n_\gamma = 2(n_3+n_4)+1$, $\zeta_3 = \zeta_1$ and $\zeta_4 = \zeta_2$).

n_1	n_2	n_3	n_4	R_3	ζ_1	R_4	ζ_2	n	$\mathcal{K}_{n_100,n_300}^{n_200,n_400}$	Error	T
1	1	1	1	6.5	2.5	2.0	1.0	9	0.1499696884D−01	0.38D−12	1.10
2	1	2	1	6.5	4.0	4.0	3.0	9	0.1131392222D+00	0.43D−10	3.23
2	2	2	2	8.0	3.5	2.0	3.0	10	0.4605249322D+01	0.17D−09	6.81
2	2	3	2	9.5	3.5	3.0	3.0	9	0.1849981521D+01	0.59D−09	5.47
2	2	3	3	7.0	2.5	3.0	3.0	9	0.1069300805D+04	0.12D−08	5.42
2	2	4	3	9.5	3.5	4.0	3.0	10	0.1097122311D+02	0.57D−09	6.86
2	2	4	4	8.0	3.0	3.5	3.5	10	0.1356218523D+02	0.29D−10	6.87

Table 9
Evaluation of $\mathcal{K}_{n_100,n_300}^{n_200,n_400}$ using $\overline{D}$ of order n. Time T is in msecs ($n_\gamma = 2(n_3+n_4)+1$, $\zeta_3 = \zeta_1$ and $\zeta_4 = \zeta_2$).

n_1	n_2	n_3	n_4	R_3	ζ_1	R_4	ζ_2	n	$\mathcal{K}_{n_100,n_300}^{n_200,n_400}$	Error	T
1	1	1	1	6.5	2.5	2.0	1.0	4	0.14996968D−01	0.11D−12	1.65
2	1	2	1	6.5	4.0	4.0	3.0	4	0.11313922D+00	0.13D−10	5.01
2	2	2	2	8.0	3.5	2.0	3.0	4	0.46052493D+01	0.37D−09	8.38
2	2	3	2	9.5	3.5	3.0	3.0	4	0.18499815D+01	0.10D−09	8.42
2	2	3	3	7.0	2.5	3.0	3.0	4	0.10693008D+04	0.11D−08	8.40
2	2	4	3	9.5	3.5	4.0	3.0	4	0.10971223D+02	0.92D−09	8.41
2	2	4	4	8.0	3.0	3.5	3.5	4	0.13562185D+02	0.76D−10	8.38

References

[1] I. Shavitt, The Gaussian function in calculation of statistical mechanics and quantum mechanics, in: *Methods in Computational Physics*, Vol. 2, *Quantum Mechanics*, eds. B. Alder, S. Fernbach and M. Rotenberg (Academic Press, New York, 1963).

[2] E.O. Steinborn and E. Filter, Translations of fields represented by spherical-harmonics expansions for molecular calculations. III. Translations of reduced Bessel functions, Slater-type s-orbitals, and other functions, Theor. Chim. Acta 38 (1975) 273.

[3] E. Filter and E.O. Steinborn, Extremely compact formulas for molecular one-electron integrals and Coulomb integrals over Slater-type orbitals, Phys. Rev. A 18 (1978) 1.

[4] E. Filter, Analytische Methoden zur Auswertung von Mehrzentren-Matrixelementen in der Theorie der Molekülorbitale bei Verwendung exponentialartiger Basissätze, Ph.D. thesis, Universität Regensburg (1978).

[5] E.J. Weniger, Reduzierte Bessel-Funktionen als LCAO-Basissatz: Analytische und numerische Untersuchungen, Ph.D. thesis, Universität Regensburg (1982).

[6] E.J. Weniger and E.O. Steinborn, The Fourier transforms of some exponential-type functions and their relevance to multicenter problems, J. Chem. Phys. 78 (1983) 6121.

[7] F.P. Prosser and C.H. Blanchard, On the evaluation of two-center integrals, J. Chem. Phys. 36 (1962) 1112.

[8] R.A. Bonham, J.L. Peacher and H.L. Cox, On the calculation of multicenter two-electron repulsion integrals involving Slater functions, J. Chem. Phys. 40 (1964) 3083.

[9] E.O. Steinborn and E.J. Weniger, Advantages of reduced Bessel functions as atomic orbitals: An application to H_2^+, Int. J. Quantum. Chem. Symp. 11 (1977) 509.

[10] E.O. Steinborn and E.J. Weniger, Reduced Bessel functions as atomic orbitals: some mathematical aspects and LCAO-MO treatment of HeH^{++}, Int. J. Quantum Chem. Symp. 12 (1978) 103.
[11] E.O. Steinborn, *Methods in Computational Molecular Physics*, eds. H.H. Dierckesen and S. Wilson (D. Reidel, Dordrecht, 1983).
[12] H.P. Trivedi and E.O. Steinborn, Fourier transform of a two-center product of exponential-type orbitals. Application to one- and two-electron multicenter integrals, Phys. Rev. A 27 (1983) 670.
[13] J. Grotendorst, Berechnung der Mehrzentren-Molekülintegrale mit Exponentialartigen Basis Funktionen durch systematische Anwendung der Fourier-Transformationsmethode, Ph.D. thesis, Universität Regensburg (1985).
[14] J. Grotendorst, E.J. Weniger and E.O. Steinborn, Efficient evaluation of infinite-series representations for overlap, two-center nuclear attraction, and Coulomb integrals using nonlinear convergence accelerators, Phys. Rev. A 33 (1986) 3706.
[15] E.J. Weniger and E.O. Steinborn, Comment on "Molecular overlap integrals with exponential-type orbitals", J. Chem. Phys. 87 (1987) 3709.
[16] J. Grotendorst and E.O. Steinborn, Numerical evaluation of molecular one- and two-electron multicenter integrals with exponential-type orbitals via the Fourier-transform method, Phys. Rev. A 38 (1988) 3857.
[17] E.J. Weniger and E.O. Steinborn, Overlap integrals of B functions. A numerical study of infinite series representations and integrals representations, Theor. Chim. Acta 73 (1988) 323.
[18] E.O. Steinborn, H.H.H. Homeier and E.J. Weniger, Recent progress on representations for Coulomb integrals of exponential-type orbitals, J. Mol. Struct. (THEOCEM) 260 (1992) 207.
[19] H.H.H. Homeier and E.O. Steinborn, Improved quadrature methods for the Fourier transform of a two-center product of exponential-type basis functions, Int. J. Quantum Chem. 41 (1992) 399.
[20] H.H.H. Homeier and E.O. Steinborn, On the evaluation of overlap integrals with exponential-type basis functions, Int. J. Quantum Chem. 42 (1992) 761.
[21] H.H.H. Homeier, E.J. Weniger and E.O. Steinborn, Program for the evaluation of overlap integrals with B functions, Comput. Phys. Commun. 72 (1992) 269.
[22] H.H.H. Homeier, *Integraltransformationsmethoden und Quadraturverfahren für Molekülintegrale mit B-Functionen* (S. Roderer Verlag, Regensburg, 1990); also: Ph.D. thesis, Universität Regensburg (1990).
[23] E.J. Weniger, Nonlinear sequence transformations for the acceleration of convergence and the summation of divergent series, Comput. Phys. Rep. 10 (1989) 189.
[24] H. Safouhi and P.E. Hoggan, Three-centre two electron Coulomb and hybrid integrals evaluated using nonlinear D- and $\overline{D}$-transformations, J. Phys. A: Math. Gen. 32 (1999) 6203.
[25] H. Safouhi, Nonlinear transformations for accelerating the convergence of molecular multicenter bielectronic integrals, Ph.D. thesis, Université de Blaise Pascal, Clermont-Ferrand, France (1999).
[26] D. Levin and A. Sidi, Two new classes of non-linear transformations for accelerating the convergence of infinite integrals and series, Appl. Math. Comput. 9 (1981) 175.
[27] A. Sidi, Extrapolation methods for oscillating infinite integrals, J. Inst. Math. Appl. 26 (1980) 1.
[28] H. Safouhi and P.E. Hoggan, Efficient and rapid evaluation of three-center two-electron Coulomb and hybrid integrals using nonlinear transformations, J. Comput. Phys. 155 (1999) 331.
[29] E.U. Condon and G.H. Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, Cambridge, UK, 1970).
[30] G.B. Arfken and H.J. Weber, *Mathematical Methods for Physicists* (Academic Press, New York, 1995).
[31] J.C. Slater, Atomic shielding constants, Phys. Rev. 36 (1930) 57.
[32] J.C. Slater, Analytic atomic wave functions, Phys. Rev. 42 (1932) 33.
[33] I.M. Gel'fand and G.E. Shilov, *Generalized Functions I. Properties and Operations* (Academic Press, New York, 1964).
[34] M. Weissbluth, *Atoms and Molecules* (Academic Press, New York, 1978).

[35] J.A. Gaunt, The triplets of heluim, Phil. Trans. Roy. Soc. Ser. A 228 (1929) 151.
[36] H.H.H. Homeier and E.O. Steinborn, Some properties of the coupling coefficients of real spherical harmonics and their relation to Gaunt coefficients, J. Mol. Struct. (THEOCEM) 368 (1996) 31.
[37] D. Sébilleau, On the computation of the integrated product of three spherical harmonics, J. Phys. A 31 (1998) 7157.
[38] E.J. Weniger and E.O. Steinborn, Programs for the coupling of spherical harmonics, Comput. Phys. Comm. 25 (1982) 149.
[39] Yu-Lin Xu, Fast evaluation of Gaunt coefficients, Math. Comput. 65 (1996) 1601.
[40] Yu-Lin Xu, Fast evaluation of Gaunt coefficients: recursive approach, J. Comput. Appl. Math. 85 (1997) 53.
[41] Yu-Lin Xu, Efficient evaluation of vector translation coefficients in multiparticle light-scattering theories, J. Comput. Phys. 139 (1998) 137.
[42] R.D. Jenks and R.S. Sutor, *Axiom, The Scientific Computation System* (Springer, New York, 1992).
[43] E.O. Steinborn and H.H.H. Homeier, Möbius-type quadrature of electron repulsion integrals with B functions, Int. J. Quantum. Chem. 24 (1990) 349.
[44] H.H.H. Homeier and E.O. Steinborn, Numerical integration of a function with a sharp peak at or near one boundary using Möbius transformations, J. Comput. Phys. 87 (1990) 61.
[45] H.H.H. Homeier and E.O. Steinborn, Improved quadrature methods for three-center nuclear attraction integrals with exponential-type basis functions, Int. J. Quantum. Chem. 39 (1991) 625.
[46] P. Wynn, On a device for computing the $e_m(S_n)$ transformation, Math. Tables Aids Comput. 10 (1956) 91.
[47] D. Levin, Development of non-linear transformations for improving convergence of sequences, Int. J. Comput. Math. B 3 (1973) 371.
[48] E.J. Weniger, J. Grotendorst and E.O. Steinborn, Unified analytical treatement of overlap, two-center nuclear attraction, and Coulomb integrals over B functions via the Fourier-transform method, Phys. Rev. A 33 (1986) 3688.
[49] A. Sidi, Some properties of a generalization of the Richardson process, J. Inst. Maths. Appl. 24 (1979) 327.
[50] A. Sidi, Convergence properties of some non-linear sequence transformations, Math. Comput. 33 (1979) 315.
[51] T. Kato, On the eigenfunctions of many-particle systems in quantum mechanics, Comm. Pure Appl. Math. 10 (1957) 151.
[52] S.F. Boys, The integral formulae for the variational solution of the molecular many-electron wave equation in terms of Gaussian functions with direct electronic correlation, Proc. Roy. Soc. Ser. A. 258 (1960) 402.
[53] C.A. Weatherford and H.W. Jones, eds., *International Conference on ETO Multicenter Integrals*, Tallahasse, 1981 (D. Reidel, Dordrecht, Holland, 1982).
[54] E.J. Weniger and E.O. Steinborn, Addition theorems for B functions and other exponentially declining functions, J. Math. Phys. 30(4) (1989) 774.
[55] E.J. Weniger and E.O. Steinborn, Numerical properties of the convolution theorems of B functions, Phys. Rev. A 28 (1983) 2026.