Journal of Computational Physics **165,** 473–495 (2000)
doi:10.1006/jcph.2000.6621, available online at http://www.idealibrary.com on IDEAL®

The *HD* and $H\bar{D}$ Methods for Accelerating the Convergence of Three-Center Nuclear Attraction and Four-Center Two-Electron Coulomb Integrals over *B* Functions and Their 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 January 24, 2000; revised August 22, 2000

Three-center nuclear attraction and four-center two-electron Coulomb integrals over Slater-type orbitals are required for *ab initio* and density functional theory (DFT) molecular structure calculations. They occur in many millions of terms, even for small molecules and require rapid and accurate evaluation. The *B* functions are used as a basis set of atomic orbitals. These functions are well adapted to the Fourier transform method that allowed analytical expressions for the integrals of interest to be developed. Rapid and accurate evaluation of these analytical expressions is now made possible by applying the *HD* and $H\bar{D}$ methods for accelerating the convergence of the semi-infinite oscillatory integrals. The convergence properties of the new methods are analysed. The numerical results section shows the high predetermined accuracy and the substantial gain in the calculation times obtained using the new methods.

Key Words: nonlinear transformations; convergence accelerators; numerical integration; three-center nuclear attraction integrals; four-center two-electron Coulomb integrals.

1. INTRODUCTION

In numerical analysis, in applied mathematics, and in physics, one must often deal with infinite series and infinite or semi-infinite integrals to represent the solutions of many problems. In practice, these series and integrals have a very poor convergence. This presents severe numerical and computational difficulties. Therefore, convergence accelerators and nonlinear transformation methods for accelerating the convergence of infinite series and

0021-9991/00 $35.00

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

Three-center nuclear attraction and four-center two-electron Coulomb integrals are the rate limiting step of *ab initio* and density functional theory (DFT) molecular structure calculations. These integrals contribute to the total energy of the molecule which is required to a precision sufficient for small fractional changes to be evaluated reliably. In practice, the precision threshold for the total energy is of order 10^{-3} atomic units and therefore individual integrals must be accurate to 10^{-8}–10^{-10} au.

The choice of a basis set for the expansion of atomic orbitals is of great importance in *ab initio* calculations. A good atomic orbital basis should decay exponentially for large distances [4–8] and should also satisfy Kato's conditions for analytical solutions of the appropriate Schrödinger equation [9].

The most popular functions used in *ab initio* calculations are the so-called gaussian-type orbitals (GTOs) [10]. With GTOs the numerous molecular integrals can be evaluated rather easily. Unfortunately, these GTO basis functions fail to satisfy the above mathematical conditions for atomic electronic distributions.

Exponential-type orbitals (ETOs) are better suited than GTOs to represent electron wave functions near the nucleus and at long range, provided that multicenter integrals using such functions could be computed efficiently. The ETOs show the same behavior as the exact solutions of atomic or molecular Schrödinger equations satisfying Kato's conditions [11].

Among the ETOs, slater-type functions (STFs) [12, 13] have a dominating position, because their analytical expression is very simple; however, the use of STFs has been prevented by the fact that their multicenter integrals are extremely difficult to evaluate for polyatomic molecules, particularly bielectronic terms. Various studies have focused on the use of B functions proposed by Shavitt [14] and introduced by Filter and Steinborn [15, 16]. These functions are analytically more complicated than STFs but they have much more appealing properties applicable to multicenter integral problems. They possess a relatively simple addition theorem [15, 17–19] and extremely compact convolution integrals [17, 20], they can be expressed as finite linear combinations of STFs [16, 17], and their Fourier transforms are exceptionally simple [18, 21]. The B functions are well adapted to the Fourier transform method [22–37], which led to analytical expressions for multicenter bielectronic integrals over B functions. These analytical expressions present severe numerical and computational difficulties due to the presence of semi-infinite very oscillatory integrals.

The molecular integrals under consideration are to be evaluated via a numerical quadrature of integral representations in terms of nonphysical integration variables. These integral representations were derived with the help of the Fourier transformation method [27, 31].

It is well known that the numerical integration of oscillatory integrands is beset with difficulties, especially when the oscillatory part is a (spherical) Bessel function and not a simple trigonometric function [38, 39]. The semi-infinite integrals can be transformed into infinite series of integrals of alternating sign. These series are slowly convergent, and this is why their use is prohibitively long for sufficient accuracy. The epsilon algorithm of Wynn [40] or Levin's u transform [41] accelerates the convergence of infinite series. In the case of the semi-infinite integrals involved in the analytical expressions of molecular integrals, however, the calculation times for a sufficient accuracy are still long, especially for large

values of λ and v, since the zeros of $j_\lambda(vx)$ become closer, and for s close to 0 or 1, since the exponential decreasing part $\hat{k}_v$ of the integrands becomes a constant. Thus the rapid oscillations of $j_\lambda(vx)$ cannot be damped and suppressed, and new numerical integration techniques are required.

In previous work [42, 43], we showed that all the conditions of applicability of the nonlinear D and $\bar{D}$ transformations [44, 45] are satisfied by the integrands of semi-infinite integrals involved in the analytical expressions of the three-center nuclear attraction and the four-center two-electron Coulomb integrals.

The D and $\bar{D}$ transformations in a sense combine the G transformation [46], the confluent ϵ algorithm [47], and the P transformation [48]. To apply these two transformations to accelerating the convergence of the semiinfinite integral $\int_0^{+\infty} f(x)\,dx$, the integrand $f(x)$ is required to satisfy a linear differential equation of order m with coefficients having asymptotic expansions in inverse powers of their argument x as $x \to +\infty$.

We demonstrated [42, 43] that the integrands of interest satisfy linear differential equations of order 4 in the case of three-center nuclear attraction integrals and of order 6 in the case of four-center two-electron Coulomb integrals, of the form required to apply the D and $\bar{D}$ transformations. The results obtained were satisfactory. Unfortunately, the calculations of the approximations using these two transformations present severe numerical and computational difficulties, in particular, for the four-center two-electron Coulomb integrals.

In [49, 50], we showed that the order of the linear differential equations satisfied by the integrands of the form $f(x) = g(x)\,j_\lambda(x)$, where $j_\lambda(x)$ is the spherical Bessel function of order λ, where $g(x)$ is of the form $h(x)e^{\phi(x)}$, where $\phi(x)$ is such that $\phi(x) \sim P_k(x)$ as $x \to +\infty$, and where $P_k(x)$ is a real polynomial in x of degree k, can be reduced to two, using some properties of reduced Bessel and spherical Bessel functions. This approach is shown to be applicable to the integrands of question.

The present work focused on the generalization of the method leading to the reduction of the order of linear differential equations required to apply D and $\bar{D}$ to two, keeping all the other conditions satisfied. This result led to an extension of the range of functions satisfying second-order linear differential equations with coefficients having asymptotic expansions in inverse powers of their arguments and satisfying all the conditions of the applicability of the D and $\bar{D}$ transformations. Great simplifications in evaluating the semi-infinite integrals are obtained using the approach presented in this work, leading to new methods that we called *HD* and $H\bar{D}$.

The convergence properties of the $H\bar{D}$ were analysed and they showed that from the numerical point of view the new approach corresponds to the most ideal situation.

The numerical results section shows the substantial simplification and the gain in the calculation times obtained using the new method compared with other alternatives.

The symbolic programming language Axiom [51] is used to confirm the analytical developments and to provide exact values of the semi-infinite integrals.

2. GENERAL DEFINITIONS AND PROPERTIES

We defined $A^{(\gamma)}$ for some 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

$$p(x) \sim x^\gamma \left(a_0 + \frac{a_1}{x} + \frac{a_2}{x^2} + \cdots \right), \tag{1}$$

and their derivatives of any order have asymptotic expansions, which can be obtained by differentiating that in Eq. (1) formally term by term.

For $\gamma \in \mathbb{R}$, we denote by $\tilde{A}^{(\gamma)}$ the set of functions $f(x)$ such that $f \in A^{(\gamma)}$ and $\lim_{x\to+\infty} x^{-\gamma} f(x) \neq 0$. Thus, $f \in \tilde{A}^{(\gamma)}$ has an asymptotic expansion in inverse powers of x as $x \to +\infty$ of the form given by Eq. (1) with $a_0 \neq 0$.

We defined the functional $\alpha_0(f)$ by $\alpha_0(f) = a_0 \neq 0$ in the case where $f \in \tilde{A}^{(\gamma)}$ for a certain γ.

We defined $e^{\tilde{A}^{(\gamma)}}$ for some γ as the set of functions $g(x)$ such that

$$g(x) = e^{f(x)} \quad \text{where} \quad f \in \tilde{A}^{(\gamma)}.$$

The reduced Bessel function $\hat{k}_{n-1/2}(\zeta r)$ is defined by [14, 15]

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

The spherical Bessel function $j_l(x)$ for order $l \in \mathbb{N}_0$ is defined by [52]

$$j_l(x) = (-1)^l x^l \left(\frac{d}{x\,dx}\right)^l \left(\frac{\sin(x)}{x}\right). \tag{3}$$

The spherical Bessel function is also defined by [52]

$$j_l(x) = [\pi/(2x)]^{1/2} J_{l+1/2}(x), \tag{4}$$

where $J_{l+1/2}(x)$ stands for the Bessel function of the first kind [52].

$j_l(x)$ and its first derivative $j_l'(x)$ satisfy the recurrence relations [52]

$$\begin{cases} x j_{l-1}(x) + x j_{l+1}(x) = (2l+1) j_l(x) \\ l j_{l-1}(x) - (l+1) j_{l+1}(x) = (2l+1) j_l'(x), \end{cases} \tag{5}$$

where

$$j_0(x) = \frac{\sin x}{x} \quad \text{and} \quad j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}. \tag{6}$$

The zeros of the spherical Bessel function $j_l(x)$ for $l \geq 1$ are identical to the zeros $j^n_{l+1/2}$, $n \geq 1$ of $J_{l+1/2}(x)$ because of the relation Eq. (4).

For the following, we set $j^n_{l,v} = j^n_{l+1/2}/v$, $n = 1, 2, \ldots$, which are the successive zeros of $j_l(vx)$. $j^0_{l+1/2}$ and $j^0_{l,v}$ are assumed to be 0.

The surface spherical harmonic $Y_l^m(\theta, \varphi)$ is defined explicitly using the Condon and Shortley phase convention as [53]

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

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

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

The Rayleigh expansion of the plane wave functions is defined by [54]

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

The Fourier integral representation of the Coulomb operator $\frac{1}{|\vec{r}-\vec{R}_1|}$ is given by [55]

$$\frac{1}{|\vec{r}-\vec{R}_1|} = \frac{1}{2\pi^2} \int_{\vec{k}} \frac{e^{-i\vec{k}\cdot(\vec{r}-\vec{R}_1)}}{k^2}\, d\vec{k}. \tag{10}$$

The Gaunt coefficients are defined as [56–62]

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

These coefficients linearize the product of two spherical harmonics,

$$\left[Y_{l_1}^{m_1}(\theta, \varphi)\right]^* Y_{l_2}^{m_2}(\theta, \varphi) = \sum_{l=l_{\min,2}}^{l_{\max}} \langle l_2 m_2 | l_1 m_1 | l m_2 - m_1 \rangle Y_l^{m_2-m_1}(\theta, \varphi), \tag{11}$$

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 $l_{\max}$. The constants $l_{\min}$ and $l_{\max}$ are given by [59]

$$l_{\max} = l_1 + l_2 \tag{12}$$

$$l_{\min} = \begin{cases} \max(|l_1 - l_2|, |m_2 - m_1|), & \text{if } l_1 + l_2 + \max(|l_1 - l_2|, |m_2 - m_1|) \text{ is even} \\ \max(|l_1 - l_2|, |m_2 - m_1|) + 1, & \text{if } l_1 + l_2 + \max(|l_1 - l_2|, |m_2 - m_1|) \text{ is odd.} \end{cases} \tag{13}$$

The Slater-type orbitals are defined in normalized form according to the relationship [12, 13]

$$\chi_{n,1}^m(\zeta\vec{r}) = N(n, \zeta) r^{n-1} e^{-\zeta r} Y_l^m(\theta_{\vec{r}}, \varphi_{\vec{r}}), \tag{14}$$

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

$$N(n, \zeta) = \zeta^{-n+1} [(2\zeta)^{2n+1}/(2n)!]^{1/2}. \tag{15}$$

The *B* functions are defined as [15, 16]

$$B_{n,l}^m(\zeta\vec{r}) = \frac{(\zeta r)^l}{2^{n+l}(n+l)!} \hat{k}_{n-\frac{1}{2}}(\zeta r) Y_l^m(\theta_{\vec{r}}, \varphi_{\vec{r}}). \tag{16}$$

The *B* function can only be used as an L.C.A.O. basis functions if $n \in \mathbb{N}$ holds. For $-l \le n \le 0$, a *B* function is singular at the origin, and if $n = -l - \nu$ with $\nu \in \mathbb{N}$ holds, then a *B* function is no longer a function in the sense of classical analysis but a derivation of the three-dimensional Dirac delta function [63].

The Slater-type orbitals can be expressed as finite linear combinations of B functions [16],

$$\chi_{n,l}^{m}(\zeta\vec{r}) = \sum_{p=\tilde{p}}^{n-l} \frac{(-1)^{n-l-p}(n-l)!2^{l+p}(l+p)!}{(2p-n-l)!(2n-2l-2p)!!} B_{p,l}^{m}(\zeta\vec{r}), \tag{17}$$

where

$$\tilde{p} = \begin{cases} (n-l)/2 & \text{if } n-l \text{ even} \\ (n-l+1)/2 & \text{if } n-l \text{ odd} \end{cases} \tag{18}$$

and where the double factorial is defined by

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

The Fourier transform $\bar{B}_{n,l}^{m}(\zeta,\vec{p})$ of $B_{n,l}^{m}(\zeta\vec{r})$ is given by [18, 21]

$$\bar{B}_{n,l}^{m}(\zeta,\vec{p}) = \sqrt{\frac{2}{\pi}}\zeta^{2n+l-1}\frac{(-i|p|)^l}{(\zeta^2+|p|^2)^{n+l+1}} Y_l^m(\theta_{\vec{p}},\varphi_{\vec{p}}). \tag{19}$$

3. THREE-CENTER NUCLEAR ATTRACTION AND FOUR-CENTER TWO-ELECTRON COULOMB INTEGRALS OVER *B* FUNCTIONS

The three-center nuclear attraction integral is

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

The four-center two-electron Coulomb integral is

$$\begin{aligned}\mathcal{J}_{n_1l_1m_1,n_3l_3m_3}^{n_2l_2m_2,n_4l_4m_4} = &\int_{\vec{R},\vec{R}'} \left[B_{n_1,l_1}^{m_1}(\zeta_1(\vec{R}-\vec{OA}))\right]^* \left[B_{n_3,l_3}^{m_3}(\zeta_3(\vec{R}'-\vec{OC}))\right]^* \\ &\times \frac{1}{|\vec{R}-\vec{R}'|} B_{n_2,l_2}^{m_2}[\zeta_2(\vec{R}-\vec{OB})] B_{n_4,l_4}^{m_4}[\zeta_4(\vec{R}'-\vec{OD})]\,d\vec{R}\,d\vec{R}'. \end{aligned}\tag{21}$$

By substituting the integral representation of the Coulomb operator Eq. (10) in the above equations, we can re-write these two integrals as

$$\mathcal{I}_{n_1,l_1,m_1}^{n_2,l_2,m_2} = \frac{1}{2\pi^2}\int \frac{e^{i\vec{x}\cdot\vec{R}_1}}{x^2} \left\langle B_{n_1,l_1}^{m_1}(\zeta_1\vec{r}')|e^{-i\vec{x}\cdot\vec{r}}|B_{n_2,l_2}^{m_2}[\zeta_2(\vec{r}-\vec{R}_2)]\right\rangle_{\vec{r}} d\vec{x}, \tag{22}$$

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

$$\begin{aligned}\mathcal{J}_{n_1l_1m_1,n_3l_3m_3}^{n_2l_2m_2,n_4l_4m_4} = &\frac{1}{2\pi^2}\int \frac{e^{i\vec{x}\cdot\vec{R}_{41}}}{x^2} \left\langle B_{n_1,l_1}^{m_1}(\zeta_1\vec{r}')|e^{-i\vec{x}\cdot\vec{r}}|B_{n_2,l_2}^{m_2}[\zeta_2(\vec{r}-\vec{R}_{21})]\right\rangle_{\vec{r}} \\ &\times \left\langle B_{n_4,l_4}^{m_4}(\zeta_4\vec{r}')|e^{-i\vec{x}\cdot\vec{r}'}|B_{n_3,l_3}^{m_3}[\zeta_3(\vec{r}'-\vec{R}_{34})]\right\rangle_{\vec{r}'}^{*} d\vec{x}, \end{aligned}\tag{23}$$

where $\vec{R}_1 = \vec{OA}$, $\vec{R}_2 = \vec{OB}$, $\vec{R}_3 = \vec{OC}$, $\vec{R}_4 = \vec{OD}$, $\vec{r} = \vec{R} - \vec{R}_1$, $\vec{r}' = \vec{R}' - \vec{R}_4$, and $\vec{R}_{ij} = \vec{R}_i - \vec{R}_j$.

By applying the Fourier transform method [27, 31] to the terms

$$\left\langle B^{m_i}_{n_i,l_i}(\zeta_i \vec{r}') | e^{-i\vec{x}\cdot\vec{r}} | B^{m_j}_{n_j,l_j}[\zeta_j(\vec{r} - \vec{R})] \right\rangle_{\vec{r}}$$

involved in the Eqs. (22) and (23), one can obtain analytical expressions for these integrals given by [27, 31]

$$\begin{aligned}
\mathcal{I}^{n_2,l_2,m_2}_{n_1,l_1,m_1} &= 8(4\pi)^2(2l_1+1)!!(2l_2+1)!! \\
&\times \frac{(n_1+l_1+n_2+l_2+1)!}{(n_1+l_1)!(n_2+l_2)!}\zeta_1^{2n_1+l_1-1}\zeta_2^{2n_2+l_2-1} \\
&\times \sum_{l'_1=0}^{l_1}\sum_{m'_1=-l'_1}^{l'_1}(i)^{l_1+l'_1}(-1)^{l_1}\frac{\langle l_1 m_1 | l'_1 m'_1 | l_1 - l'_1 m_1 - m'_1\rangle}{(2l'_1+1)!![2(l_1-l'_1)+1]!!} \\
&\times \sum_{l'_2=0}^{l_2}\sum_{m'_2=-l'_2}^{l'_2}(i)^{l_2+l'_2}(-1)^{l_2+l'_2}\frac{\langle l_2 m_2 | l'_2 m'_2 | l_2 - l'_2 m_2 - m'_2\rangle}{(2l'_2+1)!![2(l_2-l'_2)+1]!!} \\
&\times \sum_{l=l'_{\min},2}^{l'_{\max}}\langle l'_2 m'_2 | l'_1 m'_1 | l m'_2 - m'_1\rangle R_2^l Y_l^{m'_2-m'_1}\left(\theta_{\vec{R}_2},\varphi_{\vec{R}_2}\right) \\
&\times \sum_{\lambda=l''_{\min},2}^{l''_{\max}}(-i)^{\lambda}\langle l_2 - l'_2 m_2 - m'_2 | l_1 - l'_1 m_1 - m'_1 | \lambda\mu\rangle \\
&\times \sum_{j=0}^{\Delta l}\binom{\Delta l}{j}\frac{(-1)^j}{2^{n_1+n_2+l_1+l_2-j+1}(n_1+n_2+l_1+l_2-j+1)!} \\
&\times \int_{s=0}^{1} s^{n_2+l_1+l_2-l'_1}(1-s)^{n_1+l_1+l_2-l'_2}Y_\lambda^\mu(\theta_{\vec{v}},\varphi_{\vec{v}}) \\
&\times \left[\int_{x=0}^{+\infty} x^{n_x}\frac{\hat{k}_\nu[R_2\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}} j_\lambda(vx)\,dx\right] ds, \qquad (24)
\end{aligned}$$

where

$$\begin{aligned}
[\gamma(s,x)]^2 &= (1-s)\zeta_1^2 + s\zeta_2^2 + s(1-s)x^2 \\
\vec{v} &= (1-s)\vec{R}_2 - \vec{R}_1, \quad v = \|\vec{v}\|, \quad R_2 = \|\vec{R}_2\| \\
n_\gamma &= 2(n_1+l_1+n_2+l_2) - (l'_1+l'_2) - l + 1 \\
\nu &= n_1+n_2+l_1+l_2-l-j+\frac{1}{2} \\
\mu &= (m_2 - m'_2) - (m_1 - m'_1) \\
n_x &= l_1 - l'_1 + l_2 - l'_2 \\
\Delta l &= [(l'_1+l'_2-l)/2]
\end{aligned}$$

$$\begin{aligned}
\mathcal{J}_{n_1l_1m_1,n_3l_3m_3}^{n_2l_2m_2,n_4l_4m_4} &= 8(4\pi)^5(2l_1+1)!!(2l_2+1)!!\frac{(n_1+l_1+n_2+l_2+1)!}{(n_1+l_1)!(n_2+l_2)!}\\
&\times(-1)^{l_1+l_2}(2l_3+1)!!(2l_4+1)!!\frac{(n_3+l_3+n_4+l_4+1)!}{(n_3+l_3)!(n_4+l_4)!}\\
&\times\zeta_1^{2n_1+l_1-1}\zeta_2^{2n_2+l_2-1}\\
&\times\zeta_3^{2n_3+l_3-1}\zeta_4^{2n_4+l_4-1}\sum_{l_1'=0}^{l_1}\sum_{m_1'=\mu_{11}}^{\mu_{12}} i^{l_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]!!}\\
&\times\sum_{l_2'=0}^{l_2}\sum_{m_2'=\mu_{21}}^{\mu_{22}} 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]!!}\\
&\times\sum_{l_3'=0}^{l_3}\sum_{m_1'=\mu_{31}}^{\mu_{32}} i^{l_3+l_3'}\frac{\langle l_3m_3|l_3'm_3'|l_3-l_3'm_3-m_3'\rangle}{(2l_3'+1)!![2(l_3-l_3')+1]!!}\\
&\times\sum_{l_4'=0}^{l_4}\sum_{m_4'=\mu_{41}}^{\mu_{42}} i^{l_4+l_4'}(-1)^{l_4'}\frac{\langle l_4m_4|l_4'm_4'|l_4-l_4'm_4-m_4'\rangle}{(2l_4'+1)!![2(l_4-l_4')+1]!!}\\
&\times\sum_{l=l_{1,\min},2}^{l_{1,\max}}\langle l_2'm_2'|l_1'm_1'|lm'2-m_1'\rangle R_{21}^{l}Y_l^{m_2'-m_1'}\left(\theta_{\vec{R}_{21}},\varphi_{\vec{R}_{21}}\right)\\
&\times\sum_{l_{12}=l_{1,\min}',2}^{l_{1,\max}'}\langle l_2-l_2'm_2-m_2'|l_1-l_1'm_1-m_1'|l_{12}m_{21}\rangle\\
&\times\sum_{l'=l_{2,\min},2}^{l_{2,\max}}\langle l_4'm_4'|l_3'm_3'|l'm'4-m_3'\rangle R_{34}^{l'}Y_{l'}^{m_4'-m_3'}\left(\theta_{\vec{R}_{34}},\varphi_{\vec{R}_{34}}\right)\\
&\times\sum_{l_{34}=l_{2,\min}',2}^{l_{2,\max}'}\langle l_4-l_4'm_4-m_4'|l_3-l_3'm_3-m_3'|l_{34}m_4-m_4'-(m_3-m_3')\rangle\\
&\times\sum_{\lambda=l_{\min}'',2}^{l_{\max}''}(-i)^{\lambda}\langle l_{12}m_{21}|l_{34}m_4-m_4'-(m_3-m_3')|\lambda\mu\rangle\\
&\times\sum_{j_{12}=0}^{\Delta l_{12}}\sum_{j_{34}=0}^{\Delta l_{34}}\binom{\Delta l_{12}}{j_{12}}\binom{\Delta l_{34}}{j_{34}}\frac{(-1)^{j_{12}+j_{34}}}{2^{\nu_1+\nu_2+l+l'+1}\left(\nu_1+\frac{1}{2}+l\right)!\left(\nu_2+\frac{1}{2}+l'\right)!}\\
&\times\int_{s=0}^{1}\frac{s^{n_2+l_2+l_1}(1-s)^{n_1+l_1+l_2}}{s^{l_1'}(1-s)^{l_2'}}\int_{t=0}^{1}\frac{t^{n_4+l_4+l_3}(1-t)^{n_3+l_3+l_4}}{t^{l_3'}(1-t)^{l_4'}}Y_{\lambda}^{m_2-\mu}(\theta_{\vec{v}},\varphi_{\vec{v}})\\
&\times\left[\int_{x=0}^{+\infty}x^{n_x}\frac{\hat{k}_{\nu_1}[R_{21}\gamma_{12}(s,x)]}{[\gamma_{12}(s,x)]^{n_{\gamma_{12}}}}\frac{\hat{k}_{\nu_2}[R_{34}\gamma_{34}(t,x)]}{[\gamma_{34}(t,x)]^{n_{\gamma_{34}}}}j_{\lambda}(vx)\,dx\right]dt\,ds, \quad (25)
\end{aligned}$$

where

$$\mu=(m_2-m_2')-(m_1-m_1')+(m_4-m_4')-(m_3-m_3')$$

$$\mu_{1i}=\max(-l_i',m_i-l_i+l_i'),\quad \text{for } i=1,2,3,4$$

$$
\begin{aligned}
\mu_{2i} &= \min(l_i, m_i + l_i - l_i'), \quad \text{for } i = 1, 2, 3, 4 \\
[\gamma_{12}(s,x)]^2 &= (1-s)\zeta_1^2 + s\zeta_2^2 + s(1-s)x^2 \\
[\gamma_{34}(t,x)]^2 &= (1-t)\zeta_3^2 + t\zeta_4^2 + t(1-t)x^2 \\
\vec{v} &= (1-s)\vec{R}_{21} + (1-t)\vec{R}_{43} - \vec{R}_{41} \\
\nu_1 &= n_1 + n_2 + l_1 + l_2 - l - j_{12} + \frac{1}{2} \\
\nu_2 &= n_3 + n_4 + l_3 + l_4 - l' - j_{34} + \frac{1}{2} \\
\Delta l_{12} &= \frac{l_1' + l_2' - l}{2}, \quad \Delta l_{34} = \frac{l_3' + l_4' - 1'}{2} \\
n_{\gamma_{12}} &= 2(n_1 + l_1 + n_2 + l_2) - (l_1' + l_2') - l + 1 \\
n_{\gamma_{34}} &= 2(n_3 + l_3 + n_4 + l_4) - (l_3' + l_4') - l' + 1. \\
n_x &= l_1 - l_1' + l_2 - l_2' + l_3 - l_3' + l_4 - l_4' \\
m_{21} &= m_2 - m_2' - (m_1 - m_1').
\end{aligned}
$$

The constants $l_{\max}$ and $l_{\min}$ are given by Eqs. (12) and (13).

The numerical evaluation of the analytical expressions obtained has been proven to be very difficult. This is due to the presence of the semi-infinite integrals, which will be referred to as $\tilde{\mathcal{I}}(s)$ and $\tilde{\mathcal{J}}(s,t)$ respectively, and whose integrands oscillate rapidly in particular for large values of v and λ. Different approaches were used [64–67], namely the Gauss–Laguerre quadrature, the epsilon algorithm of Wynn [40], and Levin's u transform [41], which accelerate the convergence of the semi-infinite integrals after transforming them into infinite series.

In previous work [43, 50], we have shown that these methods are inefficient in the evaluation of these kinds of semi-infinite integrals especially in the regions where s and t are close to 0 or 1 where the oscillations of the integrands become very rapid.

It is shown that the integrands of interest satisfied all the conditions of the applicability of the nonlinear D and $\bar{D}$ transformations [42, 43]. These transformations are efficient in accelerating the convergence of semi-infinite oscillatory integrals $S = \int_0^{+\infty} f(t)\,dt$ whose integrands $f(t)$ satisfy linear differential equations of the form [44]

$$
f(t) = \sum_{k=1}^{m} p_k(t)\, f^{(k)}(t),
$$

where the coefficients p_k, for $k = 1, 2, \ldots, m$ should satisfy the following conditions [44]:

1. p_k are in $A^{(i_k)}$, where $i_k \leq k$, 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. $\forall l \geq -1$, $\sum_{k=1}^{m} l(l-1)\cdots(l-k+1)\,p_{k,0} \neq 1$; $p_{k,0} = \lim_{x\to+\infty} x^{-k} p_k(x)$.

Under the above conditions, one can obtain an asymptotic expansion for $\int_x^{+\infty} f(t)\,dt$ as $x \to +\infty$, which is given by [44]

$$
\int_x^{+\infty} f(t)\,dt \sim \sum_{k=0}^{m-1} f^{(k)}(x) x^{j_k} \left(\beta_{0,k} + \frac{\beta_{1,k}}{x} + \frac{\beta_{2,k}}{x^2} + \cdots \right), \tag{26}
$$

where

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

The approximation of S using the nonlinear D transformation, satisfies the $N = 1 + mn$ equations given by [44]

$$D_n^{(m)} = \int_0^{x_l} f(t)\,dt + \sum_{k=0}^{m-1} f^{(k)}(x_l) x_l^{\sigma_k} \sum_{i=0}^{n-1} \frac{\bar{\beta}_{i,k}}{x_l^i}, \quad l = 0, 1, \ldots, mn, \tag{27}$$

where $D_n^{(m)}$ and the $\bar{\beta}_{i,k}$, for $k = 0, \ldots, m-1$; $i = 0, 1, \ldots, n-1$ are the $N = mn + 1$ unknowns of the linear system. σ_k is the minimum of $k + 1$ and s_k, where s_k is the largest of the integers s for which $\lim_{x\to+\infty} x^s f^{(k)}(x) = 0$. The x_l for $l = 0, 1, \ldots, mn$ are such that $x_0 < x_1 < \cdots$ and $\lim_{l\to+\infty} x_l = +\infty$ [45].

The $\bar{\beta}_{i,k}$ for $k = 0, \ldots, m-1$ and $i = 0, 1, \ldots, n-1$ do not have to be identical to $\beta_{i,k}$ in Eq. (26) since the asymptotic series in Eq. (26) are usually infinite [44].

The order of the above linear system can be reduced by choosing x_l, $l = 0, 1, \ldots$ to be the successive zeros of $f(x)$. In this case the Eq. (27) can be re-written [45]

$$\bar{D}_n^{(m)} = \int_0^{x_l} f(t)\,dt + \sum_{k=1}^{m-1} f^{(k)}(x_l) x_l^{\sigma_k} \sum_{i=0}^{n-1} \frac{\bar{\beta}_{i,k}}{x_l^i}, \quad l = 0, 1, \ldots, (m-1)n, \tag{28}$$

where $\bar{D}_n^{(m)}$ and the $\bar{\beta}_{i,k}$, for $k = 1, \ldots, m-1$; $i = 0, 1, \ldots, n-1$ are the $N = (m-1)n + 1$ unknowns of the linear system.

In the case of the three-center nuclear attraction integral, the integrand, which will be referred to as $f_{a,s}(x)$ of $\tilde{\mathcal{I}}(s)$, satisfies a fourth-order linear differential equation of the form required to apply D and $\bar{D}$ [42]. For the four-center two-electron Coulomb integral, the integrand which will be referred to as $f_{c,s,t}(x)$ of $\tilde{\mathcal{J}}(s,t)$, satisfies a sixth-order linear differential equation of the form required to apply D and $\bar{D}$ [43]. The results obtained using these transformations were satisfactory. Unfortunately, the calculations of the approximations $\bar{D}_n^{(4)}$ of $\tilde{\mathcal{I}}(s)$ and $\bar{D}_n^{(6)}$ of $\tilde{\mathcal{J}}(s,t)$ present severe numerical and computational difficulties since we need to calculate the $(m-1)$ successive derivatives of the integrands and the linear set of equations to solve is of order $(m-1)n + 1$, which can be very large if the values of m and n are large. In [49], we demonstrated that the order of the differential equations satisfied by the integrands of the form $f(x) = g(x) j_\lambda(x)$, where $g(x) = h(x)e^{\phi(x)}$ and where $h \in A^{(\gamma)}$ for some γ and $\phi(x)$ is such that $\phi(x) \sim P_k(x)$ as $x \to +\infty$ and where $P_k(x)$ is a real polynomial in x of degree k, can be reduced to two.

In this work, we presented a general method leading to the reduction of the orders of linear differential equations to two, keeping all the conditions of the integrability and the applicability of the D and $\bar{D}$ transformations satisfied, using some useful calculation techniques and some properties of the reduced Bessel functions and Poincaré series [68]. This led to great simplifications in the application of D and $\bar{D}$ transformations.

4. THE *HD* AND *HD̄* METHODS

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

THEOREM 1. *Let $g(x)$ be a function in $C^2[0, +\infty[$ which is the set of twice continuously differentiable functions. If $g(x)$ is of the form*

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

where $h \in \tilde{A}^{(\gamma)}$ and $\phi \in \tilde{A}^{(k)}$, for some γ and k, then the function $f(x) = g(x)\, j_\lambda(x)$ satisfies a second-order linear differential equation given by

$$f(x) = p_1(x)\, f'(x) + p_2(x)\, f''(x), \tag{29}$$

where

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

Proof. $j_\lambda(x)$ satisfies a second-order differential equation given by

$$j_\lambda(x) = -\frac{2x}{x^2 - \lambda^2 - \lambda}\, j'_\lambda(x) - \frac{x^2}{x^2 - \lambda^2 - \lambda}\, j''_\lambda(x). \tag{30}$$

By replacing in the above equation $j_\lambda(x)$ by $\frac{f(x)}{g(x)}$, one can obtain a linear differential equation satisfied by $f(x)$, which is given by Eq. (29), where

$$p_1(x) = \frac{2x^2\left(\frac{h'(x)}{h(x)} + \phi'\right) - 2x}{w(x)} \quad \text{and} \quad p_2(x) = \frac{-x^2}{w(x)}, \tag{31}$$

and where

$$w(x) = -x^2\left[\left(\frac{h'(x)}{h(x)} + \phi'\right)' - \left(\frac{h'(x)}{h(x)} + \phi'\right)^2\right] - 2x\left(\frac{h'(x)}{h(x)} + \phi'\right) + x^2 - \lambda^2 - \lambda. \tag{32}$$

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 $p_2(x) \in A^{(-2k+2)}$.
We used the symbolic programming language Axiom to verify the above expressions and to obtain the analytical expressions for $\alpha_0(p_1)$ and $\alpha_0(p_2)$, which are given by

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

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

THEOREM 2. *If $g(x)$ is a function in $C^2[0, +\infty[$ and of the form $g(x) = h(x)e^{\phi(x)}$, where $h \in \tilde{A}^{(\gamma)}$, $\phi \in \tilde{A}^{(k)}$ 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 $\bar{D}$ transformations.*

We shall now state lemmas that will be useful to prove Theorem 2.

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

1. *If $g \in \tilde{A}^{(\delta)}$, then $f \cdot g \in \tilde{A}^{(\gamma+\delta)}$ and $\alpha_0(fg) = \alpha_0(f)\alpha_0(g)$.*
2. *$\forall k \in \mathbb{R}$, $x^k f \in \tilde{A}^{(k+\gamma)}$, and $\alpha_0(x^k f) = \alpha_0(f)$.*
3. *The function $c \cdot f \in \tilde{A}^{(\gamma)}$ and $\alpha_0(cf) = c\alpha_0(f)$ for all $c \neq 0$.*
4. *If $g \in \tilde{A}^{(\delta)}$ and $\gamma - \delta > 0$, then $f + g \in \tilde{A}^{(\gamma)}$ and $\alpha_0(f+g) = \alpha_0(f)$. If $\gamma = \delta$ and $\alpha_0(f) \neq -\alpha_0(g)$, then the function $f + g \in \tilde{A}^{(\gamma)}$ and $\alpha_0(f+g) = \alpha_0(f) + \alpha_0(g)$.*
5. *Let $m > 0$ be an integer. If $\alpha_0(f) > 0$, then the function $f^m \in \tilde{A}^{(m\gamma)}$ and $\alpha_0(f^m) = \alpha_0(f)^m$.*
6. *The function $1/f \in \tilde{A}^{(-\gamma)}$ and $\alpha_0(1/f) = 1/\alpha_0(f)$.*

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

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

$$\hat{k}_{n+\frac{1}{2}}(f(x)) = f_1(x) e^{-f(x)},$$

where $f_1 \in \tilde{A}^{(nk)}$ $(\alpha_0(f_1) = (\alpha_0(f))^n \neq 0)$.

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

Proof of Theorem 2. If $k > 0$ and $\alpha_0(\phi) < 0$, then $\lim_{x\to+\infty} \phi(x) = -\infty$. The function $g(x) \in C^2[0, +\infty[$. From these arguments, it follows that $f(x)$ is integrable on $[0, +\infty[$.

Using Theorem 1, we can show that the function $f(x)$ satisfies a second-order linear differential equation with coefficients $p_1(x) \in A^{(-k+1)}$ and $p_2(x) \in A^{(-2k+2)}$.

The function $f(x)$ is exponentially decreasing; thus

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

Using the fact that $p_1(x) \in A^{(-k+1)}$, $p_2(x) \in A^{(-2k+2)}$, and $k > 0$, it follows that

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

and, therefore,

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

The conditions of applicability of D and $\bar{D}$ for accelerating the convergence of $\int_0^{+\infty} f(t)\,dt$ are now shown to be satisfied.

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

$$HD_n^{(2)} = \int_0^{x_l} f(t)\,dt + \sum_{k=0}^{1} (g(x_l) j_\lambda(x_l))^{(k)} x_l^{\sigma_k} \sum_{i=0}^{n-1} \frac{\bar{\beta}_{i,k}}{x_l^i}, \quad l = 0, 1, \ldots, 2n. \tag{33}$$

The $x_l, l = 0, 1, \ldots, 2n$ are chosen to satisfy $x_0 < x_1 < \cdots < x_{2n}$ and $\lim_{n\to+\infty} x_n = +\infty$. $HD_n^{(2)}$ and $\bar{\beta}_{i,k}$, $i = 0, 1, \ldots, n-1$, and $k = 0, 1$ are the $(2n+1)$ unknowns of the above linear system.

By choosing $x_l = j_{\lambda+1/2}^{l+1}$ for $l = 0, 1, \ldots, n$, the above linear set of equations can be re-written as

$$H\bar{D}_n^{(2)} = \int_0^{x_l} f(t)\,dt + g(x_l) j'_\lambda(x_l) x_l^{\sigma_1} \sum_{i=0}^{n-1} \frac{\bar{\beta}_{i,1}}{x_l^i}, \quad l = 0, 1, \ldots, n. \tag{34}$$

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

5. EVALUATION OF THREE-CENTER NUCLEAR ATTRACTION AND FOUR-CENTER TWO-ELECTRON COULOMB INTEGRALS

The integrand $f_{a,s}(x)$ of $\tilde{\mathcal{I}}(s)$ is given by

$$f_{a,s}(x) = g_a(x) j_\lambda(vx),$$

where

$$g_a(x) = x^{n_x} \frac{\hat{k}_{n+1/2}[R_2\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}.$$

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

$$\phi(x) = R_2\gamma(s,x) = R_2\sqrt{(1-s)\zeta_1^2 + s\zeta_2^2 + s(1-s)x^2}.$$

$\phi(x)$ is in $\tilde{A}^{(1)}$ (Lemma 1 for $m = \frac{1}{2}$).

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

By using Lemmas 1 and 2, $g_a(x)$ can be re-expressed in the form

$$g_a(x) = g_1(x)e^{-\phi(x)}, \quad g_1 \in \tilde{A}^{(n+n_x-n_\gamma)}, \quad \text{and} \quad \phi \in \tilde{A}^{(1)} \quad \text{with } \alpha_0(\phi) > 0.$$

The integrand $f_{j,s,t}(x)$ of $\tilde{\mathcal{J}}(s,t)$ is given by $f_{j,s,t}(x) = g_j(x) j_\lambda(vx)$, where

$$g_j(x) = x^{n_x} \frac{\hat{k}_{n_{12}+\frac{1}{2}}[R_{21}\gamma_{12}(s,x)]}{[\gamma_{12}(s,x)]^{n_{\gamma_{12}}}} \frac{\hat{k}_{n_{34}+\frac{1}{2}}[R_{34}\gamma_{34}(t,x)]}{[\gamma_{34}(t,x)]^{v_{\gamma_{34}}}}.$$

Let the functions $\phi_1(x)$ and $\phi_2(x)$ be defined as

$$\phi_1 = R_{21}\gamma(s,x) = R_{21}\sqrt{(1-s)\zeta_1^2 + s\zeta_2^2 + s(1-s)x^2} \in \tilde{A}^{(1)}$$

$$\phi_2 = R_{34}\gamma(t,x) = R_{34}\sqrt{(1-t)\zeta_3^2 + t\zeta_4^2 + t(1-t)x^2} \in \tilde{A}^{(1)}.$$

If we let $\phi_j(x) = \phi_1(x) + \phi_2(x)$, then from Lemma 1, it follows that $\phi_j(x)$ still in $\tilde{A}^{(1)}$ and $\alpha_0(\phi_j) = \alpha_0(\phi_1) + \alpha_0(\phi_2) \neq 0$.

Using these arguments, we can re-write the function $g_j(x)$ as

$$g_j(x) = g_3(x)e^{-\phi_j(x)}, \begin{cases} g_3 \in \tilde{A}^{(n_{12}+n_{34}+n_x-n_{\gamma_{12}}-n_{\gamma_{34}})} \\ \phi_j \in \tilde{A}^{(1)} \quad \text{with } \alpha_0(\phi_j) > 0. \end{cases}$$

By using Theorem 1, we can show that $f_{a,s}(x)$ and $f_{c,s,t}(x)$ satisfy second-order linear differential equations of the form given by Eq. (29).

From Theorem 2, it follows that $f_{a,s}(x)$ and $f_{c,s,t}(x)$ are integrable on $[0,+\infty[$ and satisfy all the conditions of applicability of D and $\bar{D}$.

$f_{a,s}(x)$ and $f_{c,s,t}(x)$ are exponentially decreasing; thus $\sigma_k = k+1$.

The approximations $HD_n^{(2)}$ of $\tilde{\mathcal{I}}(s)$ and $\tilde{\mathcal{J}}(s,t)$ can be obtained by solving the linear set of equations (34) with $\sigma_1 = 2$ and $x_l = j_{\lambda,\nu}^{l+1}$, $l = 0, 1, \ldots, n$.

6. CONVERGENCE PROPERTIES

Let us consider a function $f(x)$ integrable on $[0,+\infty[$ satisfying all the conditions of applicability of the nonlinear D transformation.

Let $S = \int_0^{+\infty} f(t)\,dt$, $F(x) = \int_0^x f(t)\,dt$ and $\Phi_k(x) = x^{\sigma_k} f^{(k)}(x)$ for $k = 0, 1, \ldots, m-1$. The approximation $D_n^{(m)}$ of S satisfies the linear system of order $(mn+1)$ given by [44]

$$D_n^{(m)} = F(x_l) + \sum_{k=0}^{m-1} \Phi_k(x_l) \sum_{i=0}^{n-1} \frac{\bar{\beta}_{i,k}}{x_l^i}, \quad l = 0, 1, \ldots, mn. \tag{35}$$

COROLLARY 1 [69]. *Let $(\gamma_0, \gamma_1, \ldots, \gamma_{mn})$ be the first row of the inverse of the matrix of the linear system Eq.* (35)*. Then*

$$\left|S - D_n^{(m)}\right| \leq \left(\sum_{l=0}^{mn} |\gamma_l|\right) o(n^{-j}), \quad \forall j > 0 \quad \text{as } n \to +\infty. \tag{36}$$

COROLLARY 2 [69]. *If $\sum_{l=0}^{mn} |\gamma_l| \leq L < \infty$, then*

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

Using the fact that the first column of the matrix of the linear system Eq. (35) is the vector $(1, 1, \ldots, 1)^T$ (T denotes transpose), it follows that $\sum_{l=0}^{mn} \gamma_l = 1$ and therefore $\sum_{l=0}^{mn} |\gamma_l| \geq 1$.

Now, let us consider the linear system given by Eq. (34). We defined the function $\Phi_1(x) = x^{\sigma_1} g(x) j_\lambda'(x)$.

Using the fact that $x_l = j_{\lambda+1/2}^{l+1}$, $l = 0, 1, \ldots, n$ are the successive zeros of $j_\lambda(x)$, one can easily show that

$$\Phi_1(x_l)\Phi_1(x_{l+1}) < 0, \quad l = 0, 1, 2, \ldots \tag{38}$$

We defined the matrix M_2 by

$$M_2 = \begin{pmatrix} \frac{F(x_0)}{\Phi_1(x_0)} & \frac{F(x_1)}{\Phi_1(x_1)} & \cdots & \frac{F(x_n)}{\Phi_1(x_n)} \\ 1 & 1 & \cdots & 1 \\ x_0^{-1} & x_1^{-1} & \cdots & x_n^{-1} \\ \vdots & \vdots & & \vdots \\ x_0^{-n+1} & x_1^{-n+1} & \cdots & x_n^{-n+1} \end{pmatrix} \tag{39}$$

and let K_2 be the matrix obtained after replacing the first row of M_2 with the vector $(\frac{1}{\Phi_1(x_0)}, \frac{1}{\Phi_1(x_1)}, \ldots \frac{1}{\Phi_1(x_n)})$.

Using Cramer's rule, one can express $H\bar{D}_n^{(2)}$ as

$$H\bar{D}_n^{(2)} = \frac{\det(M_2)}{\det(K_2)} = \frac{\sum_{l=0}^{n}(-1)^l[V_l/\Phi_1(x_l)]F(x_l)}{\sum_{l=0}^{n}(-1)^l[V_l/\Phi_1(x_l)]}, \tag{40}$$

where V_l denotes the minor of $F(x_l)/\Phi_1(x_l)$ in M_2 or of $1/\Phi_1(x_l)$ in K_2.

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

$$V_0 = V\left(x_1^{-1}, \ldots, x_n^{-1}\right) \tag{41}$$

$$V_l = V\left(x_0^{-1}, \ldots, x_{l-1}^{-1}, x_{l+1}^{-1}, \ldots, x_{n-1}^{-1}\right), \quad l = 1, \ldots, n-1 \tag{42}$$

$$V_n = V\left(x_0^{-1}, \ldots, x_{n-1}^{-1}\right), \tag{43}$$

where $V(\alpha_0, \alpha_1, \ldots, \alpha_{n-1})$ is the Vandermonde determinant, which can be expressed by

$$V(\alpha_0, \alpha_1, \ldots, \alpha_{n-1}) = \prod_{0 \le i < j \le n-1} (\alpha_j - \alpha_i). \tag{44}$$

Since $\alpha_0 < \alpha_1 < \cdots < \alpha_{n-1}$, it follows that $V(\alpha_0, \alpha_1, \ldots, \alpha_{n-1}) > 0$.

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

$$\gamma_l = \frac{(-1)^l[V_l/\Phi_1(x_l)]}{\sum_{i=0}^{n}(-1)^i[V_i/\Phi_1(x_i)]}, \quad 0 \le l \le n. \tag{45}$$

As $x_0 < x_1 < \ldots$, all V_l, for $0 \le l \le n$ have the same sign. Now by using Eq. (38), we can easily show that $(-1)^l\,[V_l/\Phi_1(x_l)]$, for $0 \le l \le n$ have also the same sign. Therefore, $\forall l$, $\gamma_l > 0$ and consequently

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

Corollary 3 becomes:

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

The convergence properties of the $H\bar{D}$ method 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.

7. CONCLUSION

Analytical expressions can be obtained for the three-center nuclear attraction and the four-center two-electron Coulomb integrals by choosing the *B* functions as a basis set of atomic orbitals and applying the Fourier transform method. These analytical expressions

TABLE I
Values of $\tilde{\mathcal{I}}(s)$ Obtained with 20 Correct Decimals

s	n_1	n_2	λ	R_1	ζ_1	R_2	ζ_2	max	$\tilde{\mathcal{I}}(s)$
.005	1	1	0	6.50	2.00	2.50	1.00	201	.360140912983302D−02
.010	2	1	1	7.00	2.00	4.00	1.00	86	.481637530646112D−03
.010	2	2	2	6.50	2.00	1.00	1.00	470	.456117321707410D−02
.010	3	3	3	7.50	2.00	3.50	1.00	133	.181139626222770D−01
.010	4	4	4	8.50	2.00	3.50	1.00	167	.193274110480817D+00
.999	1	1	0	7.50	2.00	3.50	1.00	525	.161198710040904D+00
.990	2	1	1	4.50	2.00	1.50	1.00	222	.849175425774129D+00
.990	2	2	2	9.00	2.00	3.50	1.00	251	.271313806558930D+00

Note. $n_x = \lambda$ and $n_y = 2\nu$.

involve semi-infinite very oscillatory integrals whose integrands are shown to be suitable for the application of the nonlinear D and $\bar{D}$ transformations.

This work presents a general approach, using some properties of reduced Bessel, spherical Bessel functions, and Poincaré series, for reducing the order of the linear differential equations required to apply the D and $\bar{D}$ to two. This led to a great simplification in the application of D and $\bar{D}$ in calculating the approximations of semi-infinite oscillatory integrals. The calculation of the successive derivatives is avoided and the order of the linear set of equations to solve is reduced to $n + 1$, where n is the order of the accuracy. This new approach is now shown to be applicable to the semi-infinite integrals of interest.

Obviously, this great increase of rapidity of the new methods, which we called *HD* and $H\bar{D}$, is a key issue. In the molecular context, many millions of such integrals are required for close range terms; therefore, rapidity is the primordial criterion when the precision has been reached. The progress represented by the $H\bar{D}$ approach is another useful step in developing software for evaluating molecular integrals over Slater-type orbitals.

8. NUMERICAL RESULTS

The exact of $\tilde{\mathcal{I}}(s)$ and $\tilde{\mathcal{J}}(s, t)$ are computed to 20 exact decimals using the symbolic programming language Axiom (Tables I, IV, VII, and X), after transforming the integrals

TABLE II
Evaluation of $\tilde{\mathcal{I}}(s)$ Using $H\bar{D}_n^{(2)}$

s	ν	λ	R_1	ζ_1	R_2	ζ_2	n	$\tilde{\mathcal{I}}(s)$	Error	T
.005	5/2	0	6.5	2.0	2.5	1.0	7	.3601409132D−02	.59D−11	0.04
.010	7/2	1	7.0	2.0	4.0	1.0	7	.4816375329D−03	.50D−11	0.04
.010	9/2	2	6.5	2.0	1.0	1.0	9	.4561174046D−02	.27D−11	0.06
.010	13/2	3	7.5	2.0	3.5	1.0	7	.1811388162D−01	.50D−08	0.04
.010	17/2	4	8.5	2.0	3.5	1.0	8	.1932833577D+00	.96D−08	0.06
.999	5/2	0	7.5	2.0	3.5	1.0	5	.1611987095D+00	.51D−09	0.02
.990	7/2	1	4.5	2.0	1.5	1.0	9	.8491753954D+00	.74D−09	0.07
.990	9/2	2	9.0	2.0	3.5	1.0	8	.2713138630D+00	.81D−09	0.05

Note. Time T is in milliseconds. $n_x = \lambda$ and $n_y = 2\nu$.

TABLE III
Evaluation of $\tilde{\mathcal{I}}(s)$ Using $\bar{D}_n^{(4)}$

s	ν	λ	R_1	ζ_1	R_2	ζ_2	n	$\tilde{\mathcal{I}}(s)$	Error	T
.005	5/2	0	6.5	2.0	2.5	1.0	5	.3601409132D−02	.18D−11	0.18
.010	7/2	1	7.0	2.0	4.0	1.0	4	.4816375329D−03	.28D−11	0.11
.010	9/2	2	6.5	2.0	1.0	1.0	6	.4561174046D−02	.54D−11	0.30
.010	13/2	3	7.5	2.0	3.5	1.0	5	.1811388162D−01	.33D−08	0.19
.010	17/2	4	8.5	2.0	3.5	1.0	6	.1932833577D+00	.40D−07	0.30
.999	5/2	0	7.5	2.0	3.5	1.0	5	.1611987095D+00	.70D−09	0.18
.990	7/2	1	4.5	2.0	1.5	1.0	5	.8491753954D+00	.21D−09	0.18
.990	9/2	2	9.0	2.0	3.5	1.0	6	.2713138630D+00	.74D−09	0.30

Note. Time T is in milliseconds. $n_x = \lambda$ and $n_\gamma = 2\nu$.

TABLE IV
Values of $\tilde{\mathcal{J}}(s, t)$ Obtained with 20 Correct Decimals

s	t	n_{12}	λ	R_1	R_2	R_3	R_4	ζ_1	ζ_2	max	$\tilde{\mathcal{J}}(s, t)$
.999	.999	2	0	2.5	5.0	7.5	6.0	1.5	1.0	182	.1332888362507D+01
.999	.005	2	0	1.5	4.0	5.5	6.5	2.5	1.5	211	.4862207177866D−03
.005	.005	3	1	1.5	2.0	4.5	3.5	2.0	1.0	139	.2241938649088D−02
.005	.999	4	2	1.0	2.0	6.0	3.5	3.5	2.0	97	.4057636102915D−04
.999	.999	4	2	3.0	3.5	7.0	5.0	2.5	3.0	234	.1969258557126D−05
.999	.005	5	3	5.5	6.0	8.5	7.5	5.0	1.0	233	.1426496442765D−02
.005	.005	6	4	5.0	5.5	9.0	5.0	2.5	2.0	120	.4625584384664D−04
.005	.005	8	5	3.5	4.0	7.0	5.0	3.0	2.5	135	.1598600048274D−03

Note. $\nu_1 = \nu_2, n_{\gamma_{12}} = n_{\gamma_{34}} = 2\nu_1, n_x = \lambda, \zeta_3 = \zeta_1$, and $\zeta_4 = \zeta_2$.

TABLE V
Evaluation of $\tilde{\mathcal{J}}(s, t)$ Using $H\bar{D}_n^{(2)}$

s	t	ν_1	λ	R_1	R_2	R_3	R_4	ζ_1	ζ_2	n	$\tilde{\mathcal{J}}(s, t)$	Error	T
.999	.999	5/2	0	2.5	5.0	7.5	6.0	1.5	1.0	8	.1332D+01	.78D−10	0.05
.999	.005	5/2	0	1.5	4.0	6.5	5.5	2.5	1.5	4	.4862D−03	.54D−11	0.02
.005	.005	7/2	1	1.5	2.0	4.5	3.5	2.0	1.0	7	.2241D−02	.90D−10	0.04
.005	.999	9/2	2	1.0	2.0	6.0	2.5	3.5	2.0	6	.4057D−04	.81D−10	0.03
.999	.999	9/2	2	3.0	3.5	7.0	5.0	2.5	3.0	6	.1969D−05	.92D−12	0.03
.999	.005	11/2	3	5.5	6.0	8.5	7.5	5.0	1.0	8	.1426D−02	.93D−10	0.05
.005	.005	13/2	4	5.0	5.5	9.0	5.0	2.5	2.0	7	.4625D−04	.32D−09	0.04
.005	.005	17/2	5	3.5	4.0	7.0	5.0	3.0	2.5	8	.1598D−03	.36D−09	0.05

Note. Time T is in milliseconds. $\nu_1 = \nu_2, n_{\gamma_{12}} = n_{\gamma_{34}} = 2\nu_1, n_x = \lambda, \zeta_3 = \zeta_1$, and $\zeta_4 = \zeta_2$.

TABLE VI
Evaluation of $\tilde{\mathcal{J}}(s,t)$ Using $\bar{D}_n^{(6)}$

s	t	ν_1	λ	R_1	R_2	R_3	R_4	ζ_1	ζ_2	n	$\tilde{\mathcal{J}}(s,t)$	Error	T
.999	.999	5/2	0	2.5	5.0	7.5	6.0	1.5	1.0	5	.1332D+01	.27D−09	0.70
.999	.005	5/2	0	1.5	4.0	6.5	5.5	2.5	1.5	4	.4862D−03	.13D−11	0.39
.005	.005	7/2	1	1.5	2.0	4.5	3.5	2.0	1.0	3	.2241D−02	.70D−10	0.18
.005	.999	9/2	2	1.0	2.0	6.0	2.5	3.5	2.0	3	.4057D−04	.99D−09	0.19
.999	.999	9/2	2	3.0	3.5	7.0	5.0	2.5	3.0	5	.1969D−05	.58D−12	0.71
.999	.005	11/2	3	5.5	6.0	8.5	7.5	5.0	1.0	5	.1426D−02	.17D−10	0.70
.005	.005	13/2	4	5.0	5.5	9.0	5.0	2.5	2.0	4	.4625D−04	.95D−09	0.39
.005	.005	17/2	5	3.5	4.0	7.0	5.0	3.0	2.5	5	.1598D−03	.34D−09	0.71

Note. Time T is in milliseconds. $\nu_1 = \nu_2$, $n_{\gamma_{12}} = n_{\gamma_{34}} = 2\nu_1$, $n_x = \lambda$, $\zeta_3 = \zeta_1$, and $\zeta_4 = \zeta_2$.

TABLE VII
Values of $\mathcal{I}_{n_1 00}^{n_2 00}$ Obtained with 20 Exact Decimals

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	.9857079490760573D−01
2	1	7	1	1	4.50	1.50	2.50	1.00	.8761720595719150D+00
2	2	9	2	2	9.00	1.00	1.50	.50	.4459612679987856D+00
3	2	11	3	3	3.50	1.00	2.00	1.00	.2914294482354681D+01
3	3	13	3	3	8.50	4.50	5.00	3.00	.9938451545759212D−06
4	3	15	4	4	4.00	1.50	1.50	1.00	.1679864602693776D+01
4	4	17	4	4	2.50	.50	1.00	1.00	.1139978397585097D+00

Note. $\vec{R}_i = (R_i, 0, 0)$, $i = 1, 2$.

TABLE VIII
Evaluation of $\mathcal{I}_{n_1 00}^{n_2 00}$ Using $H\bar{D}_n^{(2)}$

n_1	n_2	λ	R_1	ζ_1	R_2	ζ_2	n	$\mathcal{I}_{n_1 00}^{n_2 00}$	Error	T
1	1	0	6.0	2.5	2.5	1.5	8	.985707949061D−01	.15D−11	0.80
2	1	1	4.5	1.5	2.5	1.0	7	.876172059562D+00	.95D−11	0.65
2	2	2	9.0	1.0	1.5	0.5	9	.445961267995D+00	.39D−11	1.06
3	2	3	3.5	1.0	2.0	1.0	8	.291429448235D+01	.83D−12	0.85
3	3	3	8.5	4.5	5.0	3.0	6	.993845549984D−06	.40D−12	0.50
4	3	4	4.0	1.5	1.5	1.0	8	.167986460269D+01	.32D−12	0.81
4	4	4	2.5	0.5	1.0	1.0	5	.113997839758D+00	.52D−12	0.39

Note. Time T is in milliseconds. $n_x = \lambda$ and $n_\gamma = 2(n_1 + n_2) + 1$. $\vec{R}_i = (R_i, 0, 0)$, $i = 1, 2$.

TABLE IX
Evaluation of $\mathcal{I}_{n_1 00}^{n_2 00}$ Using $\bar{D}_n^{(4)}$

n_1	n_2	λ	R_1	ζ_1	R_2	ζ_2	n	$\mathcal{I}_{n_1 00}^{n_2 00}$	Error	T
1	1	0	6.0	2.5	2.5	1.5	4	.985707949111D−01	.35D−11	1.65
2	1	1	4.5	1.5	2.5	1.0	4	.876172059573D+00	.14D−11	1.68
2	2	2	9.0	1.0	1.5	0.5	5	.445961268013D+00	.14D−10	2.94
3	2	3	3.5	1.0	2.0	1.0	4	.291429448235D+01	.53D−11	1.67
3	3	3	8.5	4.5	5.0	3.0	4	.993845773692D−06	.62D−12	1.66
4	3	4	4.0	1.5	1.5	1.0	4	.167986460270D+01	.79D−11	1.71
4	4	4	2.5	0.5	1.0	1.0	3	.113997839759D+00	.19D−12	0.89

Note. Time T is in milliseconds. $n_x = \lambda$ and $n_\gamma = 2(n_1 + n_2) + 1$. $\vec{R}_i = (R_i, 0, 0)$, $i = 1, 2$.

TABLE X
Values of $\mathcal{J}_{n_1 00, n_3 00}^{n_2 00, n_4 00}$ Obtained with 20 Exact Decimals

n_1	n_2	$n_{\gamma_{12}}$	λ	R_1	R_2	R_3	R_4	ζ_1	ζ_2	$\mathcal{J}_{n_1 00, n_3 00}^{n_2 00, n_4 00}$
1	1	5	0	1.5	3.5	6.5	4.5	3.0	2.5	.1712887759698046D−01
2	1	7	1	3.0	4.5	7.5	5.0	2.0	2.5	.1096433803364221D+00
2	2	9	2	2.5	3.0	5.5	4.0	2.0	1.5	.5077289993314878D+01
3	2	11	2	1.5	2.5	6.0	4.0	1.0	3.0	.2249496975806865D+01
3	3	13	3	2.5	4.0	6.0	5.0	2.0	3.5	.1225528163777224D+00
4	3	15	3	2.5	4.5	7.5	6.5	3.5	2.0	.2005488272296953D−03
4	4	17	4	2.5	4.5	7.0	6.0	3.0	1.5	.3653628513846506D−02

Note. $n_3 = n_1$, $n_4 = n_2$, $n_{\gamma_{34}} = n_{\gamma_{12}} = 2(n_1 + n_2) + 1$, $n_x = \lambda$, $\zeta_3 = \zeta_1$ and $\zeta_4 = \zeta_2$. $\vec{R}_i = (R_i, 0, 0)$, $i = 1, 2, 3, 4$.

TABLE XI
Evaluation of $\mathcal{J}_{n_1 00, n_3 00}^{n_2 00, n_4 00}$ Using $H\bar{D}_n^{(2)}$ to Evaluate $\tilde{\mathcal{J}}(s, t)$

n_1	n_2	λ	R_1	R_2	R_3	R_4	ζ_1	ζ_2	n	$\mathcal{J}_{n_1 00, n_3 00}^{n_2 00, n_4 00}$	Error	T
1	1	0	1.5	3.5	6.5	4.5	3.0	2.5	7	.1712887760D−01	.79D−12	9
2	1	1	3.0	4.5	7.5	5.0	2.0	2.5	5	.1096433810D+00	.61D−09	5
2	2	2	2.5	3.0	5.5	4.0	2.0	1.5	5	.5077289993D+01	.21D−10	7
3	2	2	1.5	2.5	6.0	4.0	1.0	3.0	7	.2249496976D+01	.83D−11	9
3	3	3	2.5	4.0	6.0	5.0	2.0	3.5	5	.1225528164D+00	.43D−11	6
4	3	3	2.5	4.5	7.5	6.5	3.5	2.0	6	.2005488272D−03	.37D−13	4
4	4	4	2.5	4.5	7.0	6.0	3.0	1.5	6	.3653628514D−02	.21D−14	8

Note. Time T is in milliseconds. $n_3 = n_1$, $n_4 = n_2$, $n_{\gamma_{34}} = n_{\gamma_{12}} = 2(n_1 + n_2) + 1$, $n_x = \lambda$, $\zeta_3 = \zeta_1$ and $\zeta_4 = \zeta_2$. $\vec{R}_i = (R_i, 0, 0)$, $i = 1, 2, 3, 4$.

TABLE XII
Evaluation of $\mathcal{J}_{n_1 00, n_3 00}^{n_2 00, n_4 00}$ Using $\bar{D}_n^{(6)}$ to Evaluate $\tilde{\mathcal{J}}(s, t)$

n_1	n_2	λ	R_1	R_2	R_3	R_4	ζ_1	ζ_2	n	$\mathcal{J}_{n_1 00, n_3 00}^{n_2 00, n_4 00}$	Error	T
1	1	0	1.5	3.5	6.5	4.5	3.0	2.5	3	.1712887760D−01	.80D−12	45
2	1	1	3.0	4.5	7.5	5.0	2.0	2.5	2	.1096433810D+00	.70D−09	18
2	2	2	2.5	3.0	5.5	4.0	2.0	1.5	2	.5077289993D+01	.14D−10	20
3	2	2	1.5	2.5	6.0	4.0	1.0	3.0	3	.2249496976D+01	.31D−12	53
3	3	3	2.5	4.0	6.0	5.0	2.0	3.5	2	.1225528164D+00	.13D−11	23
4	3	3	2.5	4.5	7.5	6.5	3.5	2.0	2	.2005488276D−03	.41D−12	17
4	4	4	2.5	4.5	7.0	6.0	3.0	1.5	2	.3653628514D−02	.18D−13	17

Note. Time T is in milliseconds. $n_3 = n_1$, $n_4 = n_2$, $n_{\gamma_{34}} = n_{\gamma_{12}} = 2(n_1 + n_2) + 1$, $n_x = \lambda$, $\zeta_3 = \zeta_1$, and $\zeta_4 = \zeta_2$. $\vec{R}_i = (R_i, 0, 0)$, $i = 1, 2, 3, 4$.

into infinite series $\sum_{n=0}^{+\infty} \int_{x_n}^{x_{n+1}} f(t)\, dt$, which we sum until $N = max$ (see Tables I and II) and where x_i and x_{i+1} are two successive zeros of the integrand $f(x)$ (see Tables VII–XII). The finite integrals are evaluated using the Gauss–Legendre quadrature of order 16. The LU decomposition method is used to solve the linear systems Eqs. (28) and (34).

In the analytical expression of $\mathcal{I}_{n_1 00}^{n_2 00}$ and $\mathcal{I}_{n_1 00, n_3 00}^{n_2 00, n_4 00}$ we let n_x and λ vary to compare the efficiency of the transformations in the evaluation of the semi-infinite integrals whose integrands are very oscillating.

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

ACKNOWLEDGMENTS

Special thanks 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 showing interest in this work and for their practical assistance.

REFERENCES

1. D. Shanks, Non-linear transformations of divergent and slowly convergent sequences, *J. Math. Phys.* **34**, 1 (1955).
2. C. Brezinski and M. R. Zaglia, *Extrapolation Methods: Theory and Practice* (North–Holland, Amsterdam, 1991).
3. C. Brezinski, *Algorithmes d'Accélérations de la Convergence* (Technip, Paris, 1978).
4. S. Agmon, *Lectures on Exponential Decay of Solutions of Second-order Elliptic Equations: Bounds of Eigenfunctions of N-Body Schrödinger Operators* (Princeton University, Princeton, N.J., 1982).
5. S. Agmon, Bounds on exponential decay of eigenfunctions of Schrödinger operators, in *Schrödinger Operators*, edited by S. Graffi (Springer–Verlag, Berlin, 1985), pp. 1–38.
6. R. Ahlrichs, Basic mathematical properties of electronic wave functions in momentum space, in *Numerical Determination of the Electronic Structure of Atoms, Diatomic and Polyatomic Molecules*, edited by M. Defranceschi and J. Delhalle (Kluwer, Dordrecht, 1989), pp. 1–15.
7. H. L. Cycon, R. G. Froese, W. Kirsch, and B. Simon, *Schrödinger Operators* (Springer–Verlag, Berlin, 1993).
8. I. Herbst, Perturbation theory for the decay rate of eigenfunctions in the generalized N-body problem, *Commun. Math. Phys.* **158**, 517 (1993).
9. T. Kato, On the eigenfunctions of many-particle systems in quantum mechanics, *Comm. Pure Appl. Math.* **10**, 151 (1957).

10. 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. A.* **258**, 402 (1960).
11. C. A. Weatherford and H. W. Jones, *International Conference on ETO Multicenter Integrals*, Tallahasse, 1981 (Reidel, Dordrecht, 1982).
12. J. C. Slater, Atomic shielding constants, *Phys. Rev.* **36**, 57 (1930).
13. J. C. Slater, Analytic atomic wave functions, *Phys. Rev.* **42**, 33 (1932).
14. I. Shavitt, The Gaussian function in calculation of statistical mechanics and quantum mechanics, in *Methods in Computational Physics 2. Quantum Mechanics*, edited by B. Alder, S. Fernbach, and M. Rotenberg (Academic Press, New York, 1963).
15. 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**, 273 (1975).
16. 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**, 1 (1978).
17. E. Filter, *Analytische Methoden zur Auswertung von Mehrzentren-Matrixelementen in der Theorie der Molekülorbitale bei Verwendung exponentialartiger Basissütze*, Ph.D. thesis (Universität Regensburg, 1978).
18. E. J. Weniger, *Reduzierte Bessel–Funktionen als LCAO–Basissatz: Analytische und numerische Untersuchungen*, Ph.D. thesis (Universität Regensburg, 1982).
19. E. J. Weniger and E. O. Steinborn, Addition theorems for *B* functions and other exponentially declining functions, *J. Math. Phys.* **30**(4), 774 (1989).
20. E. J. Weniger and E. O. Steinborn, Numerical properties of the convolution theorems of *B* functions, *Phys. Rev. A.* **28**, 2026 (1983).
21. 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**, 6121 (1983).
22. F. P. Prosser and C. H. Blanchard, On the evaluation of two-center integrals, *J. Chem. Phys.* **36**, 1112 (1962).
23. 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**, 3083 (1964).
24. 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**, 509 (1977).
25. 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**, 103 (1978).
26. E. O. Steinborn, *Methods in Computational Molecular Physics*, edited by H. H. Dierckesen and S. Wilson (Reidel, Holland, 1983).
27. 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**, 670 (1983).
28. J. Grotendorst, *Berechnung der Mehrzentren-Molekülintegrale mit exponentialartigen Basis Funktionen durch Systematische Anwendung der Fourier-transformationsmethode*, Ph.D. thesis (Universität Regensburg, 1985).
29. 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**, 3706 (1986).
30. E. J. Weniger and E. O. Steinborn, Comment on "Molecular overlap integrals with exponential-type orbitals," *J. Chem. Phys.* **87**, 3709 (1987).
31. J. Grotendorst and E. O. Steinborn, Numerical evaluation of molecular one- and tow-electron multicenter integrals with exponential-type orbitals via the Fourier-transform method, *Phys. Rev. A.* **38**, 3857 (1988).
32. 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**, 323 (1988).
33. 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.* **260**, 207 (1992).
34. 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**, 399 (1992).

35. H. H. H. Homeier and E. O. Steinborn, On the evaluation of overlap integrals with exponential-type basis functions, *Int. J. Quantum Chem.* **42**, 761 (1992).
36. 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**, 269 (1992).
37. H. H. H. Homeier, *Integraltransformationsmethoden und Quadraturverfahren für Molekülintegrale mit B-Functionen* (S. Roderer Verlag, Regensburg, 1990). Also: Ph.D. thesis (Universität Regensburg, 1990).
38. P. J. Davis and P. Rabinowitz, *Methods of Numerical Integration* (Academic Press, Orlando, 1994).
39. G. Evans, *Practical Numerical Integration* (Wiley, Chichester, 1993).
40. P. Wynn, On a device for computing the $e_m(S_n)$ transformation, *Math. Tables Aids Comput.* **10**, 91 (1956).
41. D. Levin, Developement of non-linear transformations for improving convergence of sequences, *Int. J. Comput. Math. B* **3**, 371 (1973).
42. H. Safouhi, D. Pinchon, and P. E. Hoggan, Efficient evaluation of integrals for density functional theory: Non-linear *D*-transformations to evaluate three-center nuclear attraction integrals over *B* functions, *Int. J. Quantum Chem.* **70**, 181 (1998).
43. H. Safouhi and P. E. Hoggan, Efficient evaluation of Coulomb integrals: The non-linear *D*- and $\bar{D}$-transformations, *J. Phys. A. Math. Gen.* **31**, 8941 (1998).
44. 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**, 175 (1981).
45. A. Sidi, Extrapolation methods for oscillating infinite integrals, *J. Inst. Math. Appl.* **26**, 1 (1980).
46. H. L. Gray, T. A. Atchison, and G. V. McWilliams, Higher order *G*-transformations, *SIAM J. Numer. Anal.* **8**, 365 (1971).
47. P. Wynn, Upon a second confluent form the ϵ-algorithm, *Proc. Glascow Math. Assoc.* **5**, 160 (1962).
48. D. Levin, Numerical inversion of the Laplace transform by accelerating the convergence of Bromwich's integrals, *J. Comput. Appl. Math.* **1**, 247 (1975).
49. H. Safouhi and P. E. Hoggan, Non-linear transformations for rapid and efficient evaluation of multicenter bielectronic integrals over *B* functions, *J. Math. Chem.* **25**, 259 (1999).
50. H. Safouhi, *Les transformations non-linéaires pour l'accélération de la convergence des intégrales biélectroniques multicentriques moléculaires*, Ph.D. thesis (Université de Blaise Pascal, Clermont–Ferrand, France, 1999).
51. R. D. Jenks and R. S. Sutor, *Axiom, the Scientific Computation System* (Springer-Verlag, New York, 1992).
52. G. B. Arfken and H. J. Weber, *Mathematical Methods for Physicists*, 4th ed. (Academic Press, New York, 1995).
53. E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge Univ. Press, Cambridge, UK, 1970).
54. M. Weissbluth, *Atoms and Molecules* (Academic Press, New York, 1978), p. 11.
55. I. M. Gel'fand and G. E. Shilov, *Generalized Functions I, Properties and Operations* (Academic press, New York, 1964), p. 194.
56. J. A. Gaunt, The triplets of heluim, *Phil. Trans. Roy. Soc. A* **228**, 151 (1929).
57. 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.* **368**, 31 (1996).
58. D. Sébilleau, On the computation of the integrated product of three spherical harmonics, *J. Phys. A.* **31**, 7157 (1998).
59. E. J. Weniger and E. O. Steinborn, Programs for the coupling of spherical harmonics, *Comput. Phys. Commun.* **25**, 149 (1982).
60. Yu-Lin Xu, Fast evaluation of Gaunt coefficients, *Math. Comput.* **65**, 1601 (1996).
61. Yu-Lin Xu, Fast evaluation of Gaunt coefficients: Recursive approach, *J. Comput. Appl. Math.* **85**, 53 (1997).
62. Yu-Lin Xu, Efficient evaluation of vector translation coefficients in multiparticle light-scattering theories, *J. Comput. Phys.* **139**, 137 (1998).
63. E. J. Weniger and E. O. Steinborn, New representations for the spherical tensor gradient and the spherical delta function, *J. Math. Phys.* **24**, 2553 (1983).

64. E. O. Steinborn and H. H. H. Homeier, Möbius-type quadrature of electron repulsion integrals with *B* functions, *Int. J. Quantum. Chem.* **24**, 349 (1990).
65. 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**, 61 (1990).
66. 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**, 625 (1991).
67. 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**, 3688 (1986).
68. T. J. l'A. Bromwich, *An Introduction to the Theory of Infinite Series* (London Macmillan, 1959).
69. A. Sidi, Some properties of a generalization of the Richardson process, *J. Inst. Math. Appl.* **24**, 327 (1979).