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Efficient and Rapid Numerical Evaluation of the Two-Electron, Four-Center Coulomb Integrals Using Nonlinear Transformations and Useful Properties of Sine and Bessel Functions

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Two-electron, four-center Coulomb integrals are undoubtedly the most difficult type involved in ab initio and density functional theory molecular structure calculations. Millions of such integrals are required for molecules of interest; therefore rapidity is the primordial criterion when the precision has been reached. This work presents an extremely efficient approach for improving convergence of semi-infinite very oscillatory integrals, based on the nonlinear $\bar{D}$-transformation and some useful properties of spherical Bessel, reduced Bessel, and sine functions. The new method is now shown to be applicable to evaluating the two-electron, four-center Coulomb integrals over B functions. The section with numerical results illustrates the unprecedented efficiency of the new approach in evaluating the integrals of interest.

Key Words: nonlinear transformations; semi-infinite integrals; molecular multi-center integrals; Bessel functions; oscillatory integrals; convergence accelerators.

1. INTRODUCTION

Coulomb integrals are present in all accurate molecular, electronic structure calculation techniques. At the ab initio level, the two-electron two-, three-, and four-center Coulomb integrals have long been the source of bottlenecks. In density functional theory, we also need the two-electron, two-center Coulomb integrals and a three-center term from the potential.

The ab initio calculations are usually carried out using the LCAO-MO approach, where molecular orbitals are built from a linear combination of atomic orbitals [1]. The choice of the

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basis set of atomic orbitals is of utmost importance in this approach. A good atomic orbital basis should satisfy two conditions for analytical solutions of the appropriate Schrödinger equation, namely the exponential decay at infinity [2] and the cusp at the origin [3].

A good basis set for molecular orbitals should also satisfy two pragmatic requirements:

1. Already short expansions of the atomic orbitals in terms of the basis functions should provide sufficiently accurate results.
2. The molecular multicenter integrals should be computed efficiently.

The Gaussian-type functions (GTFs) [4–6] are the most popular functions used in ab initio calculations. This is due to the fact that with GTFs the numerous molecular integrals can be evaluated rather easily. Unfortunately, these Gaussian basis functions fail to satisfy the aforementioned mathematical conditions satisfied by exact eigenfunctions of atomic and molecular Schrödinger equations.

The exponential-type functions (ETFs) are better suited than GTFs to represent electron wave functions near the nucleus and at long range [7]; this implies that a smaller number of ETFs than of GTFs is needed for comparable accuracy. This good convergence of ETFs can be explained by the fact that they show the same asymptotic behavior as exact solutions of atomic and molecular Schrödinger equations.

Among the ETFs, Slater-type functions (STFs) [8, 9] are certainly the simplest analytical functions. Hence, they have a dominating position in atomic electronic structure calculations. However, the use of STFs in molecular calculations has been prevented by the fact that their multicenter integrals are extremely difficult to evaluate for polyatomic molecules, particularly bielectronic terms.

Although B functions [10–12] are more complicated than STFs, they have some remarkable mathematical properties applicable to multicenter integral problems. They possess a relatively simple addition theorem [11, 13–15] and extremely compact convolution integrals [13, 16], and their Fourier transform is of exceptional simplicity [14, 17]. Note that STFs can be expressed as a linear combination of B functions [12, 13].

The B functions are well adapted to the Fourier-transform method [18–20], which is one of the most successful approaches to the evaluation of multicenter integrals. This method allowed integral representations in terms of nonphysical variables for the molecular multicenter integrals over B functions to be developed [19, 20]. The numerical evaluation of these integral representations in terms of nonphysical variables presents severe computational difficulties due to the presence of semi-infinite very oscillatory integrals.

The use of Gauss–Laguerre quadrature is inefficient for evaluating these kinds of integrals as we showed in [21–23]. These semi-infinite integrals can be transformed into infinite series. These series are convergent and alternating; thus the sum of the first N terms, for N sufficiently large, gives a good approximation of the corresponding semi-infinite integral. Unfortunately, the calculation times are prohibitive. Although we accelerate the convergence of the infinite series by using the epsilon algorithm of Wynn [24] or Levin's u transform [25], the calculation times are still prohibitive for good accuracy.

In [21–23], we showed the efficiency of the nonlinear $\bar{D}$-transformation due to Sidi [26, 28] and Levin and Sidi [27] for improving convergence of these kinds of semi-infinite oscillatory integrals. To apply the $\bar{D}$-transformation, the integrand is required to satisfy a linear differential equation of order m with coefficients having asymptotic expansions in inverse powers of their arguments. The approximation $\bar{D}_n^{(m)}$, which as n becomes large converges very quickly to the exact value of the semi-infinite integral, is obtained by solving a linear set of equations of order $n(m-1)+1$ and where it is necessary to calculate the $(m-1)$ successive derivatives of the integrands and its $n(m-1)$ successive zeros [26, 28]. In the case of the two-electron, four-center Coulomb integrals, the integrand satisfies a sixth-order differential equation of the form required to apply the $\bar{D}$-transformation [21]. This makes the application of the $\bar{D}$-transformation very difficult, especially when the values of the quantum numbers are large.

Previous work [22, 29] focused on the use of some properties of the reduced Bessel and spherical Bessel functions to reduce the order of the differential equation required to apply the $\bar{D}$-transformation to 2, keeping all the other conditions fulfilled. This led to the $H\bar{D}$ method, which greatly simplified the application of the $\bar{D}$-transformation. The calculation of the successive derivatives of integrands is avoided and the order of the linear set of equations to solve is reduced to $n+1$. The computation of the $n+1$ successive zeros of the spherical Bessel function and its first derivative is necessary for the calculations.

The purpose of the present work is to further simplify the application of the above non-linear transformations and to further reduce the calculation times keeping the same high accuracy. This is made possible by the help of some useful properties of sine, spherical Bessel, and reduced Bessel functions and the use of Cramer's rule for calculating approximations of semi-infinite highly oscillatory integrals. The computation of the successive zeros of the integrand is avoided.

The numerical results section shows the unprecedented efficiency of the new approach in evaluating the two-electron, four-center. Coulomb integral over B functions.

2. DEFINITIONS AND BASIC FORMULAE

The two-electron, four-center Coulomb integral over B functions is defined by

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

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

The B function is defined as [11, 12]

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

where n, l, m are the quantum numbers such that $n = 1, 2, \ldots, l = 0, 1, \ldots, n-1$, and $m = -l, -l+1, \ldots, l-1, l$ and where $Y^m_l(\theta, \varphi)$ stands for the surface spherical harmonic and is defined by [30]

$$Y^m_l(\theta, \varphi) = i^{m+|m|} \left[\frac{(2l+1)(l-|m|)!)}{4\pi(l+|m|)!)}\right]^{\frac{1}{2}} P^{|m|}_l(\cos\theta) e^{im\varphi}. \tag{3}$$

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

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

The reduced Bessel function $\hat{k}_{n+\frac{1}{2}}(z)$ for $n \in N_0$ is defined by [10, 11]

$$\hat{k}_{n+\frac{1}{2}}(z) - \sqrt{\frac{2}{\pi}}(z)^{n+\frac{1}{2}} K_{n+\frac{1}{2}}(z) = z^n e^{-z} \sum_{j=0}^{n} \frac{(n+j)!}{j!(n-j)!} \frac{1}{(2z)^j}, \tag{5}$$

where $K_{n+\frac{1}{2}}$ stands for the modified Bessel function of the second kind [31].

Reduced Bessel functions satisfy the recurrence relation [10]

$$\hat{k}_{n+\frac{1}{2}}(z) = (2n-1)\hat{k}_{n-\frac{1}{2}}(z) + z^2 \hat{k}_{n-\frac{3}{2}}(z). \tag{6}$$

A useful property satisfied by $\hat{k}_{n+\frac{1}{2}}(z)$ is given by [31]

$$\left(\frac{d}{z\,dz}\right)^m \left[\frac{\hat{k}_{n+\frac{1}{2}}(z)}{z^{2n+1}}\right] = \left(\frac{d}{z\,dz}\right)^m \left[\sqrt{\frac{\pi}{2}} \frac{K_{n+\frac{1}{2}}(z)}{z^{n+\frac{1}{2}}}\right] = (-1)^m \frac{\hat{k}_{n+m+\frac{1}{2}}(z)}{z^{2(n+m)+1}}. \tag{7}$$

The Slater-type function is defined in normalized form according to the relationship [8, 9]

$$\chi_{n,l}^m(\zeta, \vec{r}) = N(n,\zeta) r^{n-1} e^{-\zeta r} Y_l^m(\theta_{\vec{r}}, \varphi_{\vec{r}}), \tag{8}$$

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

The Slater-type function can be expressed as a finite linear combination of B functions [12]

$$\chi_{n,l}^m(\zeta, \vec{r}) = \sum_{p=\tilde{p}}^{n-l} \frac{(-1)^{n-l-p}(n-l)! 2^{l+p}(l+p)!}{(2p-n-l)!(2n-2l-2p)!!} B_{p,l}^m(\zeta, \vec{r}), \tag{9}$$

where

$$\tilde{p} = \begin{cases} (n-l)/2 & \text{if } n-l \text{ even} \\ (n-l+1)/2 & \text{if } n-l \text{ odd}, \end{cases} \tag{10}$$

and where the double factorial is defined by

$$\begin{aligned} (2k)!! &= 2 \times 4 \times 6 \times \cdots \times (2k) = 2^k k! \\ (2k+1)!! &= 1 \times 3 \times 5 \times \cdots \times (2k+1) = \frac{(2k+1)!}{2^k k!} \\ 0!! &= 1. \end{aligned} \tag{11}$$

The Fourier transform $\bar{B}_{n,l}^m(\zeta, \vec{p})$ of $B_{n,l}^m(\zeta, \vec{r})$ is given by [14, 17]

$$\bar{B}_{n,l}^m(\zeta, \vec{p}) = \frac{1}{(2\pi)^{3/2}} \int_{\vec{r}} e^{-i\vec{p}\cdot\vec{r}} B_{n,l}^m(\zeta, \vec{r})\, d\vec{r} \tag{12}$$

$$= \sqrt{\frac{2}{\pi}} \zeta^{2n+l-1} \frac{(-i|p|)^l}{(\zeta^2 + |p|^2)^{n+l+1}} Y_l^m(\theta_{\vec{p}}, \varphi_{\vec{p}}). \tag{13}$$

The Rayleigh expansion of the plane wave functions is given by [32]

$$e^{\pm i\vec{p}\cdot\vec{r}} = \sum_{l=0}^{+\infty} \sum_{m\neg -1}^{l} 4\pi (\pm i)^l j_l(|\vec{p}||\vec{r}|) Y_l^m(\theta_{\vec{r}}, \varphi_{\vec{r}}) \left[Y_l^m(\theta_{\vec{p}}, \varphi_{\vec{p}})\right]^*. \tag{14}$$

The spherical Bessel function $j_l(x)$ of order $l \in N$ is defined by [31, 33]

$$j_l(x) = (-1)^l x^l \left(\frac{d}{x\,dx}\right)^l j_0(x) = (-1)^l x^l \left(\frac{d}{x\,dx}\right)^l \left(\frac{\sin(x)}{x}\right), \tag{15}$$

where $j_l(x)$ and its first derivative $j_l'(x)$ satisfy the recurrence relations [33]

$$\begin{cases} x j_{l-1}(x) + x j_{l+1}(x) = (2l+1) j_l(x) \\ l j_{l-1}(x) - (l+1) j_{l+1}(x) = (2l+1) j_l'(x). \end{cases} \tag{16}$$

In the following, we denote the successive zeros of $j_l(x)$ by $j^n_{l+\frac{1}{2}}$ with $n = 1, 2, \ldots$. $j^0_{l+\frac{1}{2}}$ is assumed to be 0.

The Gaunt coefficients are defined as [34–40]

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

These coefficients linearize the product of two spherical harmonics,

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

where the subscript $l = l_{\min}, 2$ in the summation symbol implies that the summation index l runs in steps of 2 from $l_{\min}$ to $l_1 + l_2$ and the constant $l_{\min}$ is given by [37]

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

The Fourier integral representation of the Coulomb operator $\frac{1}{|\vec{r} - \vec{R}_1|}$ is given by [41]

$$\frac{1}{|\vec{r} - \vec{R}_1|} = \frac{1}{2\pi^2} \int_{\vec{K}} \frac{e^{-i\vec{K}\cdot(\vec{r} - \vec{R}_1)}}{k^2} \, d\vec{k}. \tag{20}$$

3. TWO-ELECTRON, FOUR-CENTER COULOMB INTEGRALS OVER *B* FUNCTIONS

By substituting the integral representation of the Coulomb operator (20) in the expression of the two-electron, four-center Coulomb integrals (1), we obtain

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

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

The Fourier-transform method allowed analytical expressions to be developed for the terms [19, 20]

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

This great result led to analytical expressions for one- and two-electron multicenter integrals over B functions. In the case of two-electron, four-center Coulomb integrals, this expression is given by [20]

$$\begin{aligned}
\mathcal{J}^{n_2l_2m_2,n_4l_4m_4}_{n_1l_1m_1,n_3l_3m_3} &= 8(4\pi)^5(2l_1+1)!!(2l_2+1)!!\frac{(n_1+l_1+n_2+l_2+1)!}{(n_1+l_1)!(n_2+l_2)!}\\
&\times(-1)^{l_1+l_2}(2l_3+1)!!(2l_4+1)!!\frac{(n_3+l_3+n_4+l_4+1)!}{(n_3+l_3)!(n_4+l_4)!}\zeta_1^{2n_1+l_1-1}\zeta_2^{2n_2+l_2-1}\\
&\times\zeta_3^{2n_3+l_3-1}\zeta_4^{2n_4+l_4-1}\sum_{l_1'-0}^{l_1}\sum_{m_1'=\mu_{11}}^{\mu_{12}} i^{l_1+l_1'}\frac{\langle l_1m_1|l_1'm_1'|l_1-l_1'm_1-m_1'\rangle}{(2l_1'+1)!![2(l_1-l_1')+1]!!}\\
&\times\sum_{l_2'=0}^{l_2}\sum_{m_2'=\mu_{21}}^{\mu_{22}} i^{l_2+l_2'}(-1)^{l_2'}\frac{\langle l_2m_2|l_2'm_2'|l_2-l_2'm_2-m_2'\rangle}{(2l_2'+1)!![2(l_2-l_2')+1]!!}\\
&\times\sum_{l_3'=0}^{l_3}\sum_{m_1'=\mu_{31}}^{\mu_{32}} i^{l_3+l_3'}\frac{\langle l_3m_3|l_3'm_3'|l_3-l_3'm_3-m_3'\rangle}{(2l_3'+1)!![2(l_3-l_3')+1]!!}\\
&\times\sum_{l_4'=0}^{l_4}\sum_{m_4'=\mu_{41}}^{\mu_{42}} i^{l_4+l_4'}(-1)^{l_4'}\frac{\langle l_4m_4|l_4'm_4'|l_4-l_4'm_4-m_4'\rangle}{(2l_4'+1)!![2(l_4-l_4')+1]!!}\\
&\times\sum_{l=l_{1,min},2}^{l_1'+l_2'}\langle l_2'm_2'|l_1'm_1'|lm'2-m_1'\rangle R_{21}^l Y_l^{m_2'-m_1'}\left(\theta_{\vec{R}_{21}},\varphi_{\vec{R}_{21}}\right)\\
&\times\sum_{l_{12}=l'_{1,min},2}^{l_1-l_1'+l_2-l_2'}\langle l_2-l_2'm_2-m_2'|l_1-l_1'm_1-m_1'|l_{12}m_{21}\rangle\\
&\times\sum_{l'=l_{2,min},2}^{l_3'+l_4'}\langle l_4'm_4'|l_3'm_3'|l'm_4'-m_3'\rangle R_{34}^{l'} Y_{l'}^{m_4'-m_3'}\left(\theta_{\vec{R}_{34}},\varphi_{\vec{R}_{34}}\right)\\
&\times\sum_{l_{34}=l'_{2,min},2}^{l_3-l_3'+l_4-l_4'}\langle l_4-l_4'm_4-m_4'|l_3-l_3'm_3-m_3'|l_{34}m_{43}\rangle\\
&\times\sum_{\lambda=l''_{min},2}^{l_{12}+l_{34}}(-i)^\lambda\langle l_{12}m_{21}|l_{34}m_{43}|\lambda\mu\rangle\\
&\times\sum_{j_{12}-0}^{\Delta l_{12}}\sum_{j_{34}=0}^{\Delta l_{34}}\binom{\Delta l_{12}}{j_{12}}\binom{\Delta l_{34}}{j_{34}}\frac{(-1)^{j_{12}+j_{34}}}{2^{\nu_1+\nu_2+l+l'+1}\left(\nu_1+\frac{1}{2}+l\right)!\left(\nu_2+\frac{1}{2}+l'\right)!}
\end{aligned}$$

$$\times \int_{s=0}^{1} \frac{s^{n_2+l_2+l_1}(1-s)^{n_1+l_1+l_2}}{s^{l'_1}(1-s)^{l'_2}} \int_{t=0}^{1} \frac{t^{n_4+l_4+l_3}(1-t)^{n_3+l_3+l_4}}{t^{l'_3}(1-t)^{l'_4}} Y_{\lambda}^{m_2-\mu}(\theta_{\vec{v}}, \varphi_{\vec{v}})$$

$$\times \left[\int_{x=0}^{+\infty} x^{n_x} \frac{\hat{k}_{\nu_1}[R_{21}\,\gamma_{12}(s,x)]}{[\gamma_{12}(s,x)]^{n_{\gamma_{12}}}} \frac{\hat{k}_{\nu_2}[R_{34}\,\gamma_{34}(t,x)]}{[\gamma_{34}(t,x)]^{n_{\gamma_{34}}}} j_{\lambda}(vx)\,dx \right] dt\,ds \qquad (22)$$

$$\mu - (m_2 - m'_2) - (m_1 - m'_1) + (m_4 - m'_4) - (m_3 - m'_3)$$

$$n_{\gamma_{12}} = 2(n_1 + l_1 + n_2 + l_2) - (l'_1 + l'_2) - l + 1$$

$$n_{\gamma_{34}} = 2(n_3 + l_3 + n_4 + l_4) - (l'_3 + l'_4) - l' + 1$$

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

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

$$[\gamma_{12}(s,x)]^2 = (1-s)\zeta_1^2 + s\zeta_2^2 + s(1-s)x^2$$

$$[\gamma_{34}(t,x)]^2 = (1-t)\zeta_3^2 + t\zeta_4^2 + t(1-t)x^2$$

$$n_x = l_1 - l'_1 + l_2 - l'_2 + l_3 - l'_3 + l_4 - l'_4$$

$$\nu_1 = n_1 + n_2 + l_1 + l_2 - l - j_{12} + \frac{1}{2}$$

$$\nu_2 - n_3 + n_4 + l_3 + l_4 - l' - j_{34} + \frac{1}{2}$$

$$\vec{v} = (1-s)\vec{R}_{21} + (1-t)\vec{R}_{43} - \vec{R}_{41}$$

$$\Delta' l_{12} = \frac{l'_1 + l'_2 - l}{2}, \quad \Delta' l_{34} = \frac{l'_3 + l'_4 - l'}{2}$$

$$m_{ij} = m_i - m'_i - (m_j - m'_j).$$

The principal difficulties in the numerical evaluation of the above expression arise mainly from the presence of the semi-infinite integral, which will be referred to as $\tilde{\mathcal{J}}(s,t)$, whose integrand, which will be referred to as $F_{\mathcal{J}}(x)$, oscillates rapidly due to the presence of the spherical Bessel function $j_{\lambda}(vx)$ in particular for large values of v and λ. Note that in the regions where s and t are close to 0 or 1, the oscillations become very rapid. Indeed, when we make the substitutions $s = 0$ or 1 and $t = 0$ or 1, the integrand will be reduced to the term $x^{n_x} j_{\lambda}(vx)$, because the terms

$$\frac{\hat{k}_{\nu_1}[R_{21}\,\gamma_{12}(s,x)]}{[\gamma_{12}(s,x)]^{n_{\gamma_{12}}}}$$

and

$$\frac{\hat{k}_{\nu_2}[R_{34}\,\gamma_{34}(t,x)]}{[\gamma_{34}(t,x)]^{n_{\gamma_{34}}}},$$

which are exponentially decreasing, become constants and therefore the rapid oscillations of $j_{\lambda}(vx)$ cannot be damped and suppressed by the exponential decreasing functions $\hat{k}_{\nu}$. It should be mentioned that the regions where s and t are close to 0 or 1 carry a very small weight due to factors $s^{i_2}(1-s)^{i_1}$, $t^{i_4}(1-t)^{i_3}$ in the integrands (22) [42–45].

Let us consider the semi-infinite integral $\tilde{\mathcal{J}}(s,t)$. It is given by

$$\tilde{\mathcal{J}}(s,t) = \int_0^{+\infty} x^{n_x} \frac{\hat{k}_{\nu_1}[R_{21}\,\gamma_{12}(s,x)]}{[\gamma_{12}(s,x)]^{n_{\gamma_{12}}}} \frac{\hat{k}_{\nu_2}[R_{34}\,\gamma_{34}(t,x)]}{[\gamma_{34}(t,x)]^{n_{\gamma_{34}}}}\, j_\lambda(vx)\,dx \tag{23}$$

$$- \sum_{n=0}^{+\infty} \int_{j^n_{\lambda,v}}^{j^{n+1}_{\lambda,v}} x^{n_x} \frac{\hat{k}_{\nu_1}[R_{21}\,\gamma_{12}(s,x)]}{[\gamma_{12}(s,x)]^{n_{\gamma_{12}}}} \frac{\hat{k}_{\nu_2}[R_{34}\,\gamma_{34}(t,x)]}{[\gamma_{34}(t,x)]^{n_{\gamma_{34}}}}\, j_\lambda(vx)\,dx, \tag{24}$$

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

The above infinite series is convergent and alternating therefore the sum of the first N terms, for N sufficiently large, gives a good approximation of the semi-infinite integral, but the use of this approach has been prevented by the fact that the calculation times for a sufficient accuracy are prohibitive. We have shown [21, 22] that the use of the Gauss-Laguerre quadrature for evaluating these kinds of integrals gives inaccurate results in the regions where s and t are close to 0 or 1 since the integrand cannot be represented by a function of the form $g(x)e^{-\lambda x}$ where $g(x)$ is not a rapidly oscillating function. The use of the epsilon algorithm of Wynn [24] or Levin's u transform [25] accelerates the convergence of the infinite series but the calculation times are still prohibitive [21, 22].

4. THE $\bar{\text{D}}$ AND H$\bar{\text{D}}$ METHODS FOR ACCELERATING CONVERGENCE OF SEMI-INFINITE OSCILLATORY INTEGRALS

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

$$p(x) \sim x^\gamma \left(a_0 + \frac{a_1}{x} + \frac{a_2}{x^2} + \cdots \right) \tag{25}$$

and their derivatives of any order have asymptotic expansions, which can be obtained by differentiating that in (25) term by term.

From (25) it follows that $A^{(\gamma)} \supset A^{(\gamma-1)} \supset \cdots$.

We denote $\tilde{A}^{(\gamma)}$ for some γ, the set of functions $p(x)$ such that $p(x) \in A^{(\gamma)}$ and $\lim_{x\to+\infty} x^{-\gamma}\, p(x) \neq 0$. Thus, $p \in \tilde{A}^{(\gamma)}$ has an asymptotic expansion in inverse powers of x as $x \to +\infty$ of the form given by (25) with $a_0 \neq 0$.

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

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

THEOREM 1 [26]. *Let $f(x)$ be integrable on* $[0, +\infty]$ (*i.e.*, $\int_0^{+\infty} f(t)\,dt$ *exists*) *and let it satisfy a linear differential equation of order m of the form*

$$f(x) = \sum_{k-1}^{m} p_k(x)\, f^{(k)}(x), \quad p_k \in A^{(i_k)}, \quad i_k \leq k. \tag{26}$$

If for every integer $l \geq -1$,

$$\sum_{k-1}^{m} l(l-1)\cdots(l-k+1)\, p_{k,0} \neq 1,$$

where

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

and for $i \leq k \leq m,\ 1 \leq i \leq m,\ \lim_{x\to+\infty} p_k^{(i-1)}(x) f^{(k-i)}(x) = 0$, *then the approximation* $\bar{D}_n^{(m)}$ *of* $\int_0^\infty f(t)\,dt$, *using the nonlinear* $\bar{D}$*-transformation, satisfies the* $n(m-1)+1$ *equations given by* [26]

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

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

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

In previous work [21], we showed that the integrand $F_{\mathcal{J}}(x)$ of $\tilde{\mathcal{J}}(s,t)$ satisfies a sixth-order, linear differential equation with coefficients having asymptotic expansion in inverse powers of their argument x as $x \to +\infty$ and all the conditions to apply the $\bar{D}$-transformation are fulfilled.

The results obtained by applying this transformation were very satisfactory. Unfortunately the computation of the fifth successive derivatives of the integrand and its $5n$ successive zeros is necessary for the calculations as can be seen from (27). This presents severe numerical and computational difficulties in particular when the values of the quantum numbers n_i, l_i, and m_i are large. The order of the linear set of equations to solve for calculating the approximations $\bar{D}_n^{(m)}$ is equal to $5n+1$; thus when the value of n is large, the calculations become very difficult.

In [23, 29], we showed by using some helpful properties of spherical Bessel, reduced Bessel, and Poincaré series [46] that we can obtain a second-order, linear differential equation of the form required to apply the $\bar{D}$-transformation for a function $f(x)$ of the form $f(x) = g(x) j_\lambda(x)$, where $j_\lambda(x)$ stands for the spherical Bessel function and $g(x) = h(x)e^{\phi(x)}$, and where $h(x) \in \tilde{A}^{(\gamma)}$ for some γ and $\phi(x) \in \tilde{A}^{(k)}$ for $k > 0$ and $\alpha_0(\phi) < 0$. The reduction of the order of the linear differential equation to 2 led to the $H\bar{D}$ method that greatly simplified the application of the $\bar{D}$-transformation. The approximation $H\bar{D}_n^{(2)}$ of $\int_0^{+\infty} f(t)\,dt$ is given by [23, 29]

$$H\bar{D}_n^{(2)} = \int_0^{x_l} f(t)\,dt + g(x_l) j'_\lambda(x_l) x_l^2 \sum_{i=0}^{n-1} \frac{\bar{\beta}_{1,i}}{x_l^i}, \quad l = 0, 1, \ldots, n, \tag{28}$$

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

It is shown that that the integrand $F_{\mathcal{J}}(x)$ of $\tilde{\mathcal{J}}(s,t)$ satisfies all the conditions for applying the $H\bar{D}$ method [22, 29], and consequently a good approximation of the semi-infinite integral $\tilde{\mathcal{J}}(s,t)$ can be obtained by solving the linear system (28).

As can be seen from (28), calculation of the successive derivatives is avoided, and we only need to calculate the first derivative of the spherical Bessel function $j_\lambda(x)$. The order of the linear system to solve using the $H\bar{D}$ method is reduced to $n+1$. This leads to a substantial reduction in the calculation times for high predetermined accuracy, but it is still necessary to compute the n successive zeros of $j_\lambda(x)$ and to solve the linear system (28).

The purpose of this work is to further simplify the application of the above nonlinear transformations to evaluating the two-electron, four-center Coulomb integral and to further reduce the calculation times, keeping the same high predetermined accuracy.

5. THE $S\bar{D}$ APPROACH TO EVALUATING SEMI-INFINITE HIGHLY OSCILLATORY INTEGRALS AND APPLICATION

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

1. *If $\gamma \neq 0$, then $p'(x) \in \tilde{A}^{(\gamma-1)}$; otherwise $p'(x) \in A^{(-2)}$.*
2. *If $q(x) \in \tilde{A}^{(\delta)}$, then $p(x)q(x) \in \tilde{A}^{(\gamma+\delta)}$ and $\alpha_0(pq) = \alpha_0(p)\alpha_0(q)$.*
3. *$\forall k \in \mathbb{R}$, $x^k p(x) \in \tilde{A}^{(k+\gamma)}$ and $\alpha_0(x^k p) = \alpha_0(p)$.*
4. *The function $cp(x) \in \tilde{A}^{(\gamma)}$ and $\alpha_0(cp) = c\alpha_0(p)$ for all $c \neq 0$.*
5. *If $q(x) \in A^{(\delta)}$ and $\gamma - \delta > 0$, then the function $p(x) + q(x) \in \tilde{A}^{(\gamma)}$ and $\alpha_0(p+q) = \alpha_0(p)$. If $\gamma = \delta$ and $\alpha_0(p) \neq -\alpha_0(q)$, then the function $p(x)+q(x) \in \tilde{A}^{(\gamma)}$ and $\alpha_0(p+q) = \alpha_0(p) + \alpha_0(q)$.*
6. *For $m > 0$ an integer, $p^m(x) \in \tilde{A}^{(m\gamma)}$ and $\alpha_0(p^m) = \alpha_0(p)^m$.*
7. *The function $1/p(x) \in \tilde{A}^{(-\gamma)}$ and $\alpha_0(1/p) = 1/\alpha_0(p)$.*

The proof of Lemma 1 follows from the properties of Poincaré series [46].

LEMMA 2. *Let $\phi \in \tilde{A}^{(k)}$ where k is a positive integer and $k \neq 0$. The function*

$$\hat{k}_{n+\frac{1}{2}}(\phi(x)) \in \tilde{A}^{(nk)} e^{\tilde{A}^{(k)}}$$

and can be written in the following form:

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

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

By using the analytical expression of the reduced Bessel function which is given by Eq. (5) and using some properties of Poincaré series, one can easily demonstrate the validity of Lemma 2.

THEOREM 2. *Let $f(x)$ be a function of the form $f(x) - g(x) j_\lambda(x)$, where $g(x)$ is in $\mathcal{C}^2([0,+\infty])$ which is the space of functions that are twice continuously differentiable on $[0,+\infty]$, and of the form $g(x) = h(x)e^{\phi(x)}$ and where $h(x) \in \tilde{A}^{(\gamma)}$ and $\phi(x) \in \tilde{A}^{(k)}$ for some γ and k. If $k > 0$, $\alpha_0(\varphi) < 0$ and for all $l = 0, \ldots, \lambda - 1$, $\lim_{x\to 0} x^{l-\lambda+1}[(\frac{d}{x\,dx})^l (x^{\lambda-1} g(x))] j_{\lambda-1-l}(x) = 0$, then $f(x)$ is integrable on $[0,+\infty]$ (i.e., $\int_0^{+\infty} f(t)\,dt$ exists) and an approximation of $\int_0^{+\infty} f(x)\,dx$ is given by*

$$S\bar{D}_n^{(2,j)} = \frac{\sum_{i=0}^{n+1} \binom{n+1}{i} (x_0/\pi + i + j)^n F(x_{i+j}) \big/ \left[x_{i+j}^2 G(x_{i+j})\right]}{\sum_{i=0}^{n+1} \binom{n+1}{i} (x_0/\alpha + i + j)^n \big/ \left[x_{i+j}^2 G(x_{i+j})\right]}, \tag{29}$$

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

Proof. Let us consider $\int_0^{+\infty} f(x)\,dx = \int_0^{+\infty} g(x)\, j_\lambda(x)$. By replacing the spherical Bessel function $j_\lambda(x)$ with its analytical expression given by (15), we obtain

$$\int_0^{+\infty} f(x)\,dx = (-1)^\lambda \int_0^{+\infty} x^\lambda g(x) \left[\left(\frac{d}{x\,dx}\right)^\lambda j_0(x)\right] dx. \tag{30}$$

By integrating by parts until all the derivatives of $j_0(x)$ with respect to $x\,dx$ disappear in the last term on the right-hand side of (30), one can obtain

$$\int_0^{+\infty} f(x)\,dx = (-1)^\lambda \left[\sum_{l=0}^{\lambda-1} (-1)^l \left(\left(\frac{d}{x\,dx}\right)^l (x^{\lambda-1} g(x))\right)\left(\left(\frac{d}{x\,dx}\right)^{\lambda-1-l} j_0(x)\right)\right]_0^{+\infty} + \int_0^{+\infty} \left[\left(\frac{d}{x\,dx}\right)^\lambda (x^{\lambda-1} g(x))\right] j_0(x)\, x\,dx. \tag{31}$$

Using Eq. (15) and replacing $j_0(x)$ by $\frac{\sin(x)}{x}$, the above equation can be rewritten as

$$\int_0^{+\infty} f(x)\,dx = -\left[\sum_{l=0}^{\lambda-1} x^{l-\lambda+1}\left(\left(\frac{d}{x\,dx}\right)^l (x^{\lambda-1} g(x))\right) j_{\lambda-1-l}(x)\right]_0^{+\infty} + \int_0^{+\infty} \left[\left(\frac{d}{x\,dx}\right)^\lambda (x^{\lambda-1} g(x))\right] \sin(x)\,dx, \tag{32}$$

where $g(x)$ is exponentially decreasing as $x \to +\infty$. From this it follows that $(\frac{d}{x\,dx})^l (x^{\lambda-1} g(x))$ is also exponentially decreasing as $x \to +\infty$ and consequently $\lim_{x\to+\infty} x^{l-\lambda+1} [(\frac{d}{x\,dx})^l (x^{\lambda-1} g(x))] j_{\lambda-1-l}(x) = 0$ for all $l \geq 0$.

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

$$\int_0^{+\infty} f(x)\,dx = \int_0^{+\infty} \left[\left(\frac{d}{x\,dx}\right)^\lambda (x^{\lambda-1} g(x))\right] \sin(x)\,dx. \tag{33}$$

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

$$G(x) = \sum_{i=0}^{\lambda} \frac{\lambda!!}{(\lambda-2i)!!} x^{\lambda-2i} \left(\frac{d}{x\,dx}\right)^{\lambda-i} g(x) - \sum_{i=0}^{\lambda}\sum_{m=0}^{\lambda-i} \frac{\lambda!!}{(\lambda-2i)!!} \binom{\lambda-i}{m} x^{\lambda-2i} \left[\left(\frac{d}{x\,dx}\right)^m h(x)\right]\left[\left(\frac{d}{x\,dx}\right)^{\lambda-i-m} e^{\phi(x)}\right]. \tag{34}$$

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

$$\begin{cases} \left(\frac{d}{x\,dx}\right)^m h(x) \in A^{(\gamma-2m)} \\ \left(\frac{d}{x\,dx}\right)^\alpha e^{\phi(x)} \neg\, \varphi(x)\, e^{\phi(x)}, \end{cases}$$

where $\varphi \in A^{(\alpha(k-2))}$ and consequently

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

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

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

$$G(x) = H(x)\, e^{\phi(x)}, \tag{35}$$

where $H(x) \in \tilde{A}^{(\gamma+\lambda k-\lambda)}$.

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

$$\sin(x) = -\sin''(x). \tag{36}$$

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

$$\mathcal{F}(x) = q_1(x)\mathcal{F}'(x) + q_2(x)\mathcal{F}''(x), \tag{37}$$

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

$$\begin{aligned} q_1(x) &= \frac{2\left(\phi'(x) + \frac{H'(x)}{H(x)}\right)}{1 + \left(\phi'(x) + \frac{H'(x)}{H(x)}\right)^2 - \left(\phi'(x) + \frac{H'(x)}{H(x)}\right)'} \\ q_2(x) &= \frac{-1}{1 + \left(\phi'(x) + \frac{H'(x)}{H(x)}\right)^2 - \left(\phi'(x) + \frac{H'(x)}{H(x)}\right)'}. \end{aligned} \tag{38}$$

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

If $k > 0$ and $\alpha_0(\phi_1) < 0$, then $\mathcal{F}(x)$ is exponentially, decreasing as $x \to +\infty$ and consequently is integrable on $[0, +\infty]$ and for all $l = i, 2$, $i = 1, 2$,

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

It is easy to show that $q_{i,0} = \lim_{x\to+\infty} x^{-i} q_i(x) = 0$ for $i = 1, 2$; thus for every integer $l \geq -1$

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

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

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

$$S\bar{D}_n^{(2)} = \int_0^{x_l} \mathcal{F}(x)\,dx + (-1)^{l+1} G(x_l) x_l^2 \sum_{i=0}^{n-1} \frac{\bar{\beta}_{1,i}}{x_l^i}, \quad l - 0, 1, \ldots n, \tag{39}$$

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

Following Levin in [25], we can use Cramer's rule, since the zeros of $\sin(x)$ are equidistant, to obtain the simple solution which is given by (29) for the unknown $S\bar{D}_n^{(2)}$. ■

Now let us consider the integrand $F_{\mathcal{J}}(x) = g(x)\, j_\lambda(vx)$ of $\tilde{\mathcal{J}}(s,t)$, where $g(x)$ is defined by

$$g(x) = x^{n_x} \frac{\tilde{k}_{\nu_1}[R_{21}\gamma_{12}(s,x)]}{[\gamma_{12}(s,x)]^{n_{\gamma_{12}}}} \frac{\hat{k}_{\nu_2}[R_{34}\gamma_{34}(t,x)]}{[\gamma_{34}(s,x)]^{n_{\gamma_{34}}}} \in \mathcal{C}^2([0,+\infty]).$$

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

$$\phi_1 = R_{21}\gamma_{12}(s,x) = R_{21}\sqrt{(1-s)\zeta_1^2 + s\zeta_2^2 + s(1-s)x^2} \in \tilde{A}^{(1)}$$
$$\phi_2 = R_{34}\gamma_{34}(t,x) = R_{34}\sqrt{(1-t)\zeta_3^2 + t\zeta_4^2 + t(1-t)x^2} \in \tilde{A}^{(1)}.$$

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

Using these arguments, we can rewrite the function $g(x)$ as

$$g(x) = h(x)e^{-\phi(x)} \begin{cases} h(x) \in \tilde{A}^{(\nu_1+\nu_2-1+n_x-n_{\gamma 12}-n_{\gamma 34})} \\ \phi \in \tilde{A}^{(1)} \quad \text{with } \alpha_0(\phi) > 0. \end{cases}$$

Let l be in $\{0, 1, \ldots, \lambda - 1\}$:

$$\begin{aligned} x^{l-\lambda+1}\left(\frac{d}{x\,dx}\right)^l (x^{\lambda-1}g(x)) = {} & \sum_{i=0}^{l}\sum_{j=0}^{l-i}\binom{l}{i}\frac{(n_x+\lambda-1)!!}{(n_x+\lambda-1-2i)!!}x^{n_x+l-2i} \\ & \times \binom{l-i}{j}\left(\frac{d}{x\,dx}\right)^i \left(\frac{\hat{k}_{\nu_1}[R_{21}\gamma_{12}(s,x)]}{[\gamma_{12}(s,x)]^{n_{\gamma_{12}}}}\right) \\ & \times \left(\frac{d}{x\,dx}\right)^{l-i-j}\left(\frac{\hat{k}_{\nu_2}[R_{34}\gamma_{34}(t,x)]}{[\gamma_{34}(t,x)]^{n_{\gamma_{34}}}}\right). \end{aligned} \tag{40}$$

The two last terms on the right-hand side of the above equation are defined for $x = 0$ and for all $l,\ i$, and j.

The integers λ vary from $l_{\min}$, which is given by (19) to n_x; thus for all $l = 0, 1, \ldots, \lambda - 1$, $n_x - l > 0$ and consequently for all $i = 0, 1, \ldots, l$, the integer $n_x + l - 2i \geq 1$.

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

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

All the conditions of Theorem 2 are now shown to be fulfilled by the integrand $F_{\mathcal{J}}(x)$. The semi-infinite integral $\tilde{\mathcal{J}}(s,t)$ can be rewritten as

$$\begin{aligned} \tilde{\mathcal{J}}(s,t) = \frac{1}{v^{\lambda+1}} \int_0^{+\infty} & \left[\left(\frac{d}{x\,dx}\right)^\lambda \left(x^{n_x+\lambda-1}\frac{\hat{k}_{\nu_1}[R_{21}\gamma_{12}(s,x)]}{[\gamma_{12}(s,x)]^{n_{\gamma_{12}}}}\right.\right. \\ & \times \left.\left.\frac{\hat{k}_{\nu_2}[R_{34}\gamma_{34}(t,x)]}{[\gamma_{34}(t,x)]^{n_{\gamma_{34}}}}\right)\right] \sin(vx)\, dx \end{aligned} \tag{41}$$

$$= \frac{1}{v^{\lambda+1}} \sum_{n=0}^{+\infty} \int_{n\pi/v}^{(n+1)\pi/v} \left[\left(\frac{d}{x\,dx} \right)^{\lambda} \left(x^{n_x+\lambda'-1} \frac{\hat{k}_{\nu_1}[R_{21}\gamma_{12}(s,x)]}{[\gamma_{12}(s,x)]^{n_{\gamma_{12}}}} \right.\right.$$
$$\left.\left. \times \frac{\hat{k}_{\nu_2}[R_{34}\gamma_{34}(t,x)]}{[\gamma_{34}(t,x)]^{n_{\gamma_{34}}}} \right) \right] \sin(vx)\,dx. \tag{42}$$

The approximation of $\tilde{\mathcal{J}}(s,t)$ is given by

$$S\bar{D}_n^{(2,j)} = \frac{1}{v^{\lambda+1}} \frac{\sum_{i=0}^{n+1} \binom{n+1}{i} (1+i+j)^n F(x_{i+j}) \big/ \left[x_{i+j}^2 G(x_{i+j})\right]}{\sum_{i=0}^{n+1} \binom{n+1}{i} (1+i+j)^n \big/ \left[x_{i+j}^2 G(x_{i+j})\right]}, \tag{43}$$

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

The function $G(x)$ can be easily computed by using Eq. (7), the Leibnitz formula, and the fact that $\frac{d}{dx} = \frac{dz}{dx}\frac{d}{dz}$.

Let j be in N; if $n_{\gamma 12} = 2\nu_1$, then

$$\left(\frac{d}{x\,dx}\right)^j \left[\frac{\hat{k}_{\nu_1}[R_{21}\gamma_{12}(s,x)]}{[\gamma_{12}(s,x)]^{2\nu_1}} \right] = (-1)^j s^j (1-s)^j \frac{\hat{k}_{\nu_1+j}[R_{21}\gamma_{12}(s,x)]}{[\gamma_{12}(s,x)]^{2(\nu_1+j)}}. \tag{44}$$

For $n_{\gamma 12} < 2\nu_1$, we obtain

$$\left(\frac{d}{x\,dx}\right)^j \left[\frac{\hat{k}_{\nu_1}[R_{21}\gamma_{12}(s,x)]}{[\gamma_{12}(s,x)]^{n_{\gamma_{12}}}} \right]$$
$$= \sum_{i=0}^{j} \binom{j}{i} (-1)^{j-i} \frac{(2\nu_1 - n_{\gamma_{12}})!!}{(2\nu_1 - n_{\gamma_{12}} - 2i)!!} s^i (1-s)^i \frac{\hat{k}_{\nu_1+j-i}[R_{21}\gamma_{12}(s,x)]}{[\gamma_{12}(s,x)]^{n_{\gamma_{12}}+2i}}. \tag{45}$$

6. NUMERICAL RESULTS

The finite integrals involved in Eqs. (28) and (43) are transformed into finite sums $\int_0^{x_n} f(x)\,dx = \sum_{l=0}^{n-1} \int_{x_l}^{x_{l+1}} f(x)\,dx$ and each term of the finite sum is evaluated using the Gauss–Legendre quadrature of order 16. The finite integrals involved in Eqs. (24) and (42) are evaluated using the Gauss–Legendre quadrature of order 16. Numerical results are presented on Tables I–VIII.

TABLE I

Values of $\tilde{\mathcal{J}}(s,t)$ Obtained with 15 Correct Decimals Using the Infinite Series (24)

s	t	ν_1	$n_{\gamma_{12}}$	λ	R_1	R_2	R_3	R_4	ζ_1	ζ_2	max	$\tilde{\mathcal{J}}(s,t)$
0.999	0.999	5/2	5	0	2.5	5.0	7.5	6.0	1.5	1.0	182	0.133288836250D+01
0.999	0.005	5/2	3	1	2.5	4.0	5.0	6.5	2.0	1.0	173	0.713647099798D−01
0.005	0.005	7/2	7	1	1.5	1.7	3.7	3.5	2.0	1.0	172	0.536376822348D−02
0.005	0.999	9/2	5	2	1.5	2.0	6.0	3.5	3.0	2.0	157	0.391621109662D+00
0.999	0.999	9/2	9	3	4.0	6.0	6.5	7.5	1.5	2.0	343	0.189344506463D−02
0.999	0.005	11/2	11	3	5.5	6.0	8.5	7.5	5.0	1.0	215	0.142649644276D−02
0.005	0.005	13/2	11	4	3.5	6.5	9.0	5.0	2.5	2.0	70	0.121634061600D−02
0.005	0.005	17/2	17	4	2.0	3.0	7.0	5.0	3.0	2.5	135	0.100732525411D−04

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

TABLE II
Values of $\tilde{\mathcal{J}}(s, t)$ Obtained with 15 Correct Decimals Using the Infinite Series (42)

s	t	ν_1	$n_{\gamma_{12}}$	λ	R_1	R_2	R_3	R_4	ζ_1	ζ_2	max	$\tilde{\mathcal{J}}(s,t)$
0.999	0.999	5/2	5	0	2.5	5.0	7.5	6.0	1.5	1.0	181	0.133288836250D+01
0.999	0.005	5/2	3	1	2.5	4.0	5.0	6.5	2.0	1.0	192	0.713647099798D−01
0.005	0.005	7/2	7	1	1.5	1.7	3.7	3.5	2.0	1.0	152	0.536376822348D−02
0.005	0.999	9/2	5	2	1.5	2.0	6.0	3.5	3.0	2.0	196	0.391621109662D+00
0.999	0.999	9/2	9	3	4.0	6.0	6.5	7.5	1.5	2.0	272	0.189344506462D−02
0.999	0.005	11/2	11	3	5.5	6.0	8.5	7.5	5.0	1.0	174	0.142649644276D−02
0.005	0.005	13/2	11	4	3.5	6.5	9.0	5.0	2.5	2.0	77	0.121634061600D−02
0.005	0.005	17/2	17	4	2.0	3.0	7.0	5.0	3.0	2.5	127	0.100732525411D−04

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

TABLE III
Evaluation of $\tilde{\mathcal{J}}(s, t)$ Using $S\bar{D}_n^{(2,5)}$ (43)

s	t	ν_1	$n_{\gamma_{12}}$	λ	R_1	R_2	R_3	R_4	ζ_1	ζ_2	n	$\tilde{\mathcal{J}}(s,t)$	Error
0.999	0.999	5/2	5	0	2.5	5.0	7.5	6.0	1.5	1.0	4	0.1333D+01	0.53D−10
0.999	0.005	5/2	3	1	2.5	4.0	5.0	6.5	2.0	1.0	6	0.7136D−01	0.62D−10
0.005	0.005	7/2	7	1	1.5	1.7	3.7	3.5	2.0	1.0	7	0.5364D−02	0.19D−10
0.005	0.999	9/2	5	2	1.5	2.0	6.0	3.5	3.0	2.0	9	0.3916D+00	0.64D−10
0.999	0.999	9/2	9	3	4.0	6.0	6.5	7.5	1.5	2.0	5	0.1893D−02	0.19D−10
0.999	0.005	11/2	11	3	5.5	6.0	8.5	7.5	5.0	1.0	7	0.1426D−02	0.51D−10
0.005	0.005	13/2	11	4	3.5	6.5	9.0	5.0	2.5	2.0	6	0.1216D−02	0.44D−10
0.005	0.005	17/2	17	4	2.0	3.0	7.0	5.0	3.0	2.5	5	0.1007D−04	0.13D−12

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

TABLE IV
Evaluation of $\tilde{\mathcal{J}}(s, t)$ Using $H\bar{D}_n^{(2)}$ (28)

s	t	ν_1	$n_{\gamma_{12}}$	λ	R_1	R_2	R_3	R_4	ζ_1	ζ_2	n	$\tilde{\mathcal{J}}(s,t)$	Error
0.999	0.999	5/2	5	0	2.5	5.0	7.5	6.0	1.5	1.0	8	0.1333D+01	0.72D−09
0.999	0.005	5/2	3	1	2.5	4.0	5.0	6.5	2.0	1.0	9	0.7136D−01	0.28D−09
0.005	0.005	7/2	7	1	1.5	1.7	3.7	3.5	2.0	1.0	9	0.5364D−02	0.53D−10
0.005	0.999	9/2	5	2	1.5	2.0	6.0	3.5	3.0	2.0	9	0.3916D+00	0.15D−07
0.999	0.999	9/2	9	3	4.0	6.0	6.5	7.5	1.5	2.0	9	0.1893D−02	0.10D−09
0.999	0.005	11/2	11	3	5.5	6.0	8.5	7.5	5.0	1.0	8	0.1426D−02	0.93D−10
0.005	0.005	13/2	11	4	3.5	6.5	9.0	5.0	2.5	2.0	9	0.1216D−02	0.80D−09
0.005	0.005	17/2	17	4	2.0	3.0	7.0	5.0	3.0	2.5	9	0.1007D−04	0.52D−11

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

TABLE V

Values of $\mathcal{J}^{n_2 00, n_4 00}_{n_1 00, n_3 00}$ Obtained with 15 Exact Decimals Using the Infinite Series (24)

n_1	n_2	$n_{\gamma_{12}}$	n_x	λ	R_1	R_2	R_3	R_4	ζ_1	ζ_2	$\mathcal{J}^{n_2 00, n_4 00}_{n_1 00, n_3 00}$
1	1	5	0	0	1.5	3.5	6.5	4.5	3.0	2.5	0.171288775969805D−01
2	1	7	1	1	3.0	4.5	7.5	5.0	2.0	2.5	0.109643380336422D+00
2	2	9	2	2	2.5	3.5	5.5	4.5	2.0	1.5	0.550614613833544D+01
3	2	11	2	2	2.0	3.5	5.0	4.5	1.0	3.0	0.803372062349496D+01
3	3	13	3	3	1.0	3.0	5.0	4.5	2.0	1.5	0.524493460602543D+00
4	3	15	3	3	2.0	5.0	8.5	6.0	1.5	2.0	0.138426701495125D+00
4	4	17	4	4	4.5	5.0	9.0	6.5	3.5	1.5	0.127171435604003D−02

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

TABLE VI

Values of $\mathcal{J}^{n_2 00, n_4 00}_{n_1 00, n_3 00}$ Obtained with 15 Exact Decimals Using the Infinite Series (42)

n_1	n_2	$n_{\gamma_{12}}$	n_x	λ	R_1	R_2	R_3	R_4	ζ_1	ζ_2	$\mathcal{J}^{n_2 00, n_4 00}_{n_1 00, n_3 00}$
1	1	5	0	0	1.5	3.5	6.5	4.5	3.0	2.5	0.171288775969805D−01
2	1	7	1	1	3.0	4.5	7.5	5.0	2.0	2.5	0.109643380336422D+00
2	2	9	2	2	2.5	3.5	5.5	4.5	2.0	1.5	0.550614613833540D+01
3	2	11	2	2	2.0	3.5	5.0	4.5	1.0	3.0	0.803372062349499D+01
3	3	13	3	3	1.0	3.0	5.0	4.5	2.0	1.5	0.524493460602543D+00
4	3	15	3	3	2.0	5.0	8.5	6.0	1.5	2.0	0.138426701495125D+00
4	4	17	4	4	4.5	5.0	9.0	6.5	3.5	1.5	0.127171435604001D−02

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

TABLE VII

Evaluation of $\mathcal{J}^{n_2 00, n_4 00}_{n_1 00, n_3 00}$ Using $S\bar{D}^{(2,5)}_n$ (43) for Evaluating the Semi-Infinite Integrals $\tilde{\mathcal{J}}(s, t)$

n_1	n_2	$n_{\gamma_{12}}$	n_x	λ	R_1	R_2	R_3	R_4	ζ_1	ζ_2	n	$\mathcal{J}^{n_2 00, n_4 00}_{n_1 00, n_3 00}$	Error
1	1	5	0	0	1.5	3.5	6.5	4.5	3.0	2.5	4	0.1712D−01	0.69D−13
2	1	7	1	1	3.0	4.5	7.5	5.0	2.0	2.5	5	0.1096D+00	0.46D−11
2	2	9	2	2	2.5	3.5	5.5	4.5	2.0	1.5	6	0.5506D+01	0.12D−12
3	2	11	2	2	2.0	3.5	5.0	4.5	1.0	3.0	4	0.8033D+01	0.92D−12
3	3	13	3	3	1.0	3.0	5.0	4.5	2.0	1.5	4	0.5244D+00	0.29D−11
4	3	15	3	3	2.0	5.0	8.5	6.0	1.5	2.0	3	0.1384D+00	0.78D−11
4	4	17	4	4	4.5	5.0	9.0	6.5	3.5	1.5	3	0.1271D−02	0.55D−14

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

TABLE VIII

Evaluation of $\mathcal{J}^{n_2 00, n_4 00}_{n_1 00, n_3 00}$ Using $H\bar{D}^{(2)}_n$ (28) for Evaluating the Semi-Infinite Integrals $\tilde{\mathcal{J}}(s, t)$

n_1	n_2	$n_{\gamma_{12}}$	n_x	λ	R_1	R_2	R_3	R_4	ζ_1	ζ_2	n	$\mathcal{J}^{n_2 00, n_4 00}_{n_1 00, n_3 00}$	Error
1	1	5	0	0	1.5	3.5	6.5	4.5	3.0	2.5	6	0.1712D−01	0.10D−10
2	1	7	1	1	3.0	4.5	7.5	5.0	2.0	2.5	6	0.1096D+01	0.39D−10
2	2	9	2	2	2.5	3.5	5.5	4.5	2.0	1.5	6	0.5506D+01	0.23D−11
3	2	11	2	2	2.0	3.5	5.0	4.5	1.0	3.0	6	0.8033D+01	0.26D−11
3	3	13	3	3	1.0	3.0	5.0	4.5	2.0	1.5	5	0.5244D+00	0.47D−11
4	3	15	3	3	2.0	5.0	8.5	6.0	1.5	2.0	5	0.1384D+00	0.51D−11
4	4	17	4	4	4.5	5.0	9.0	6.5	3.5	1.5	4	0.1271D−02	0.43D−13

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

The values with 15 correct decimals are obtained for the integrals by using the infinite series (24) and (42), which we sum until $N = \max$ (see Tables I, II, V, and VI).

The linear set of Eqs. (28) is solved using the LU decomposition method.

The numerical values of the semi-infinite integrals $\tilde{\mathcal{J}}(s,\ t)$, are obtained for $s = 0.005$ or 0.999 and $t = 0.005$ or 0.999. Note that in these regions, the oscillations of the integrand become very rapid.

In the evaluation of $\mathcal{J}^{n_2 00, n_4 00}_{n_1 00, n_3 00}$ (see Tables V–VIII) we let n_x and λ vary to compare the efficiency of the new method in evaluating semi-infinite integrals whose integrands are very oscillating.

7. CONCLUSION

The Fourier-transform method allowed analytical expressions to be developed for the two-electron, four-center Coulomb integrals by choosing the B functions as a basis set of atomic orbitals. The numerical evaluation of these analytical expressions presents severe computational difficulties due to the presence of semi-infinite, very oscillatory integrals.

It was shown that these semi-infinite integrals are suitable for application of the nonlinear $\bar{D}$-transformation and the $H\bar{D}$ method.

In the present work, we showed that we can further simplify the application of the above methods with the help of useful properties of the sine, spherical Bessel, and reduced Bessel functions.

The use of Cramer's rule for calculating the approximations $SD^{(2,j)}_n$ of the semi-infinite integrals is made possible by the fact that the zeros of the sine function are equidistant. The computation of the successive zeros of the integrands and a method to solve the linear systems are avoided.

The computation of the function $G(x) = (\frac{d}{x\,dx})^{\lambda}(x^{\lambda-1} g(x))$ does not present any difficulty as can be seen from Eqs. (44) and (45).

The numerical results section shows the unprecedented accuracy obtained using the $S\bar{D}$ approach to evaluating the two-electron, four-center Coulomb integrals (see Tables IV and VIII), which are the most difficult type involved in ab initio and density functional theory molecular structure calculations.

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