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Efficient evaluation of Coulomb integrals: the nonlinear D- and $\bar{D}$-transformations

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Abstract. The two-electron multicentre Coulomb integrals constitute the rate-limiting step of *ab initio* and density functional theory (DFT) molecular structure calculations. Speed-up can be achieved by limiting the number of integrals to evaluate analytically but these analytical evaluations remain rate-limiting for large molecules. Here we apply the nonlinear D- and $\bar{D}$-transformations to evaluate Coulomb integrals over B-functions more rapidly than the alternative transformation methods to a given predetermined high accuracy.

1. Introduction

Coulomb integrals are present in all the accurate molecular electronic structure calculation techniques. At the *ab initio* level, the two-, three- and four-centre two-electron integrals have long been the source of bottlenecks, particularly over the otherwise preferable Slater-type orbital basis [1, 2].

This paper aims at rapid and accurate analytic evaluation of multicentre two electron integrals. It can be applied *ab initio* (with a partition into analytic and asymptotic evaluation regions). In DFT, we also need two-centre Coulomb integrals and a three-centre term from the potential. The neglect of diatomic differential overlap (NDDO) (semi-empirical) Hamiltonians include the two-centre integrals [3–6]. We present a method applicable to all two-electron multicentre integrals including evidence of its efficiency compared with the routine alternatives.

A basis set of B-functions that was introduced in quantum chemistry calculations by Shavitt, Steinborn, Weniger, Filter and Groterndorst [7–13] is used. These functions are well adapted to the Fourier transform method [10, 15], which is still one of the most successful methods for the evaluation of multicentre integrals: where the integrals are transformed into inverse Fourier integrals. Evaluation of two-electron multicentre integrals by this method involves oscillatory semi-infinite integrals [12, 17, 20, 21], which present severe mathematical and computational difficulties.

The approach to these integrals in this paper is to apply the nonlinear transformations D (due to Levin and Sidi) and $\bar{D}$ (due to Sidi) [22–27], to accelerate their convergence. These transformations are efficient in the evaluation of oscillatory infinite integrals whose integrands satisfy linear differential equations with coefficients that have asymptotic expansions in inverse powers of their arguments. To apply these transformations successfully, we only need to show the existence of such a differential equation and its order.

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To demonstrate the superiority of these transformations, we compared the numerical results with others obtained using Gauss–Laguerre quadrature, the epsilon algorithm of Wynn [28, 29] and Levin's u-transform [29, 30], after transforming the infinite integral into infinite series. We also compared the calculation times for a given accuracy.

2. Definitions and basic formulae

The Slater orbitals are given in normalized form [12, 13, 17–22] by

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

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

The B-functions are defined [12, 13, 17–22] as follows:

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

where the reduced Bessel function $\hat{k}_{n-\frac{1}{2}}$ is defined [31] as

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

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

The reduced Bessel functions satisfy the three-term recurrence relation [31]:

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

The regular solid harmonic is given [12, 16, 20, 21] by

$$\mathcal{Y}_l^m(r) = r^l Y_l^m(\theta_r, \varphi_r) \tag{5}$$

$$= \mathrm{i}^{m+|m|} r^l \left[\frac{(2l+1)(l-|m|)!)}{4\pi(l+|m|)!)} \right]^{\frac{1}{2}} P_l^{|m|} \cos(\theta_r) \mathrm{e}^{\mathrm{i}m\varphi_r} \tag{6}$$

where $Y_l^m(\theta, \varpi)$ is the spherical harmonic and $P_l^m(x)$ is an associated Legendre polynomial.

The Gaunt coefficients are defined [12, 20, 21] as

$$\langle l_1 m_1 | l_2 m_2 | l_3 m_3 \rangle = \int_{\omega=0}^{4\pi} [Y_{l_1}^{m_1}(\omega)]^* Y_{l_2}^{m_2}(\omega) Y_{l_3}^{m_3}(\omega)\, \mathrm{d}\omega. \tag{7}$$

The STFs (and their Fourier transforms) can be expressed as a finite linear combination of B-functions (or of Fourier transforms of B-functions) [13–15, 18, 19]:

$$\chi_{n,l}^{m}(\zeta \boldsymbol{r}) = \sum_{p=\tilde{p}}^{n-l} \frac{(-1)^{n-l-p}(n-l)! 2^{l+p}(l+p)!}{(2p-n-l)!(2n-2l-2p)!!} B_{p,l}^{m}(\zeta \boldsymbol{r}) \tag{8}$$

where

$$\tilde{p} = \begin{cases} (n-l)/2 & \text{if } n-l \text{ is even} \\ (n-l+1)/2 & \text{if } n-l \text{ is odd.} \end{cases} \tag{9}$$

The double factorial is defined by

$$(2k)!! = 2 \times 4 \times 6 \times \cdots \times (2k) = 2^k k! \tag{10}$$

$$(2k+1)!! = 1 \times 3 \times 5 \times \cdots \times (2k+1) = \frac{(2k+1)!}{2^k k!} \tag{11}$$

$$0!! = 1. \tag{12}$$

The Fourier transform $\bar{B}_{n,l}^{m}(\zeta, \boldsymbol{p})$ of $B_{n,l}^{m}(\zeta \boldsymbol{r})$ is given [14, 15, 17–21] by

$$\bar{B}_{n,l}^{m}(\zeta, \boldsymbol{p}) = \frac{1}{(2\pi)^{3/2}} \int_{\boldsymbol{r}} \mathrm{e}^{-\mathrm{i}\boldsymbol{p}.\boldsymbol{r}} B_{n,l}^{m}(\zeta \boldsymbol{r})\, \mathrm{d}\boldsymbol{r} \tag{13}$$

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

This analytical form of the Fourier transform of $B_{n,l}^{m}(\zeta \boldsymbol{r})$ is obtained by inserting the well known Rayleigh expansion of the plane wavefunction [12, 32] in equation (13):

$$\mathrm{e}^{\pm \mathrm{i}\boldsymbol{p}.\boldsymbol{r}} = \sum_{\lambda=0}^{+\infty} \sum_{\mu=-\lambda}^{\lambda} 4\pi (\pm \mathrm{i})^{\lambda} j_{\lambda}(|\boldsymbol{p}||\boldsymbol{r}|) Y_{\lambda}^{\mu}(\theta_{\boldsymbol{r}}, \varphi_{\boldsymbol{r}}) [Y_{\lambda}^{\mu}(\theta_{\boldsymbol{p}}, \varphi_{\boldsymbol{p}})]^{*} \tag{15}$$

where j_{λ} is the spherical Bessel function of λth-order [31] and $|\boldsymbol{r}|$ is the modulus of vector $\boldsymbol{r}$.

The integral representation of the Coulomb operator $\frac{1}{|\boldsymbol{r}-\boldsymbol{R}_1|}$ is given [19, 33] by

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

3. Two electron multicentre integrals over B-functions

These integrals are defined [12, 17, 20, 21] as

$$\mathcal{J}_{n_1 l_1 m_1, n_3 l_3 m_3}^{n_2 l_2 m_2, n_4 l_4 m_4} = \langle B_{n_1 l_1}^{m_1}[\zeta_1(\boldsymbol{r} - \boldsymbol{R}_1)] B_{n_3 l_3}^{m_3}[\zeta_3(\boldsymbol{r}' - \boldsymbol{R}_3)] \left| \frac{1}{|\boldsymbol{r} - \boldsymbol{r}'|} \right| \times B_{n_2 l_2}^{m_2}[\zeta_2(\boldsymbol{r} - \boldsymbol{R}_2)] B_{n_4 l_4}^{m_4}[\zeta_4(\boldsymbol{r}' - \boldsymbol{R}_4)] \rangle \tag{17}$$

$$= \int_{\boldsymbol{r},\boldsymbol{r}'} [B_{n_1 l_1}^{m_1}(\zeta_1(\boldsymbol{r} - \boldsymbol{R}_1))]^{*} [B_{n_3 l_3}^{m_3}(\zeta_3(\boldsymbol{r}' - \boldsymbol{R}_3))]^{*} \frac{1}{|\boldsymbol{r} - \boldsymbol{r}'|} \times B_{n_2 l_2}^{m_2}[\zeta_2(\boldsymbol{r} - \boldsymbol{R}_2)]\, \mathrm{d}\boldsymbol{r}\, B_{n_4 l_4}^{m_4}[\zeta_4(\boldsymbol{r}' - \boldsymbol{R}_4)]\, \mathrm{d}\boldsymbol{r}\, \mathrm{d}\boldsymbol{r}'. \tag{18}$$

We apply the Fourier transform method after substituting the integral representation of the Coulomb operator, equation (16). We substitute the analytical expression of B-functions, equation (2), into the above equation, and using the Rayleigh expansion of the plane wavefunctions, equation (15), the expression for these integrals involving a three-dimensional integral representation [12, 17, 20, 21, 36, 37] is

$$\mu = m_2' + (m_1 - m_1') - (m_4 - m_4') + (m_3 - m_3')$$
$$|(l_1 - l_1') - (l_2 - l_2')| \leqslant l_{12} \leqslant (l_1 - l_1') + (l_2 - l_2')$$
$$|(l_3 - l_3') - (l_4 - l_4')| \leqslant l_{34} \leqslant (l_3 - l_3') + (l_4 - l_4')$$
$$\mu_{1i} = \max(-l_i'; m_i - l_i + l_i') \qquad \text{for } i = 1, 2, 3, 4$$
$$\mu_{2i} = \min(l_i; m_i + l_i - l_i') \qquad \text{for } i = 1, 2, 3, 4$$
$$[\gamma_{12}(s, x)]^2 = (1 - s)\zeta_1^2 + s\zeta_2^2 + s(1 - s)x^2$$
$$[\gamma_{34}(t, x)]^2 = (1 - t)\zeta_3^2 + t\zeta_4^2 + t(1 - t)x^2$$
$$v = |(1 - s)R_{21} - (1 - t)R_{43} - R_{31}|$$
$$n_{12} = n_1 + n_2 + l_1 + l_2 - l - j_{12}$$
$$n_{34} = n_3 + n_4 + l_3 + l_4 - l' - j_{34}$$
$$\Delta l_{12} = \frac{l_1' + l_2' - l}{2} \qquad \Delta l_{34} = \frac{l_3' + l_4' - l'}{2}$$
$$R_{ij} = R_i - R_j \qquad i, j = 1, 2, 3, 4$$

$$
\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)!}\zeta_1^{2n_1+l_1-1}\zeta_2^{2n_2+l_2-1}\\
&\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_3^{2n_3+l_3-1}\zeta_4^{2n_4+l_4-1}\\
&\times\sum_{l_1'=0}^{l_1}\sum_{m_1'=\mu_{11}}^{\mu_{12}} \mathrm{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}} \mathrm{i}^{l_2+l_2'}(-1)^{l_2'}\frac{\langle l_2m_2|l_2'm_2'|l_2-l_2'm_2-m_2'\rangle}{(2l_2'+1)!![2(l_2-l_2')+1]!!}\\
&\times\sum_{l_3'=0}^{l_3}\sum_{m_1'=\mu_{31}}^{\mu_{32}} \mathrm{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}} \mathrm{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'-l_2'|}^{l_1'+l_2'}\langle l_2'm_2'|l_1'm_1'|lm'2-m_1'\rangle\mathcal{Y}_l^{m_2'-m_1'}(R_{21})\\
&\times\sum_{l_{12}}\langle l_2-l_2'm_2-m_2'|l_1-l_1'm_1-m_1'|l_{12}m_2-m_2'-(m_1-m_1')\rangle\\
&\times\sum_{l'=|l_3'-l_4'|}^{l_3'+l_4'}\langle l_4'm_4'|l_3'm_3'|l'm'4-m_3'\rangle\mathcal{Y}_{l'}^{m_4'-m_3'}(R_{43})\\
&\times\sum_{l_{34}}\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_{12}-l_{34}|}^{l_{12}+l_{34}}(-\mathrm{i})^{\lambda}\langle l_{12}m_2-m_2'-(m_1-m_1')|\\
&\times l_{34}m_4-m_4'-(m_3-m_3')|\lambda m_2-\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^{n_{12}+1+l+n_{34}+1+l'}(n_{12}+1+l)!(n_{34}+1+l')!}\\
&\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_v,\varphi_v)\\
&\times\int_{x=0}^{+\infty}x^{l_1-l_1'+l_2-l_2'+l_3-l_3'+l_4-l_4'}j_\lambda(vx)\frac{\hat{k}_{n_{12}+\frac{1}{2}}[R_{21}\gamma_{12}(s,x)]}{[\gamma_{12}(s,x)]^{2(n_1+l_1+n_2+l_2)-(l_1'+l_2')-l+1}}\\
&\times\frac{\hat{k}_{n_{34}+\frac{1}{2}}[R_{43}\gamma_{34}(t,x)]}{[\gamma_{34}(t,x)]^{2(n_3+l_3+n_4+l_4)-(l_3'+l_4')-l'+1}}\,\mathrm{d}x\,\mathrm{d}t\,\mathrm{d}s. \qquad (19)
\end{aligned}
$$

The inner semi-infinite x integral was evaluated by Gauss–Laguerre quadrature and the outer s and t integrals by Gauss–Legendre formulae [12, 34]. Unfortunately, as we showed in previous work [22], for three-centre nuclear attraction integrals, the use of Gauss–Laguerre quadrature presents severe numerical difficulties for this kind of integral, especially for large values of v since the inner integrand oscillates very rapidly due to the spherical Bessel function, and therefore new numerical integration techniques are required. In this work, we focus our attention on the nonlinear D- and $\bar{D}$-transformations [22–27].

They are efficient in evaluating semi-infinite integrals of rapidly oscillating functions which satisfy linear differential equations of the form $f(t) = \sum_{k=1}^{m} p_k(t) f^{(k)}(t)$, where p_k are in $A^{(i_k)}$, $i_k \leqslant k$ for $k = 1, 2, \ldots, m$; and where $A^{(\gamma)}$ is the set of infinitely differentiable functions $a(x)$, which as $x \to +\infty$, have an asymptotic expansion in inverse powers of x of the form: $a(x) \sim x^{\gamma}(\alpha_0 + \frac{\alpha_1}{x} + \frac{\alpha_2}{x^2} + \cdots)$. $\lim_{x\to+\infty} p_k^{(i-1)}(x) f^{(k-i)}(x) = 0$, with $k = i, i+1, \ldots, m$, and $i = 1, 2, \ldots, m$, $\forall l \geqslant -1$, $\sum_{k=1}^{m} l(l-1)\ldots(l-k+1)p_{k,0} \neq 1$ where $p_{k,0} = \lim_{x\to+\infty} x^{-k} p_k(x)$.

In order to apply these transformations successfully, there is no need to know explicitly the differential equation that the integrand satisfies: knowledge of its existence and its order is sufficient. In [22] we showed the superiority of these transformations in the evaluation of three-centre nuclear attraction integrals.

For simplicity, we shall focus our attention on the the simple case of s-functions corresponding to $l_1 = l_2 = l_3 = l_4 = m_1 = m_2 = m_3 = m_4 = 0$, but we will let the order of the spherical Bessel function λ vary. The equation (19) can then be rewritten as

$$\mathcal{J}_{n_1 00, n_3 00}^{n_2 00, n_4 00} = \frac{\zeta_1^{2n_1-1}\zeta_2^{2n_2-1}\zeta_3^{2n_3-1}\zeta_4^{2n_4-1}}{\pi n_1! n_2! n_3! n_4! 2^{n_1+n_2+n_3+n_4}} \int_0^1 s^{n_1}(1-s)^{n_2} \int_0^1 t^{n_3}(1-t)^{n_4} \times \int_0^{+\infty} \frac{\hat{k}_{\nu_{12}}[R_{21}\gamma_{12}(s,x)]}{[\gamma_{12}(s,x)]^{2\nu_{12}}} \frac{\hat{k}_{\nu_{34}}[R_{43}\gamma_{34}(t,x)]}{[\gamma_{34}(t,x)]^{2\nu_{34}}} j_\lambda(vx)\, \mathrm{d}x\, \mathrm{d}t\, \mathrm{d}s \tag{20}$$

where $\nu_{12} = n_1 + n_2 + \frac{1}{2}$ and $\nu_{34} = n_3 + n_4 + \frac{1}{2}$.

Now, we consider the inner semi-infinite x integral involved in the above equation. It is defined as

$$\tilde{\mathcal{J}}_{n_1 00, n_3 00}^{n_2 00, n_4 00}(s,t) = \int_0^{+\infty} \frac{\hat{k}_{\nu_{12}}[R_{21}\gamma_{12}(s,x)]}{[\gamma_{12}(s,x)]^{2\nu_{12}}} \frac{\hat{k}_{\nu_{34}}[R_{43}\gamma_{34}(t,x)]}{[\gamma_{34}(t,x)]^{2\nu_{34}}} j_\lambda(vx)\, \mathrm{d}x \tag{21}$$

$$= \sum_{n=0}^{+\infty} \int_{j_\lambda^n}^{j_\lambda^{n+1}} \frac{\hat{k}_{\nu_{12}}[R_{21}\gamma_{12}(s,x)]}{[\gamma_{12}(s,x)]^{2\nu_{12}}} \frac{\hat{k}_{\nu_{34}}[R_{43}\gamma_{34}(t,x)]}{[\gamma_{34}(t,x)]^{2\nu_{34}}} j_\lambda(vx)\, \mathrm{d}x. \tag{22}$$

j_λ^n is the root of order n of the spherical Bessel function j_λ. j_λ^0 is assumed to be 0.

In the following, this integral will be referred to as $\tilde{\mathcal{J}}(s,t)$, and the corresponding integrand as $F(x) = f_1(x) f_2(x) j_\lambda(vx)$, where

$$f_1(x) = \frac{\hat{k}_{\nu_{12}}[R_{21}\gamma_{12}(s,x)]}{[\gamma_{12}(s,x)]^{2\nu_{12}}} \qquad f_2(x) = \frac{\hat{k}_{\nu_{34}}[R_{43}\gamma_{34}(t,x)]}{[\gamma_{34}(t,x)]^{2\nu_{34}}}.$$

$j_\lambda(vx)$ satisfies a linear second-order differential equation given [31, 35] by

$$j_\lambda(vx) = -\frac{2x}{(vx)^2 - \lambda^2 - \lambda} j_\lambda^{(1)}(vx) - \frac{x^2}{(vx)^2 - \lambda^2 - \lambda} j_\lambda^{(2)}(vx) \tag{23}$$

$$= p_{1,1}(x) j_\lambda^{(1)}(vx) + p_{2,1}(x) j_\lambda^{(2)}(vx). \tag{24}$$

Assuming that $R_{21}\gamma_{12}(s,x) = R_{21}\sqrt{(1-s)\zeta_1^2 + s\zeta_2^2 + s(1-s)x^2} = \sqrt{\beta_1 + \alpha_1 x^2}$ and $R_{43}\gamma_{34}(s,x) = R_{43}\sqrt{(1-s)\zeta_3^2 + s\zeta_4^2 + t(1-t)x^2} = \sqrt{\beta_2 + \alpha_2 x^2}$, the functions $f_1(x)$ and $f_2(x)$ satisfy linear second-order differential equations given [31, 35] by

$$f_1(x) = x^{-1}\left[(2\nu_1 + 1)\tau_1 + \frac{\delta_1\tau_1}{x^2}\right] f_1^{(1)}(x) + \left[\tau_1 - \frac{\delta_1\tau_1}{x^2}\right] f_1^{(2)}(x) \tag{25}$$

$$= p_{1,2}(x) f_1^{(1)}(x) + p_{2,2}(x) f_1^{(2)}(x) \tag{26}$$

$$f_2(x) = x^{-1}\left[(2\nu_2 + 1)\tau_2 + \frac{\delta_2\tau_2}{x^2}\right] f_2^{(1)}(x) + \left[\tau_2 - \frac{\delta_2\tau_2}{x^2}\right] f_2^{(2)}(x) \tag{27}$$

$$= p_{1,3}(x) f_2^{(1)}(x) + p_{2,3}(x) f_2^{(2)}(x) \tag{28}$$

where

$$\delta_1 = -\frac{\beta_1}{\alpha_1} \qquad \tau_1 = \frac{1}{\alpha_1} \qquad \delta_2 = -\frac{\beta_2}{\alpha_2} \qquad \text{and} \qquad \tau_2 = \frac{1}{\alpha_2}.$$

The $p_{1,i}$ are in $A^{(-1)}$ and $p_{2,i}$ are in $A^{(0)}$ for $i = 1, 2, 3$.

We shall now state a lemma and corollary which are proven in [26, 27] and that will be useful in determining the order of the differential equation which the integrand $F(x)$ satisfies.

Lemma. If the functions f and g satisfy linear differential equations of order m and n respectively, then their product fg satisfies a linear differential equation of order less than or equal to mn.

Corollary. If the coefficients of the linear differential equations that f and g satisfy have asymptotic expansions in inverse powers of x as $x \to +\infty$, then so do the coefficients of the linear differential equation that fg satisfies.

Now, we can easily show that the function $F(x)$ satisfies a linear differential equation of order 6 or less, of the form required to apply the D-transformation. In a previous work [22] we gave the linear fourth-order differential equation satisfied by a function of the form $f_1(x) j_\lambda(vx)$, explicitly.

The coefficients p_k for $k = 1, 2, \ldots, 6$ of the linear differential equation that $F(x)$ satisfies are linear combinations of $p_{1,i}, p_{2,i}$, $i = 1, 2, 3$ and their successive derivatives, thus $p_k \in A^{(i_k)}$ where $i_k \leqslant 0$ for $k = 1, 2, \ldots, 6$.

The behaviour of $F(x)$ and its successive derivatives are dominated by the exponentially decreasing $\hat{k}_\nu$ and its successive derivatives, thus $\lim_{x\to+\infty} p_k^{(i-1)}(x) F^{(k-i)}(x) = 0$, for $k = i, i+1, \ldots, 6$, and $i = 1, 2, \ldots, 6$. One can easily show that $p_{k,0} = \lim_{x\to+\infty} x^{-k} p_k(x) = 0$, then $\forall l \geqslant -1$, $\sum_{k=1}^{6} l(l-1)\ldots(l-k+1) p_{k,0} = 0 \neq 1$.

The conditions required to apply the nonlinear D-transformation are satisfied. The approximations $D_m^{(6)}$ to $\tilde{\mathcal{J}}(s,t)$ satisfies $M = 6m+1$ equations given [26, 27] by

$$D_m^{(6)} = \int_0^{x_n} F(t)\,\mathrm{d}t + \sum_{k=0}^{5} F^{(k)}(x_n) x_n^{k+1} \sum_{i=0}^{m-1} \frac{\bar{\beta}_{k,i}}{x_n^i} \qquad n = 0, 1, 2, \ldots, 6m. \tag{29}$$

The x_n are chosen to satisfy $0 < x_0 < x_1 < \cdots < x_{6m}$, and $\lim_{n\to+\infty} x_n = +\infty$. $D_m^{(6)}$ and the $\bar{\beta}_{k,i}$ for $k = 0, 1, \ldots, 5$; $i = 0, 1, \ldots, m-1$ are the M unknowns.

Now if we choose $x_n = j_\lambda^{n+1}$, for $n = 0, 1, 2, \ldots$, which are the zeros of $F(x)$, then we can reduce the order of the above set of equations to $M = 5m+1$ which can be rewritten [23–25] as

$$\bar{D}_m^{(6)} = \int_0^{x_n} F(t)\,\mathrm{d}t + \sum_{k=1}^{5} F^{(k)}(x_n)\, x_n^{k+1} \sum_{i=0}^{m-1} \frac{\bar{\beta}_{k,i}}{x_n^i} \qquad n = 0, 1, 2, \ldots, 5m. \tag{30}$$

$\bar{D}_m^{(6)}$ and the $\bar{\beta}_{k,i}$ for $k = 1, 2, \ldots, 5$; $i = 0, 1, \ldots, m-1$ are the M unknowns. These expressions are implemented in an original set of Fortran 77 subroutines.

4. The general case

In the general case, the semi-infinite x integral involved in the two-electron multicentre integrals $\tilde{\mathcal{J}}^{n_2l_2m_2,n_4l_4m_4}_{n_1l_1m_1,n_3l_3m_3}(s,t)$ which will be referred as $\tilde{\mathcal{J}}_G(s,t)$ is of the form [12, 17, 20, 21]

$$\tilde{\mathcal{J}}_G(s,t) = \int_0^{+\infty} x^{m_x} j_\lambda(vx) \frac{\hat{k}_{n_{12}+\frac{1}{2}}[R_{21}\gamma_{12}(s,x)]}{[\gamma_{12}(s,x)]^{m_{12}}} \frac{\hat{k}_{n_{34}+\frac{1}{2}}[R_{43}\gamma_{34}(t,x)]}{[\gamma_{34}(t,x)]^{m_{34}}}\,\mathrm{d}x \tag{31}$$

$$= \sum_{n=0}^{+\infty} \int_{j_\lambda^n}^{j_\lambda^{n+1}} x^{m_x} j_\lambda(vx) \frac{\hat{k}_{n_{12}+\frac{1}{2}}[R_{21}\gamma_{12}(s,x)]}{[\gamma_{12}(s,x)]^{m_{12}}} \frac{\hat{k}_{n_{34}+\frac{1}{2}}[R_{43}\gamma_{34}(t,x)]}{[\gamma_{34}(t,x)]^{m_{34}}}\,\mathrm{d}x. \tag{32}$$

$m_x, \lambda, n_{12}, n_{34}, m_{12}, m_{34}, \gamma_{12}(s,x)$ and $\gamma_{34}(t,x)$ are defined according to equation (19).

Using the previous arguments, one can easily show that the integrand of the semi-infinite x integral involved in equation (31) satisfies a sixth-order linear differential equation of the form required to apply the D- and $\bar{D}$-transformations. The order of the set of equations which gives the approximation $D_m^{(6)}$ is $M = 6m + 1$ but it can be reduced to $5m + 1$ by choosing the $x_n = j_\lambda^{n+1}$ for $n = 0, 1, 2, \ldots, 5m$.

5. Discussion

The exact values of integrals (21) and (32) are computed to 20 correct decimals using the series expansions given by equations (22) and (32) (see tables 4 and 5). (A Fortran 77 routine has been specially devised for this purpose.)

The finite $\int_{j_\lambda^n}^{j_\lambda^{n+1}} F(x)\,\mathrm{d}x$ involved in equations (22) and (32) and $\int_0^{j_\lambda^n} F(x)\,\mathrm{d}x = \sum_{i=0}^{n-1} \int_{j_\lambda^i}^{j_\lambda^{i+1}} F(x)\,\mathrm{d}x$ involved in equation (30) are evaluated using Gauss–Legendre quadrature of order 16. The set of equations (30) is solved using Gaussian elimination with maximal column pivoting.

The calculation time using the $\bar{D}$-transformation computed with an IBM RS6000 340 is noted (see tables 1 and 5). We also used the epsilon algorithm of Wynn [28, 29] and the Levin u-transform [29, 30] to evaluate the semi-infinite x integral $\tilde{\mathcal{J}}(s,t)$ (equation (21)) and $\tilde{\mathcal{J}}_G(s,t)$ (equation (31)) by accelerating the convergence of the infinite series given by equations (22) and (32). The calculation time is also computed to show the superiority of $\bar{D}$-transformation (see tables 2, 3 and 6). The integral $\mathcal{I}^{n_200,n_400}_{n_100,n_300}$ (equation (20)) is evaluated for different values of n_1, n_2, n_3, n_4 and λ, using the $\bar{D}$-transformation of order 2, Levin's

Table 1. Evaluation of $\tilde{\mathcal{J}}(s,t)$ (equation (21)) using the $\bar{D}$-transformation (equation (30)). Time is in milliseconds. ($\zeta_1 = 2.1$, $\zeta_2 = 2.6$, $\zeta_3 = 3.1$, $\zeta_4 = 1.8$, $R_1 = 1.2$, $R_2 = 3.25$, $R_3 = 4.25$, $R_4 = 6.75$ and $s = 0.01$).

t	m	n_{12}	n_{34}	λ	$\bar{D}_m^{(6)}$	Error	Time
0.01	1	2	2	0	0.693 350 864 597 446 916D-06	0.1812D-07	0.05
0.01	2	3	2	2	0.594 119 031 449 745 757D-06	0.2319D-11	0.19
0.01	3	3	3	3	0.579 443 696 446 507 191D-06	0.1294D-14	0.48
0.01	4	4	4	4	0.138 323 510 330 356 551D-05	0.1778D-16	0.98
0.99	1	2	2	0	0.335 139 744 246 110 843D-03	0.4174D-06	0.04
0.99	2	3	2	2	0.260 138 750 356 833 778D-03	0.2036D-14	0.19
0.99	3	3	3	3	0.461 713 233 934 115 124D-03	0.5421D-19	0.49
0.99	4	4	4	4	0.191 325 914 385 519 213D-02	0.6505D-18	0.97

Table 2. Evaluation of $\tilde{\mathcal{J}}(s,t)$ (equation (21)), Levin's u-transform. Time is in milliseconds. ($\zeta_1 = 2.1$, $\zeta_2 = 2.6$, $\zeta_3 = 3.1$, $\zeta_4 = 1.8$, $R_1 = 1.2$, $R_2 = 3.25$, $R_3 = 4.25$, $R_4 = 6.75$ and $s = 0.01$).

t	m	n_{12}	n_{34}	λ	$u_m(S_0)$	Error	Time
0.01	2	2	2	0	0.668 576 020 932 511 367D-06	0.6651D-08	0.55
0.01	4	3	2	2	0.594 087 778 432 344 762D-06	0.2893D-10	1.30
0.01	6	3	3	3	0.579 443 844 056 614 544D-06	0.1463D-12	2.23
0.01	8	4	4	4	0.138 323 514 777 015 398D-05	0.4448D-13	3.84
0.99	2	2	2	0	0.333 367 847 810 568 435D-03	0.1355D-05	0.57
0.99	4	3	2	2	0.260 139 032 317 670 401D-03	0.2820D-09	1.31
0.99	6	3	3	3	0.461 713 233 441 734 898D-03	0.4924D-12	2.24
0.99	8	4	4	4	0.191 325 914 385 478 339D-02	0.4094D-15	3.82

Table 3. Evaluation of $\tilde{\mathcal{J}}(s,t)$ (equation (21)), the epsilon algorithm of Wynn. Time is in milliseconds. ($\zeta_1 = 2.1$, $\zeta_2 = 2.6$, $\zeta_3 = 3.1$, $\zeta_4 = 1.8$, $R_1 = 1.2$, $R_2 = 3.25$, $R_3 = 4.25$, $R_4 = 6.75$ and $s = 0.01$).

t	m	n_{12}	n_{34}	λ	ϵ_m^0	Error	Time
0.01	2	2	2	0	0.678 328 605 359 331 317D-06	0.3102D-08	0.56
0.01	4	3	2	2	0.594 143 016 808 293 294D-06	0.2630D-10	1.30
0.01	6	3	3	3	0.579 483 040 814 865 933D-06	0.3934D-10	2.23
0.01	8	4	4	4	0.138 323 522 632 148 885D-05	0.1230D-12	3.88
0.99	2	2	2	0	0.334 526 801 546 043 326D-03	0.1955D-06	0.55
0.99	4	3	2	2	0.260 140 497 449 965 564D-03	0.1747D-08	1.31
0.99	6	3	3	3	0.461 713 234 344 733 115D-03	0.4106D-12	2.23
0.99	8	4	4	4	0.191 325 914 385 569 651D-02	0.5037D-15	3.85

Table 4. Evaluation of $\tilde{\mathcal{J}}(s,t)$ (equation (21)) using the DGLGQ routine (Gauss–Laguerre quadrature of order N_{GL}) available from IBM–ESSL mathematical library [38]. ($\zeta_1 = 2.1$, $\zeta_2 = 2.6$, $\zeta_3 = 3.14$, $\zeta_4 = 1.8$, $R_1 = 1.2$, $R_2 = 3.25$, $R_3 = 4.25$, $R_4 = 6.75$ and $s = 0.01$.)

t	N_{GL}	n_{12}	n_{34}	λ	DGLDQ	Exact values
0.01	40	2	2	0	0.626 353 439 912 286D-06	0.675 226 987 571 87D-06
0.01	20	3	2	2	0.684 327 058 147 507D-06	0.594 116 712 565 53D-06
0.01	10	3	3	3	0.648 248 032 098 591D-06	0.579 443 697 740 71D-06
0.01	40	4	4	4	0.116 766 324 234 304D-05	0.138 323 510 328 57D-05
0.99	32	2	2	0	0.367 771 794 129 447D-03	0.334 722 351 034 20D-03
0.99	64	3	2	2	0.200 636 251 584 565D-03	0.260 138 750 354 79D-03
0.99	48	3	3	3	0.479 123 239 274 658D-03	0.461 713 233 934 11D-03
0.99	64	4	4	4	0.200 161 369 995 836D-02	0.191 325 914 385 51D-02

u-transform of order 6 and the epsilon algorithm of Wynn of order 6 (see tables 7 and 8).

From the values reported in table 4, note that the use of Gauss–Laguerre quadrature even to high order (for instance 64) gives inaccurate results, especially for s and t close to 0 or 1. If we let $s, t = 0$ or 1, the integrand $F(x)$, and equations (21) and (31) will be reduced to the term $j_\lambda(vx)$, because the terms $f_i(x), i = 1, 2$ become constants and hence the asymptotic behaviour of the integrand $F(x)$ cannot be represented by a function of the form $e^{-\alpha x} g(x)$ where $g(x)$ is not a rapidly oscillating function. We also note that the regions close to $s = t = 0$ and $s = t = 1$ carry very small weight because of their

Table 5. Evaluation of $\mathcal{J}_G(s,t)$ (equation (31)). The inner semi infinite integral was evaluated using the $\bar{D}$-transformation of order 3 ($\bar{D}_3^{(6)}$). Time is in milliseconds. ($\zeta_1 = 2.1$, $\zeta_2 = 2.6$, $\zeta_3 = 3.1$, $\zeta_4 = 1.8$, $R_1 = 1.2$, $R_2 = 3.25$, $R_3 = 4.25$, $R_4 = 6.75$, $m_{12} = 2n_{12} + 1$, $m_{34} = 2n_{34} + 1$ and $s = t = 0.01$.)

n_{12}	n_{34}	m_x	λ	$\bar{D}_3^{(6)}$	Exact values	Error	Time
2	2	2	3	0.811 031D-07	0.811 009 169 633 874 602D-07	0.2D-11	0.47
2	2	3	1	0.286 313D-06	0.286 312 754 031 869 044D-06	0.1D-14	0.49
3	3	4	3	0.982 144D-06	0.982 155 428 849 900 776D-06	0.1D-10	0.48
4	4	3	2	0.157 213D-05	0.157 213 518 681 928 447D-05	0.7D-11	0.48
4	4	4	3	0.268 975D-05	0.268 976 960 759 980 355D-05	0.2D-10	0.48
5	5	4	4	0.960 641D-05	0.960 686 068 198 986 670D-05	0.4D-09	0.49
6	6	5	5	0.113 655D-03	0.113 661 593 530 865 794D-03	0.7D-08	0.48
6	6	6	6	0.357 697D-03	0.357 682 012 033 322 643D-03	0.1D-07	0.49

Table 6. Evaluation of $\mathcal{J}_G(s,t)$ in the general case (equation (31)) using Levin's u-transform of order 8 ($u_8(S_0)$) and the epsilon algorithm of order 8 ($\epsilon_8^{(0)}$). Time is in milliseconds. ($\zeta_1 = 2.1$, $\zeta_2 = 2.6$, $\zeta_3 = 3.1$, $\zeta_4 = 1.8$, $R_1 = 1.2$, $R_2 = 3.25$, $R_3 = 4.25$, $R_4 = 6.75$, $m_{12} = 2n_{12} + 1$, $m_{34} = 2n_{34} + 1$ and $s = t = 0.01$.)

n_{12}	n_{34}	m_x	λ	$u_8(S_0)$	Error	Time	$\epsilon_8^{(0)}$	Error	Time
2	2	2	3	0.811 039D-07	0.3D-11	2.12	0.811 031D-07	0.2D-11	2.10
2	2	3	1	0.286 313D-06	0.6D-13	2.35	0.286 313D-06	0.8D-13	2.33
3	3	4	3	0.982 162D-06	0.7D-11	3.20	0.982 196D-06	0.4D-10	3.24
4	4	3	2	0.157 214D-05	0.3D-11	3.57	0.157 213D-05	0.7D-11	3.54
4	4	4	3	0.268 979D-05	0.2D-10	3.87	0.268 984D-05	0.7D-10	3.83
5	5	4	4	0.960 736D-05	0.5D-09	4.62	0.960 742D-05	0.6D-09	4.59
6	6	5	5	0.113 679D-03	0.2D-07	5.79	0.113 696D-03	0.3D-07	5.82
6	6	6	6	0.357 823D-03	0.1D-06	6.26	0.358 112D-03	0.4D-06	6.20

Table 7. Evaluation of $\mathcal{J}^{n_2 00, n_4 00}_{n_1 00, n_3 00}$ (equation (20)). The inner semi-infinite integral was evaluated using the $\bar{D}$-transformation of order 2 ($\bar{D}_2^{(6)}$). The outer finite s and t integrals were evaluated using the Gauss–Legendre quadrature of order 8. Time is in milliseconds. ($R_1 = (1.2, 0, 0)$, $R_2 = (3.25, 0, 0)$, $R_3 = (4.25, 0, 0)$ and $R_4 = (6.75, 0, 0)$. $\zeta_1 = 2.1$, $\zeta_2 = 2.6$, $\zeta_3 = 3.1$ and $\zeta_4 = 1.8$.)

n_1	n_2	n_3	n_4	λ	Exact values	$\bar{D}_2^{(6)}$	Error	Time
1	1	1	1	0	0.114 695 794 283 946D-06	0.114 695D-06	0.5D-16	7.0
2	1	2	1	1	0.850 849 767 895 866D-07	0.850 849D-07	0.1D-16	9.0
2	2	2	2	2	0.392 236 030 612 953D-07	0.392 236D-07	0.2D-18	11.0
3	2	3	2	3	0.370 453 241 022 581D-07	0.370 453D-07	0.5D-19	12.0
3	3	3	3	3	0.145 388 237 339 498D-07	0.145 388D-07	0.6D-21	14.0

expressions $s^{n_2}(1-s)^{n_1}$, $t^{n_4}(1-t)^{n_3}$.

6. Conclusion

The use of the series expansion given by equations (22) and (32) is prohibitively long for sufficient accuracy, especially for s, t close to 0 or 1.

Table 8. Evaluation of $\mathcal{J}_{n_1 00, n_3 00}^{n_2 00, n_4 00}$ (equation (20)). The inner semi-infinite integral was evaluated using Levin's u-transform of order 6 ($u_6(S_0)$) and the epsilon algorithm of order 6 ($\epsilon_6^{(0)}$). The outer finite s and t integrals are evaluated using the Gauss–Legendre quadrature of order 8. Time is in milliseconds. ($R_1 = (1.2, 0, 0)$, $R_2 = (3.25, 0, 0)$, $R_3 = (4.25, 0, 0)$ and $R_4 = (6.75, 0, 0)$. $\zeta_1 = 2.1$, $\zeta_2 = 2.6$, $\zeta_3 = 3.1$ and $\zeta_4 = 1.8$.)

n_1	n_2	n_3	n_4	λ	$u_6(S_0)$	Error	Time	$\epsilon_6^{(0)}$	Error	Time
1	1	1	1	0	0.114 69D-06	0.6D-16	47.0	0.114 69D-06	0.2D-15	48.0
2	1	2	1	1	0.850 84D-07	0.3D-17	63.0	0.850 84D-07	0.6D-16	64.0
2	2	2	2	2	0.392 23D-07	0.7D-18	83.0	0.392 23D-07	0.3D-17	89.0
3	2	3	2	3	0.370 45D-07	0.2D-18	115.0	0.370 45D-07	0.2D-18	120.0
3	3	3	3	3	0.145 38D-07	0.1D-19	132.0	0.145 38D-07	0.4D-19	141.0

Using the epsilon algorithm and Levin u-transform, we accelerate the convergence of the infinite oscillating series given by equations (22) and (32), but the accuracy is still insufficient compared with the accuracy obtained using the $\bar{D}$-transformation (see tables 1–3, 5–8).

In tables 1–3 for $s = 0.01$, $t = 0.01$, $n_{12} = n_{34} = 3$ and $\lambda = 3$ we obtain 14 exact decimals in 0.48 ms using $\bar{D}_3^{(6)}$, 13 exact decimals in 3.48 ms using Levin's u-transform of order 8, and 12 exact decimals in 3.88 ms using the epsilon algorithm of order 8. For $s = 0.01$, $t = 0.99$, $n_{12} = 3$, $n_{34} = 2$ and $\lambda = 2$ we obtain 14 exact decimals in 0.19 ms using $\bar{D}_2^{(6)}$, 12 exact decimals in 2.24 ms using Levin's u-transform of order 6 and 12 exact decimals in 2.23 ms using the epsilon algorithm of order 6. The evaluation using the $\bar{D}$-transformation is thus shown to be 10–12 times faster than the alternatives and even more accurate.

In tables 5 and 6, for $n_{12} = n_{34} = 2$, $m_x = 2$ and $\lambda = 3$ we obtain 11 exact decimals in 0.47 ms using $\bar{D}_3^{(6)}$, 2.12 ms using Levin's u-transform of order 8 and 2.10 ms using the epsilon algorithm of order 8. For $n_{12} = n_{34} = 6$, $m_x = 5$ and $\lambda = 5$ we obtain eight exact decimals in 0.48 ms using $\bar{D}_3^{(6)}$, seven exact decimals in 5.79 ms using Levin's u-transform of order 8 and in 5.82 using the epsilon algorithm of order 8.

From the results listed in tables 7 and 8, note that the use of $\bar{D}$- and D-transformations is more accurate for the evaluation of $\mathcal{I}_{n_1 00, n_3 00}^{n_2 00, n_4 00}$ given by equation (20) than the use of Levin u-transform, the epsilon algorithm and the series expansion, since the $\bar{D}$ of order 2 yields to better accuracy (more than 15 exact decimals) than the Levin's u-transform of order 6 and the Epsilon-Algorithm of order 6, with major run-time saving.

In most cases, the D- and $\bar{D}$-transformations are very efficient in evaluating rapidly oscillatory infinite integrals. They produce approximations $D_m^{(n)}$ and $\bar{D}_m^{(n)}$ which as m becomes large converge very quickly to the exact value.

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