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Digital erosion in the evaluation of molecular integrals

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Abstract. In the course of checking our work on the symbolic calculation of molecular integrals over Slater orbitals, we obtained some results in substantial disagreement with two recent articles that describe numerical schemes. We believe that these schemes suffer from digital erosion, possibly because recurrence formulas were used outside their regions of stability. Our results were obtained using the ζ-function method, which expands the orbital on one atom onto the other, and integrates in polar coordinates. They were checked using elliptic coordinates. Both sets of calculations were performed symbolically. We summarize these calculations and discuss the impact of symbolic calculation on the accuracy of molecular computations.

Key words: Integrals – Symbolic computation – Accuracy

1 Background

A recent article in this journal by Öztekin, Yavuz and Atalay [1] described a new scheme to compute overlap integrals over Slater orbitals. They addressed the problem of computing overlap integrals with very high quantum numbers, for use in expansions of three- and four-center integrals, and they gave spot values for overlap integrals over orbitals with quantum numbers as high as 75. Table 1, below, contrasts the results in their Table 1 with values that we constructed, for comparison, by techniques that use symbolic computation [2]. Agreement is excellent for low quantum numbers, but deteriorates rapidly. For one integral, we get a value that rounds to -8×10^{-78} compared with a value that rounds to -5×10^{-8} in Ref. [1]. The authors of Ref. [1] computed their results by three different routes. They state that agreement between their second and third methods is a measure of the accuracy. It is possible, however, that

1. These two methods start with the same set of auxiliary functions and form the same linear combinations, by different paths, with a precision that achieves consistency whatever the starting values of the auxiliary functions, and
2. These values were constructed by a recurrence scheme which accumulates errors.

An earlier, related scheme was reported by Guseinov and Mamedov [3]. Table 2, below, compares the sample results in their Table 1 with values from our formulas. Here, too, there are discrepancies that we ascribe to digital erosion in the cited work. For conciseness, we refer to Refs. [1, 3] and to their authors as OYA and GM, and to the integrals in Tables 1 and 2 as oya01–oya20 and gm01–gm21, respectively. Also, because this note is largely a commentary on OYA and GM, we do not repeat many of the references in their bibliographies.

2 The symbolic computations

Our primary approach to the evaluation of Slater integrals uses the "ζ-function" method. This is based on the Gegenbauer addition theorem [4], extended and applied by Coulson and Barnett, separately and jointly, in several articles that include Refs. [5, 6, 7, 8, 9] prior to Ref. [2]. Several other authors have explored similar expansions. The equivalence is discussed in Refs. [10, 11]. The basic ζ-function formalism is described in Refs. [5, 6, 8]. We gave general formulas for overlap (and other) integrals over Slater orbitals in Refs. [2, 7, 8]. The symbolic calculation of the relevant auxiliary functions is discussed in Ref. [9] and was applied to all the types of non-exchange two-center integrals in [2]. The calculations in the present note follow from Eq. (89) of the latter paper. They were coded in MATHEMATICA [12].

We consider the non-zero overlap integrals

$$\int \Psi_{n_a,l_a,m,\sigma}(k_a,\vec{r}_a)\Psi_{n_b,l_b,m,\sigma}(k_b,\vec{r}_b)\mathrm{d}V \quad , \tag{1}$$

Table 1. Comparison with the results of Öztekin et al. [1]

id	n_a	l_a	n_b	l_b	m	p	Overlap integral from [1]	Value from our formulas
1	4	2	3	2	1	25	$-5.65554\ 47149\ 2814 \times 10^{-6}$	$-5.65554\ 47149\ 28136\ 43477 \times 10^{-6}$
2	15	4	8	4	4	25	$2.54324\ 13255\ 908 \times 10^{-3}$	$2.54324\ 13255\ 99050\ 25346 \times 10^{-3}$
3	18	10	18	17	9	20	$-1.14908\ 69323\ 4024 \times 10^{-2}$	$-1.14908\ 69466\ 02953\ 11841 \times 10^{-2}$
4	25	12	20	17	11	30	$4.88129\ 71401\ 6814 \times 10^{-2}$	$4.88129\ 74127\ 09633\ 67291 \times 10{-}2$
5	30	15	29	10	8	50	$7.36659\ 17323\ 7904 \times 10^{-2}$	$7.36627\ 18636\ 87158\ 42865 \times 10^{-2}$
6	34	14	34	12	10	75	$1.30016\ 39359\ 0254 \times 10^{-4}$	$1.35279\ 99157\ 49023\ 94424 \times 10^{-4}$
7	40	29	40	15	15	15	$-6.64155\ 43654\ 4458 \times 10^{-8}$	$-1.19808\ 92914\ 94799\ 80851 \times 10^{-7}$
8	45	29	44	19	17	0.05	$-5.10576\ 63167\ 5415 \times 10^{-4}$	$1.47153\ 43433\ 38187\ 12078 \times 10^{-28}$
9	48	8	15	3	3	100	$1.79326\ 01304\ 6145 \times 10^{-7}$	$1.79326\ 01542\ 13879\ 83111 \times 10^{-7}$
10	50	15	15	13	11	10	$2.90100\ 70720\ 5215 \times 10^{-4}$	$2.90100\ 70720\ 05887\ 45053 \times 10^{-4}$
11	50	17	25	15	13	10	$2.67465\ 65012\ 0232 \times 10^{-2}$	$2.67465\ 65009\ 98301\ 24907 \times 10^{-2}$
12	50	17	35	17	16	25	$-1.22862\ 34623\ 0312 \times 10^{-1}$	$-1.22862\ 33664\ 18743\ 26573 \times 10^{-1}$
13	50	17	50	17	15	5	$7.91990\ 10468\ 7359 \times 10^{-1}$	$7.91990\ 10468\ 08083\ 06681 \times 10^{-1}$
14	55	20	52	23	20	35	$-1.78167\ 72801\ 6314 \times 10^{-2}$	$-2.58332\ 56897\ 62251\ 52663 \times 10^{-1}$
15	60	14	52	17	12	35	$-7.50777\ 78114\ 6405 \times 10^{-2}$	$-2.62097\ 24834\ 73092\ 31335 \times 10^{-2}$
16	62	19	52	17	15	10	$3.16515\ 41484\ 5183 \times 10^{-1}$	$3.16515\ 41484\ 60412\ 40431 \times 10^{-1}$
17	65	24	65	20	18	1×10^{-2}	$-1.26130\ 79035\ 3512 \times 10^{-10}$	$2.95052\ 48866\ 02063\ 27282 \times 10^{-14}$
18	70	15	65	13	10	1×10^{-4}	$3.35027\ 78817\ 9863 \times 10^{-11}$	$3.34993\ 30690\ 23695\ 02366 \times 10^{-11}$
19	70	25	70	15	14	25	$3.65666\ 73244\ 8635 \times 10^{-3}$	$-3.46058\ 31366\ 47395\ 18445 \times 10^{-6}$
20	75	30	75	20	18	1×10^{-6}	$-4.92600\ 26460\ 7547 \times 10^{-8}$	$-8.19297\ 54962\ 16878\ 82025 \times 10^{-78}$

Table 2. Comparison with results of Guseinov and Mamedov [3]

id	n_a	l_a	n_b	l_b	m	p	t	Overlap integral from [3,13]	Value from our formulas
1	3	2	3	2	1	25	0.6	$-4.42287\ 76698\ 8261 \times 10^{-4}$	$-4.42287\ 76698\ 82608\ 80679 \times 10^{-4}$
2	4	2	4	3	1	80	0.4	$4.03505\ 95032\ 6382 \times 10^{-17}$	$4.03505\ 95032\ 63822\ 98108 \times 10^{-17}$
3	5	4	5	4	4	100	0.7	$1.56200\ 59915\ 3976 \times 10^{-14}$	$1.56200\ 60274\ 57891\ 03745 \times 10^{-14}$
4	7	3	4	3	2	150	0.7	$-1.76861\ 05069\ 7887 \times 10^{-18}$	$-1.76861\ 05069\ 22648\ 59080 \times 10^{-18}$
5	9	5	8	4	3	45	0.2	$-5.46510\ 24302\ 2867 \times 10^{-8}$	$-5.46510\ 24302\ 27040\ 17382 \times 10^{-8}$
6	10	7	8	2	1	60	0.2	$-1.84189\ 02617\ 3558 \times 10^{-10}$	$-1.84189\ 02617\ 31981\ 06424 \times 10^{-10}$
7	10	9	10	9	9	15	0.6	$6.23122\ 31819\ 6866 \times 10^{-4}$	$6.23122\ 31819\ 11249\ 46475 \times 10^{-4}$
8	13	12	13	12	12	25	0.01	$1.35310\ 56039\ 2189 \times 10^{-4}$	$1.35310\ 57870\ 24712\ 38186 \times 10^{-4}$
9	14	13	14	13	13	15	0.4	$4.53551\ 31215\ 6525 \times 10^{-3}$	$4.53551\ 28510\ 67909\ 11552 \times 10^{-3}$
10	15	14	15	14	14	15	0	$3.74722\ 49703\ 8009 \times 10^{-2}$	$3.74722\ 49703\ 81891\ 95430 \times 10^{-2}$
11	16	15	16	15	15	35	0	$1.21686\ 56225\ 3236 \times 10^{-6}$	$1.21686\ 52185\ 90198\ 18856 \times 10^{-6}$
12	17	8	8	7	4	50	0.1	$-1.00640\ 06135\ 4258 \times 10^{-6}$	$-1.00640\ 06411\ 71881\ 72346 \times 10^{-6}$
13	17	16	17	16	16	25	−0.5	$3.06769\ 56518\ 5575 \times 10^{-5}$	$3.06770\ 32557\ 90193\ 60938 \times 10^{-5}$
14	18	12	18	12	12	20	−0.6	$6.63931\ 81365\ 1240 \times 10^{-5}$	$6.63931\ 81369\ 66506\ 77513 \times 10^{-5}$
15	21	10	9	8	6	45	0	$5.38980\ 68535\ 0612 \times 10^{-5}$	$5.38980\ 68533\ 81437\ 73017 \times 10^{-5}$
16	27	8	9	8	7	35	−0.2	$-1.73300\ 98279\ 9699 \times 10^{-4}$	$-1.74423\ 80751\ 96959\ 09193 \times 10^{-4}$
17	30	10	14	10	8	35	0	$1.35074\ 70959\ 2800 \times 10^{-2}$	$1.35074\ 70959\ 32433\ 38875 \times 10^{-2}$
18	37	8	12	10	6	10	−0.6	$3.98219\ 84900\ 4259 \times 10^{-14}$	$3.98228\ 00437\ 70915\ 73596 \times 10^{-14}$
19	40	4	12	4	3	15	0.6	$9.48379\ 26559\ 9810 \times 10^{-2}$	$9.48379\ 22083\ 22556\ 78538 \times 10^{-2}$
20	43	10	18	8	6	60	−0.4	$-1.15907\ 68712\ 3104 \times 10^{-4}$	$-1.15825\ 65326\ 71748\ 14660 \times 10^{-4}$
21	50	4	50	4	4	25	0.7	$1.84395\ 90103\ 7228 \times 10^{-12}$	$1.84395\ 87993\ 24363\ 40310 \times 10^{-12}$

containing the real orbitals

$$\Psi_{n,l,m,\sigma}(k,\vec{r}_s) = \mathcal{N}_{n,l,m}(k) r_s^{n-1} e^{-kr_s} P_l^m(\cos\theta_s) \times \left\{ \begin{matrix} \cos m\phi_s \\ \sin m\phi_s \end{matrix} \right\}_{\sigma=-1} . \tag{2}$$

The subscript s specifies the atomic center. The polar axes of the (r_a, θ_a, ϕ_a) and (r_b, θ_b, ϕ_b) coordinate systems are colinear and point in the direction AB. The azimuthal planes coincide. Nucleus B has coordinates $(\rho, 0, 0)$ in the (r_a, θ_a, ϕ_a) system. The index σ takes values -1 and 1 for $\cos m\phi_s$ and $\sin m\phi_s$, respectively. The normalizing factor $\mathcal{N}$ is

$$\mathcal{N}_{n,l,m}(k) = \begin{cases} \sqrt{\dfrac{2^{2n}(2l+1)(l-m)!k^{2n+1}}{(l+m)!(2n)!\pi}} & \text{if } m > 0; \\ \sqrt{\dfrac{2^{2n-1}(2l+1)k^{2n+1}}{(2n)!\pi}} & \text{if } m = 0 \ . \end{cases} \tag{3}$$

The integral in Eq. (1) is zero if $m_a \neq m_b$, or if $\sigma_a \neq \sigma_b$, or if $m_a = m_b = 0$ and $\sigma_a = \sigma_b = 1$. For the non-zero integrals we write $m_a = m_b = m, \sigma_a = \sigma_b = \sigma$. The value of the integral does not depend on σ when $m > 0$.

Although these integrals depend ostensibly on the two screening constants (k_a, k_b) and the inter-nuclear

separation ρ, they can be written as functions of the two variables $\kappa = k_a/k_b$ and $\tau = k_b\rho$, or the equivalent $t = (k_a - k_b)/(k_a + k_b)$ and $p = \rho(k_a + k_b)/2$. Shortly before OYA was published, we constructed a table of formulas for the individual overlap integrals with $(n_a, n_b) \leq 8$. For equal screening constants, these formulas depend on the single variable ρ. For example, the $(4d_{xz}, 3d_{xz})$ integral that is particularized in oya01 is given by

$$\frac{e^{-\rho}}{210\sqrt{14}}\left(735 + 735\rho + 255\rho^2 + 10\rho^3 - 20\rho^4 - 7\rho^5 - \rho^6\right) \tag{4}$$

To check the other integrals in OYA, we assigned the appropriate numerical values to ρ as well as to the quantum numbers of the concomitant orbitals, before starting the process to reduce the general expression for an overlap integral symbolically. The result for oya02 is typical.

$$\frac{1474\ 29590\ 74464\ 50752\ 82029\ 15877\ \ e^{-25}}{10\ 25623\ 22267\ 30490\sqrt{616\ 16126}} \tag{5}$$

Any overlap integral with equal screening constants can be reduced to the form

$$\frac{ae^{-\rho}}{b\sqrt{c}} \tag{6}$$

where a is a polynomial in ρ with integer coefficients, and b and c are integers. For oya20, ρ is the rational 1×10^{-6}, and the numerical values of a, b and c contain 965, 1037 and 8 digits, respectively.

For unequal screening constants, too, we use tables of formulas for $(n_a, n_b) \leq 8$. Thus, the $(3d_{zx}, 3d_{zx})$ integral that is particularized by gm01 is given by

$$\begin{aligned}
&\frac{-128\kappa^{7/2}}{(\kappa^2-1)^7\tau^5} \\
&\quad\times\big\{\kappa\big(-11520 - 11520\tau + 480(\kappa^2-11)\tau^2 \\
&\quad + 480(\kappa^2-3)\tau^3 + 240(\kappa^2-1)\tau^4 \\
&\quad - (\kappa^2-1)^2(\kappa^2+23)\tau^5 + (\kappa^2-1)^3\tau^6\big)e^{-\tau} \\
&\quad + \big(\tau^5 + 23\kappa^6\tau^5 + \kappa^7\tau^6 - 3\kappa^5\tau^4(-80+\tau^2) \\
&\quad - 45\kappa^4\tau^3(\tau^2-32) + 3\kappa^3\tau^2(\tau^4 - 80\tau^2 + 1760) \\
&\quad + 3\kappa^2\tau(7\tau^4 - 160\tau^2 + 3840) \\
&\quad - \kappa(\tau^6 + 480\tau^2 - 11520)\big)e^{-\kappa\tau}\big\}
\end{aligned} \tag{7}$$

For $(n_a, n_b) > 8$, we assigned values to (κ, τ) or (p, t) and then performed the computation. This led, for example, to the following expression for the integral gm06 $(n_a = 10, l_a = 7, n_b = 8, l_b = 2, m = 1, p = 60, t = 1/5)$.

$$\begin{aligned}
&\frac{75\ 58272}{3\ 81851\ 19628\ 90625\sqrt{33915}} \\
&\quad\times\big(28\ 79825\ 09811\ 37028\ 95638\ 78731\ \ e^{-72} \\
&\qquad -120\ 24494\ 41944\ 08965\ 88195\ \ e^{-48}\big)
\end{aligned} \tag{8}$$

Any overlap integral with unequal screening parameters can be reduced to the form

$$\frac{\kappa^{v_1+1/2}(ae^{-\tau} + be^{-\kappa\tau})}{c\sqrt{d}(\kappa^2-1)^{v_2}\tau^{v_3}} \tag{9}$$

where (v_1, v_2, v_3, c, d) are integers, and (a, b) are polynomials in (κ, τ) with integer coefficients.

When referring to Table 1 of GM, it should be noted that the values of l', the angular quantum number of the orbital on nucleus B, were omitted from their published work. The column that is headed l' in Ref. [3] actually contains the values of the quantum number m. Also, since publishing their paper, the authors have amended the values of gm04 (in sign), gm11 (in the 3rd digit), gm12 (in the 5th digit) and gm18 (from order 10^{-1} to order 10^{-14}) [13]. While we get 15-digit agreement with a few of their results, mismatch still occurs as high as the 3rd digit amongst the others.

3 Checking our formulas

A detailed account of our process that applies the ζ-function method to the tabulation of formulas for overlap integrals is in preparation [14]. Its development has included an exploration of the use of computer algebra to optimize both symbolic and numeric computations. The relative simplicity of the overlap integrals facilitated this study. It has provided results that we will use in further work on molecular integrals of greater complexity and related problems.

However, even when dealing with objects as simple as the overlap integrals by computer algebra, checking is essential – hence our interest in a diversity of numerical results of other authors and, where possible, formulas from other sources. Very early in our use of MATHEMATICA for this work, we tried to regenerate a table of formulas for two-center one-particle integrals that Coulson derived manually [15]. These did not have a uniform structure and, in consequence, we could not design an algorithm to generate the expressions that he published. The manual transformation of our immediate results to the formulas in [16] was tedious and error prone. This showed the need for interactive resources to fine tune formulas produced by computer algebra, which led us to develop the "hierarchical addressing" scheme in the suite of MATHEMATICA procedures that we call MATHSCAPE [16, 17]. As mentioned in Ref. [2], this let us produce results that matched those in Ref. [16] precisely, except for two of the expressions. Further checking confirmed our formulas throughout. Numerically, we verified some results of Kennedy and Zhao [18], using other formulas which we had tabulated [9]. Also, we calculated spot values for all the Coulomb integrals containing K and L shell orbitals, from appropriate formulas, which matched the values which we computed numerically using the programs of Rico et al. [19]. This was reported in Ref. [2].

When using the values in GM to check our overlap integral formulas, we repeated each asymmetric case with the orbitals interchanged, and we recalculated gm03 using elliptic coordinates. This confirmed our expression of the form of Eq. (9). In principle, the test does not exclude possible errors in the exponential and square

root functions, or in the manipulation of the specific very long integers that are involved. Because errors have occurred for exceptional arguments historically, e.g. in square roots on the EDSAC computer [20], in e^{-2} on the ATLAS computer [21], and in division on the PENTIUM chip [22], we ran further checks. These excluded such errors as the cause of discrepancy here.

After recalculating the OYA integrals using the ζ-function procedures, we repeated the calculations in elliptic coordinates, using simple coding. The integrands were converted to the (λ, μ, ϕ) coordinate system using the basic formulas in [15]. The integrands were expanded and the integrations were distributed using elementary MATHSCAPE and built-in MATHEMATICA functions. Then the built-in `Integrate` function was used to work outwards through the integrations over ϕ, μ and λ in succession. The function was used for expediency, and its use was inefficient computationally. However, it had the advantage of avoiding any commonality with the ζ-function calculation, as regards intermediary mathematical functions, except for exponentials, square roots and the normalizing factors in the final conversion to numerical form. We have now run corresponding checks on all the GM integrals, confirming the results that we obtained using ζ-functions. We will try to develop faster procedures using elliptic coordinates in due course.

4 Simplified calculations

We are exploring the construction of bounds and asymptotic formulas, using the fact that $r^n e^{-r}$ peaks very sharply at $r = n$ for high quantum numbers. The approximation $\exp(-r_b) \approx \exp(-r_a) \times \exp(\rho \cos\theta_a - \rho^2 \sin^2\theta_a / 2r_a)$ worked well in some preliminary tests for integrals containing s orbitals. For $(21s, 1s)$ at $\rho = 1$, we expanded the second exponential about the origin, and took the first three terms. This gave 0.00002 42095 32395 27782 17497 for the integral, which differs by 3 units in the rightmost digit from the value found from the precise formula. Attempts to use this approach for high angular quantum numbers have not succeeded, so far. Maslov and Niukkanen have reported an approach to the computation of molecular integrals [24] that may help in this regard.

5 Explaining the discrepancies

Calculations that take differences of relatively large quantities may be a source of error in both OYA and GM. Neither work addresses the issue. The differencing problem is discussed in relation to the evaluation of molecular integrals by Jones [23]. He advocates using the unrestricted precision arithmetic resources of computer algebra systems when performing molecular calculations. Other authors also take this view. Weniger, Čížek and Vinette [25] used 1000-digit precision arithmetic in studies of high order anharmonic oscillators. We use rational arithmetic throughout our molecular integrals work, and we used rational arithmetic and 100-digit floating–point arithmetic in a study of parameterized secular equations [26]. Also, at one point in the molecular integrals studies, symbolic calculation removed paired terms of identical magnitude and opposite sign that had dominated the prior piecewise numerical computation of certain auxiliary functions [9]. Working in a symbolic computation environment facilitates the monitoring of digital erosion [26]. Also it helps in the mechanical production of reports and papers by techniques that avoid any manual transcription. This issue is discussed in Ref. [2]. As well as converting the direct results of our MATHSCAPE sessions to LaTeX mechanically [27], we now convert the encoded formulas back to symbolic and numerical forms, to ensure that no errors were introduced in the coding.

Both OYA and GM stress their use of recurrence schemes. Such schemes provide fertile ground for digital erosion. The standard literature of numerical analysis cautions against the indiscriminate use of recurrence formulas (see, e.g., page 21 of Ref. [28], page 25 of Ref. [29]). The accounts of rigorous numerical tabulations of mathematical functions state the region of stability of each formula that is used (see, e.g., [30]). We discussed this issue in connection with the evaluation of molecular integrals half a century ago in the comments accompanying Eq. (35f) on page 329 of Ref. [6]. Antolović and Delhalle [31], Weniger and Steinborn [32], Bhattacharya and Dhabal [33], Li, Dong and Pan [34], Sébilleau [35] and other authors have also discussed the numerical stability of the functions that are used to compute molecular integrals, too. Neither OYA nor GM, however, give detailed, explicit attention to this topic.

The discrepancies that are noted in Tables 1 and 2 reflect a more general problem that affects computational science. The recency of the field has not yet allowed the accumulation and systematization of experience comparable to the experimental lore of traditional scientific research. Often, numbers are accepted unless they are in conspicuous violation of physical principles because there is no real alternative. Numerical analysis is a well established field and has an extensive literature that deals with error bounds, but many scientific computations are reported without any attention to this. Symbolic computation offers new ways to check, but it is not a simple panacea. We have found it to be fraught with error, too. For example, when streamlining part of our overlap integral calculation recently, we generated a set of results that showed consistency in the differentiation check that raises n_a and n_b, but that were completely wrong. The expressions had been reconstructed, consistently, as linear combinations of a damaged file of Gaunt coefficients. Another test, which checked the limit $\rho \to 0$, detected the error. Numerical and symbolic calculations, however, do provide powerful cross checks on each other and, if used cautiously, can be combined to give greater accuracy and confidence in theoretical research.

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