

Reply to "Comment on 'Analysis of some integrals arising in the atomic four-electron problem'" [J. Chem Phys. 99, 3622 (1993)]

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The comment by Harris *et al.* makes three principal points on the paper cited in the title. The authors point out that the seventh and 21st W_4 auxiliary functions contain an incorrect argument. I have checked the formulas and I am in agreement. These are both typographical errors; τ_7 should have read τ_8 in the seventh W_4 term in Eq. (42), and τ_4 should have read τ_6 in the 21st W_4 term. The calculated results reported in Table I were based on the correct formula.

Harris *et al.* have produced an elegant simplification of the angular integral that occurs in Eq. (34). The computational approach that I employed makes substantial use of tabled values for a significant number of the $3-j$ symbols that arise. This makes the calculation of the angular integral a very minor component of the computational cost of a single I_4 integral evaluation. This is particularly the situation with the more difficult integrals involving a multiple number of r_{ij}^n factors with odd values for the exponent indices, cases that are important in practical calculations. Every computational simplification should be exploited, and the improved formula given in the comment may allow for some minor gains in evaluation speed. With the continuing reduction in the cost of computer memory, the formula of Harris *et al.* offers an alternative evaluation strategy for I_Ω by tabling a large number of $6-j$ symbols. The radial integral contribution consumes the most significant fraction of the computer resources when evaluating an individual I_4 integral. Substantial improvements in computational speed depend on continuing refinements and proper selection of convergence acceleration techniques, Richardson extrapolations, and the related asymptotic series expansion techniques.^{1–5}

The final comment by Harris *et al.* concerns a way to set

up the various argument lists to carry out the required permutations for the ordering of the distance factors r_i so that $r_i \leq r_j \leq r_k \leq r_l$. This suggestion is potentially useful for the generation of the formulas using symbolic algebra packages. The permutation structure associated with this ordering is an important complication to the evaluation of the I_4 integrals. The number of auxiliary W_N integrals scales as $N!$, where N is the number of electrons. Clearly, the complexity spirals significantly with increasing N , and the resulting correlated integrals are likely to be rather intractable. It is possible to circumvent this problem entirely for the case $N=4$ by employing a different form of the Sack expansion.⁶ This leads to additional infinite series to contend with, but judicious application of convergence acceleration techniques may resolve these infinite series issues. The auxiliary functions that arise have not been previously studied, and the general cases lead to some recalcitrant integration problems. They are currently under investigation.

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