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Symmetry-adapted integrals over many-electron basis functions and operators

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Abstract. We consider integrals over symmetry-adapted basis functions that involve the coordinates of more than one electron. We focus on basis functions that can be written as products of one-electron functions and (say) a two-electron function. We show first that the two-electron parts of the basis functions can be absorbed into the operator, resulting in an integral over only one-electron basis functions, but a more complicated many-electron operator. We then prove a general formula for expressing such integrals in terms of symmetry-distinct integrals only.

Introduction

One of the strategies that can be used to reduce the computational effort in quantum-chemical calculations is to exploit molecular symmetry. Symmetry serves to reduce the number of non-vanishing terms that must be processed, as well as to relate quantities that are equal and thus need be calculated only once, reducing redundant work. The first stage of most calculations is the computation of integrals involving various operators over some form of one-electron basis. The molecular Hamiltonian comprises one- and two-electron operators, and for a one-electron basis this leads to one- and two-electron integrals. The greatest economy from symmetry in later stages of the calculation is obtained if the one-electron basis is symmetry-adapted, that is, the elements of this basis transform as basis functions for irreducible representations of the molecular point group. Integrals over such symmetry-adapted basis functions will be referred to as *symmetry-adapted integrals* in this work. Typically, the basis functions used in molecular calculations are centered on individual atoms, and thus symmetry-adapted basis functions must be formed as appropriate linear combinations of the original basis. We shall refer to the original basis functions as *atomic orbitals* (AOs) and the symmetry-adapted combinations as *symmetry orbitals* (SOs) in what follows.

Probably the most elegant and powerful technique for obtaining symmetry-adapted integrals is the method of double coset decompositions introduced by Davidson [1]. This approach unifies the enumeration of *symmetry-distinct integrals* – the list of distinct integrals over AOs – with the construction of symmetry-adapted integrals by combining these distinct integrals with appropriate weights. In his original paper Davidson considered one- and two-electron integrals over *totally symmetric* operators O, that is operators for which

$$G^{-1}\mathcal{O}G = \mathcal{O}\ \forall G \in \mathcal{G} \ , \tag{1}$$

where $\mathcal{G}$ is the molecular point group, of order g. Integrals over operators that are not totally symmetric have been discussed by one of the present authors [2], as have integrals over basis functions that are differentiated with respect to certain parameters, such as the coordinates of their centres [3].

Recently, there has been a resurgence of interest in the use of basis functions that depend on the coordinates of more than one electron. Such methods go back to Hylleraas [4], with the inclusion of the interelectronic coordinate for helium. Current approaches include the use of *Gaussian-type geminals* (see, e.g., [5]), of the form

$$\begin{aligned}
&(i, j, k, l.m, n, \eta, \theta, \kappa, \vec{A}, \vec{B}) \\
&\quad = x_{1A}^{i} y_{1A}^{j} z_{1A}^{k} x_{2B}^{l} y_{2B}^{m} z_{2B}^{n} \exp\left(-\eta r_{1A}^{2} - \theta r_{2B}^{2} - \kappa r_{12}^{2}\right) \\
&\quad \equiv x_{1A}^{i} y_{1A}^{j} z_{1A}^{k} \exp\left(-\eta r_{1A}^{2}\right) x_{2B}^{l} y_{2B}^{m} z_{2B}^{n} \\
&\qquad \times \exp\left(-\theta r_{2B}^{2}\right) \exp\left(-\kappa r_{12}^{2}\right) \ .
\end{aligned} \tag{2}$$

and of wave functions that include factors of linear r_{12}, the interelectronic coordinate (see, e.g., [6]). We may note that all of these approaches can be viewed as using two-electron basis functions of the general product form

$$\phi_a(\vec{r}_{1A})\phi_b(\vec{r}_{2B})w(r_{12}) \ . \tag{3}$$

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In current applications of these functions, the two-electron part w – the "correlation factor" – is totally symmetric:

$$Gw(r_{12}) = w(r_{12})\ \forall\ G \in \mathcal{G}\ . \tag{4}$$

In general, we shall assume this to be the case, although we will discuss briefly the situation where it is not.

Even for a Hamiltonian comprising only one- and two-electron operators, a much richer set of integrals arises once two-electron basis functions are admitted. For the simplest treatment of electron correlation, second-order perturbation theory, at least three-electron integrals are needed, and as the correlation treatment becomes more elaborate four-electron integrals and even five-electron and higher integrals can appear. The scaling of the computational effort for these many-electron integrals is very great, and indeed it is difficult to see that a method that requires, say, four-electron integrals can find wide applicability. Nevertheless, for any desired order of integrals there are the same opportunities to use molecular symmetry to reduce the work needed to calculate the integrals and the work performed using them in later stages of the calculation. As part of our on-going efforts [7] to use two-electron basis functions in practical calculations we have therefore generalized the double coset decomposition (DCD) procedure to integrals of any order. In this paper we first review DCDs and their application to one- and two-electron integrals, in part to establish notation. We then develop a general formula, proved by induction. Finally, we use this general formula to discuss computational considerations and the example of three-electron integrals, which we have recently programmed in the Dalton package [8] for computational quantum chemistry.

Symmetry-adapted integrals over one-electron basis functions

At the outset of this work we found ourselves in a notational quandary. There is a rather well-established notation for all of the various quantities that comprise the formulas for symmetry-adapted integrals, and all of the previous work has consistently used these conventions. Unfortunately, this notation makes heavy use of different alphabetical sequences for different quantities, and there are simply not enough letters in the (Roman) alphabet to do the job for higher-order integrals. After many attempts to use different fonts for different quantities and endless difficulties with multiple levels of subscripts, we have reluctantly concluded that a change in notation is unavoidable. In this section, therefore, we will briefly review one- and two-electron integrals over one-electron basis functions in the usual notation, and then make a transition to the more general notation we shall use later, in order to make clear the connections to earlier work.

In most computational implementations of DCDs, the molecular symmetry treated has been restricted to $D_{2\mathrm{h}}$ and its subgroups. These are Abelian groups in which each element is its own inverse. Further, any function on a given center is taken into a single "image" function on another center under any group operation, rather than a linear combination of functions. Let an AO on center A be denoted f_{aA}, where all other properties of the AO (angular type, s, p_x, etc., Gaussian or Slater exponent or exponents and contraction coefficients) are subsumed into the index a. Then

$$Gf_{aA} = p_a(G) f_{aG(A)}\ , \tag{5}$$

where $G(A)$ is the transformed center obtained by applying G to center A, and $p_a(G)$ is a parity factor (for D_{2h} and its subgroups) that depends on the angular behaviour of f_{aA}. An SO F^{α}_{aA} for irreducible representation (irrep) α can be constructed from this AO and its images by projection:

$$F^{\alpha}_{aA} = g^{-1} \sum_{G} \chi^{\alpha}(G) G f_{aA}\ ; \tag{6}$$

where g is the order of the group and χ^{α} the group character for the desired irrep.

We note that there is some subgroup $\mathcal{U} \subset \mathcal{G}$ for which $U(A) = A$. $\mathcal{U}$ is known as the *stabilizer* of A. If the order of $\mathcal{U}$ is denoted u. Under the stabilizer AOs on A transform as

$$Uf_{aA} = p_a(U) f_{aA}\ . \tag{7}$$

In fact, each f_{aA} transforms as a basis function for some irrep υ of the subgroup $\mathcal{U}$, giving

$$\sum_{U} \chi^{\upsilon}(U) p_a(U) = u\ . \tag{8}$$

Consider now another AO, f_{bB}, with stabilizer $\mathcal{V}$. From two subgroups $\mathcal{U}$ and $\mathcal{V}$ we can form *double cosets*

$$\mathcal{U}G\mathcal{V} \quad \forall\ G \in \mathcal{G}\ . \tag{9}$$

Two double cosets are either distinct (no elements in common) or identical. Unlike cosets, GU or UG, a given element of $\mathcal{G}$ may occur multiple times in a given double coset. For D_{2h} and its subgroups this degeneracy is independent of G in Eq. (9) and is given by the expression $\lambda_{\mathrm{G}} = |\mathcal{U} \cap \mathcal{V}|$. A group can thus be decomposed into distinct double cosets in this way: a double coset decomposition. By selecting a set of operators R chosen one from each *distinct* double coset, a sum over group elements can be replaced with a sum over elements of $\mathcal{U}$, $\mathcal{V}$, and R, with a weighting factor of λ_{R}. The elements of R are termed *double coset representatives*. For example

$$F^{\alpha}_{aA} = g^{-1} \lambda_{\mathrm{R}}^{-1} \sum_{U} \sum_{R} \sum_{V} \chi^{\alpha}(URV) URV f_{aA}\ . \tag{10}$$

Using DCDs, it is possible to write a symmetry-adapted integral as a sum of symmetry-distinct integrals with appropriate weight factors. The most important cases are totally symmetric one- and two-electron operators, whose integrals over SOs take the form

$$\begin{aligned}&\left(F^{\alpha}_{aA}|O|F^{\alpha}_{aB}\right)\\ &\quad = uvg^{-1}\lambda_{\mathrm{R}}^{-1} I_{\alpha\beta} \sum_{R} \chi^{\beta}(R) p_b(R) \left(f_{aA}|O|f_{bR(B)}\right)\end{aligned} \tag{11}$$

and

$$\left(F^{\alpha}_{aA}F^{\beta}_{bB}|F^{\gamma}_{cC}F^{\delta}_{dD}\right)$$
$$= g^{-3}uvwxI_{\alpha\beta\gamma\delta}\lambda_{\mathrm{T}}^{-1}\sum_{R}\sum_{S}\sum_{T}\chi^{\beta}(R)\chi^{\gamma}(T)\chi^{\delta}(TS)$$
$$\times p_b(R)p_c(T)p_d(TS)\left(f_{aA}f_{bR(B)}|f_{cT(C)}f_{dTS(D)}\right) \ . \tag{12}$$

Here the selection rule factor $I_{\alpha\beta\ldots}$ is given by

$$I_{\alpha\beta\ldots} = g^{-1}\sum_{G}\chi^{\alpha}(G)\chi^{\beta}(G)\ldots \ ; \tag{13}$$

which vanishes unless the direct product $\alpha\otimes\beta\otimes\ldots$ contains the totally symmetric irrep, and the DCR *R*, *S*, and T are obtained from DCDs involving respectively $\mathcal{U}$ and $\mathcal{V}$, $\mathcal{W}$ and $\mathcal{X}$, and $\mathcal{U}\cap\mathcal{V}$ and $\mathcal{W}\cap\mathcal{X}$. $\mathcal{U}$, $\mathcal{V}$, $\mathcal{W}$, and $\mathcal{X}$ are the respective stabilizers of centers *A*, *B*, *C*, and *D*. $\mathcal{U}\cap\mathcal{V}$ is the stabilizer of the *pair* of centers *A* and *B*, and thus of the charge distribution $f_{aA}f_{bB}$, and similarly $\mathcal{W}\cap\mathcal{X}$ for $f_{cC}f_{dD}$. Finally, we may note that if the charge distribution $f_{cC}f_{dD}$ is the same as $f_{aA}f_{bB}$ the DCD defining T can be expanded; see [1, 2].

We will later make use of a particular property of the selection rule at Eq. (13) for D_{2h} and its subgroups. We note first that since all irreps are one-dimensional, it follows that any direct product of irreps is one-dimensional. Further, for the totally symmetric irrep all characters are unity, of course, whereas for all other irreps half of the *g* characters are $+1$ and half are -1. The result is that when Eq. (13) is satisfied we have the stronger condition

$$\chi^{\alpha}(G)\chi^{\beta}(G)\ldots = 1 \ \forall\, G\in\mathcal{G} \ . \tag{14}$$

We may term this stronger condition a superselection rule.

The formulas of Eqs. (11) and (12) are relatively straightforward. Each comprises a set of summations over group operators that generate distinct AO integrals, and a product of selection rule and parity factor terms that give the weight with which each distinct integral contributes to the nonvanishing symmetry-adapted integrals. Computational implementation is also relatively straightforward: Almlöf's MOLECULE program [9] computed symmetry-adapted integrals in this way almost 30 years ago, although the author arrived at the necessary formulas via a quite different route. Several current integral programs use an implementation very close to that described here, including the program SEWARD [10] as well as the integral routines in the package Dalton [8].

As noted above the notation used in this brief review is exactly that introduced by Davidson [1], and in retrospect it can be seen to be profligate in its use of alphabetical symbols even though it is economical of subscripts and superscripts. In order to generalize these formulas to higher-order integrals we will have to revise the notation. Going forward, then, we will denote different AOs by $f[a_i,A_i]$, with different choice of subscripts *i*, and similarly the possible SOs derived from $f[a_i,A_i]$ and its images as $F[a_i,A_i,\alpha_p]$, where irreps are now labeled as α_p. Group operators in $\mathcal{G}$ will be denoted G_j ; the stabilizer of center A_i becomes $\mathcal{U}^i$ with elements U^i and order u_i. Here *i*, *j*, and *p* are integers, counting from one up. The selection rule $I_{\alpha\beta\ldots}$ becomes $I(\alpha_1\alpha_2\ldots)$; the parity factors become $\mathrm{p}_{a_i}(\mathrm{G}_k)$. Each set of DCR will be denoted T^k, with *k* again an integer counting index. It is essential to understand that the superscript notation denotes a specific *set* of DCR or a subgroup of $\mathcal{G}$, and not an *element* of a set. That is, the elements of the set T^1 are labeled T^1, and similarly for an element $U^i\in\mathcal{U}^i$. The factor λ associated with each set of DCR is written as λ_{T^i}.

In this notation the one- and two-electron symmetry-adapted integrals introduced above would become

$$(F[a_1,A_1,\alpha_1]|O|F[a_2,A_2,\alpha_2])$$
$$= u_1u_2g^{-1}\lambda_{\mathrm{T}^1}^{-1}I(\alpha_1\alpha_2)\times\sum_{T^1}\chi^{\alpha_2}(T^1)p_{a_2}(T^1)$$
$$\times\left(f[a_1,A_1]|O|f\left[a_2,T^1(A_2)\right]\right) \tag{15}$$

and

$$(F[a_1,A_1,\alpha_1]F[a_2,A_2,\alpha_2]|F[a_3,A_3,\alpha_3]F[a_4,A_4,\alpha_4])$$
$$= g^{-3}u_1u_2u_3u_4I(\alpha_1\alpha_2\alpha_3\alpha_4)\lambda_{\mathrm{T}^3}^{-1}$$
$$\times\sum_{T^1}\sum_{T^2}\sum_{T^3}\chi^{\alpha_2}(T^1)\chi^{\alpha_3}(T^3)\chi^{\alpha_4}(T^3T^2)$$
$$\times P_{a_2}(T^1)P_{a_3}(T^3)P_{a_4}(T^3T^2)$$
$$\times\left(f[a_1,A_1]f[a_2,T^1(A_2)]|f[a_3,T^3(A_3)]f[a_4,T^3T^2(A_4)]\right) \ . \tag{16}$$

Comparison with Eqs. (11) and (12) should make all of the notational changes clear. With this notation we can now establish a general formula for symmetry-adapted integrals.

General formula for symmetry-adapted integrals

We begin by reminding the reader that we are using two-electron basis functions of the general form of Eq. (3). We then redefine the operator in a general many-electron integral so that the two-electron factors are absorbed into the operator. For example, if we have a two-electron operator $\mathcal{O}_{12}$ and a "cyclic" three-electron integral

$$\iiint \phi_i(r_1)\phi_j(r_3)w_a(r_1,r_3)\phi_k(r_2)\mathcal{O}_{12}\phi_m(r_2)\phi_n(r_3)$$
$$\times w_b(r_2,r_3)\phi_l(r_1)\mathrm{d}r_1\,\mathrm{d}r_2\,\mathrm{d}r_3 \ , \tag{17}$$

we define a new operator

$$\mathcal{O}^{ab}_{123} = w_a(r_1,r_3)\mathcal{O}_{12}w_b(r_2,r_3) \tag{18}$$

and rewrite the integral as

$$\iiint \phi_i(r_1)\phi_j(r_3)\phi_k(r_2)\mathcal{O}^{ab}_{123}\phi_m(r_2)$$
$$\times \phi_n(r_3)\phi_l(r_1)\mathrm{d}r_1\,\mathrm{d}r_2\,\mathrm{d}r_3 \ . \tag{19}$$

Assuming for the moment that $\mathcal{O}_{12}$ is a totally symmetric operator, and that the correlation factors are also totally symmetric, it follows that the new operator $\mathcal{O}^{ab}_{123}$ is also totally symmetric. (We will relax these restrictions subsequently.) This is of course also true for any operator we construct in this way, irrespective of how many correlation factors appear. We can therefore write a general symmetry-adapted integral over such a many-electron operator (say n -electron) as

$$\int\ldots\int F[a_1,A_1,\alpha_1](r_1)F[a_3,A_3,\alpha_3](r_2)$$
$$\ldots F[a_{2n-1},A_{2n-1},\alpha_{2n-1}](r_n)$$
$$\times\,\mathcal{O}^{ab}_{12\ldots n}F[a_2,A_2,\alpha_2](r_1)F[a_4,A_4,\alpha_4](r_2)$$
$$\ldots F[a_{2n},A_{2n},\alpha_{2n}](r_n)\mathrm{d}r_1\ldots\mathrm{d}r_n\ , \tag{20}$$

where we have specifically indicated the electron coordinates associated with each symmetry orbital, or in a more convenient charge distribution notation as

$$(F[a_1,A_1,\alpha_1]F[a_2,A_2,\alpha_2]|F[a_3,A_3,\alpha_3]F[a_4,A_4,\alpha_4]|$$
$$\ldots|F[a_{2n-1},A_{2n-1},\alpha_{2n-1}]F[a_{2n},A_{2n},\alpha_{2n}])\ , \tag{21}$$

by analogy with the LHS of Eq. (16). Here each pair of symmetry orbitals between vertical bars involves a single electron coordinate: a charge distribution.

We now assert that the integral of Eq. (21) can be written in terms of distinct integrals over AO charge distributions as

$$(F[a_1,A_1,\alpha_1]F[a_2,A_2,\alpha_2]|F[a_3,A_3,\alpha_3]F[a_4,A_4,\alpha_4]|$$
$$\ldots|F[a_{2n-1},A_{2n-1},\alpha_{2n-1}]F[a_{2n},A_{2n},\alpha_{2n}])$$
$$=g^{-(2n-1)}u_1\ldots u_{2n}I(\alpha_1\ldots\alpha_{2n})\lambda^{-1}_{\mathrm{T}^{2n-1}}$$
$$\times\sum_{T^1}\cdots\sum_{T^{2n-1}}\chi^{\alpha_2}(T^1)\chi^{\alpha_3}(T^{2n-1})\chi^{\alpha_4}(T^{2n-1}T^2)$$
$$\ldots\chi^{\alpha_{2n}}(T^{2n-1}T^{2n-2}\cdots T^n)$$
$$\times p_{a_2}(T^1)p_{a_3}(T^{2n-1})p_{a_4}(T^{2n-1}T^2)\ldots p_{a_{2n}}(T^{2n-1}T^{2n-2}\cdots T^n)$$
$$\times\left(f[a_1,A_1]f\left[a_2,T^1(A_2)\right]\middle|\,f\left[a_3,T^{2n-1}(A_3)\right]\right.$$
$$\times f\left[a_4,T^{2n-1}T^2(A_4)\right]|\ldots f\left[a_{2n-1},T^{2n-1}\ldots T^{n+1}(A_{2n-1})\right]$$
$$\left.\times f\left[a_{2n},T^{2n-1}\ldots T^n(A_{2n})\right]\right)\ . \tag{22}$$

In this expression we have adopted the following numbering convention for the DCRs. DCR T^1 generates distinct charge distributions from the orbital pair $f[a_1,A_1]$ $f[a_2,A_2]$, DCR T^2 generates distinct charge distributions from $f[a_3,A_3]$ $f[a_4,A_4]$, and so on through T^n for $f[a_{2n-1},A_{2n-1}]$ $f[a_{2n},A_{2n}]$. The DCR T^{n+1} arises from a DCD involving the respective stabilizers of $f[a_{2n-3},\mathrm{A}_{2n-3}]$ $f[\mathrm{a}_{2n-2},\mathrm{T}^{\mathrm{n}-1}(\mathrm{A}_{2n-2})]$ and $f[A_{2n-1},A_{2n-1}]$ $f[A_{2n},\mathrm{T}^n(A_{2n})]$, then DCR T^{n+2} arises from the stabilizers of $f[\mathrm{A}_{2n-5},A_{2n-5}]$ $f[A_{2n-4},\mathrm{T}^{n-2}(A_{2n-4})]$ and the *quadruplet*

$$f[a_{2n-3},A_{2n-3}]f\left[a_{2n-2},T^{n-1}(A_{2n-2})\right]$$
$$\times f\left[a_{2n-1},T^{n+1}(A_{2n-1})\right]f\left[a_{2n},T^{n+1}T^n(A_{2n})\right]\ , \tag{23}$$

and so on recursively back to T^{2n-1}.

We shall prove Eq. (22) by induction, by constructing from this n-electron integral and an additional pair of symmetry orbitals an $n+1$ -electron symmetry-adapted integral.

For further manipulation we make some indexing changes in the integral, numbering orbitals from 3 to $2n + 2$ instead of 1 to $2n$, with a corresponding shift in DCR numbering from 2 to $2n$ instead of 1 to $2n$−1. We also expand the selection rule (after resequencing) as

$$I(\alpha_3\ldots\alpha_{2n+2})=g^{-1}\sum_i\chi^{\alpha_3}(G_i)\ldots\chi^{\alpha_{2n+2}}(G_i) \tag{24}$$

and multiply the AO integral by G_i for each term in this sum. The integral is a scalar and unaffected by this operation, of course. We thus rewrite Eq. (22) as

$$(F[a_3,A_3,\alpha_3]F[a_4,A_4,\alpha_4]|F[a_5,A_5,\alpha_5]F[a_6,A_6,\alpha_6]\ |$$
$$\ldots|F[a_{2n+1},A_{2n+1},\alpha_{2n+1}]F[a_{2n+2},A_{2n+2},\alpha_{2n+2}])$$
$$=g^{-(2n)}u_3\ldots u_{2n+2}\sum_i\chi^{\alpha_3}(G_i)\ldots\chi^{\alpha_{2n+2}}(G_i)\lambda^{-1}_{\mathrm{T}^{2n}}$$
$$\times\sum_{T^2}\cdots\sum_{T^{2n}}\chi^{\alpha_4}(T^2)\chi^{\alpha_5}(T^{2n})\chi^{\alpha_6}(T^{2n}T^3)$$
$$\ldots\chi^{\alpha_{2n+2}}(T^{2n}T^{2n-1}\ldots T^{n+1})$$
$$\times p_{a_4}(T^2)p_{a_5}(T^{2n})p_{a_6}(T^{2n}T^3)$$
$$\ldots p_{a_{2n+2}}(T^{2n}T^{2n-1}\ldots T^{n+1})$$
$$\times\left(G_if[a_3,A_3]G_if\left[a_4,T^2(A_4)\right]\ \middle|\ G_if\left[a_5,T^{2n}(A_5)\right]\right.$$
$$\times G_if\left[a_6,T^{2n}T^3(A_6)\right]\ |$$
$$\ldots G_if\left[a_{2n+1},T^{2n}\ldots T^{n+2}(A_{2n+1})\right]$$
$$\left.\times G_if\left[a_{2n+2},T^{2n}\ldots T^{n+1}(A_{2n+2})\right]\right)\ . \tag{25}$$

We now wish to develop an $n+1$ -electron integral by extending the existing integral with an additional charge distribution, which in SOs we take to be $F[a_1,A_1,\alpha_1]$ $F[a_2,A_2,\alpha_2]$. This gives

$$(F[a_1,A_1,\alpha_1]F[a_2,A_2,\alpha_2]|F[a_3,A_3,\alpha_3]F[a_4,A_4,\alpha_4]\,|$$
$$\ldots|F[a_{2n+1},A_{2n+1},\alpha_{2n+1}]F[a_{2n+2},A_{2n+2},\alpha_{2n+2}])$$
$$=g^{-(2n)}u_3\ldots u_{2n+2}\sum_i\chi^{\alpha_3}(G_i)\ldots\chi^{\alpha_{2n+2}}(G_i)\lambda^{-1}_{\mathrm{T}^{2n}}$$
$$\times\sum_{T^2}\cdots\sum_{T^{2n}}\chi^{\alpha_4}(T^2)\chi^{\alpha_5}(T^{2n})\chi^{\alpha_6}(T^{2n}T^3)$$
$$\ldots\chi^{\alpha_{2n+2}}(T^{2n}T^{2n-1}\ldots T^{n+1})$$
$$\times p_{a_4}(T^2)p_{a_5}(T^{2n})p_{a_6}(T^{2n}T^3)$$
$$\ldots p_{a_{2n+2}}(T^{2n}T^{2n-1}\ldots T^{n+1})$$
$$\times(F[a_1,A_1,\alpha_1]F[a_2,A_2,\alpha_2]\,|\,G_if[a_3,A_3]$$
$$\times G_if\left[a_4,T^2(A_4)\right]|\,G_if\left[a_5,T^{2n}(A_5)\right]G_if\left[a_6,T^{2n}T^3(A_6)\right]|$$
$$\ldots G_if\left[a_{2n+1},T^{2n}\ldots T^{n+2}(A_{2n+1})\right]$$
$$\times G_if\left[a_{2n+2},T^{2n}\ldots T^{n+1}(A_{2n+2})\right])\ . \tag{26}$$

We expand the charge distribution $F[a_1,A_1,\alpha_1]$ $F[a_2,A_2,\alpha_2]$ using a DCD as

$$F[a_1,A_1,\alpha_1]F[a_2,A_2,\alpha_2]$$
$$=g^{-2}u_1u_2\lambda^{-1}_{\mathrm{T}^1}\sum_j\sum_{T^1}\chi^{\alpha_1}(G_j)\chi^{\alpha_2}(G_j)\chi^{\alpha_2}(T^1)p_{a_2}(T^1)$$
$$\times G_jf[a_1,A_1]G_jf\left[a_2,T^1(A_2)\right] \tag{27}$$

and substitute this into the RHS of Eq. (26) to give

$$(F[a_1,A_1,\alpha_1]F[a_2,A_2,\alpha_2]|F[a_3,A_3,\alpha_3]F[a_4,A_4,\alpha_4]\,|$$
$$\ldots|F[a_{2n+1},A_{2n+1},\alpha_{2n+1}]F[a_{2n+2},A_{2n+2},\alpha_{2n+2}])$$

$$
\begin{aligned}
&= g^{-(2n+2)} u_1 \ldots u_{2n+2} \sum_i \sum_j \chi^{\alpha_1}(G_j)\chi^{\alpha_2}(G_j)\chi^{\alpha_3}(G_i) \\
&\quad \ldots \chi^{\alpha_{2n+2}}(G_i)\lambda_{\mathrm{T}^1}^{-1}\lambda_{\mathrm{T}^{2n}}^{-1} \\
&\quad \times \sum_{T^1}\sum_{T^2}\cdots\sum_{T^{2n}} \chi^{\alpha_2}(T^1)\chi^{\alpha_4}(T^2)\chi^{\alpha_5}(T^{2n})\chi^{\alpha_6}(T^{2n}T^3) \\
&\quad \ldots \chi^{\alpha_{2n+2}}(T^{2n}T^{2n-1}\ldots T^{n+1}) \\
&\quad \times p_{a_2}(T^1)p_{a_4}(T^2)p_{a_5}(T^{2n})p_{a_6}(T^{2n}T^3) \\
&\quad \ldots p_{a_{2n+2}}(T^{2n}T^{2n-1}\ldots T^{n+1}) \\
&\quad \times \big(G_j f[a_1,A_1] G_i f\big[a_2, T^1(A_2)\big]\big| G_j f[a_3,A_3] \\
&\quad \times G_i f\big[a_4, T^2(A_4)\big]\big| \\
&\quad \times G_i f\big[a_5, T^{2n}(A_5)\big] G_i f\big[a_6, T^{2n}T^3(A_6)\big]\big| \\
&\quad \ldots G_i f\big[a_{2n+1}, T^{2n}\ldots T^{n+2}(A_{2n+1})\big] \\
&\quad \times G_i f\big[a_{2n+2}, T^{2n}\ldots T^{n+1}(A_{2n+2})\big]\big) \; . \qquad (28)
\end{aligned}
$$

We replace G_i with G_jG_i using the Rearrangement Theorem and then rotate the AO integral by G_j, giving

$$
\begin{aligned}
&(F[a_1,A_1,\alpha_1]F[a_2,A_2,\alpha_2]|F[a_3,A_3,\alpha_3]F[a_4,A_4,\alpha_4]| \\
&\quad \ldots |F[a_{2n+1},A_{2n+1},\alpha_{2n+1}]F[a_{2n+2},A_{2n+2},\alpha_{2n+2}]) \\
&= g^{-(2n+2)} u_1 \ldots u_{2n+2} \sum_i \sum_j \chi^{\alpha_1}(G_j) \\
&\quad \ldots \chi^{\alpha_{2n+2}}(G_j)\chi^{\alpha_3}(G_i)\ldots\chi^{\alpha_{2n+2}}(G_i)\lambda_{\mathrm{T}^1}^{-1}\lambda_{\mathrm{T}^{2n}}^{-1} \\
&\quad \times \sum_{T^1}\sum_{T^2}\cdots\sum_{T^{2n}} \chi^{\alpha_2}(T^1)\chi^{\alpha_4}(T^2)\;\chi^{\alpha_5}(T^{2n})\chi^{\alpha_6}(T^{2n}T^3) \\
&\quad \ldots \chi^{\alpha_{2n+2}}(T^{2n}T^{2n-1}\ldots T^{n+1}) \\
&\quad \times p_{a_2}(T^1)p_{a_4}(T^2)p_{a_5}(T^{2n})p_{a_6}(T^{2n}T^3) \\
&\quad \ldots p_{a_{2n+2}}(T^{2n}T^{2n-1}\ldots T^{n+1}) \\
&\quad \times \big(f[a_1,A_1] f\big[a_2, T^1(A_2)\big]\big| G_i f[a_3,A_3] G_i f\big[a_4, T^2(A_4)\big]\big| \\
&\quad \times G_i f\big[a_5, T^{2n}(A_5)\big] G_i f\big[a_6, T^{2n}T^3(A_6)\big]\big| \\
&\quad \ldots G_i f\big[a_{2n+1}, T^{2n}\ldots T^{n+2}(A_{2n+1})\big] \\
&\quad \times G_i f\big[a_{2n+2}, T^{2n}\ldots T^{n+1}(A_{2n+2})\big]\big) \; . \qquad (29)
\end{aligned}
$$

We now use a DCD derived from the stabilizer (denoted $\mathscr{U}^I$) of $f[a_1,A_1]\,f[a_2,A_2]$ and the stabilizer (denoted $\mathscr{U}^{II}$) of the set of centers $A_3\ldots A_{2n+2}$, with DCR T^{2n+1}. (We note that this notation for the stabilizers can be arbitrary since they do not appear in any final expressions.) From the properties of the stabilizers we have

$$
U^{II} f[a_k,A_k] = p_{a_k}(U^{II}) f[a_k,A_k] \quad \forall\; k \geq 3 \text{ and } U^{II} \in \mathscr{U}^{II} \; . \qquad (30)
$$

We replace the sum over G_i using this DCD, and note that we can collapse the sum over G_j into the usual selection rule to give

$$
\begin{aligned}
&(F[a_1,A_1,\alpha_1]F[a_2,A_2,\alpha_2]|F[a_3,A_3,\alpha_3]F[a_4,A_4,\alpha_4]| \\
&\quad \ldots |F[a_{2n+1},A_{2n+1},\alpha_{2n+1}]F[a_{2n+2},A_{2n+2},\alpha_{2n+2}]) \\
&\quad = g^{-(2n+1)} u_1 \ldots u_{2n+2} I(\alpha_1\ldots\alpha_{2n+2})\lambda_{\mathrm{T}^1}^{-1}\lambda_{T^{2n}}^{-1}\lambda_{T^{2n+1}}^{-1} \\
&\quad \times \sum_{U^I}\sum_{U^{II}}\sum_{T^{2n+1}}\sum_{T^1}\sum_{T^2}\cdots\sum_{T^{2n}} \chi^{\alpha_3}(U^I)\cdots\chi^{\alpha_{2n+2}}(U^I) \\
&\quad \times \chi^{\alpha_3}(U^{II})\cdots\chi^{\alpha_{2n+2}}(U^{II})\chi^{\alpha_3}(T^{2n+1})\cdots\chi^{\alpha_{2n+2}}(T^{2n+1}) \\
&\quad \times \chi^{\alpha_2}(T^1)\chi^{\alpha_4}(T^2)\chi^{\alpha_5}(T^{2n})\chi^{\alpha_6}(T^{2n}T^3) \\
&\quad \ldots \chi^{\alpha_{2n+2}}(T^{2n}T^{2n-1}\ldots T^{n+1}) \\
&\quad \times p_{a_2}(T^1)p_{a_4}(T^2)p_{a_5}(T^{2n})p_{a_6}(T^{2n}T^3) \\
&\quad \ldots p_{a_{2n+2}}(T^{2n}T^{2n-1}\ldots T^{n+1}) \\
&\quad \times (f[a_1,A_1]f[a_2,T^1(A_2)]|U^I T^{2n+1} U^{II} f[a_3,A_3] \\
&\quad \times U^I T^{2n+1} U^{II} f[a_4,T^2(A_4)]|U^I T^{2n+1} U^{II} f[a_5,T^{2n}(A_5)] \\
&\quad \times U^I T^{2n+1} U^{II} f[a_6,T^{2n}T^3(A_6)]| \\
&\quad \ldots U^I T^{2n+1} U^{II} f[a_{2n+1},T^{2n}\ldots T^{2n+2}(A_{2n+1})] \\
&\quad \times U^I T^{2n+1} U^{II} f[a_{2n+2},T^{2n}\ldots T^{n+1}(A_{2n+2})]) \; . \qquad (31)
\end{aligned}
$$

If we carry out the transformations by T^{2n+1} and U^{II} we obtain

$$
\begin{aligned}
&(F[a_1,A_1,\alpha_1]F[a_2,A_2,\alpha_2]|F[a_3,A_3,\alpha_3]F[a_4,A_4,\alpha_4]| \\
&\quad \ldots |F[a_{2n+1},A_{2n+1},\alpha_{2n+1}]F[a_{2n+2},A_{2n+2},\alpha_{2n+2}]) \\
&= g^{-(2n+1)} u_1 \ldots u_{2n+2} I(\alpha_1\ldots\alpha_{2n+2})\lambda_{\mathrm{T}^1}^{-1}\lambda_{\mathrm{T}^{2n}}^{-1}\lambda_{\mathrm{T}^{2n+1}}^{-1} \\
&\quad \times \sum_{U^I}\sum_{U^{II}}\sum_{T^{2n+1}}\sum_{T^1}\sum_{T^2}\cdots\sum_{T^{2n}} \chi^{\alpha_3}(U^I)\cdots\chi^{\alpha_{2n+2}}(U^I) \\
&\quad \times \chi^{\alpha_3}(U^{II})\cdots\chi^{\alpha_{2n+2}}(U^{II})\chi^{\alpha_3}(T^{2n+1})\cdots\chi^{\alpha_{2n+2}}(T^{2n+1}) \\
&\quad \times \chi^{\alpha_2}(T^1)\chi^{\alpha_4}(T^2)\chi^{\alpha_5}(T^{2n})\chi^{\alpha_6}(T^{2n}T^3) \\
&\quad \ldots \chi^{\alpha_{2n+2}}(T^{2n}T^{2n-1}\ldots T^{n+1}) \\
&\quad \times p_{a_2}(T^1)p_{a_4}(T^2)p_{a_5}(T^{2n})p_{a_6}(T^{2n}T^3) \\
&\quad \ldots p_{a_{2n+2}}(T^{2n}T^{2n-1}\ldots T^{n+1}) \\
&\quad \times p_{a_3}(T^{2n+1})\ldots p_{a_{2n+2}}(T^{2n+1})p_{a_3}(U^{II})\ldots p_{a_{2n+2}}(U^{II}) \\
&\quad \times (f[a_1,A_1]f\big[a_2,T^1(A_2)\big]|U^I f\big[a_3,T^{2n+1}(A_3)\big] \\
&\quad \times U^I[a_4,T^{2n+1}T^2(A_4)]|U^I f[a_5,T^{2n+1}T^{2n}(A_5)] \\
&\quad \times U^I f[a_6,T^{2n+1}T^{2n}T^3(A_6)] \\
&\quad \ldots U^I f[a_{2n+1},T^{2n+1}T^{2n}\ldots T^{n+2}(A_{2n+1})] \\
&\quad \times U^I f[a_{2n+2},T^{2n+1}T^{2n}\ldots T^{n+1}(A_{2n+2})] \qquad (32)
\end{aligned}
$$

and by rotating the AO integral by U^I we obtain

$$
\begin{aligned}
&(F[a_1,A_1,\alpha_1]F[a_2,A_2,\alpha_2]|F[a_3,A_3,\alpha_3]F[a_4,A_4,\alpha_4]| \\
&\quad \ldots |F[a_{2n+1},A_{2n+1},\alpha_{2n+1}]F[a_{2n+2},A_{2n+2},\alpha_{2n+2}]) \\
&= g^{-(2n+1)} u_1 \ldots u_{2n+2} I(\alpha_1\ldots\alpha_{2n+2})\lambda_{\mathrm{T}^1}^{-1}\lambda_{\mathrm{T}^{2n}}^{-1}\lambda_{\mathrm{T}^{2n+1}}^{-1} \\
&\quad \times \sum_{U^I}\sum_{U^{II}}\sum_{T^{2n+1}}\sum_{T^1}\sum_{T^2}\cdots\sum_{T^{2n}} \chi^{\alpha_3}(U^I)\cdots\chi^{\alpha_{2n+2}}(U^I) \\
&\quad \times \chi^{\alpha_3}(U^{II})\cdots\chi^{\alpha_{2n+2}}(U^{II})\chi^{\alpha_3}(T^{2n+1})\cdots\chi^{\alpha_{2n+2}}(T^{2n+1}) \\
&\quad \times \chi^{\alpha_2}(T^1)\chi^{\alpha_4}(T^2)\chi^{\alpha_5}(T^{2n})\chi^{\alpha_6}(T^{2n}T^3) \\
&\quad \ldots \chi^{\alpha_{2n+2}}(T^{2n}T^{2n-1}\ldots T^{n+1}) \\
&\quad \times p_{a_2}(T^1)p_{a_4}(T^2)p_{a_5}(T^{2n})p_{a_6}(T^{2n}T^3) \\
&\quad \ldots p_{a_{2n+2}}(T^{2n}T^{2n-1}\ldots T^{n+1})p_{a_3}(T^{2n+1})\ldots \\
&\quad \times p_{a_{2n+2}}(T^{2n+1})p_{a_3}(U^{II})\ldots p_{a_{2n+2}}(U^{II})p_{a_1}(U^I)p_{a_2}(U^I) \\
&\quad \times (f[a_1,A_1]f[a_2,T^1(A_2)]\,|\,f[a_3,T^{2n+1}(A_3)]
\end{aligned}
$$

$$
\begin{aligned}
&\times f[a_4, T^{2n+1}T^2(A_4)] \mid f[a_5, T^{2n+1}T^{2n}(A_5)]\\
&\times f[a_6, T^{2n+1}T^{2n}T^3(A_6)]|\\
&\ldots f[a_{2n+1}, T^{2n+1}T^{2n} \ldots T^{n+2}(A_{2n+1})]f[a_{2n+2}, T^{2n+1}T^{2n}\\
&\ldots T^{n+1}(A_{2n+2})]) \ . \qquad (33)
\end{aligned}
$$

Now, from the superselection rule at Eq. (14)

$$\chi^{\alpha_1}(G_i) \cdots \chi^{\alpha_{2n+2}}(G_i) = 1 \ \forall \ G_i \in \mathscr{G} \ , \qquad (34)$$

or the integral would anyway vanish under Eq. (13). Hence

$$\chi^{\alpha_1}(G_i)\chi^{\alpha_2}(G_i) = \chi^{\alpha_3}(G_i) \cdots \chi^{\alpha_{2n+2}}(G_i) \ . \qquad (35)$$

In turn, then,

$$
\begin{aligned}
&\sum_{U^I} \chi^{\alpha_3}(U^I) \cdots \chi^{\alpha_{2n+2}}(U^I) p_{a_1}(U^I) p_{a_2}(U^I)\\
&\quad = \sum_{U^I} \chi^{\alpha_1}(U^I)\chi^{\alpha_2}(U^I) p_{a_1}(U^I) p_{a_2}(U^I) = \lambda_{\mathrm{T}^1} \ , \qquad (36)
\end{aligned}
$$

(cf. Eq. 8 and [1, 2]), and also

$$\sum_{U^{II}} \chi^{\alpha_3}(U^{II}) \cdots \chi^{\alpha_{2n+2}}(U^{II}) p_{a_3}(U^{II}) \cdots p_{a_{2n+2}}(U^{II}) = \lambda_{\mathrm{T}^{2n}} \ , \qquad (37)$$

yielding finally

$$
\begin{aligned}
&(F[a_1, A_1, \alpha_1]F[a_2, A_2, \alpha_2]|F[a_3, A_3, \alpha_3]F[a_4, A_4, \alpha_4]|\\
&\ldots |F[a_{2n+1}, A_{2n+1}, \alpha_{2n+1}]F[a_{2n+2}, A_{2n+2}, \alpha_{2n+2}])\\
&= g^{-(2n+1)} u_1 \ldots u_{2n+2} I(\alpha_1 \ldots \alpha_{2n+2}) \lambda^{-1}_{T^{2n+1}}\\
&\quad \times \sum_{T^1} \cdots \sum_{T^{2n+1}} \chi^{a_2}(T^1)\chi^{a_3}(T^{2n+1})\chi^{a_4}(T^{2n+1}T^2)\\
&\quad \ldots \chi^{a_{2n+2}}(T^{2n+1}T^{2n} \ldots T^{n+1})\\
&\quad \times p_{a_2}(T^1) p_{a_3}(T^{2n+1}) p_{a_4}(T^{2n+1}T^2)\\
&\quad \ldots p_{a_{2n+2}}(T^{2n+1}T^{2n} \ldots T^{n+1})\\
&\quad \times (f[a_1, A_1] f[a_2, T^1(A_2)]|\\
&\quad \times f[a_3, T^{2n+1}(A_3)] f[a_4, T^{2n+1}T^2(A_4)]|\\
&\quad \ldots f[a_{2n+1}, T^{2n+1} \ldots T^{n+2}(A_{2n+1})]\\
&\quad \times f[a_{2n+2}, T^{2n+1} \ldots T^{n+1}(A_{2n+2})]) \ . \qquad (38)
\end{aligned}
$$

This is exactly the same as the formula of Eq. (22) except that the index ranges are larger. Hence coupling a new charge distribution into the *n* -electron integral formula has produced the same formula as extending the indices in the original formula. This, together with the observation that we obtain the correct result for the two-electron case from the one-electron case, is sufficient to establish Eq. (22) as correct by induction.

The above derivation assumed a totally symmetric many-electron operator in the integral, which allowed us to ignore the operator itself in our derivation. If the many-electron operator is of symmetry species α_0, say, not necessarily the totally symmetric irrep, then provided the operator does not depend on any center coordinates the only change to the symmetry-adapted integral formula is that the selection rule I becomes $I(\alpha_0\alpha_1 \ldots \alpha_{2n})$, that is, includes an extra factor for α_0. This allows us to generalize the two-electron function $w(1,2)$ in Eq. (3) to include angular terms like x_{12}. If $w(1,2)$ depends on any center coordinates, then in order to obtain an expression that involves no redundant terms in the summation it is necessary to introduce another double coset decomposition, based on the stabilizer of the center(s) appearing in the operator and the stabilizer of *all* the charge distributions [1, 2].

Discussion

It is edifying to look at a specific case to illustrate the formulas. The most obvious new case would be a three-electron integral. We see from above that a cyclic three-electron integral over the electron repulsion operator would be given by

$$
\begin{aligned}
&\iiint F[a_1, A_1, \alpha_1](r_1) F[a_3, A_3, \alpha_3](r_2) F[a_5, A_5, \alpha_5](r_3)\\
&\quad \times w(r_1, r_3) r_{12}^{-1} w'(r_2, r_3) F[a_2, A_2, \alpha_2](r_1)\\
&\quad \times F[a_4, A_4, \alpha_4](r_2) F[a_6, A_6, \alpha_6](r_3) dr_1\, dr_2\, dr_3\\
&\equiv (F[a_1, A_1, \alpha_1]F[a_2, A_2, \alpha_2]|F[a_3, A_3, \alpha_3]\\
&\quad \times F[a_4, A_4, \alpha_4]|F[a_5, A_5, \alpha_5]F[a_6, A_6, \alpha_6])\\
&= g^{-5} u_1 u_2 u_3 u_4 u_5 u_6 I(\alpha_1\alpha_2\alpha_3\alpha_4\alpha_5\alpha_6) \lambda^{-1}_{\mathrm{T}^5}\\
&\quad \times \sum_{T^1} \sum_{T^2} \sum_{T^3} \sum_{T^4} \sum_{T^5} \chi^{a_2}(T^1)\chi^{a_3}(T^5)\chi^{a_4}(T^5T^2)\\
&\quad \times \chi^{a_5}(T^5T^4)\chi^{a_6}(T^5T^4T^3)\\
&\quad \times p_{a_2}(T^1) p_{a_3}(T^5) p_{a_4}(T^5T^2) p_{a_5}(T^5T^4) p_{a5}(T^5T^4T^3)\\
&\quad \times \left(f[a_1, A_1] f\left[a_2, T^1(A_2)\right] | f\left[a_3, T^5(A_3)\right]\right.\\
&\quad \left. \times f\left[a_4, T^5T^2(A_4)\right] | f\left[a_5, T^5T^4(A_5)\right] f\left[a_6, T^5T^4T^3(A_6)\right]\right) \ . \qquad (39)
\end{aligned}
$$

This expression is long but not complicated. It comprises a selection rule, some numerical factors which weight each integral according to the irreps it contributes to, with what phase, and how many equivalent integrals are accounted for. The various DCR ensure first that only distinct charge distributions appear, and then that only distinct *combinations* of those charge distributions appear. The five sets of DCR arise as follows. T^1, T^2, and T^3 generate distinct charge distributions from the original pairs $f[a_1,A_1]$ $f[a_2,A_2]$, $f[a_3,A_3]$ $f[a_4,A_4]$, and $f[a_5,A_5] f[a_6,A_6]$, respectively. Then T^4 generates distinct quadruplets from $f[a_3,A_3]$ $f[a_4,T^2(A_4)]$ and $f[a_5,A_5]$ $f[a_6,T^3(A_6)]$, and finally T^5 generates distinct hextuplets from $f[a_1,A_1]$ $f[a_2,T^1(A_2)]$ and $f[a_3,A_3]$ $f[a_4,T^2(A_4)]$ $f[a_5,T^4(A_5)]$ $f[a_6,T^4T^3(A_6)]$. There is no structural difference between the three-electron formula and the two-electron formula. For example, Dalton [8] includes a matrix multiplication formulation of the two-electron integral formula, developed by Helgaker (unpublished), and we have had little trouble implementing the appropriate loop structure and formulas to extend this to the case of three-electron integrals over Gaussian-type geminal basis functions.

In applications such as MP2 calculations with correlation factors of Gaussian or linear r_{12} type, three- and perhaps four-electron integrals appear in partial trace expressions where they are contracted with the SCF density matrix. It is possible to simplify symmetry processing in such trace calculations somewhat by defining new density matrices that include some of the phase and weighting factors [2].

Conclusions

A general formula has been developed for computing integrals over symmetry-adapted basis functions to any order, extending existing work for one- and two-electron integrals. The formula expresses integrals over symmetry-adapted two-electron basis functions of the general form of Eq. (3) in terms of symmetry-distinct integrals. The formula has been proved by induction and holds for arbitrarily many electrons. This approach has been programmed for three-electron integrals in the Dalton program as part of our efforts to explore the use of GTGs in molecular calculations.

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