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# Traces of $p$ th-order reduced density matrices: symmetric group approach

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**Abstract.** This paper describes a general procedure for calculating the traces of reduced density matrices of any order  $p$  of an  $N$ -electron system, in the basis of the irreducible representations of the symmetric group  $S_p$ , in a spin-free formalism. The numerical values of these traces are determined by useful formulae. This approach provides a suitable study of the  $N$ - and  $S$ -representability of the reduced density matrices.

## 1. Introduction

The  $p$ th-order reduced density matrices ( $p$ -RDM) have proved to be powerful tools in the calculation of physical properties of many-body systems (McWeeny 1960, Davidson 1976). These matrices are particularly used in atomic and molecular physics or in quantum chemistry as they avoid the explicit use of the  $N$ -electron wavefunctions which are always more difficult to deal with. Most of the physical situations are described through the first- and second-order reduced density matrices (1-RDM) and (2-RDM). However, there are also some treatments, as in coupled-cluster theory (Paldus and Jeziorski 1988), in spin-adapted reduced Hamiltonian theory (Lain *et al* 1988) or in the spin-coupled valence approach (Cooper *et al* 1991), where higher-order  $p$ -RDMs ( $p > 2$ ) are required.

From a computational point of view, it is always convenient to reduce the size of the  $p$ -RDMs as much as possible. Hence, the spin-free formulation, which deals with orbital functions instead of spin-orbitals, is the most advisable formalism to describe systems out of magnetic fields. However, a block factorization of the spin-free  $p$ -RDMs can be achieved when those matrices are expressed according to the basis functions of the irreducible representations of the symmetric group  $S_p$ , the group constituted by the permutations on  $p$  objects (Pauncz 1995). In this way, each of the factorized blocks can be dealt with independently.

The traces of the different blocks of the spin-free  $p$ -RDM, expressed according to the irreducible representations of the symmetric group  $S_p$ , are functions of the number of electrons  $N$  and the spin  $S$  of the system which they represent. These relationships constitute necessary conditions for the  $N$ - and  $S$ -representability of the  $p$ -RDM (Coleman 1963). In the case of the 2-RDM, this kind of relation for the traces of each of the two blocks obtained according to the  $S_2$  group is well established (Bingel and Kutzelnigg 1970). Recently, a relationship between both traces has been used in studies of population analysis which try to visualize chemical bonds (Ponec and Bochicchio 1995). However, similar expressions for higher orders ( $p > 2$ ) have not been described. The aim of this paper is to report a simple and general procedure which allows the calculation of the partial traces of a

$p$ -RDM, corresponding to an  $N$ -electron state with a defined spin  $S$ , factorized according to the irreducible representations of the group  $S_p$ . Our approach does not need the evaluation of matrix elements of the  $p$ -RDM and leads to a general expression that fits for any value of the reduced order  $p$  and the spin  $S$  of the  $N$ -electron system represented by that  $p$ -RDM. The method is based on our previous studies of traces of  $p$ th-order replacement operators ( $p$ -RO) calculated over finite-dimensional  $N$ -electron spin-adapted spaces (Torre *et al* 1993, Torre and Lain 1995, Lain and Torre 1995a, Planelles and Karwowski 1997) which have been used in the determination of spin-adapted reduced Hamiltonians (Lain *et al* 1988) as well as in the calculation of moments of spectral density distributions (Lain and Torre 1995b).

The organization of the paper is as follows. In section 2 a review of traces of  $p$ -ROs is reported. Section 3 describes the procedure to determine the traces of permutation symmetry-adapted  $p$ -RDMs. Finally, the appendix describes the results for the four lowest orders of the  $p$ -RDM.

## 2. Traces of $p$ -ROs

We will refer to an  $N$ -electron system described by a nonrelativistic, clamped nuclei and spin-independent Hamiltonian which, in a spin-free second quantized formalism, can be written as

$$\hat{H} = \frac{1}{2} \sum_{i,j,k,l} {}^2H_{jl}^{ik} {}^2E_{jl}^{ik} \quad (1)$$

where

$${}^2H_{jl}^{ik} = (ij|kl) + \frac{1}{N-1}(\delta_{kl} \epsilon_{ij} + \delta_{ij} \epsilon_{kl}) \quad (2)$$

$(ij|kl)$  are the standard two-electron integrals (in the (11|22) convention) and  $\epsilon_{ij}$  are the one-electron integrals.  ${}^2E_{jl}^{ik}$  are the second-order spin-free replacement operators (2-RO) whose  $p$ -order version is (Kutzelnigg 1985, Paldus and Jeziorski 1988)

$${}^pE_{j_1 \dots j_p}^{i_1 \dots i_p} = \sum_{\sigma_1} \dots \sum_{\sigma_p} b_{i_1 \sigma_1}^+ \dots b_{i_p \sigma_p}^+ b_{j_p \sigma_p} \dots b_{j_1 \sigma_1} \quad (3)$$

where  $b_{i_k \sigma_k}^+ / b_{j_k \sigma_k}$  are the usual creation/annihilation fermion operators;  $\sigma_1, \dots, \sigma_p$  are the spin coordinates and  $i_1, \dots, i_p, j_1, \dots, j_p \dots$  are the  $K$  orbital functions of an orthonormal basis set.

The Hamiltonian  $\hat{H}$  is projected onto an antisymmetric and spin-adapted model space  $H^A(N, K, S, S_z)$  which is a subspace of a finite-dimensional Hilbert space ( $S$  and  $S_z$  are the standard spin quantum numbers and  $A$  stands for antisymmetric). The subspace  $H^A(N, K, S, S_z)$ , which is known as the full configuration-interaction space (Paldus 1976), is defined as the antisymmetric and spin-adapted part of the  $N$ -fold tensorial product of a one-electron space

$$H^A(N, K, S, S_z) = (V_{2K}^{\otimes N})_{S, S_z}^A. \quad (4)$$

The one-electron space  $V_{2K}$  is spanned by a set of  $2K$  spin-orbitals and is a product of the  $K$ -dimensional orbital space

$$V_K = \{\Phi_k\}_{k=1}^K \quad (5)$$

spanned by a set of  $K$  orthonormal orbitals and the two-dimensional spin space.

We will denote with  $|\mathcal{L}_S\rangle$  the  $N$ -electron eigenstates of the Hamiltonian (1) corresponding to a defined spin  $S$  and a determined  $S_z$  value. As is well known, the

expectation value of a  $p$ -RO generates the corresponding element of the  $p$ -RDM of that state, so that

$${}^p D_{j_1 \dots j_p}^{i_1 \dots i_p}(\mathcal{L}_S) = \frac{\langle \mathcal{L}_S | {}^p E_{j_1 \dots j_p}^{i_1 \dots i_p} | \mathcal{L}_S \rangle}{p!}. \quad (6)$$

The elements of the  $p$ -RDM can also be expressed in the basis functions of the irreducible representations of the symmetry group  $S_p$ , as linear combinations of the matrix elements in the basis of the product of orbitals. It is well known (Pauncz 1995) that the spatial part of the  $p$ -electron eigenfunctions of the spin operator  $\hat{S}^2$  (as well as the pure spin functions) are basis functions of those irreducible representations, so that the permutation symmetry-adapted  $p$ -RDM is factorized into blocks, each of them related to one value of the spin of the  $p$  electrons. Consequently, the traces of this kind of block depend on the corresponding  $p$ -electron spin as well as on the spin  $S$  of the  $N$ -electron system that the  $p$ -RDM represents. The values of these traces, for any order  $p$  of the RDM, will be investigated in the next section.

We have called spin-adapted trace of a determined  $p$ -RO,  $\langle {}^p E_{j_1 \dots j_p}^{i_1 \dots i_p} \rangle_{N,K,S}$  (Torre *et al* 1993), to

$$\langle {}^p E_{j_1 \dots j_p}^{i_1 \dots i_p} \rangle_{N,K,S} = \sum_{\mathcal{L}_S} \langle \mathcal{L}_S | {}^p E_{j_1 \dots j_p}^{i_1 \dots i_p} | \mathcal{L}_S \rangle \quad (7)$$

where the subscripts  $N, K, S$  mean that the numerical value of that trace depends on those parameters. Although the eigenstates  $|\mathcal{L}_S\rangle$  refer to a fixed  $S_z$  quantum number, the value of the trace (7) is independent of it so that it has not been considered.

As was mentioned in the introduction, an optimized calculation of expression (7) has been carried out in previous papers, both for the  $p = N$  case (Lain and Torre 1995b) and for the  $p < N$  one (Lain and Torre 1995a). Consequently, it can easily be determined, even in a systematic way on a computer. In the next section we apply our approach for the determination of spin-adapted traces of  $p$ -ROs to the calculation of the traces of permutation symmetry-adapted  $p$ -RDMs

### 3. Traces of permutation symmetry-adapted $p$ -RDMs

Let us define the  $p$ -electron operator

$${}^p \hat{M} = \frac{1}{p!} \sum_{\substack{(i_1 \dots i_p) \\ (j_1 \dots j_p)}} {}^p M_{j_1 \dots j_p}^{i_1 \dots i_p} {}^p E_{j_1 \dots j_p}^{i_1 \dots i_p} \quad (8)$$

in which the matrix element  ${}^p M_{j_1 \dots j_p}^{i_1 \dots i_p}$  is

$${}^p M_{j_1 \dots j_p}^{i_1 \dots i_p} = \sum_{\mathcal{L}_S} {}^p D_{j_1 \dots j_p}^{i_1 \dots i_p}(\mathcal{L}_S). \quad (9)$$

In what follows, we will represent the spin quantum numbers of  $p$ -electron functions by  $j$  and  $j_z$  to distinguish from those of the  $N$ -electron ones,  $S$  and  $S_z$ . In this way, we will consider the trace of the  ${}^p \hat{M}$  operator defined by

$$\text{Tr}[{}^p \hat{M}]_j = \sum_{\mathcal{L}_j} \langle \mathcal{L}_j | {}^p \hat{M} | \mathcal{L}_j \rangle \quad (10)$$

where  $|\mathcal{L}_j\rangle$  are the  $p$ -electron functions, eigenstates of the  $\hat{S}^2$  operator, corresponding to the spin quantum numbers  $j$  and  $j_z$ . From equations (9) and (10)

$$\text{Tr}[{}^p\hat{M}]_j = \frac{1}{p!} \sum_{\mathcal{L}_j} \sum_{\substack{(i_1\dots i_p) \\ (j_1\dots j_p)}} \sum_{\mathcal{L}_S} {}^pD_{j_1\dots j_p}^{i_1\dots i_p}(\mathcal{L}_S) \langle \mathcal{L}_j | {}^pE_{j_1\dots j_p}^{i_1\dots i_p} | \mathcal{L}_j \rangle. \quad (11)$$

Equation (11) is a projection of the  $\sum_{\mathcal{L}_S} {}^pD_{j_1\dots j_p}^{i_1\dots i_p}(\mathcal{L}_S)$  matrix over the  $p$ -electron functions  $|\mathcal{L}_j\rangle$ , whose orbital functions are basis functions of the irreducible representation of the group  $S_p$  related to the spin quantum number  $j$ . Consequently,  $\text{Tr}[{}^p\hat{M}]_j$  is identical to the trace of the corresponding permutation symmetry-adapted block when the matrix defined by equation (9) is factorized according to the irreducible representations of the group  $S_p$ . If we represent by  $[{}^pD(\mathcal{L}_S)]_j$  the block of the  $p$ -RDM of the  $N$ -electron state  $|\mathcal{L}_S\rangle$  expressed in that same basis, equation (11) can be written as

$$\sum_{\mathcal{L}_S} \text{Tr}[{}^pD(\mathcal{L}_S)]_j = \frac{1}{p!^2} \sum_{\mathcal{L}_j} \sum_{\substack{(i_1\dots i_p) \\ (j_1\dots j_p)}} \sum_{\mathcal{L}_S} \langle \mathcal{L}_S | {}^pE_{j_1\dots j_p}^{i_1\dots i_p} | \mathcal{L}_S \rangle \langle \mathcal{L}_j | {}^pE_{j_1\dots j_p}^{i_1\dots i_p} | \mathcal{L}_j \rangle \quad (12)$$

where equation (6) has been taken into account.

The value of the trace  $\text{Tr}[{}^pD(\mathcal{L}_S)]_j$  is, obviously, independent of the  $|\mathcal{L}_S\rangle$  state, for a defined  $S$  value. Consequently, the trace of the block related to the  $p$ -electron spin  $j$ , of a  $p$ -RDM corresponding to a  $N$ -electron state with spin  $S$ , expressed in the basis of the irreducible representations of the group  $S_p$ , is

$$\text{Tr}[{}^pD(\mathcal{L}_S)]_j = \sum_{\substack{(i_1\dots i_p) \\ (j_1\dots j_p)}} \frac{\langle {}^pE_{j_1\dots j_p}^{i_1\dots i_p} \rangle_{N,K,S} \langle {}^pE_{j_1\dots j_p}^{i_1\dots i_p} \rangle_{p,j}}{(p!)^2 D(N, K, S)} \quad (13)$$

where  $D(N, K, S)$  is the number of  $N$ -electron states of spin  $S$ ,  $|\mathcal{L}_S\rangle$  that can be constructed with  $K$  orbitals (the dimension of the  $H^A(N, K, S, S_z)$  subspace). Its value is independent of the  $S_z$  quantum number and it is given by the well known Weyl–Paldus formula (Paldus 1974),

$$D(N, S, K) = \frac{2S+1}{K+1} \binom{K+1}{\frac{1}{2}N-S} \binom{K+1}{\frac{1}{2}N+S+1} \quad (14)$$

where  $\langle {}^pE_{j_1\dots j_p}^{i_1\dots i_p} \rangle_{N,K,S}$  has been defined in equation (7) and, in a similar way

$$\langle {}^pE_{j_1\dots j_p}^{i_1\dots i_p} \rangle_{p,j} = \sum_{\mathcal{L}_j} \langle \mathcal{L}_j | {}^pE_{j_1\dots j_p}^{i_1\dots i_p} | \mathcal{L}_j \rangle \quad (15)$$

that is, the trace of the  $p$ -RO  ${}^pE_{j_1\dots j_p}^{i_1\dots i_p}$ , calculated over the functions of  $p$  electrons with spin  $j$ . The value of this trace is independent of the number of orbitals  $K$  (Torre and Lain 1995) as well as the parameter  $j_z$  so that they have not been considered.

The trace of any  $p$ -RO can easily be calculated through the general expressions reported previously (Lain and Torre 1995a, b) and, consequently, equation (13) provides a suitable way to construct a simple and general computer program for the calculation of the numerical values of the traces of any permutation symmetry-adapted  $p$ -RDM. However, we will transform equation (13) to obtain simpler explicit expressions of the partial traces of any factorized  $p$ -RDM in terms of only the number of electrons  $N$  and the spin  $S$  of the system.

As has been reported previously (Torre *et al* 1993), the sets  $(i_1 \dots i_p)$  and  $(j_1 \dots j_p)$  must be composed of identical orbitals (one is a permutation of the other), otherwise the traces  $\langle^p E_{j_1 \dots j_p}^{i_1 \dots i_p} \rangle_{N,K,S}$  and  $\langle^p E_{j_1 \dots j_p}^{i_1 \dots i_p} \rangle_{p,j}$  are zero and, as we are dealing with fermions, a determinate index in those sets can be repeated only once (otherwise the Pauli principle would be violated). Furthermore, the value of a  $p$ -RO trace is invariant with respect to numbering orbitals, it only depends on their ordering. Consequently, it is possible to reduce the number of addends of the sum  $\sum_{\substack{(i_1 \dots i_p) \\ (j_1 \dots j_p)}}$ , in formula (13), so that only the nonequivalent ones are calculated. In this sense, we will represent by  $Q_0$  the number of possibilities of constructing, with  $K$  orbitals, creation sets  $(i_1 \dots i_p)$ , without any repetition of indices, that is,  $Q_0 = K(K-1) \dots (K-p+1)$ . Similarly,  $Q_1$  will be an identical concept when the set  $(i_1 \dots i_p)$  has one repeated index and, in general,  $Q_r$  when there are  $r$  repeated indices. With these considerations, formula (13) can be rewritten as

$$\text{Tr}[^p D(\mathcal{L}_S)]_j = \sum_{r=0}^{r_{\max}} \sum_{P_r} \frac{Q_r \langle^p E_{P_r(11\dots rr\dots(p-r))}^{11\dots rr\dots(p-r)} \rangle_{N,K,S} \langle^p E_{P_r(11\dots rr\dots(p-r))}^{11\dots rr\dots(p-r)} \rangle_{p,j}}{(p!)^2 D(N, K, S)} \quad (16)$$

where  $r_{\max}$  is the maximum number of repeated indices that can appear in the  $p$ -RO ( $r_{\max} = \frac{1}{2}p$  ( $p$  even) or  $r_{\max} = \frac{1}{2}p - 1$  ( $p$  odd)) and  $P_r$  is a permutation of the set  $(1, 1, \dots, r, r \dots (p-r))$  (with  $r$  repeated indices). Obviously, the traces of  $p$ -ROs with  $P_r$  belonging to the same class of the group  $S_p$  are identical, so that only one trace out of each class need be evaluated.

A more useful version of formula (16) can be obtained taking into account that the value of  $\text{Tr}[^p D(\mathcal{L}_S)]_j$  is independent of the number of orbitals  $K$  (that independence arises from a cancellation among the factors  $Q_r$ , the Weyl–Paldus formula  $D(N, K, S)$  and the traces  $\langle^p E_{P_r(11\dots rr\dots(p-r))}^{11\dots rr\dots(p-r)} \rangle_{N,K,S}$ ). As any value of  $K$  can be used, we propose the lowest one, that is,  $K = \frac{1}{2}N + S$ . With that condition,  $D(N, K, S) = \binom{\frac{1}{2}N+S}{2S}$  and the evaluation of traces  $\langle^p E_{P_r(11\dots rr\dots(p-r))}^{11\dots rr\dots(p-r)} \rangle_{N,(\frac{1}{2}N+S),S}$  is considerably simplified. Consequently, formula (16) will be used in the form

$$\text{Tr}[^p D(\mathcal{L}_S)]_j = \sum_{r=0}^{r_{\max}} \sum_{P_r} \frac{Q_r \langle^p E_{P_r(11\dots rr\dots(p-r))}^{11\dots rr\dots(p-r)} \rangle_{N,(\frac{1}{2}N+S),S} \langle^p E_{P_r(11\dots rr\dots(p-r))}^{11\dots rr\dots(p-r)} \rangle_{p,j}}{(p!)^2 \binom{\frac{1}{2}N+S}{2S}} \quad (17)$$

which constitutes a practical version of equation (13). In equation (17), the factors  $Q_r$  obviously refer to  $\frac{1}{2}N + S$  orbitals and their calculation is trivial. Following the procedure described previously (Torre *et al* 1993), the traces  $\langle^p E_{P_r(11\dots rr\dots(p-r))}^{11\dots rr\dots(p-r)} \rangle_{N,(\frac{1}{2}N+S),S}$  and  $\langle^p E_{P_r(11\dots rr\dots(p-r))}^{11\dots rr\dots(p-r)} \rangle_{p,j}$  can easily be reduced to simple relations between binomial coefficients, involving only the parameters  $N$  and  $S$ . Hence equation (17) allows us to derive the particular expressions for the partial traces of any  $p$ -RDM, in the symmetric group approach, through simple functions of those parameters.

The appendix shows the relations obtained in this way for the four lower orders of the permutation symmetry-adapted reduced density matrices. Obviously, the results corresponding to the cases  ${}^1D_{j=\frac{1}{2}}$ ,  ${}^2D_{j=1}$  and  ${}^2D_{j=0}$  are equivalent to previously reported ones (Bingel and Kutzelnigg 1970). Using our methodology, the derivation of the relations for higher orders is straightforward. The simple dependence of the traces of these matrices on the number of electrons of the system,  $N$ , and its spin  $S$ , provides a suitable study of the  $N$ - and  $S$ -representability which are necessary conditions that  $p$ -electron tools must fulfil to represent  $N$ -electron systems properly.

In conclusion, this paper has described a new, simple and general approach to calculating the numerical values of the traces of permutation symmetry-adapted reduced density matrices of any order  $p$ . The procedure, which is based on the determination of traces of replacement operators, does not need a previous evaluation of the  $p$ -RDM elements. Our treatment also leads to formulae providing a simple analysis of the  $N$ - and  $S$ -representability properties which are useful in methods which approximate high-order reduced density matrices.

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### Appendix. Traces of the four lowest-order permutation symmetry-adapted reduced density matrices

$$\text{Tr}[{}^1\text{D}]_{j=\frac{1}{2}} = \left( \frac{\frac{1}{2}N + S}{2S} \right)^{-1} (\frac{1}{2}N + S) \sum_{i=0}^1 \left( \frac{\frac{1}{2}N + S - i}{2S} \right) \quad (\text{A1})$$

$$\text{Tr}[{}^2\text{D}]_{j=1} = \left( \frac{\frac{1}{2}N + S}{2S} \right)^{-1} \binom{\frac{1}{2}N + S}{2} \sum_{i=0}^2 \left( \frac{\frac{1}{2}N + S - i}{2S} \right) \quad (\text{A2})$$

$$\text{Tr}[{}^2\text{D}]_{j=0} = \left( \frac{\frac{1}{2}N + S}{2S} \right)^{-1} \binom{\frac{1}{2}N + S + 1}{2} \left( \frac{\frac{1}{2}N + S - 1}{2S} \right) \quad (\text{A3})$$

$$\text{Tr}[{}^3\text{D}]_{j=\frac{3}{2}} = \left( \frac{\frac{1}{2}N + S}{2S} \right)^{-1} \binom{\frac{1}{2}N + S}{3} \sum_{i=0}^3 \left( \frac{\frac{1}{2}N + S - i}{2S} \right) \quad (\text{A4})$$

$$\text{Tr}[{}^3\text{D}]_{j=\frac{1}{2}} = \left( \frac{\frac{1}{2}N + S}{2S} \right)^{-1} \binom{\frac{1}{2}N + S + 1}{3} \sum_{i=1}^2 \left( \frac{\frac{1}{2}N + S - i}{2S} \right) \quad (\text{A5})$$

$$\text{Tr}[{}^4\text{D}]_{j=2} = \left( \frac{\frac{1}{2}N + S}{2S} \right)^{-1} \binom{\frac{1}{2}N + S}{4} \sum_{i=0}^4 \left( \frac{\frac{1}{2}N + S - i}{2S} \right) \quad (\text{A6})$$

$$\text{Tr}[{}^4\text{D}]_{j=1} = \left( \frac{\frac{1}{2}N + S}{2S} \right)^{-1} \binom{\frac{1}{2}N + S + 1}{4} \sum_{i=1}^3 \left( \frac{\frac{1}{2}N + S - i}{2S} \right) \quad (\text{A7})$$

$$\text{Tr}[{}^4\text{D}]_{j=0} = \left( \frac{\frac{1}{2}N + S}{2S} \right)^{-1} \frac{(\frac{1}{2}N + S)^2 [(\frac{1}{2}N + S)^2 - 1]}{24} \left( \frac{\frac{1}{2}N + S - 2}{2S} \right). \quad (\text{A8})$$

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