Calculation of traces of p-order replacement operators over N-electron spin-adapted spaces

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We present here a simple method for the direct evaluation of traces of p-order replacement operators (p-RO's) calculated in a finite-dimensional, antisymmetric, and spin-adapted N-electron space. The procedure is based on the reduction of the operator order together with a performance of the summations through Slater determinants. Very useful and general formulas, which can be applied to RO's of any order $p \leq N$, are then derived.

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I. INTRODUCTION

The calculation of traces of p-order replacement operators (p-RO's) over finite N-electron spaces with definite spin S plays an important role in some theoretical developments in physics and chemical physics. These traces are needed in studies of spectral distribution both in atomic and nuclear physics [1–7] as well as in the construction of algorithms to describe the electronic structure of atoms and molecules. The development of the spin-adapted reduced Hamiltonian theory [8–12] has required carrying out a systematic study of these traces due to one of its steps, consisting of the evalution of spin-adapted traces of products of replacement operators.

The summation of these kind of traces is performed over the N-electron basis functions corresponding to the spin quantum numbers S and M (eigenfunctions of $\hat{S}^2$ and $\hat{S}_z$ operators). In other words, these traces are taken over the functions that constitute a basis set of a full configuration-interaction (FCI) space corresponding to the case of K orbitals, N electrons, and a spin S. In Refs. [10,12] a rigorous study is reported that allows one to express the spin-adapted trace of an arbitrary p-RO in terms of spin-adapted traces of diagonal p-RO's [6,7] (the traces of products of the occupation number operators). This paper tries to go beyond showing a simple algorithm that leads to the direct evaluation of spin-adapted traces of all p-RO's (diagonal and off-diagonal) by a progressive reduction in the order of the p-RO's. The foundation of the method consists of transforming the summations taken over the eigenfunctions of $\hat{S}^2$ and $\hat{S}_z$ operators into those of the simpler eigenfunctions of $\hat{S}_z$ operator. The final results are expressed in terms of binomial coefficients, which is useful for programming purposes.

In Secs. II and III, several aspects related with spin-adapted traces of p-RO are considered. In Sec. IV, an appropriate notation and a discussion of the different cases that can occur are presented. Finally, the Appendix shows some illustrative practical examples.

II. THE DIMENSION OF THE FCI SPACE

Let us consider an N-electron system and its spin functions, the spin eigenfunctions of the $(\hat{S}^2,\hat{S}_z)$ operators. We will denote by S the spin quantum number and by M the biggest eigenvalue of the $\hat{S}_z$ operator for a determined S. The spin function defined by the quantum numbers S and M fulfills $M=S=\frac{1}{2}(N_\alpha-N_\beta)$; $N_\alpha=(N/2)+S$ and $N_\beta=(N/2)-S$, where N_α and N_β are the number of α and β electrons, respectively.

The dimension of the spin degeneracy for $\hat{S}^2$ eigenfunctions, with spin quantum number S, is given by [13,14]

$$\begin{bmatrix} N \\ N_\alpha \end{bmatrix} - \begin{bmatrix} N \\ N_\alpha+1 \end{bmatrix} = \begin{bmatrix} N \\ N_\beta \end{bmatrix} - \begin{bmatrix} N \\ N_\beta-1 \end{bmatrix} . \tag{1}$$

Note that although the parameters N_α and N_β have a clear physical meaning referring to the spin function with the spin quantum numbers (S,M), formula (1) describes the degeneracy of the $\hat{S}^2$ eigenfunctions, independently of the eigenvalues of the $\hat{S}_z$ operator.

In the left-hand side (lhs) of this equation the first and second binomial coefficients mean the number of primitive spin functions, $(\sigma_1(1)\sigma_2(2)\cdots\sigma_N(N))$ (with $\sigma_i\,\alpha$ or β), that can be built having the quantum numbers M and $(M+1)$, respectively.

It is well known that the Slater determinants, eigenfunctions of the $\hat{S}_z$ operator, are formed by suitable linear combinations of all the primitive spin functions corresponding to a M value, and orbital functions. So, for a given basis set of K orbital functions, the number of Slater determinants corresponding to an eigenvalue M is $\binom{K}{N_\alpha}\binom{K}{N_\beta}$ and, consequently, the number of the wave functions having spin quantum number S, eigenfunctions of $(\hat{S}^2,\hat{S}_z)$ operators, is, according with formula (1)

$$\begin{bmatrix} K \\ N_\alpha \end{bmatrix} \begin{bmatrix} K \\ N_\beta \end{bmatrix} - \begin{bmatrix} K \\ N_\alpha+1 \end{bmatrix} \begin{bmatrix} K \\ N_\beta-1 \end{bmatrix} . \tag{2}$$

Obviously, a simple algebra shows that formula (2) is

equivalent to the well-known Weyl-Paldus formula [15]

$$\frac{2S+1}{K+1}\begin{bmatrix}K+1\\N_\beta\end{bmatrix}\begin{bmatrix}K+1\\N_\alpha+1\end{bmatrix}, \tag{3}$$

which is commonly used in the literature. The interest of the equivalent formula (2) is that the number of wave functions with a $\hat{S}^2$ eigenvalue $S(S+1)$ is calculated through the number of the Slater determinants with eigenvalues M and $(M+1)$. Formulas (2) and (3) express the dimension of the full configuration-interaction (FCI) space [15].

III. SPIN-ADAPTED TRACES OF p-RO

Expression (2) and the simple properties of the Slater determinants are very useful in the calculation of spin-adapted traces of p-order replacement operators (p-RO's). The spin-free expression of these operators is [10,16–19]

$${}^pE^{i_1\cdots i_p}_{j_1\cdots j_p}=\sum_{\sigma_1}\cdots\sum_{\sigma_p}b^\dagger_{i_1\sigma_1}\cdots b^\dagger_{i_p\sigma_p}b_{j_p\sigma_p}\cdots b_{j_1\sigma_1}, \tag{4}$$

where $b^\dagger_{i_k\sigma_k}$ and $b_{j_k\sigma_k}$ are the fermion creation and annihilation operators. The RO's have also been called in the literature [10–12] reduced density operators due to the expectation values of these operators generating the matrix elements of the p-order reduced density matrices. For a given N-electron state $|\mathcal{L}\rangle$ of a Hamiltonian $\hat{H}$, a $(i_1\cdots i_p,j_1\cdots j_p)$ element of the p-order reduced density matrix is

$${}^pD^{i_1\cdots i_p}_{j_1\cdots j_p}=\frac{\langle\mathcal{L}|{}^pE^{i_1\cdots i_p}_{j_1\cdots j_p}|\mathcal{L}\rangle}{p!}. \tag{5}$$

In the following, $\Lambda,\Omega,\ldots$ will be the eigenfunctions of $(\hat{S}^2,\hat{S}_z)$ in the N-electron space, corresponding to a quantum number S, constructed with K orbitals (the basis set of the FCI space). Closing both sides of a determined operator given by formula (4), a matrix is obtained whose (Λ,Ω) elements are

$$\langle\Lambda|{}^pE^{i_1\cdots i_p}_{j_1\cdots j_p}|\Omega\rangle \tag{6}$$

and so, the trace of this matrix, labeled by (Λ,Ω), is

$$\sum_\Lambda\langle\Lambda|{}^pE^{i_1\cdots i_p}_{j_1\cdots j_p}|\Lambda\rangle. \tag{7}$$

As has been previously reported [8], the value of this trace does not depend on the value of the indices denoting the orbitals but only on their ordering. The reason for this is that the sum is carried out over the whole space, therefore all the indices play equivalent roles.

The simplest case dealing with the calculation of these kind of traces is when ${}^pE^{i_1\cdots i_p}_{j_1\cdots j_p}\equiv 1$. In this particular case the trace is expressed, according to formula (2), as

$$\sum_\Lambda\langle\Lambda|\Lambda\rangle=\sum_{\mathcal{S}(M)}\langle\mathcal{S}(M)|\mathcal{S}(M)\rangle-\sum_{\mathcal{S}(M+1)}\langle\mathcal{S}(M+1)|\mathcal{S}(M+1)\rangle, \tag{8}$$

where we denote by $\mathcal{S}(M)$ the Slater determinants corresponding to a $\hat{S}_z$ eigenvalue M.

Formula (8) can be easily generalized to any p-RO without any difficulty. We will consider a simple example to show the procedure. Using the identity

$$\sum_i\sum_j\frac{{}^2E^{ij}_{ij}}{N(N-1)}=1, \tag{9}$$

formula (8) can be written

$$\sum_\Lambda\sum_{i,j}\langle\Lambda|{}^2E^{ij}_{ij}|\Lambda\rangle=\sum_{\mathcal{S}(M)}\sum_{i,j}\langle\mathcal{S}(M)|{}^2E^{ij}_{ij}|\mathcal{S}(M)\rangle-\sum_{\mathcal{S}(M+1)}\sum_{i,j}\langle\mathcal{S}(M+1)|{}^2E^{ij}_{ij}|\mathcal{S}(M+1)\rangle. \tag{10}$$

Some exact manipulations of this equation based on the possibilities that the indices are equal or different allow us to write

$$\sum_\Lambda\langle\Lambda|{}^2E^{12}_{12}|\Lambda\rangle_{N,K}=\sum_{\mathcal{S}(M)}\langle\mathcal{S}(M)|{}^2E^{12}_{12}|\mathcal{S}(M)\rangle_{N,K}-\sum_{\mathcal{S}(M+1)}\langle\mathcal{S}(M+1)|{}^2E^{12}_{12}|\mathcal{S}(M+1)\rangle_{N,K} \tag{11}$$

and

$$\sum_\Lambda\langle\Lambda|\Lambda\rangle_{(N-2),(K-1)}=\sum_{\mathcal{S}(M)}\langle\mathcal{S}(M)|\mathcal{S}(M)\rangle_{(N-2),(K-1)}-\sum_{\mathcal{S}(M+1)}\langle\mathcal{S}(M+1)|\mathcal{S}(M+1)\rangle_{(N-2),(K-1)}, \tag{12}$$

where indices 1 and 2 in the ${}^2E$ operator mean any pair of orbital functions of the basis set. This simplification derives from the above-mentioned invariance of the traces with respect to the numbering of the orbitals [8]. The symbols $N,K,(N-2)$, and $(K-1)$ as subscripts denote the parameters over which the eigenfunctions included in the summations are built.

The above example refers to the trace of a diagonal RO, but since the traces of off-diagonal operators can be expressed as simple linear combinations of the diagonal ones [10,12], we conclude that a general procedure to calculate spin-adapted p-RO traces is

$$\sum_\Lambda\langle\Lambda|{}^pE^{i_1\cdots i_p}_{j_1\cdots j_p}|\Lambda\rangle=\sum_{\mathcal{S}(M)}\langle\mathcal{S}(M)|{}^pE^{i_1\cdots i_p}_{j_1\cdots j_p}|\mathcal{S}(M)\rangle-\sum_{\mathcal{S}(M+1)}\langle\mathcal{S}(M+1)|{}^pE^{i_1\cdots i_p}_{j_1\cdots j_p}|\mathcal{S}(M+1)\rangle. \tag{13}$$

IV. CASES, GRAPHS, AND FORMULAS

In the following we will use the angular brackets $\langle\ \rangle_{N,K}$ as a shorthand notation for $\sum_\Lambda \langle |\ | \rangle_{N,K}$, where $|\Lambda\rangle$ are again the wave functions, eigenfunctions of $(\hat{S}^2,\hat{S}_z)$ operators, constructed with K orbital functions in a spin-adapted N-electron space, so that

$$\langle {}^pE^{i_1\cdots i_p}_{j_1\cdots j_p}\rangle_{N,K}=\sum_\Lambda \langle \Lambda|{}^pE^{i_1\cdots i_p}_{j_1\cdots j_p}|\Lambda\rangle_{N,K}\ . \tag{14}$$

Since we have proposed the calculation of these kinds of traces through the difference of traces defined by Slater determinants, we will denote

$$\|{}^pE^{i_1\cdots i_p}_{j_1\cdots j_p}\|^{N_\alpha,K}_{N_\beta,K}=\sum_{\mathcal{S}(M)}\langle \mathcal{S}(M)|{}^pE^{i_1\cdots i_p}_{j_1\cdots j_p}|\mathcal{S}(M)\rangle^{N_\alpha,K}_{N_\beta,K}-\sum_{\mathcal{S}(M+1)}\langle \mathcal{S}(M+1)|{}^pE^{i_1\cdots i_p}_{j_1\cdots j_p}|\mathcal{S}(M+1)\rangle^{(N_\alpha+1),K}_{(N_\beta-1),K}\ , \tag{15}$$

where the superscripts N_α,K mean the number of α electrons and functions employed in the construction of Slater determinants. The same meaning is given to the subscripts N_β,K for the β electrons. So, Eq. (13) will be written as

$$\langle {}^pE^{i_1\cdots i_p}_{j_1\cdots j_p}\rangle_{N,K}=\|{}^pE^{i_1\cdots i_p}_{j_1\cdots j_p}\|^{N_\alpha,K}_{N_\beta,K}\ . \tag{16}$$

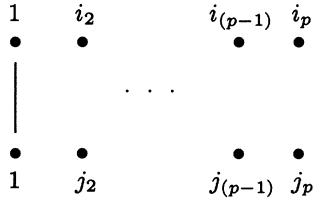
For the particular case of ${}^pE^{i_1\cdots i_p}_{j_1\cdots j_p}\equiv 1$ we will call

$$||1||^{N_\alpha,K}_{N_\beta,K}=T^{N_\alpha,K}_{N_\beta,K}=\begin{bmatrix}K\\N_\alpha\end{bmatrix}\begin{bmatrix}K\\N_\beta\end{bmatrix}-\begin{bmatrix}K\\N_\alpha+1\end{bmatrix}\begin{bmatrix}K\\N_\beta-1\end{bmatrix}\ . \tag{17}$$

The spin-adapted traces of p-RO are nil unless the creation set $\{i_1,\ldots,i_p\}$ contains identical indices to the annihilation one $\{j_1,\ldots,j_p\}$ [8]. So, the differences between all nonvanishing traces are established comparing the permutations $(i_1,\ldots,i_p)$ and $(j_1,\ldots,j_p)$. The permutation $(1,2,\ldots,p)$ will be used as reference for the set $\{i_1,\ldots,i_p\}$ if it has no repetition of indices.

We will show that the spin-adapted trace of any p-RO can be expressed in terms of traces of lower-order RO's, so that finally the original trace is calculated as a function of T expressions given by formula (17). The reduction procedure presents several cases that can be represented by simple graphs described as follows.

(a)



which means $i_1=j_1=1$ and $\{i_2,\ldots,i_p\}=\{j_2,\ldots,j_p\}$. We exclude any repetition of indices in any of the sets.

The corresponding operator is

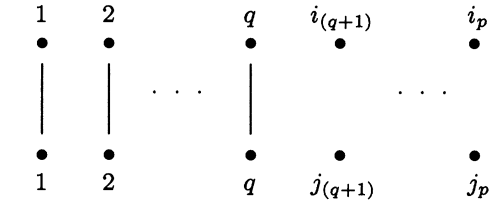
$$\begin{aligned}{}^pE^{1,i_2\cdots i_p}_{1,j_2\cdots j_p}&=\sum_{\sigma_1}\cdots\sum_{\sigma_p}b^\dagger_{1\sigma_1}\cdots b^\dagger_{i_p\sigma_p}b_{j_p\sigma_p}\cdots b_{1\sigma_1}\\&=\sum_{\sigma_1}b^\dagger_{1\sigma_1}{}^{(p-1)}E^{i_2\cdots i_p}_{j_2\cdots j_p}b_{1\sigma_1}\\&=b^\dagger_1{}^{(p-1)}E^{i_2\cdots i_p}_{j_2\cdots j_p}b_1\\&\quad+b^\dagger_{\bar 1}{}^{(p-1)}E^{i_2\cdots i_p}_{j_2\cdots j_p}b_{\bar 1}\ ,\end{aligned} \tag{18}$$

where 1 and $\bar 1$ mean the spin functions 1^α and 1^β, respectively. According to Eq. (15) and after applying the $b^\dagger_1,b_1,b^\dagger_{\bar 1}$, and $b_{\bar 1}$ operators, we have

$$\begin{aligned}\langle {}^pE^{1,i_2\cdots i_p}_{1,j_2\cdots j_p}\rangle_{N,K}&=\|{}^{(p-1)}E^{i_2\cdots i_p}_{j_2\cdots j_p}\|^{(N_\alpha-1),(K-1)}_{N_\beta,K}\\&\quad+\|{}^{(p-1)}E^{i_2\cdots i_p}_{j_2\cdots j_p}\|^{N_\alpha,K}_{(N_\beta-1),(K-1)}\ ,\end{aligned} \tag{19}$$

which shows that the p order of the original trace has been reduced in one unit.

Formula (19) can be generalized for q equal indices in the same position whose graph is

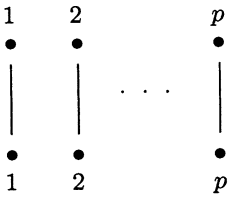


which mean $i_1=j_1=1$, $i_2=j_2=2,\ldots,i_q=j_q=q$, and $\{i_{(q+1)},\ldots,i_p\}=\{j_{(q+1)},\ldots,j_p\}$.

The corresponding trace is

$$\langle {}^pE^{1,2,\ldots,q,i_{(q+1)}\cdots i_p}_{1,2,\ldots,q,j_{(q+1)}\cdots j_p}\rangle_{N,K}=\sum_{i=0}^{q}\begin{bmatrix}q\\i\end{bmatrix}\|{}^{(p-q)}E^{i_{(q+1)}\cdots i_p}_{j_{(q+1)}\cdots j_p}\|^{(N_\alpha-q+i),(K-q+i)}_{(N_\beta-i),(K-i)}\ . \tag{20}$$

An important application of Eq. (20) is the direct calculation of spin-adapted traces of diagonal p-RO's, so that, when the graph is

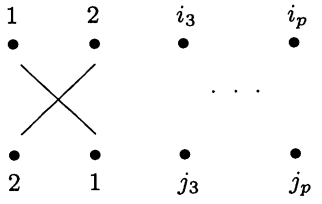


the trace is

$$\langle {}^pE^{1,2,\ldots,p}_{1,2,\ldots,p}\rangle_{N,K}=\sum_{i=0}^{p}\binom{p}{i}T^{(N_\alpha-p+i),(K-p+i)}_{(N_\beta-i),(K-i)}\,, \tag{21}$$

which is very handy for computational purposes.

(b) In this case we again exclude any repetition of indices in any of the sets. We refer to situations where the equal indices do not have the same position; for example, the graph



where $i_1=j_2=1$, $i_2=j_1=2$, and $\{i_3,\ldots,i_p\}=\{j_3,\ldots,j_p\}$. The p-RO is

$$\begin{aligned}{}^pE^{1,2,i_3\cdots i_p}_{2,1,j_3\cdots j_p}=&-b_1^\dagger b_2^\dagger\,{}^{(p-2)}E^{i_3\cdots i_p}_{j_3\cdots j_p}b_2b_1\\&-b_{\bar1}^\dagger b_{\bar2}^\dagger\,{}^{(p-2)}E^{i_3\cdots i_p}_{j_3\cdots j_p}b_{\bar2}b_{\bar1}\end{aligned} \tag{22}$$

and so, its trace calculated through the Slater determinants is

$$\langle {}^pE^{1,2,i_3\cdots i_p}_{2,1,j_3\cdots j_p}\rangle_{N,K}=-\|{}^{(p-2)}E^{i_3\cdots i_p}_{j_3\cdots j_p}\|^{(N_\alpha-2),(K-2)}_{N_\beta,K}-\|{}^{(p-2)}E^{i_3\cdots i_p}_{j_3\cdots j_p}\|^{N_\alpha,K}_{(N_\beta-2),(K-2)}\,. \tag{23}$$

This equation shows again the reduction of the order in the RO.

The procedure is also applied to the case of p-RO's having two blocks of equal indices, one with q indices and another with $(p-q)$ ones, for example $\{i_1,\ldots,i_q\}=\{j_1,\ldots,j_q\}$ and $\{i_{(q+1)},\ldots,i_p\}=\{j_{(q+1)},\ldots,j_p\}$. The result is

$$\langle {}^pE^{i_1,\ldots,i_q,i_{(q+1)},\ldots,i_p}_{j_1,\ldots,j_q,j_{(q+1)},\ldots,j_p}\rangle_{N,K}=(-1)^\nu(\|{}^{(p-q)}E^{i_{(q+1)}\cdots i_p}_{j_{(q+1)}\cdots j_p}\|^{(N_\alpha-q),(K-q)}_{N_\beta,K}+\|{}^{(p-q)}E^{i_{(q+1)}\cdots i_p}_{j_{(q+1)}\cdots j_p}\|^{N_\alpha,K}_{(N_\beta-q),(K-q)})\,, \tag{24}$$

where ν is the number of permutations required to pass from $(j_1,\ldots,j_q)$ to $(i_1,\ldots,i_q)$.

In the particular case of only one block being formed with the p indices, formula (24) is transformed into

$$\langle {}^pE^{i_1\cdots i_p}_{j_1\cdots j_p}\rangle_{N,K}=(-1)^\nu(T^{(N_\alpha-p),(K-p)}_{N_\beta,K}+T^{N_\alpha,K}_{(N_\beta-p),(K-p)})\,, \tag{25}$$

which again allows a direct calculation of the trace.

(c) Finally, we briefly refer to spin-adapted traces of RO's having repeated indices. Since a direct procedure has been reported to remove the repeated indices [10,12], once those indices have been eliminated, we can apply cases (a) or (b).

In conclusion, we have presented a straightforward method for the calculation of spin-adapted traces of p-RO. It carries out a reduction of p-RO's to lower orders. The final formulas are simple relationships between binomial coefficients $T^{N_\alpha,K}_{N_\beta,K}$ [see Eq. (17)] which is very useful in a computational point of view. Some application examples are given in the Appendix.

Previous calculations of these kind of traces are based on a classification of the corresponding p-RO [10,12]. In a second step, the spin-adapted trace of a determined p-RO is expressed as a function of several traces of products of occupation number operators (the traces of the diagonal p-RO's) and, finally, the evaluation of the last trace is carried out as described in Ref. [7]. The procedure that has been described above allows a simpler classification and a direct evaluation of the spin-adapted trace of any p-RO, diagonal or off-diagonal. This simplifies the algorithms in those fields where these traces are needed. In particular, in the spin-adapted reduced Hamiltonian theory, p-RO traces are required in the calculation of the p-order spin-adapted reduced Hamiltonian matrices. The eigenvectors of these matrices allow the direct approximation of the p-order reduced density matrix [12,20,21].

Furthermore, the method reported here is needed in the calculation of traces of p-RO's taken over wave functions of spin and other symmetries, where the previous procedure cannot be applied. That is the case for traces $\sum_{\Lambda_g}\langle\Lambda_g|{}^pE^{i_1\cdots i_p}_{j_1\cdots j_p}|\Lambda_g\rangle$ and $\sum_{\Lambda_u}\langle\Lambda_u|{}^pE^{i_1\cdots i_p}_{j_1\cdots j_p}|\Lambda_u\rangle$, where Λ_g and Λ_u are gerade and ungerade eigenfunctions of $(\hat S^2,\hat S_z)$ operators. A study of spin and gerade (or ungerade) adapted traces are planned to be given elsewhere [22].

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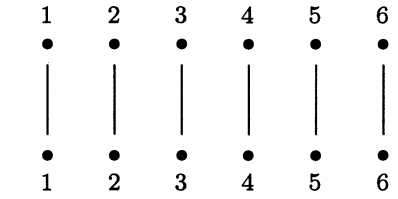


APPENDIX: EXAMPLES

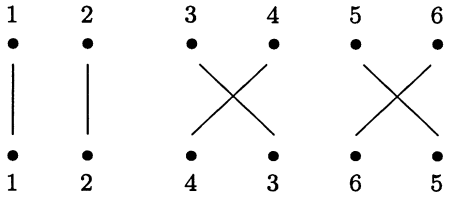
Several spin-adapted traces of p-RO are given for the system $N=6, K=10, S=1$ ($N_\alpha=4$ and $N_\beta=2$). We have

$$\langle {}^6E^{1,2,3,4,5,6}_{1,2,3,4,5,6}\rangle_{6,10} = \|{}^6E^{1,2,3,4,5,6}_{1,2,3,4,5,6}\|^{4,10}_{2,10} = T^{-2,4}_{2,10} + 6.\,T^{-1,5}_{1,9} + 15.\,T^{0,6}_{0,8} + \cdots$$

$$= 6\left[\begin{bmatrix}5\\-1\end{bmatrix}\begin{bmatrix}9\\1\end{bmatrix} - \begin{bmatrix}5\\0\end{bmatrix}\begin{bmatrix}9\\0\end{bmatrix}\right] + 15\left[\begin{bmatrix}6\\0\end{bmatrix}\begin{bmatrix}8\\0\end{bmatrix} - \begin{bmatrix}6\\1\end{bmatrix}\begin{bmatrix}8\\-1\end{bmatrix}\right]$$

$$= 9\,, \tag{A1}$$

where, obviously, the binomial coefficients with negative indices are zero. We also have

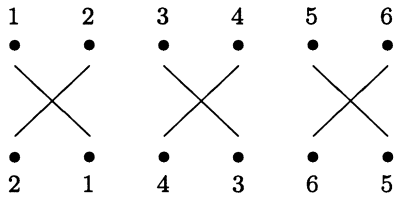


$$\langle {}^6E^{1,2,3,4,5,6}_{1,2,4,3,6,5}\rangle_{6,10} = \|{}^6E^{1,2,3,4,5,6}_{1,2,4,3,6,5}\|^{4,10}_{2,10} = \|{}^4E^{3,4,5,6}_{4,3,6,5}\|^{2,8}_{2,10} + 2\|{}^4E^{3,4,5,6}_{4,3,6,5}\|^{3,9}_{1,9} + \|{}^4E^{3,4,5,6}_{4,3,6,5}\|^{4,10}_{0,8}$$

$$= -\|{}^2E^{5,6}_{6,5}\|^{0,6}_{2,10} - \|{}^2E^{5,6}_{6,5}\|^{2,8}_{0,8} - 2\,|\,|{}^2E^{5,6}_{6,5}\|^{1,7}_{1,9} - 2\|{}^2E^{5,6}_{6,5}\|^{3,9}_{-1,7} - \|{}^2E^{5,6}_{6,5}\|^{2,8}_{0,8} - \|{}^2E^{5,6}_{6,5}\|^{4,10}_{-2,6}$$

$$= T^{-2,4}_{2,10} + T^{0,6}_{0,8} + T^{0,6}_{0,8} + T^{2,8}_{-2,6} + 2T^{-1,5}_{1,9} + 2T^{1,7}_{-1,7} + T^{0,6}_{0,8} + T^{2,8}_{-2,6} = 1 \tag{A2}$$

and



$$\langle {}^6E^{1,2,3,4,5,6}_{2,1,4,3,6,5}\rangle_{6,10} = \|{}^6E^{1,2,3,4,5,6}_{2,1,4,3,6,5}\|^{4,10}_{2,10} = -\|{}^4E^{1,2,3,4}_{2,1,4,3}\|^{2,8}_{2,10} - \|{}^4E^{1,2,3,4}_{2,1,4,3}\|^{4,10}_{0,8}$$

$$= \|{}^2E^{1,2}_{2,1}\|^{0,6}_{2,10} + \|{}^2E^{1,2}_{2,1}\|^{2,8}_{0,8} + \|{}^2E^{1,2}_{2,1}\|^{2,8}_{0,8} + \|{}^2E^{1,2}_{2,1}\|^{4,10}_{-2,6}$$

$$= \|{}^2E^{1,2}_{2,1}\|^{0,6}_{2,10} + 2\,|\,|{}^2E^{1,2}_{2,1}\|^{2,8}_{0,8} = -T^{-2,4}_{2,10} - T^{0,6}_{0,8} - 2T^{0,6}_{0,8} - 2T^{2,8}_{-2,6} \tag{A3}$$

$$= -3\,.$$

[1] J. Karwowski and M. Bancewicz, J. Phys. A **20**, 6309 (1987).
[2] M. Bancewicz, G. H. F. Diercksen, and J. Karwowski, Phys. Rev. A **40**, 5507 (1989).
[3] J. Bauche and C. Bauche-Arnoult, Comput. Phys. Rep. **12**, 1 (1990).
[4] M. Nomura, Prog. Theor. Phys. **51**, 489 (1974).
[5] M. Nomura, J. Math. Phys. **27**, 536 (1986).
[6] M. Nomura, Phys. Rev. A **37**, 2709 (1988).
[7] J. Karwowski and C. Valdemoro, Phys. Rev. A **37**, 2712 (1988).
[8] J. Karwowski, W. Duch, and C. Valdemoro, Phys. Rev. A **33**, 2254 (1986).
[9] L. Lain, A. Torre, J. Karwowski, and C. Valdemoro, Phys. Rev. A **38**, 2721 (1988).
[10] J. Planelles, C. Valdemoro, and J. Karwowski, Phys. Rev. A **41**, 2391 (1990).
[11] J. Planelles, C. Valdemoro, and J. Karwowski, Phys. Rev.

A **43**, 3392 (1991).
[12] C. Valdemoro, A. Torre, and L. Lain, in *Structure, Interactions and Reactivity,* edited by S. Fraga (Elsevier, Amsterdam, 1992).
[13] R. Pauncz, *Spin Eigenfunctions: Construction and Use* (Plenum, New York, 1979).
[14] M. Kibler and J. Katriel, Phys. Lett. A **147**, 417 (1990).
[15] J. Paldus, J. Chem. Phys. **61**, 5321 (1974).
[16] J. Paldus, in *Theoretical Chemistry: Advances and Perspectives,* edited by H. Eyring and D. J. Henderson (Academic, New York, 1976).
[17] J. Koutecky and A. Laforgue, Int. J. Quantum. Chem. **11**, 505 (1977).
[18] W. Kutzelnigg, J. Chem. Phys. **82**, 4166 (1985).
[19] J. Paldus and B. Jeziorski, Theor. Chim. Acta **73**, 81 (1988).
[20] L. Lain, C. Valdemoro, A. Torre, and M. Reguero, Phys. Rev. A **35**, 3132 (1987).
[21] L. Lain, A. Torre, and C. Valdemoro, Phys. Rev. A **37**, 2868 (1988).
[22] J. Millan, A. Torre, and L. Lain (unpublished).