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

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In our previous studies with the evaluation of traces of p-order replacement operators calculated in finite-dimensional, antisymmetric, and spin-adapted N-electron spaces ($p \leq N$), we described a technique for the calculation of those expressions based on the reduction of the operator order [A. Torre, L. Lain, and J. Millan, Phys. Rev. A **47**, 923 (1993)]. Now, we report a general formula which, condensing all the reduction steps, leads to the direct evaluation of those traces. Some examples for illuminating the usefulness of that formula are reported.

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I. INTRODUCTION

In a previous paper [1] we described a technique to evaluate traces of p-order replacement operators (p-RO's), calculated over finite-dimensional, antisymmetric, and spin-adapted N-electron spaces ($p \leq N$). The procedure is based on a progressive reduction in the order of the p-RO's so that, in the final step, those operators are reduced to the unity one. Using the foundations of that technique, this report derives a general formula that directly calculates the numerical values of this kind of trace for any p-RO, avoiding all the intermediate reduction steps. This achievement complements and improves the previous approaches to the calculation of spin-adapted traces of p-RO's [1–4] and, since the derived formula can easily be programmed, it renders feasible the task of evaluating these tools with a computer.

There are several areas in physics where the calculation of this kind of trace is needed and, consequently, where the application of the formula we present here is useful. In particular, we must mention the determination of moments of spectral density distributions, which are used in statistical theories of nuclear and atomic spectra [5–7], as well as some computational approaches to many-electron theories [8,9]. In the next section, a brief summary of the concepts and the arguments for deriving the computing formula are described. Section III shows some examples of calculation of S_z-adapted traces of p-RO's, according to the structure of those operators. That leads to the evaluation of the corresponding spin-adapted traces [1].

II. THE EVALUATION OF S_z-ADAPTED TRACES OF p-RO'S

The spin-free p-RO's are [10]

$$ {}^pE^{i_1\cdots i_p}_{j_1\cdots j_p} = \sum_{\sigma_1}\cdots\sum_{\sigma_p} b^+_{i_1\sigma_1}\cdots b^+_{i_p\sigma_p} b_{j_p\sigma_p}\cdots b_{j_1\sigma_1}, \tag{1} $$

where $b^+_{i_k\sigma_k}$ ($b_{j_k\sigma_k}$) are the usual creation (annihilation) fermion operators; $\sigma_1,\ldots,\sigma_p$ are the spin coordinates and $i_1,\ldots,i_p$, $j_1,\ldots,j_p,\ldots$ are the K one-electron orbital functions of an orthonormal basis set.

The spin-adapted traces of a p-RO are defined as [1]

$$ \sum_{\Lambda}\langle\Lambda|{}^pE^{i_1\cdots i_p}_{j_1\cdots j_p}|\Lambda\rangle_{N,K,S}, \tag{2} $$

where Λ are the N-electron eigenfunctions of the $(\hat{S}^2,\hat{S}_z)$ operators, constructed with K orbitals, corresponding to a spin quantum number S. The value of expression (2) is independent of the S_z quantum number, so it has been omitted [1].

The most suitable calculation of expression (2) is carried out through the relation [1]

$$ \begin{aligned} \sum_{\Lambda}\langle\Lambda|{}^pE^{i_1\cdots i_p}_{j_1\cdots j_p}|\Lambda\rangle_{N,K,S} &= \sum_{D(S)}\langle D(S)|{}^pE^{i_1\cdots i_p}_{j_1\cdots j_p}|D(S)\rangle_{N,K} \\ &\quad - \sum_{D(S+1)}\langle D(S+1)|{}^pE^{i_1\cdots i_p}_{j_1\cdots j_p}|D(S+1)\rangle_{N,K} \end{aligned} \tag{3} $$

where $D(S)$ are the Slater determinants (the N-electron eigenfunctions of the $\hat{S}_z$ operator), which can be constructed with the K orbital functions of the basis set, having $N_\alpha = \frac{N}{2} + S$ α-spin orbitals and $N_\beta = \frac{N}{2} - S$ β-spin orbitals. Similarly, the $D(S+1)$ determinants are composed of $N_\alpha = \frac{N}{2} + S + 1$ α-spin orbitals and $N_\beta = \frac{N}{2} - S - 1$ β-spin orbitals. Consequently, $\sum_{D(S)}\langle D(S)|{}^pE^{i_1\cdots i_p}_{j_1\cdots j_p}|D(S)\rangle_{N,K}$ is the S_z-adapted trace of the RO ${}^pE^{i_1\cdots i_p}_{j_1\cdots j_p}$, corresponding to the eigenvalue $S_z = S$.

Formula (3) implies that the calculation of a spin-adapted trace of a given p-RO is carried out through a difference of S_z-adapted traces of that operator. The main object of this report is to express the value of

$$ \sum_{D(S)}\langle D(S)|{}^pE^{i_1\cdots i_p}_{j_1\cdots j_p}|D(S)\rangle_{N,K} \tag{4} $$

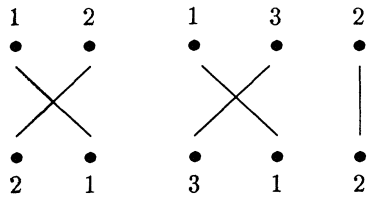
through a general formula which can be used for computational purposes. Obviously, the evaluation of formula

(4) provides the calculation of the spin-adapted traces of p-RO's given in formula (2).

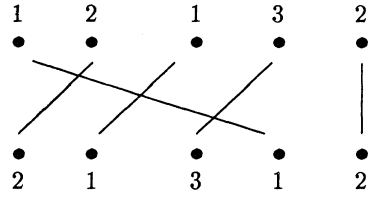
As mentioned above, the Slater determinants in sum (4) are composed of $N_\alpha = \frac{N}{2} + S$ α-spin orbitals and $N_\beta = \frac{N}{2} - S$ β-spin orbitals. Hence, the problem to consider is the determination of the number of Slater determinants in that sum that contain all the spin-orbitals that are included in the creation operators (and in the annihilation ones) of any of the terms derived from the expansion of the p-RO, given in Eq. (1). The number of these determinants depends on the structure of the p-RO and each of them contributes to the sum (4) as $(-1)^\nu$, where ν is the number of transpositions needed to pass from the set $(i_1, \ldots, i_p)$ to the $(j_1, \ldots, j_p)$ one. Obviously, both sets must be composed of the same orbitals [otherwise trace (4) will be zero], although they can be ordered in different ways.

In dealing with the p-RO's, it is convenient to classify the indices in the creation and annihilation sets into diagonal indices (identical indices occupying the same position in both sets) and blocks of indices, that is, subsets of creation indices $(i_k, \ldots, i_l)$ and annihilation ones $(j_k, \ldots, j_l)$ both containing identical indices but in different positions (otherwise they would be diagonal indices). The expansion of fermion operators expressed by formula (1) shows that indices occupying the same position in the creator and annihilator sets have identical spin coordinates. Consequently, the diagonal indices have the same spin (α or β) in the creation and in the annihilation sets, in all terms of the p-RO expansion. Since the expansion (1) is closed on both sides by the same Slater determinant, the creation and annihilation indices that constitute a block must have also identical spin coordinates; otherwise their contribution to sum (4) will be zero. Blocks and diagonal indices provide a structure for the p-RO's, which will be represented by graphs.

If there is no repetition of indices in the creation set (and in the annihilation one) the p-RO is represented by only one graph. However, when the creation and annihilation sets have nondiagonal repeated indices, there are different ways to set up blocks of indices with the same spin. Each of these ways corresponds to some terms of expansion (4) and is represented by a graph. Due to the Pauli principle, a determined index can be repeated only once in the creation and annihilation sets. Consequently, a p-RO with g nondiagonal repeated indices will be able to be represented by 2^g graphs (2^g ways of relating g pairs of creation indices to g pairs of annihilation ones). In order to clarify this aspect, let us consider the 5-RO ${}^5E^{12132}_{21312}$, where $1, 2, 3, \ldots$ mean different orbitals. This 5-RO can be represented by the graphs



and



where the lines link identical indices with the same spin. Obviously, the last graph must be neglected since it has repeated indices in the same block.

A quantitative description of each graph arising from a determined p-RO is given by the parameters m (the number of blocks in the graph), b_i [the number of creation (or annihilation) indices in the block i], r_{id} (the number of indices in the block i that are also present in the diagonal part of the p-RO), r_d (the number of repeated indices in the diagonal part of the p-RO), q (the number of diagonal indices without any repetition), $x_i = 1$ when the spin coordinate of the block i is β and $x_i = 0$ when it is α, $c^i_j = 1$ for the blocks i and j when $i \cap j \neq \emptyset$ and $c^i_j = 0$ otherwise, and ν [the number of transpositions required to pass from the ordered set $(i_1, \ldots, i_p)$ to the $(j_1, \ldots, j_p)$ one].

For each graph corresponding to a determined p-RO, the number of Slater determinants that contribute with a nonzero value to sum (4) is obtained through the appropriate distributions of all the blocks and diagonal indices to the α and β parts of the determinants. For given values of the parameters $x_1, \ldots, x_m$, which characterize the corresponding blocks as α or β, and assigning β spin to $t \leq q$ fixed diagonal indices without any repetition, the number of possibilities $B(t, x_1, \ldots, x_m)$ to construct the β-part of that kind of determinants is expressed in terms of the resultant binomial coefficient, as follows

$$B(t, x_1, \ldots, x_m) = \begin{pmatrix} K - \sum_i [x_i b_i + (1 - x_i) r_{id}] - r_d - t \\ \frac{N}{2} - S - \sum_i [x_i b_i + (1 - x_i) r_{id}] - r_d - t \end{pmatrix} \tag{5}$$

and, similarly, the number of possibilities $A(t, x_1, \ldots, x_m)$, for the α-part is

$$A(t, x_1, \ldots, x_m) = \begin{pmatrix} K - \sum_i [(1 - x_i) b_i + x_i r_{id}] - r_d - q + t \\ \frac{N}{2} + S - \sum_i [(1 - x_i) b_i + x_i r_{id}] - r_d - q + t \end{pmatrix}. \tag{6}$$

Consequently, the sum for all the possible values of the parameters $x_1, \ldots, x_m$, and all the possible ways to distribute the q diagonal indices without any repetition, $[\sum_{t=0}^{q} \binom{q}{t}]$, as well as the (2^{r_d}) ways to distribute the r_d pairs of diagonal

repeated indices to the α and β parts of the determinants, calculate the contribution of a determined graph of the p-RO to the value of trace (4), so that one finally finds

$$(-1)^{\nu}\, 2^{r_d} \sum_{x_1} \cdots \sum_{x_m} \prod_{i<j} (1-\delta_{x_i x_j} c_j^i) \sum_{t=0}^{q} \binom{q}{t} A(t, x_1, \ldots, x_m) B(t, x_1, \ldots, x_m), \tag{7}$$

where the factor $\prod_{i<j} (1-\delta_{x_i x_j} c_j^i)$ excludes determinants having blocks with common indices and the same spin.

The task of determining the graphs corresponding to a given p-RO, and the values of their parameters m, b_i, c_j^i, r_{id}, r_d, q, and ν, as well as the exclusion of the graphs having repeated indices in the same block, can be easily programmed for a computer. Hence, the sum of formula (7) for all the possible graphs leads to the direct computation of the S_z-adapted traces and, consequently, according to formula (3), to the calculation of the spin-adapted trace of any p-RO.

In conclusion, this report describes a formula that allows the direct calculation of the spin-adapted traces of any p-RO as a function of the parameters N, S, and K which characterize the model space. In this way, we go beyond the previous treatments which require classification of the p-RO, then removal of the repeated indices, and, finally, carring out several reduction steps [1,4]. The procedure described here avoids all these stages so that it generalizes and simplifies the calculation of those traces. Some examples are considered in the next section.

III. EXAMPLES

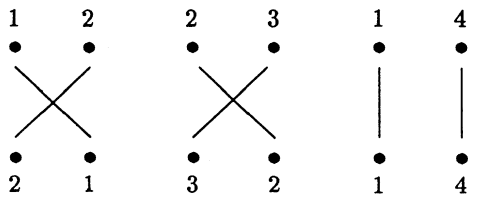
As a first example, we will show the calculation of the S_z-adapted trace of the 6-RO, ${}^6E^{122314}_{213214}$, for the case of $S_z = 0$, $N = 8$ electrons, and $K = 10$ orbitals.

This 6-RO has $g = 1$ nondiagonal repeated indices so that it has two graphs according to the following relationships between the creation and the annihilation indices.

(a) Graph 1, block 1: $i_1 = j_2 = 1$, $i_2 = j_1 = 2$; block 2: $i_3 = j_4 = 2$, $i_4 = j_3 = 3$, diagonal indices: $i_5 = j_5 = 1$, $i_6 = j_6 = 4$.

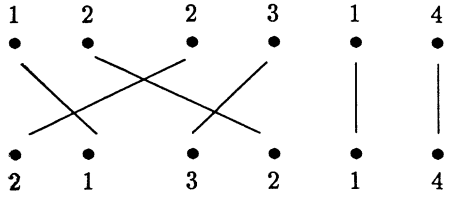
(b) Graph 2, block 1: $i_1 = j_2 = 1$, $i_2 = j_4 = 2$, $i_3 = j_1 = 2$, $i_4 = j_3 = 3$ diagonal indices: $i_5 = j_5 = 1$, $i_6 = j_6 = 4$.

Starting with the first graph, we have



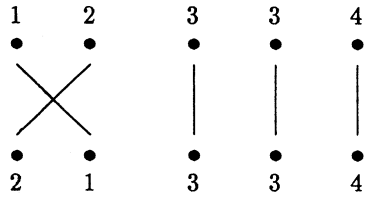
which is characterized by the parameters $m = 2$, $b_1 = 2$, $b_2 = 2$, $c_2^1 = 1$, $r_{1d} = 1$, $r_{2d} = 0$, $q = 1$, $r_d = 0$, $\nu = 2$. The application of formula (7) for $S_z = S = 0$, $\frac{N}{2}+S = 4$, $\frac{N}{2} - S = 4$, and $K = 10$ leads to the value 154.

The second graph is as follows



Since as it has a block with repeated indices, it must be neglected so that it does not contribute to the value of that S_z-adapted trace.

Let us consider a second example, related to the 5-RO ${}^5E^{12334}_{21334}$ for $S_z = \frac{1}{2}$, $N = 7$ electrons, and, again, $K = 10$ orbitals. Since this 5-RO has no nondiagonal repeated indices ($g = 0$) it will be represented by one unique graph, that is block 1: $i_1 = j_2 = 1$, $i_2 = j_1 = 2$; diagonal indices: $i_3 = j_3 = 3$, $i_4 = j_4 = 3$, $i_5 = j_5 = 4$.



This graph is defined by the parameters $m = 1$, $b_1 = 2$, $r_{1d} = 0$, $q = 1$, $r_d = 1$, $\nu = 1$.

Hence, for $S_z = S = \frac{1}{2}$, $\frac{N}{2} + S = 4$, $\frac{N}{2} - S = 3$, and $K = 10$, formula (7) leads to the value -240.

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