Symmetric-group approach to the study of the traces of p-order reduced-density operators and of products of these operators

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(Received 14 July 1989)

In this work we give the values of traces of p-order reduced-density operators. These traces are obtained by application of the spin functions and of the symmetric-group properties. The relations obtained here will allow an easy and fast evaluation of the high-order spin-adapted reduced Hamiltonian matrix elements and high-order Hamiltonian moments.

I. INTRODUCTION

In the spin-adapted reduced Hamiltonian (SRH) theory[1,2] a crucial step is the evaluation of traces of products of replacement[3] operators. In these traces the summation is performed over the basis of a subspace $H^A(N,K,S,M)$ defined as the antisymmetric and spin-adapted part of the N-fold tensorial product of one-electron space

$$H^A(N,K,S,M)=(V_{2K}^N)_{SM}^A ,$$

where A stands for antisymmetric, S and M refer to the eigenvalues of the N-electron spin operators, and K is the dimension of the orbital space. Evaluating this kind or closely related traces is a general problem occurring in different theoretical developments, in particular, in atomic and nuclear spectral density distribution analysis.[4-9]

When approaching the building of high-order SRH matrices or Hamiltonian moments a very powerful tool has to be devised from the very starting point, otherwise the task becomes so complicated that it cannot be attempted. To build such a tool is the aim of this work. We will show that the generalized reduced-density operators (RDO) whose general properties have been recently reviewed[10] have a series of other properties which render them very adequate for our purpose. It will also be shown here that the product of these operators, which is known to be equal to a sum of higher-order RDO's (Refs. 11 and 12), can be carried out in a very effective way by using a new graphical technique which can be easily applied and programmed for a computer. Finally, an extremely fast technique is described for evaluating traces of any RDO's. This technique renders feasible the task of building high-order Hamiltonian moments and SRH matrices.

As our interest lies mainly in obtaining close form expressions for the matrix elements of the fourth-order SRH (4-SRH), we focus our attention on examples of traces appearing in this particular case, but all the techniques are general and cover all the possibilities that may appear in an atomic or molecular problem.

In the following section we describe the notation and basic relations used. By using a graphical procedure we show in Sec. III how to transform a product of p-RDO's into a sum of single t-RDO's. Then, in Sec. IV and V we give a closed-form procedure for obtaining the value of the trace for any single t-RDO in terms of traces of products of p occupation number operators.[3,8,9] Products of occupation number operators are referred to as diagonal RDO's.

II. NOTATION AND BASIC RELATIONS AMONG GENERALIZED OPERATORS

A. p-electron creation $B^\dagger$, and annihilation B, operators

We denote a p-electron creator $B^\dagger$ and annihilator B as

$$\begin{aligned} B^\dagger_{(i_1,i_2,\ldots,i_p),\sigma_1,\sigma_2,\ldots,\sigma_p} &\equiv b^\dagger_{i_1\sigma_1} b^\dagger_{i_2\sigma_2} \cdots b^\dagger_{i_p\sigma_p} , \\ B_{(i_1,i_2,\ldots,i_p)\sigma_1,\sigma_2,\ldots,\sigma_p} &\equiv b_{i_p\sigma_p} \cdots b_{i_2,\sigma_2} b_{i_1\sigma_1} , \end{aligned} \tag{1}$$

where $(i_1,\ldots,i_p)$ are orbitals and $\sigma_1,\sigma_2,\ldots,\sigma_p$ are spin functions.

This notation can be further generalized as

$$B^\dagger_{(i_1,i_2,\ldots,i_p)j_1,j_2,\ldots,j_q}, \quad q \le p \tag{2}$$

where $(i_1,\ldots,i_p)$ denotes the spatial function of the p-electron state and $j_1,j_2,\ldots,j_q$ define the spin coupling.

If $B^\dagger$ represents a p-electron eigenstate of $\hat{S}^2$ and $\hat{S}_z$, the total spin quantum number S and its projection M are

among the indices $j_1, \ldots, j_q$.

B. p-order reduced-density operators (p-RDO)

The 1-RDO, also called in the literature replacement operator,[13–16] is

$$E_{ij} \equiv \sum_{\sigma} b^{\dagger}_{i\sigma} b_{j\sigma} \ . \tag{3}$$

The p-order operator is written as

$${}^{p}E^{ijk,\ldots}_{acd,\ldots} \equiv \sum_{\sigma_1,\ldots,\sigma_p} b^{\dagger}_{i\sigma_1} b^{\dagger}_{j\sigma_2} b^{\dagger}_{k\sigma_3} \cdots b_{d\sigma_3} b_{c\sigma_2} b_{a\sigma_1} \tag{4}$$

These operators generate the p-order reduced-density matrix (p-RDM) elements of any given N-electron state $|\mathcal{L}\rangle$ as

$${}^{p}D^{\mathcal{L}}_{ijk,\ldots;\ldots,acd} \equiv \frac{\langle \mathcal{L}|\, {}^{p}E^{ijk,\ldots}_{acd,\ldots}\, |\mathcal{L}\rangle}{p!} \ . \tag{5}$$

In what follows the superscript p will be omitted unless it is needed for clarity.

C. p-RDO written in terms of spin-adapted $B^{\dagger}$ and B operators

It is known that

$$B^{\dagger}_{(ijkl)SM(j_1j_2)} = \sum_{m_1,m_2} \langle SMj_1j_2|j_1m_1j_2m_2\rangle \times B^{\dagger}_{(ij)j_1m_1} B^{\dagger}_{(kl)j_2m_2} \ , \tag{6}$$

and that, in general,

$$\{B^{\dagger}_{(i_1,\ldots,i_p)\sigma_1,\ldots,\sigma_p}\} = \{C^{SM\lambda}_{\sigma_1,\ldots,\sigma_N}\}\{B^{\dagger}_{(i_1,\ldots,i_p)SM\lambda}\} \ , \tag{7}$$

where $\{C^{SM\lambda}_{\sigma_1,\ldots,\sigma_N}\}$ is a unitary matrix. Thus

$$\begin{aligned} {}^{p}E^{ij,\ldots}_{ab,\ldots} &\equiv \sum_{SM\lambda} B^{\dagger}_{(ij,\ldots)SM\lambda} B_{(ab,\ldots)SM\lambda} \\ &\equiv \sum_{\sigma_1,\ldots,\sigma_p} B^{\dagger}_{(ij,\ldots)\sigma_1,\ldots,\sigma_p} B_{(ab,\ldots)\sigma_1,\ldots,\sigma_p} \ , \end{aligned} \tag{8}$$

where λ labels different spin functions corresponding to a given S and M.

D. Spin-independent many-body Hamiltonian and the 4-SRH matrix written in terms of these operators

The many-body Hamiltonian operator $\hat{H}$ takes the following form when written in terms of 2-RDO operators:

$$\hat{H} = \tfrac{1}{2} \sum_{i,j,k,l} \{ij|kl\}\, {}^{2}E^{ik}_{jl} \ , \tag{9}$$

where the symbol $\{ij|kl\}$ represent generalized two-electron integrals, defined previously,[3] which are referred to hereafter as electronic integrals.

Following the rules given previously,[1,3,17] the 4-SRH elements take the form

$$H^{prtw}_{qsuv} = \frac{1}{2!4!} \sum_{i,j,k,l} \{ij|kl\} \langle {}^{2}E^{ik}_{jl}\, {}^{4}E^{prtw}_{qsuv} \rangle \ , \tag{10}$$

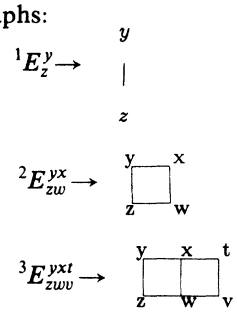
where the angular brackets $\langle\ \rangle$ are a shorthand notation for $\sum_{\Lambda}\langle\Lambda|\ |\Lambda\rangle$ where $|\Lambda\rangle$ are eigenfunctions of $\hat{S}^2$ and $\hat{S}_z$ in the N-electron space. They define a spin-adapted subspace of the N-fold tensorial product of a $2K$-dimensional one-electron space.

The values of traces such as those appearing in (10) depend only upon N (number of electrons), K (number of orbitals), and S (total spin).[3] In the next section we will consider how to transform a product of RDO's to a sum of single RDO's.

III. A GRAPHICAL REPRESENTATION OF PRODUCTS OF RDO'S

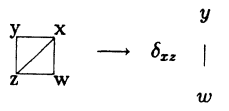
A product of RDO's yields a linear combination of single RDO's.[11,12] Except for the highest-order term, every other RDO is multiplied by one or more Kronecker δ's. The indices labeling these δ's and the RDO's have different ordering in each term. This is what renders it too complex to be applied when many indices appear. In this section a simple graphical technique is described to overcome this difficulty.

We start by representing the RDO's by the following graphs:



(11)

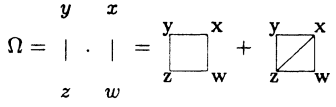
and so on. Now, by a diagonal line we mean a Kronecker δ involving the two indices linked by this line. Thus



(12)

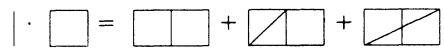
Let us see how this works in the simplest example of RDO's products:

$$\Omega = E^{y}_{z} \cdot E^{x}_{w} = E^{yx}_{zw} + \delta_{xz} E^{y}_{w} \ ,$$

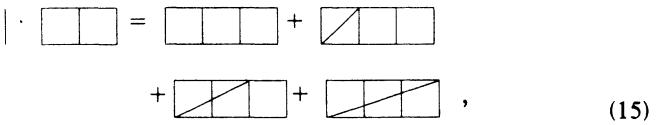


(13)

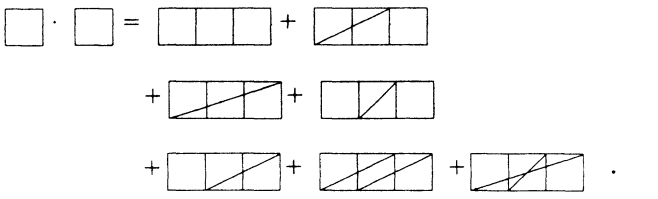
Let us now see a series of examples which will give the general rule. The indices are obviously not needed because their places in the diagrams are always the same. Thus we omit them:



(14)



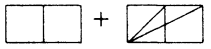
(15)



(16)

Note that as no index appears simultaneously in more than one δ, all graphs can be superimposed into a single one. We will show it in two steps. Thus

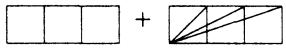
Eq. (14)=



and since one ${}^3E$ and two ${}^2E\cdot\delta$ terms must appear, it can be further contracted into

In the same way,

Eq. (15)=



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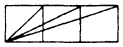
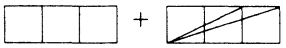
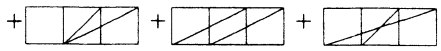


Eq. (16)=





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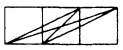


Thus all the terms are created by linking annihilator vertices of the operator on the left to the different creators of the operator on the right with zero, one, two, etc. δ lines. Each Kronecker δ reduces by 1 the order of the RDO. The annihilator index below the creator one, which disappears by contraction, takes the place of the annihilator, which also disappears [see, for instance, Eq. (13)]. In this way the multiplication of RDO's becomes a routine and it may easily be programmed.

Once the products of RDO's are converted into a sum of single RDO's, the next step is to evaluate their traces. Let us start by recalling the following properties of these traces:[3] (a)

$$\langle {}^pE^{ijk,\ldots,r}_{tux,\ldots,s}\rangle \equiv \langle {}^pE^{jk,\ldots,ri}_{ux,\ldots,st}\rangle \equiv \langle {}^pE^{ikr,\ldots,j}_{txs,\ldots,u}\rangle \cdots . \quad (17)$$

(b) As a whole, the set of creator indices $\{i,j,k,\ldots,r\}$ must be the same as the annihilators one $\{t,u,x,\ldots,s\}$, otherwise the trace will be zero. In what follows, this is always assumed. Because of these properties only three main cases appear: (i) the RDO is a diagonal operator, i.e., the order of the creator and of the annihilator indices is the same; (ii) all the indices appearing simultaneously in the creator and annihilator sets are different and the ordering of indices in both sets is different; (iii) a similar case to (ii) but when some of the indices are repeated.

Case (i) has been satisfactorily solved previously.[3,9] Therefore in the next two sections we will study cases (ii) and (iii), respectively.

IV. TRACES OF OPERATORS HAVING INDICES WITHOUT ANY REPETITION

Here we will describe an efficient technique to obtain the value of traces of any RDO without repetition of indices, while in Sec. V we will describe the last case. Let us start by enumerating a series of general properties that the spin-dependent RDO's and state operators, or their traces, possess.

A. λ-independent relation

A property of traces is that

$$\langle B^\dagger_{(1,\ldots,n)\hat{P}(\sigma_1,\ldots,\sigma_n)} B_{(1,\ldots,n)\hat{P}(\sigma_1,\ldots,\sigma_n)}\rangle = \langle B^\dagger_{(1,\ldots,n)\hat{Q}(\sigma_1,\ldots,\sigma_n)} B_{(1,\ldots,n)\hat{Q}(\sigma_1,\ldots,\sigma_n)}\rangle , \quad (18)$$

where $\hat{P},\hat{Q}\in S_n$. (Note that the ordering of the orbital labels does not need to be the same in the creator and in the annihilator.) Equation (18) implies that

$$\langle B^\dagger_{(1,\ldots,n)\hat{P}(SM\lambda_i)} B_{(1,\ldots,n)\hat{P}(SM\lambda_i)}\rangle = \langle B^\dagger_{(1,\ldots,n)\hat{Q}(SM\lambda_i)} B_{(1,\ldots,n)\hat{Q}(SM\lambda_i)}\rangle . \quad (19)$$

Now, bearing in mind that for a pair of quantum numbers S and M the set of $|SM\lambda_i\rangle$ spin functions is a basis of an irreducible representation of S_n, we get

$$\hat{P}|SM\lambda_i\rangle = \sum_j \Gamma(P)_{ij}|SM\lambda_j\rangle .$$

Let us now rewrite, as an example, Eq. (19) for the particular values $i=1$; $\hat{P}$ is the identity; operator $\hat{Q}$ is an operation such that all the elements of its matrix representation of a_{1j} type are zero for $j\neq 1,2$ (as, for instance, $\hat{Q}=(34)$ for [3,1] irreducible representation of S_4, $\hat{Q}=(13)$ for $[2,1^2]$ of S_4, $\hat{Q}=(45)$ for [4,1] of S_5, etc.[18]). With this choice, Eq. (19) becomes

$$\langle B^\dagger_{(1,\ldots,n)SM\lambda_1} B_{(1,\ldots,n)SM\lambda_1}\rangle = \Gamma(\hat{Q})^2_{11}\langle B^\dagger_{(1,\ldots,n)SM\lambda_1} B_{(1,\ldots,n)SM\lambda_1}\rangle + \Gamma(\hat{Q})^2_{12}\langle B^\dagger_{(1,\ldots,n)SM\lambda_2} B_{(1,\ldots,n)SM\lambda_2}\rangle , \quad (20)$$

where $\Gamma(\hat{Q})^2_{11}+\Gamma(Q)^2_{12}=1$. It can be rewritten as

$$\langle B^\dagger_{(1,\ldots,n)SM\lambda_1} B_{(1,\ldots,n)SM\lambda_1}\rangle = \langle B^\dagger_{(1,\ldots,n)SM\lambda_2} B_{(1,\ldots,n)SM\lambda_2}\rangle . \quad (21)$$

The previous proof is not a particular case. Indeed, it can be repeated for any given pair (λ_1,λ_3), (λ_1,λ_4),..., etc. Therefore Eq. (21) says that the trace is λ independent.

B. Freezing relation

Let us consider a trace

$$\langle B^{\dagger}_{12;0,0}\hat{O}_{(3,4,5,\ldots)}B_{12;0,0}\rangle_{N,K} , \tag{22}$$

where N is the number of electrons of the states over which the trace is performed, K is the number of orbitals from which these states are built, and $\hat{O}_{(3,4,5,\ldots)}$ is any operator involving $3,4,5,\ldots$ indices. It can easily be proved that

$$E_{12}E_{21}-(E_{11}-E_{22})E_{11} \equiv (E_{11}-1)E_{11}+2B^{\dagger}_{12;0,0}B_{12;0,0} . \tag{23}$$

Therefore, because of Eq. (19) and Eq. (49) in (Ref. 3),

$$\langle B^{\dagger}_{12;0,0}B_{12;0,0}\hat{O}_{(3,4,5,\ldots)}\rangle = \tfrac{1}{2}\langle E_{11}(E_{11}-1)\hat{O}_{(3,4,5,\ldots)}\rangle . \tag{24}$$

But $E_{11}^2-E_{11}$ means that orbital 1 is doubly occupied. Therefore the right-hand side of Eq. (24) becomes

$$\tfrac{1}{2}\langle E_{11}(E_{11}-1)\hat{O}_{(3,4,5,\ldots)}\rangle=\langle \hat{O}_{(3,4,5,\ldots)}\rangle_{N-2,K-1} . \tag{25}$$

Hence

$$\langle B^{\dagger}_{12;0,0}\hat{O}_{(3,4,\ldots)}B_{12;0,0}\rangle_{N,K}=\langle \hat{O}_{(3,4,\ldots)}\rangle_{N-2,K-1} . \tag{26}$$

C. A useful *character* relation

Let us consider a trace

$$\left\langle \sum_{\lambda_1} B^{\dagger}_{(ijk,\ldots)SM\lambda_1}B_{(kli,\ldots)SM\lambda_1}\right\rangle , \tag{27}$$

where the spin part is the same in both operators, but the space indices have different ordering, and the sum does not run over S and M but just λ. Let us also take into account the relation

$$B_{(jnk,\ldots)SM\lambda_1}=B_{\hat{P}(j,k,\ldots,n)SM\lambda_1} =(-1)^p B_{(j,k,\ldots,n)\hat{P}(SM\lambda_1)} , \tag{28}$$

which is due to the fact that except for the factor $(-1)^p$, it is equivalent to interchange the spin or the orbital labels. (This is a consequence of the duality of the irreducible representations of which the spin and the space parts of a fermion function constitute a basis.)

Then we may write Eq. (27) as

$$\left\langle \sum_{\lambda_1} B^{\dagger}_{(ijk,\ldots)SM\lambda_1}B_{(kli,\ldots)SM\lambda_1}\right\rangle = \sum_{\lambda_1\lambda_2}\langle B^{\dagger}_{(ijk,\ldots)SM\lambda_1}B_{(ijk,\ldots)SM\lambda_2}\rangle \times\Gamma^S(\hat{P})_{\lambda_1\lambda_2}(-1)^p . \tag{29}$$

Note that the traces do not depend on λ_i, but they vanish unless $\lambda_1=\lambda_2$. Hence we have Eq. (29) identically equal to

$$(-1)^p\langle B^{\dagger}_{(ijk,\ldots)SM\lambda_0}B_{(ijk,\ldots)SM\lambda_0}\rangle\sum_{\lambda_1}\Gamma^S(\hat{P})_{\lambda_1\lambda_1} , \tag{30}$$

which gives the important character χ relation

$$\left\langle \sum_{\lambda_1} B^{\dagger}_{(ijk,\ldots)SM\lambda_1}B_{(kli,\ldots)SM\lambda_1}\right\rangle =(-1)^p\chi^S(P)\langle B^{\dagger}_{(ijk,\ldots)SM\lambda_0}B_{(ijk,\ldots)SM\lambda_0}\rangle . \tag{31}$$

V. TRACES OF THE q-ORDER REDUCED-DENSITY OPERATORS

We shall now apply these relations to evaluating traces of an arbitrary q-RDO

$$\langle {}^qE^{ijk,\ldots}_{lkj,\ldots}\rangle=\langle {}^qE^{ijk,\ldots}_{\hat{P}(ikj,\ldots)}\rangle=\left\langle \sum_{SM\lambda} B^{\dagger}_{(ijk,\ldots)SM\lambda}B_{\hat{P}(ijk,\ldots)SM\lambda}\right\rangle =(-1)^p\sum_S\chi^S(P)\left\langle \sum_{|M|<S} B^{\dagger}_{(ijk,\ldots)SM\lambda_0}B_{ijk,\ldots,SM\lambda_0}\right\rangle . \tag{32}$$

As we know how to evaluate the trace of ${}^qE$ when it is diagonal,[11,12] let us write

$$\chi^S(P)=\chi^S(E)+[\chi^S(P)-\chi^S(E)] , \tag{33}$$

where $\chi(E)$ is the character of the identity operator. Then,

$$\langle {}^qE^{ijk,\ldots}_{lkj,\ldots}\rangle=(-1)^p\left[\langle {}^qE^{ijk,\ldots}_{ijk,\ldots}\rangle+\sum_{S,M}[\chi^S(P)-\chi^S(E)]\langle B^{\dagger}_{(ijk,\ldots)SM\lambda_0}B_{(ijk,\ldots)SM\lambda_0}\rangle\right] . \tag{34}$$

For the maximum value of S the spin functions are totally symmetric and hence all the characters are equal to 1. So the contribution to Eq. (34) of $S_{\max}$ is null.

What we shall do now is to use, in an alternate and systematic way, relations Eqs. (21), (26), and (31). Thus, denoting

$$c_q^S=\chi(P)-\chi(E) , \tag{35}$$

we rewrite Eq. (34) as

$$\langle {}^{q}E^{ijk,\cdots}_{lkj,\cdots}\rangle=(-1)^{p}\left[\langle {}^{q}E^{ijk,\cdots}_{ijk,\cdots}\rangle_{N,K}+\sum_{S}^{S_{\max}-1}c_q^{S}\left\langle\sum_{M}B^{\dagger}_{(ijk,\ldots)SM\mu_0}B_{(ijk,\ldots)SM\mu_0}\right\rangle_{N,K}\right]. \tag{36}$$

The first trace is

$$\langle {}^{q}E^{ijk,\cdots}_{ijk,\cdots}\rangle=\langle n_1n_2n_3\cdots n_q\rangle_{N,K}\ . \tag{37}$$

This relation has been obtained previously.[3,9]

Now let us consider

$$T_1=\sum_{S}^{S_{\max}-1}c_q^{S}\left\langle\sum_{M}B^{\dagger}_{(ijk,\ldots)SM\mu_0}B_{(ijk,\ldots)SM\mu_0}\right\rangle\ . \tag{38}$$

Because the term $S_{\max}$ does not exist, we may always express T_1 as

$$T_1=\sum_{S}^{S_{\max}-1}c_q^{S}\left\langle B^{\dagger}_{ij;0,0}\sum_{M}B^{\dagger}_{(kl,\ldots)SM\gamma_0}B_{(kl,\ldots)SM\gamma_0}B_{ij;0,0}\right\rangle\ ,$$

and because of the freezing relation Eq. (26),

$$T_1=\sum_{S}^{S_{\max}-1}c_q^{S}\left\langle\sum_{M}B^{\dagger}_{(kl,\cdots)SM\gamma_0}B_{(kl,\cdots)SM\gamma_0}\right\rangle_{N-2,K-1}\ . \tag{39}$$

Let us now multiply and divide this term by the $c_q^{S_{\max}-1}$. In this way, when $\mathcal{S}=S_{\max}-1$, the coefficient in front of the trace becomes 1. Then we apply again Eq. (33) and we get

$$\begin{aligned}T_1&=c_q^{S_{\max}-1}\left[\langle {}^{(q-2)}E_{\text{diagonal}}\rangle+\sum_{S}^{S_{\max}-1}\left[\frac{c^{\mathcal{S}}}{c_q^{S_{\max}-1}}-c_{q-2}^{\mathcal{S}_{\max}}\chi^{\mathcal{S}}(E)\right]\langle B^{\dagger}\cdots B\cdots\rangle_{N-2,K-1}\right]\\&=c_q^{S_{\max}-1}(\langle {}^{(q-2)}E_{\text{diagonal}}\rangle+T_2)\ ,\end{aligned} \tag{40}$$

and we can see how a new sum T_2 appears. This procedure can be pursued up to the last term, which is always either $\langle E_{ii}\rangle$ or $\langle I\rangle$. The trace of unity is equal to the dimension of the space.

All this process seems to be complicated. However, by using Table I in which all these steps have been summarized, it becomes a trivial task. Table I is built up to S_6, which is what is needed for the construction of the 4-HRS, but it can be easily expanded for higher orders. We have used in the first column of Table I the standard notation for the group classes.[18] In order to learn how to use this table, let us calculate the trace $\langle {}^{4}E^{1234}_{2314}\rangle$ as an example. The ordering of annihilators can be written as

$$2314=(1\hat{2}3)1234\ ,$$

where (123) is the simultaneous permutation of three indices and belongs to class [3]. Therefore from Table I we know that 1 and -3 are the coefficients multiplying the traces of ${}^{4}E$ and ${}^{2}E$, respectively. Consequently,

$$\begin{aligned}\langle {}^{4}E^{1234}_{2314}\rangle&=\langle {}^{4}E^{1234}_{1234}\rangle_{N,K}-3\langle E^{12}_{12}\rangle_{N-2,K-1}\\&=\langle n_1n_2n_3n_4\rangle_{N,K}-3\langle n_1n_2\rangle_{N-2,K-1}\ .\end{aligned}$$

This example shows clearly how trivial the calculation of RDO's traces becomes when all indices are different. In the next section we will show how to transform the case of repeated indices into this one.

TABLE I. Linear combination coefficients linking traces of the diagonal RDO's with the traces of nondiagonal RDO's.

Class \ Order	n	$n-2$	$n-4$	$n-6$
[1]	1			
[2]	−1	2		
[3]	1	−3		
[2^2]	1	−4	4	
[4]	−1	4	−2	
[2,3]	−1	5	−6	
[5]	1	−5	5	
[2^3]	−1	6	−12	8
[2,4]	1	−6	10	−4
[3^2]	1	−6	9	0
[6]	−1	6	−9	2

VI. TRACES OF RDO'S WITH REPEATED INDICES

In what follows we show how to express a trace of a RDO having one or several equal index labels in terms of traces of RDO's without repeated labels. For clarity this section is subdivided into two subsections.

A. Description of graphs

It is well known that due to the Pauli principle a given orbital index cannot appear more than twice in the crea-

tor or annihilator set of a RDO. A label that appears twice in the set of annihilator (or creator) indices corresponds to a doubly occupied orbital. We also know that RDO's with nonzero traces must have the same sets of the creator and annihilator indices.

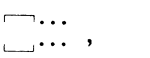
Another property of the RDO's that we apply is

$$E^{ijkl,\cdots}_{abcd,\cdots} \equiv E^{iklj,\cdots}_{acdb,\cdots} \ . \tag{41}$$

That is, we may change simultaneously the positions of a creator and its corresponding annihilator in the double string of indices.

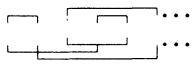
All these properties are at the basis of the graphic technique described in the three following paragraphs.

(a) The first type of RDO that will be considered is of the type $E^{ii,\cdots}_{ii,\cdots}$. We represent this operator by the graph



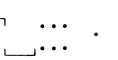
(42)

where every creator repeated index has as a partner an annihilator index which is also repeated *even if it is not the same label.* Another illustration of this type of RDO and corresponding graph might be, for instance,

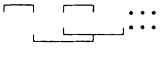
$E^{iijkkj,\cdots}_{ijkikj,\cdots} \rightarrow$  (43)

We call this kind of graph *a closed loop* and it is characterized by having *no loose ends.*

(b) The second type will have *two loose ends* corresponding to an annihilator and to a creator appearing only once in the string but whose partners are repeated indices. The simplest example of this type of RDO is

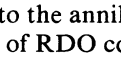
$E^{iil,\cdots}_{kii,\cdots} \rightarrow$  (44)

A more complex example of this kind is

$E^{iijjk,\cdots}_{lijij,\cdots} \rightarrow$  (45)

We call this type of graph *open opposite loop* and it has *two loose ends,* one corresponding to the creator string and the other one to the annihilator string.

(c) The last type of RDO considered is

$E^{iikl}_{pvii} \rightarrow$  (46)

Clearly here we have *four loose ends.* Two of them correspond to the creator string and the two others to the annihilator string. We call this kind of graph *parallel open loop.* Another more complex example is

$E^{iijjkklm,\cdots}_{tiijjvkk,\cdots} \rightarrow$  (47)

All the RDO's that may occur are combination of these three types. Therefore what we need now is to learn how to evaluate quickly these three kinds of traces.

Finally, by using Eq. (41) it becomes obvious that all loops belonging to the same type (closed, opposite, or parallel open) and having the same number of indices represent the same RDO. So, we can choose always the following kind of pictures for the RDO (it reminds a crenel):

closed loop 

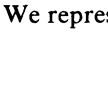
opposite open loop 

parallel open loop 

B. Computing the traces of these RDO's

1. Closed loops

The closed loop



$$\Rightarrow \sum_{\sigma} b^{\dagger}_{1\sigma} b^{\dagger}_{1\bar{\sigma}} \left[\sum_{\sigma_2} b^{\dagger}_{i\sigma_2} \cdots b_{k\sigma_2} \right] b_{1\bar{\sigma}} b_{1\sigma}$$

$$\equiv 2B^{\dagger}_{11;0,0}(E^{ij,\cdots}_{kl,\cdots}) B_{11;0,0} \ , \tag{48}$$

and its trace is

$$= 2\langle B^{\dagger}_{11;0,0} B_{11;0,0} E^{ij,\cdots}_{kl,\cdots} \rangle$$

$$= 2(-1)^0 \langle E^{ij,\cdots}_{kl,\cdots} \rangle_{N-2,K-1} \ . \tag{49}$$

Let us consider another example of this kind of loop:

$$\Rightarrow \sum_{\sigma} b^{\dagger}_{1\sigma} b^{\dagger}_{1\bar{\sigma}} b^{\dagger}_{2\sigma} b^{\dagger}_{2\bar{\sigma}} \left[\sum_{\sigma_2} b^{\dagger}_{i\sigma_2} \cdots b_{k\sigma_2} \right] b_{2\bar{\sigma}} b_{1\sigma} b_{1\bar{\sigma}} b_{2\sigma}$$

$$= 2B^{\dagger}_{11;0,0} B^{\dagger}_{22;0,0} (E^{ij,\cdots}_{kl,\cdots})(-B_{22;0,0} B_{11;0,0}) \ . \tag{50}$$

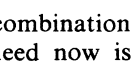
Consequently, the trace is

$$= 2(-1)^1 \langle E^{ij,\cdots}_{kl,\cdots} \rangle_{N-4,K-2} \ . \tag{51}$$

Note that the power of (-1) in these formulas coincides with the number of transpositions needed to get the ordering of the creator labels of the loop consistent with that of their annihilation labels.

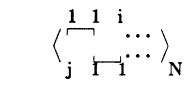
2. Opposite open loop

Let us consider

$E^{11i,\cdots}_{j11,\cdots} \Rightarrow$ 

$$= \sum_{\sigma} b^{\dagger}_{1\sigma} b^{\dagger}_{1\bar{\sigma}} b^{\dagger}_{i\sigma} \left[\sum \cdots \right] b_{1\sigma} b_{1\bar{\sigma}} b_{j\sigma}$$

$$= B^{\dagger}_{11;0,0} \sum_{\sigma} b^{\dagger}_{i\sigma} \left[\sum \cdots \right] b_{j\sigma} (-B_{11;0,0}) \ , \tag{52}$$



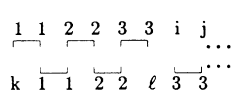
$$=(-1)^{1}\langle E^{i,\cdots}_{j,\cdots}\rangle_{N-2,K-1}\ . \tag{53}$$

The power of (-1) is again equal to the number of transpositions needed to get the same order of the creator and annihilator labels in the loop: $P_{13}(j11)=11j$.

3. *Parallel open loop*

A sufficiently general example for this last case is

$E^{112233ij}_{k1122l33}=$

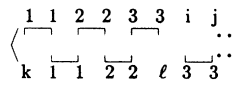


$$=\sum_{\sigma} B^{\dagger}_{11;0,0}B^{\dagger}_{22;0,0}B^{\dagger}_{33;0,0}(b^{\dagger}_{i\sigma}b^{\dagger}_{j\bar{\sigma}}B_{33;0,0}-b^{\dagger}_{i\bar{\sigma}}b^{\dagger}_{j\sigma}B_{33;0,0})b_{l\bar{\sigma}}(-B_{22;0,0})(-B_{11;0,0})b_{k\sigma}$$

$$=B^{\dagger}_{11;0,0}B_{11;0,0}B^{\dagger}_{22;0,0}B_{22;0,0}B^{\dagger}_{33;0,0}B_{33;0,0}\sum_{\sigma}b^{\dagger}_{i\sigma}b^{\dagger}_{j\bar{\sigma}}(b_{l\bar{\sigma}}b_{k\sigma}+b_{k\bar{\sigma}}b_{l\sigma})$$

$$=B^{\dagger}_{11;0,0}\cdots B_{33;0,0}\sum_{\sigma_1\sigma_2}b^{\dagger}_{i\sigma_1}b^{\dagger}_{j\sigma_2}(b_{l\sigma_2}b_{k\sigma_1}+b_{k\sigma_2}b_{l\sigma_1})\ . \tag{54}$$

Then we get



$$=(-1)^{4}\langle E^{ij,\cdots}_{kl,\cdots}+E^{ij,\cdots}_{lk,\cdots}\rangle_{N-6,K-3}\ . \tag{55}$$

The power of (-1) is now 4 because $P_{68}P_{57}P_{35}P_{13}(k1122l33)=112233lk$ and four transpositions are needed.

In summary, this diagramatic technique transforms immediately the traces of RDO's with repeated labels into traces of other RDO's containing only nonrepeated labels (but computed in a subspace of the original spin adapted Hilbert space).

ACKNOWLEDGMENTS

One of us (J.P.) wishes to acknowledge the financial support of the Caja de Ahorros y Monte de Piedad de Castellón. This work has been supported by the Comisión Interministerial de Ciencia y Tecnologia (Spain) under Grant No. PB0355 and by the Polish Academy of Sciences under Project No. CPBP-01-12.

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