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Traces of symmetry-adapted reduced density operators

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Abstract. Formulae are derived for traces of symmetry-adapted reduced density operators in a finite-dimensional, antisymmetric and spin-adapted space. The traces are expressed in terms of traces of products of the orbital occupation number operators.

1. Introduction

Traces of p-order reduced density operators (pRDOs) calculated in N-electron spin-adapted model spaces spanned by cartesian products of orthonormal spin-orbitals (also known as full configuration interaction spaces) are of importance in the theory of spin-adapted reduced Hamiltonians (Valdemoro 1989 and references therein), in statistical theories of spectra (Bauche and Bauche-Arnoult 1990, Karwowski 1989, Bancevicz *et al* 1989, Karwowski and Bancewicz 1987) and also in computational approaches to many-electron system theory (Diercksen and Karwowski 1987). Similar kinds of traces are also needed to calculate the propagation coefficients in the statistical theory of nuclear spectra (Brody *et al* 1981, Ginocchio 1973, Nomura 1985, 1986). Traces of certain kinds of the reduced density and related operators were recently calculated by Karwowski *et al* (1986), Karwowski and Bancewicz (1987), Karwowski (1989), Duch (1989), Nomura (1988), Karwowski and Valdemoro (1988). The most complete work on this subject, where traces of arbitrary pRDOs have been expressed in terms of traces of the occupation number operators was published by Planelles *et al* (1990a).

In several areas of theory of N-electron systems, including many-body perturbation theory, the coupled cluster method (Kutzelnigg 1985) and the theory of spin-adapted reduced Hamiltonians (Lain *et al* 1988, Planelles *et al* 1990a) permutation-symmetry-adapted pRDOs are of importance. In this note a method of calculation traces of the symmetry-adapted pRDOs is presented.

2. Symmetry-adapted pRDOs

A primitive pRDO is defined as (Kutzelnigg 1985)

$$ {}^{p}E^{i_1 i_2 \ldots i_p}_{a_1 a_2 \ldots a_p} = \sum_{\sigma_1 \sigma_2 \ldots \sigma_p} b^{+}_{i_1\sigma_1} b^{+}_{i_2\sigma_2} \ldots b^{+}_{i_p\sigma_p} b_{a_p\sigma_p} \ldots b_{a_2\sigma_2} b_{a_1\sigma_1} \tag{1} $$

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where $b^+_{i\sigma}/b_{i\sigma}$ are the Fermion creation/annihilation operators. Alternatively, the pRDO may be expressed in terms of the spin-adapted p-electron creation and annihilation operators (Planelles *et al* 1990a)

$$ {}^{p}E^{\alpha}_{\alpha} = \sum_{J=J_{\min}}^{J=J_{\max}} \sum_{M_J=-J}^{J} \sum_{\lambda=1}^{f(S,p)} B^{+}_{\alpha,JM_J\lambda} B_{\beta,JM_J\lambda} \tag{2} $$

where α and β are strings of the orbital indices ($i_1 i_2 \ldots i_p$, and $a_1 a_2 \ldots a_p$, respectively). Each of the strings consists of p indices. Some of them appear once in a string and they are referred to as singles and some appear twice and they are referred to as doubles. The Pauli principle does not allow an index to appear more than twice. J and M_J are the total spin quantum numbers, $J_{\min} = 0, 1/2$ depending on whether p is even or odd, $J_{\max} = p/2 - q$ where q is the larger of the number of doubles in the α and β strings of the orbital labels; λ is to distinguish different independent spin couplings leading to the same J and M_J values and, $f(S, p)$ represents the number of different spin coupling schemes. The number of different spin coupling schemes is given by the Heisenberg formula

$$ f(J, p') = \frac{2J+1}{p'+1} \binom{p'+1}{p'/2 - J} \tag{3} $$

where $p' = 2J_{\max}$.

A spin-adapted p-particle creation operator acting on the vacuum state creates an antisymmetric, p-electron, spin eigenfunction corresponding to a given orbital configuration, i.e.

$$ B^{+}_{\alpha,JM_J\lambda}|0\rangle = |\alpha, JM_J\lambda\rangle. \tag{4} $$

If $\mathcal{R}$ is a permutation operator acting in the orbital space only, then

$$ \mathcal{R}|\alpha, JM_J\lambda\rangle = \sum_{\mu=1}^{f(J,p)} U^{p}_{J}(\mathcal{R})_{\mu\lambda} |\alpha, JM_J\mu\rangle \tag{5} $$

where the $U^p_J(\mathcal{R})$ matrices form an irreducible representation of $p!$ element permutation group S_p, if only singles appear in α. Otherwise $U^p_J(\mathcal{R})$ stand for appropriate blocks of these matrices (cf Pauncz 1979).

The symmetry-adapted RDOs are defined as (Kutzelnigg 1985)

$$ {}^{[J]}E^{\alpha[\mu]}_{\beta[\nu]} = \frac{f(J,p)}{p!} \sum_{\mathcal{R}\in S_p} U^{p}_{J}(\mathcal{R})_{\mu\nu} \, {}^{p}E^{\mathcal{R}\alpha}_{\beta} \tag{6} $$

where $\mathcal{R}\alpha$ means permutation of the orbitals in the string α. It may be shown by combining (2) and (4)-(6) that

$$ {}^{[J]}E^{\alpha[\mu]}_{\beta[\nu]} = \sum_{M_J=-J}^{J} B^{+}_{\alpha,JM_J\mu} B_{\beta,JM_J\nu} \tag{7} $$

and

$$ {}^{p}E^{\mathcal{R}\alpha}_{\beta} = \sum_{J=J_{\min}}^{J=J_{\max}} \sum_{\nu=1}^{f(J,p)} {}^{[J]}E^{\mathcal{R}\alpha[\nu]}_{\beta[\nu]} \tag{8} $$

where

$$ {}^{[J]}E^{\mathcal{R}\alpha[\mu]}_{\beta[\nu]} = \sum_{\lambda=1}^{f(J,p)} U^{p}_{J}(\mathcal{R})_{\lambda\mu} \, {}^{[J]}E^{\alpha[\lambda]}_{\beta[\nu]}. \tag{9} $$

3. Traces of symmetry-adapted *p*RDOs

Let us consider the trace

$$\mathrm{Tr}(J;\, \alpha\mu,\, \beta\nu)_{NK} = \sum_{A,JMk} \langle A, JMk|^{[J]}E^{\alpha[\mu]}_{\beta[\nu]}|A, JMk\rangle \tag{10}$$

where the sum runs over the N-electron basis of spin-adapted antisymmetrized products of orthonormal orbitals. K is the number of orbitals, J and M are the total spin quantum numbers, k distinguishes different spin functions of the same J M, and A stands for the orbital configuration. For more details concerning structure of this space, see e.g. Karwowski and Bancewicz (1987) and references therein. Its dimension is (Paldus 1974)

$$D(N, J, K) = \frac{2J+1}{K+1}\binom{K+1}{N/2-J}\binom{K+1}{N/2-J+1}. \tag{11}$$

Since the orbitals are assumed to be orthonormal, the traces are equal to 0 if sets α and β are not the same. In other words, a necessary condition for the trace to be different from 0 is that $\beta = \mathscr{R}\alpha$, where $\mathscr{R}$ is a permutation. Hence, (9) yields

$$\mathrm{Tr}(J;\, \alpha\mu,\, \beta\nu)_{NK} = \delta(\alpha, \beta) \sum_{\lambda=1}^{f(J,p)} U^p_J(\mathscr{R})_{\lambda\mu}\, \mathrm{Tr}(J;\, \alpha\lambda,\, \alpha\nu)_{NK} \tag{12}$$

where $\delta(\alpha, \beta) = 1$ if $\beta = \mathscr{R}\alpha$ and $\delta(\alpha, \beta) = 0$ otherwise.

As one can check, $\mathrm{Tr}(J;\, \alpha\lambda,\, \alpha\lambda)_{NK}$ is λ independent (cf Planelles *et al* 1990a). In order to proof this property let consider the identity

$$\mathrm{Tr}(J;\, \alpha\lambda,\, \alpha\lambda)_{NK} = \frac{1}{p!} \sum_{\mathscr{R}\in S_p} \mathscr{R}\, \mathrm{Tr}(J;\, \alpha\lambda,\, \alpha\lambda)_{NK} \tag{13}$$

where $\mathscr{R}$ acts on all orbitals in the RDO. The right-hand side of this equation may be transformed using (10), (5), (7), (9) and the orthogonality relation for irreducible representation matrices. Finally we obtain

$$\mathrm{Tr}(J;\, \alpha\lambda,\, \alpha\lambda)_{NK} = \frac{1}{f(J, p)} \sum_{\mu=1}^{f(J,p)} \mathrm{Tr}(J;\, \alpha\mu,\, \alpha\mu)_{NK}. \tag{14}$$

Since the right-hand side of this equation is λ independent, we can write

$$\mathrm{Tr}(J;\, \alpha\lambda,\, \alpha\lambda)_{NK} = \mathrm{Tr}(J, \alpha)_{NK}. \tag{15}$$

Equation (15) states, that in the matrix $\mathrm{Tr}(J;\, \alpha\lambda,\, \alpha\nu)_{NK}$ with rows/columns numbered by λ/ν all diagonal elements are the same. This property remains valid independently of the representation chosen, i.e. independently of a unitary transformation of the matrix. Therefore the matrix $\mathrm{Tr}(J;\, \alpha\lambda,\, \alpha\nu)_{NK}$ must be a scalar matrix, i.e.

$$\mathrm{Tr}(J;\, \alpha\lambda,\, \alpha\nu)_{NK} = \delta_{\lambda\nu}\, \mathrm{Tr}(J, \alpha)_{NK} = \frac{\delta_{\lambda\nu}}{f(J, p)} \sum_{\lambda=1}^{f(J,p)} \mathrm{Tr}(J;\, \alpha\lambda,\, \alpha\lambda)_{NK}. \tag{16}$$

Substituting the last result into (12) we get

$$\mathrm{Tr}(J;\, \alpha\mu,\, \beta\nu)_{NK} = \delta(\alpha, \beta)\, U^p_J(\mathscr{R})_{\nu\mu}\, \mathrm{Tr}(J, \alpha)_{NK}. \tag{17}$$

The structure of the last equation is similar to that of the Wigner–Eckart theorem. The trace of a symmetry-adapted RDO is factorized in such a way that all the information connected with the specific symmetry properties is carried by a universal coefficient

$(U_J^p(\mathscr{R})_{\nu\mu}$ in (17), the Clebsch-Gordan coefficient in the Wigner-Eckart theorem) while the remaining factor contains information about the system under consideration ($\mathrm{Tr}(J,\alpha)_{NK}$—the reduced matrix element).

Taking trace of (8) with $\alpha=\beta$ and $\mathscr{R}=1$ and by using (16) we have

$$\langle {}^pE^\alpha_\alpha\rangle_{N,K}=\sum_{j=J_{\min}}^{J_{\max}} f(j,p)\,\mathrm{Tr}(j,\alpha)_{NK} \tag{18}$$

where the symbol $\langle\ \rangle_{N,K}$ stands for a trace in the N-electron, K-orbital model space.

According to Planelles *et al* (1990a), if there are q doubles in the string α of the orbital labels, then

$$\langle {}^pE^\alpha_\alpha\rangle_{N,K}=\langle n_1n_2\ldots n_{p'}\rangle_{N-2q,K-q} \tag{19}$$

where $p'=p-2q$, n_i, $i=1,2,\ldots p'$ are occupation number operators. Explicit formulae for traces of products of the occupation number operators have been given by Karwowski and Bancewicz (1987), Nomura (1988), Karwowski and Valdemoro (1988).

Let us come back to (18). If α contains q doubles, then $J_{\max}=p/2-q=p'/2$ and $f(j,p)$ has to be replaced by $f(j,p')$. Let us note, that $f(J_{\max},p')=1$. Thus, (18) and (19) yield

$$\mathrm{Tr}(J=J_{\max},\alpha)_{NK}=\langle n_1n_2\ldots n_{p'}\rangle_{N-2p,K-q}-\mathop{K}_{j=J_{\min}}^{J-1} f(j,p')\,\mathrm{Tr}(j,\alpha)_{N,K}. \tag{20}$$

The subsequent calculation of $\mathrm{Tr}(j,\alpha)$ is based on the fact that j is smaller than $J_{\max}$ allowed for p particles, and therefore the freezing relation (Planelles *et al* 1990a) can be used to remove from the string α singlet-coupled pairs of orbitals (i.e. two singles coupled to a singlet or a double). Thus, if there are p' singles and $(p-p')/2$ doubles in α, then (20) may be written as

$$\mathrm{Tr}(J_{\max},\alpha)_{NK}=\langle n_1n_2\ldots n_{p'}\rangle_{N-2q,K-q}-\sum_{j=J_{\min}}^{J-1} f(j,p')\,\mathrm{Tr}(j,\alpha')_{N-2q,K-q} \tag{21}$$

where α' is the string with no doubles. In particular, if α consists of doubles only, then

$$\mathrm{Tr}({}^pE^\alpha_\alpha)_{N,K}\equiv\langle {}^pE^\alpha_\alpha\rangle_{N,K}=\langle 1\rangle_{N-p,K-p/2}=D(N-p,S,K-p/2). \tag{22}$$

In order to continue computing $\mathrm{Tr}(J-1,\alpha')_{N-2q,K-q}$ we use the freezing theorem, again taking out the singlet-coupled pairs:

$$\mathrm{Tr}(J-1;\alpha')_{N-2q,K-q}=\mathrm{Tr}(J-1;\alpha'')_{N-2q-2,K-q-1}. \tag{23}$$

Then, since $J-1$ is the highest value of spin attainable for α'', by using (21) we arrive at

$$\begin{aligned}\mathrm{Tr}(J-1,\alpha'')_{N-2q-2,K-q-1}&\\ &=\langle n_1n_2\ldots n_{p'-2}\rangle_{N-2q-2,K-q-1}\\ &\quad-\sum_{j=J_{\min}}^{J-2} f(j,p'-2)\,\mathrm{Tr}(j,\alpha'')_{N-2q-2,K-q-1}.\end{aligned} \tag{24}$$

Combining together (11), (23) and (24) we get

$$\begin{aligned}\mathrm{Tr}(J,\alpha)_{N,K}&=\langle n_1n_2\ldots n_{p'}\rangle_{N-2q,K-q}-f(J-1,p')\langle n_1n_2\ldots n_{p'-2}\rangle_{N-2q-2,K-q-1}\\ &\quad-\sum_{j=J_{\min}}^{J-2}[f(j,p')-f(j,p'-2)]\,\mathrm{Tr}(j,\alpha'')_{N-2q-2,K-q-1}.\end{aligned} \tag{25}$$

The procedure is continued until it terminates after $J-J_{\min}$ steps. The final result can be expressed as

$$\mathrm{Tr}(J,\alpha)_{NK}=\sum_{i=J_{\max}-J}^{J_{\max}-J_{\min}} m_i^J\langle n_1n_2\ldots n_{p'-2i}\rangle_{N-2q-2i,K-q-i}. \tag{26}$$

An example of using the formalism is given in the appendix. Values of m_i^J coefficients for $J\leqslant 3$ are collected in table 1. The utilization of this table is quite easy. Let us take as an example the evaluation of the trace

$$T=\langle {}^{[2]}E^{123456[1]}_{123456[1]}\rangle_{N,K}.$$

In this case $J=2$, $J_{\max}=3$, $J_{\min}=0$. Then (26) reads

$$T=m_1^2\langle n_1n_2n_3n_4\rangle_{N-2,K-1}+m_2^2\langle n_1n_2\rangle_{N-4,K-2}+m_3^2\langle 1\rangle_{N-6,K-3}.$$

Taking the corresponding m_i^J values from $J=2$ row of table and using (22) we get

$$T=\langle n_1n_2n_3n_4\rangle_{N-2,K-1}-3\langle n_1n_2\rangle_{N-4,K-2}+D(N-6,J,K-3).$$

Table 1. Values of m_i^J coefficients, $r=J-J_{\min}$.

$J(\downarrow)i(\rightarrow)$	r	$r-1$	$r-2$	$r-3$
0	1			
$\frac{1}{2}$	1			
1	−1	1		
$\frac{3}{2}$	−2	1		
2	1	−3	1	
$\frac{5}{2}$	3	−4	1	
3	−16	6	−5	1

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Appendix. An example

As an illustration of the described formalism, let us calculate trace of ${}^{[2]}E^{1234[1]}_{1234[1]}$. According to (8)

$${}^{[2]}E^{1234[1]}_{1234[1]}={}^4E^{1234}_{1234}-\sum_{\nu=1}^{3}{}^{[1]}E^{1234[\nu]}_{1234[\nu]}-\sum_{\nu=1}^{2}{}^{[0]}E^{1234[\nu]}_{1234[\nu]}.$$

Equations (16) and (19) yield

$$\mathrm{Tr}({}^{[2]}E^{1234[1]}_{1234[1]})=\langle n_1n_2n_3n_4\rangle_{N,K}-3\,\mathrm{Tr}(1;1234)_{N,K}-2\,\mathrm{Tr}(0;1234)_{N,K}.$$

Now, from the freezing relation (Planelles *et al* 1990a) we have

$$\mathrm{Tr}(1;1234)_{N,K}=\mathrm{Tr}(1;12)_{N-2,K-1}$$

and

$$\mathrm{Tr}(0;\,1234)_{N,K} = D(N-4, J, K-2).$$

Again using (8) we obtain

$$\mathrm{Tr}(1;\,12)_{N-2,K-1} = \langle n_1 n_2 \rangle_{N-2,K-1} - D(N-4, J, K-2).$$

Finally,

$$\mathrm{Tr}({}^{[2]}E^{1234[1]}_{1234[1]}) = \langle n_1 n_2 n_3 n_4 \rangle_{N,K} - 3\langle n_1 n_2 \rangle_{N-2,K-1} + 2D(N-4, J, K-2).$$

Explicit expressions for $\langle n_1 n_2 n_3 n_4 \rangle_{N,K}$ and $\langle n_1 n_2 \rangle_{N-2,K-1}$ are given by Karwowski and Valdemoro (1988).

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