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Traces of the reduced density operators revisited: closed-form formulae

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Abstract. Closed-form expressions for traces of the qth-order reduced density operators, q-RDOs, and symmetry-adapted q-RDOs calculated in an N-electron and spin-adapted subspace of a K-orbital Fock space are derived. The asymptotic form of the expression for traces of the q-RDOs, corresponding to $K \gg N$ and $K \gg N \gg q$ limits, is discussed in detail. Several identities fulfilled by some quantities related to the traces are derived.

1. Introduction

The qth-order reduced density operators (q-RDOs) [1] (also referred to as the excitation operators [2], the replacement operators [3] and, in the case of $q = 1$, the unitary group generators [4]) and their traces belong to the most helpful tools in designing algorithms for the evaluation of matrix elements and averages in many areas of the N-electron system theory, such as for instance: in the statistical theory of electronic spectra [5], in the theory of spin-adapted reduced Hamiltonians [6], in some computational approaches [7], in the statistical theory of nuclear spectra [8] and in computational methods of quantum chemistry [2]. Discussion of some properties of these operators and of their traces calculated in the N-electron and spin-adapted (i.e. spanned by eigenfunctions of the total spin operators $\widehat{S^2}$ and $\widehat{S_z}$ corresponding to a fixed pair of their eigenvalues, S and M respectively) subspaces $\mathcal{H}^A(K, N, S)$ of a K-orbital Fock space may be found in [5], [9–16]. In particular two relations in which traces of q-RDOs and traces of symmetry-adapted q-RDOs are expressed as linear combinations of traces of the occupation number operators have been reported in [13] and [14], respectively. The coefficients of these combinations have been determined through rather complicated recurrence relations. In this paper we present a surprisingly simple, closed-form formula for the coefficients. As a consequence, several properties of the traces, in particular in their asymptotic limit of $K \gg N$ and $K \gg N \gg q$ are also derived.

2. Traces of q-RDOs

The trace of a q-RDO in $\mathcal{H}^A(K, N, S)$ may be expressed as [13]§

$$\mathrm{Tr}({}^qE^{12\ldots q}_{\mathcal{P}(12\ldots q)}) = \varepsilon(\mathcal{P}) \sum_{k=0}^{t} c_k^q(\mathcal{P}) W_{q-2k}(k) \tag{1}$$

§ In table 1 of [13] $\varepsilon(\mathcal{P})$ is included in the definition of $c_k^q(\mathcal{P})$.

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where $\mathcal{P} \in S_q$ is a permutation belonging to the $q!$-element symmetric group S_q, $\varepsilon(\mathcal{P}) = \pm 1$ is its parity,

$$t = \begin{cases} \frac{1}{2}s & \text{if } s \text{ is even} \\ \frac{1}{2}(s-1) & \text{if } s \text{ is odd} \end{cases} \tag{2}$$

s is the number of indices affected by $\mathcal{P}$, $c_k^q(\mathcal{P})$ is a K- and N-independent integer and

$$W_q(k) = \langle n_1 n_2 \ldots n_q \rangle_{S,N-2k,K-k} \tag{3}$$

denotes a trace of a product of the orbital occupation number operators

$$n_1 \cdot n_2 \cdot \ldots \cdot n_q \equiv {}^qE^{12\ldots q}_{12\ldots q} \tag{4}$$

in $\mathcal{H}^A(K-k, N-2k, S)$. This trace may be expressed according to (17) of [12] or (24) of [9] as

$$W_q(k) = \sum_{j=0}^{[q/2]} A_j(N-2k, q) \frac{(K-k-q)!}{(K-k-j)!} D(S, N-2k-2j, K-k-j) \tag{5}$$

where

$$A_j(N, q) = (-1)^j \frac{q!(N-2j)!}{j!(q-2j)!(N-q)!} \tag{6}$$

and

$$D(S, N, K) = \frac{2S+1}{K+1} \begin{pmatrix} K+1 \\ N/2-S \end{pmatrix} \begin{pmatrix} K+1 \\ N/2+S+1 \end{pmatrix} \tag{7}$$

is the dimension of $\mathcal{H}^A(K, N, S)$.

In this paper we are concerned with properties of $c_k^q(\mathcal{P})$ coefficients which, for simplicity, are referred to as *the c coefficients*. In [13] the c coefficients have been determined using a recurrence procedure, which may be expressed by the following equation

$$c_k^q(\mathcal{P}) = \chi_{\mathcal{P}}^{[q-k,k]} - \sum_{i=0}^{k-1} c_i^q(\mathcal{P}) f\left(\frac{q-2k}{2}, q-2i\right) \tag{8}$$

where $\chi_{\mathcal{P}}^{[a,b]}$ is the character of the irreducible representation of S_q labelled by a two-row Young tableau with a boxes in the first row and b boxes in the second row, and

$$f(x, y) = \frac{2x+1}{y+1} \begin{pmatrix} y+1 \\ \frac{1}{2}y - x \end{pmatrix}. \tag{9}$$

Let us note that the $\mathcal{P}$-dependence of the coefficients $c_k^q(\mathcal{P})$ is defined by the appropriate irrep. characters [13]. Therefore $c_k^q(\mathcal{P})$ are the same for all permutations belonging to the same class and (8) may be rewritten as

$$c_k^q(\pi) = \chi_{\pi}^{[q-k,k]} - \sum_{i=0}^{k-1} c_i^q(\pi) f\left(\frac{q-2k}{2}, q-2i\right) \tag{10}$$

where π is the partition of q defining the appropriate class of S_q. Since $W_{q-2k}(k)$ is $\mathcal{P}$-independent, according to (1), $\mathrm{Tr}({}^qE^{12\ldots q}_{\mathcal{P}(12\ldots q)})$ also depends on the class of S_q rather than on a specific permutation.

3. A closed-form expression for the c coefficients

Let us consider $\mathrm{Tr}({}^{q}E^{12\ldots q}_{\mathcal{P}(12\ldots q)})$ with $\mathcal{P}=\mathcal{Q}\mathcal{R}$, where $\mathcal{Q}$ and $\mathcal{R}$ commute, i.e. they act on different sets of indices. The trace does not depend upon the numbers (the orbital labels) assigned to the orbitals and therefore, without any loss of generality, we may assume that $\mathcal{Q}$ acts on the first s indices and $\mathcal{R}$ acts on the remaining $q-s$ indices. Since the product of RDOs without common labels yields an RDO for which the orbital labels are the collection of the primitive RDOs labels preserving the relative ordering between creation and annihilation indices, we may write that

$$\mathrm{Tr}({}^{q}E^{12\ldots q}_{\mathcal{P}(12\ldots q)})=\mathrm{Tr}({}^{s}E^{12\ldots s}_{\mathcal{Q}(12\ldots s)}\,{}^{q-s}E^{s+1,s+2,\ldots q}_{\mathcal{R}(s+1,s+2,\ldots q)}). \tag{11}$$

The application of the prescription given in [13] to the RDOs on the right-hand side of (11) transforms the trace on the left-hand side as a linear combination of traces of occupation number operators

$$\mathrm{Tr}({}^{q}E^{12\ldots q}_{\mathcal{P}(12\ldots q)})=\varepsilon(\mathcal{P})\sum_{m_1=0}^{t_1}\sum_{m_2=0}^{t_2}c^{s}_{m_1}(\mathcal{Q})c^{q-s}_{m_2}(\mathcal{R})W_{q-2(m_1+m_2)}(m_1+m_2) \tag{12}$$

where t_1 and t_2 are defined according to (2).

Let us assume $\mathcal{R}=\mathcal{I}$, where $\mathcal{I}$ is the identity operator. Then $t_2=0$ and, since $c^{q}_{0}=1$,

$$\mathrm{Tr}({}^{q}E^{12\ldots q}_{\mathcal{P}(12\ldots q)})=\varepsilon(\mathcal{P})\sum_{m_1=0}^{t_1}c^{s}_{m_1}(\mathcal{Q})W_{q-2m_1}(m_1). \tag{13}$$

If we replace in (13) the summation index m_1 by k and remember that in this case $\mathcal{P}=\mathcal{Q}$ then, by comparing (1) and (13), we can see that

$$c^{q}_{k}(\mathcal{P})=c^{s}_{k}(\mathcal{P}) \tag{14}$$

i.e. the c coefficients are q-independent. Consequently we shall drop the superfluous superscript and write $c_k(\mathcal{P})$ rather than $c^{q}_{k}(\mathcal{P})$.

Introducing in (12) a new summation index $k=m_1+m_2$, we transform this equation into a form which is identical to (1). By comparing the coefficients of the same $W_{q-2k}(k)$ in both equations, we get

$$c_k(\mathcal{P})=\sum_{m=0}^{t}c_m(\mathcal{Q})c_{k-m}(\mathcal{R}). \tag{15}$$

Now, if either $\mathcal{Q}$ or $\mathcal{R}$ is composed of more than one cycle (i.e. may be expressed as a product of two commuting permutations), then the same procedure may be repeated for the appropriate coefficients. Proceeding in this way we finally may express an arbitrary coefficient $c_k(\mathcal{P})$ as a linear combination of products of the coefficients corresponding to single cycles. Then, if $\mathcal{P}$ belongs to a class π of S_q composed of p cycles $\pi_1,\pi_2,\ldots,\pi_p$, then

$$c_k(\mathcal{P})=\sum_{m_1,m_2,\ldots,m_p}{}^{\prime}\;c_{m_1}(\pi_1)c_{m_2}(\pi_2)\ldots c_{m_p}(\pi_p) \tag{16}$$

where the prime means that the summation is extended over partitions of k, i.e. the summation indices are constrained by the condition $m_1+m_2+\cdots+m_p=k$.

As an example, let us calculate the coefficients for the case when $\pi=[24]$, i.e. it is composed of two cycles: $\pi_1=[2]$ and $\pi_2=[4]$. For all permutations $c_0=1$. The only

other non-vanishing coefficients for the single cycles are: $c_1([2]) = -2$, $c_1([4]) = -4$ and $c_2([4]) = 2$. Now, according to (15),

$$c_0([24]) = c_0([2])c_0([4]) = 1$$
$$c_1([24]) = c_0([2])c_1([4]) + c_1([2])c_0([4]) = -6$$
$$c_2([24]) = c_0([2])c_2([4]) + c_2([2])c_0([4]) + c_1([2])c_1([4]) = 10$$
$$c_3([24]) = c_0([2])c_3([4]) + c_3([2])c_0([4]) + c_1([2])c_2([4]) + c_2([2])c_1([4]) = -4$$

and the remaining coefficients vanish.

Now let us consider the case of $\pi = [1^{q-n}n]$. In this case $\chi_{[n]}^{[n]} = 1$, $\chi_{[n]}^{[n-1,1]} = -1$ and $\chi_{[n]}^{[n-k,k]} = 0$ if $k > 1$. Then, (10) yields

$$c_0([n]) = 1 \tag{17}$$
$$c_1([n]) = -\frac{n}{n-1}\binom{n-1}{1} \tag{18}$$

and, by induction,

$$c_k([n]) = \varepsilon(k)\frac{n}{n-k}\binom{n-k}{k}. \tag{19}$$

The last equation, combined with (16), gives us a very simple closed-form expression for an arbitrary coefficient $c_k(\mathcal{P})$.

4. A generating function for $c_k[n]$

For $0 \leqslant x \leqslant 1$ the following identity is fulfilled

$$(1-x)^n + x^n = \sum_{k=0}^{(n-\delta)/2} \varepsilon(k)\binom{n-k}{k} x^k(1-x)^k \tag{20}$$

where

$$\delta = \begin{cases} 0 & \text{if } n \text{ is even} \\ 1 & \text{if } n \text{ is odd.} \end{cases} \tag{21}$$

Let $z = x(1-x)$. Then $x = \frac{1}{2} - \sqrt{\frac{1}{4} - z}$ and (19) and (20) yield

$$\sum_{k=0}^{(n-\delta)/2} c_k([n])\, z^k = \left(\tfrac{1}{2} - \sqrt{\tfrac{1}{4} - z}\right)^n + \left(\tfrac{1}{2} + \sqrt{\tfrac{1}{4} - z}\right)^n. \tag{22}$$

Then the right-hand side of (22) is the generating function for the coefficients $c_k([n])$, i.e. coefficients associated with one-cycle permutations.

Using (22) one may easily demonstrate several interesting and important summation properties of $c_k(\mathcal{P})$ coefficients. For example, if $z = \frac{1}{4}$ then the right-hand side of (22) is equal to 2^{1-n}. If the class π to which $\mathcal{P}$ belongs is composed of p cycles, i.e. if $\pi = [1^{\alpha_1}2^{\alpha_2}\ldots r^{\alpha_r}]$ with $p = \sum_{i=1}^{r}\alpha_i$, then from (16) and (22)

$$\sum_{k=0}^{t} c_k(\pi)\, 2^{-2k} = \prod_{i=1}^{r} 2^{(1-i)\alpha_i} = 2^{p-q} \tag{23}$$

where $q = \sum_{i=1}^{r} i\alpha_i$ and t is defined according to (2). By setting $z = 1$ we have

$$\left(\frac{1}{2} - \frac{\sqrt{3}}{2}i\right)^n + \left(\frac{1}{2} + \frac{\sqrt{3}}{2}i\right)^n = 2\cos(60\,n)$$
$$= \begin{cases} -2, & \text{if } n = 3i,\ i = 1, 2, 3, \ldots, \\ 1, & \text{otherwise.} \end{cases} \tag{24}$$

Therefore if the class π to which $\mathcal{P}$ belongs is composed of p cycles, we get $2^p \prod_{i=1}^{r} \cos(60i) = (-2)^d$, where $d = \alpha_3 + \alpha_6 + \alpha_9 + \cdots = \sum_i \alpha_{3i}$, i.e.

$$\sum_{k=0}^{t} c_k(\mathcal{P}) = (-2)^d. \tag{25}$$

5. The low-density limit of q-RDO traces

The case when $K \gg N$ is of a special interest and is referred to as the low-density limit [8, 9]. The closed-form formulae and the summation properties of the c coefficients allow us to perform a simple derivation of the asymptotic equations for traces of q-RDOs. Let us define

$$R_{SN}^{(q)}(\mathcal{P}) = \frac{\mathrm{Tr}({}^{q}E^{123\ldots q}_{\mathcal{P}(123\ldots q)})}{\mathrm{Tr}({}^{q}E^{123\ldots q}_{123\ldots q})} \tag{26}$$

and

$$r_{SN}^{k} = \frac{W_{q-2k}(k)}{W_q(0)}. \tag{27}$$

Equations (1), (3), (4) and (26) yield

$$R_{SN}^{(q)}(\mathcal{P}) = \varepsilon(\mathcal{P}) \sum_{k=0}^{t} c_k^q(\mathcal{P}) r_{SN}^{k}. \tag{28}$$

If $K \gg m$, then

$$\binom{K}{m} \Rightarrow \frac{K^m}{m!}. \tag{29}$$

From this and from (7) one gets that in the limit $K \gg N$,

$$D(S, N, K) \Rightarrow \frac{f(S, N)}{N!} K^N. \tag{30}$$

Similarly, (29) and (5) lead to

$$r_{SN}^{k} \Rightarrow \frac{f(S, N-2k)}{f(S, N)}. \tag{31}$$

In addition, if $N \gg k$, after some simple algebra we get

$$r_{SN}^{k} \Rightarrow 2^{-2k}(1 - g^2)^k \tag{32}$$

where $g = 2S/N$. In particular, if $S/N \to 0$, i.e. for the low-spin systems, $r_{SN}^{k} \to 2^{-2k}$. For the high-spin system, i.e. for $S/N \to \frac{1}{2}$, we have $r_{SN}^{k} \to \delta_{k0}$. If the traces are calculated in a space spanned by Slater determinants, also $r_{SN}^{k} = 2^{-2k}$ [16].

A space of N-electron eigenfunctions of the square and of the projection of the total spin operator form a basis for the two-row irrep $[a, b]$ of the symmetric group S_N, with

$a = \frac{1}{2}N + S$ and $b = \frac{1}{2}N - S$, where S is the total spin quantum number. Then, $g = (a-b)/(a+b) = (a-b)/N$ and

$$z = x(1-x) = \tfrac{1}{4}(1+g)(1-g) = \frac{a}{N}\frac{b}{N} \tag{33}$$

where $x = a/N$ fulfils the condition $0 \leqslant x \leqslant 1$. From (28), (31), (32), (33) and (13) we get

$$R^{(q)}_{SN}(\mathcal{P}) = \sum_{k=0}^{t} c_k[\pi] z^k. \tag{34}$$

Finally, (20) and (22) and the independent action of the cycles in a permutation $\mathcal{P}$ belonging to the class $\pi = [1^{\alpha_1}2^{\alpha_2}\ldots r^{\alpha_r}]$, yield

$$R^{(q)}_{SN}(\mathcal{P}) = \varepsilon(\mathcal{P}) \prod_{i=1}^{r} \left[\left(\frac{a}{N}\right)^i + \left(\frac{b}{N}\right)^i \right]^{\alpha_i}. \tag{35}$$

6. A closed-form expression for traces of spin-adapted q-RDOs

The symmetry-adapted qth-order reduced density operators are defined as [2]

$${}^{[J]}E^{\alpha[\mu]}_{\beta[\nu]} = \frac{f(J,q)}{q!} \sum_{\mathcal{P}\in S_q} U^q_J(\mathcal{P})_{\mu\nu}\, {}^{q}E^{\mathcal{P}\alpha}_{\beta} \tag{36}$$

where $\mathcal{P}\alpha$ means permutation of the orbitals in the string α of q orbital labels. Their traces in an N-electron and spin-adapted subspace of a K-orbital Fock space may be expressed as [14]

$$\mathrm{Tr}({}^{[J]}E^{\alpha[\mu]}_{\beta[\nu]}) \equiv \mathrm{Tr}(J;\alpha[\mu],\beta[\nu])_{NK} = \delta(\alpha\beta)\, U^q_J(\mathcal{P})_{\nu\mu}\, \mathrm{Tr}(J,\alpha)_{NK} \tag{37}$$

where $\delta(\alpha\beta) = 1$ if $\beta = \mathcal{P}\alpha$ and $\delta(\alpha\beta) = 0$ otherwise; $U^q_J(\mathcal{P})_{\nu\mu}$ is the $\nu\mu$-matrix element of the S_q irrep labelled by J, and $\mathrm{Tr}(J,\alpha)_{NK} = \mathrm{Tr}(J;\alpha[\lambda],\alpha[\lambda])_{NK}$ is λ-independent [14]. The structure of the last equation is similar to that of the Wigner–Eckart theorem. The trace of a symmetry-adapted q-RDO is factorized in such a way that all information connected with specific symmetry properties is carried by a universal coefficient ($U^q_J(\mathcal{P})_{\nu\mu}$ in (37), 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).

In the calculation of $\mathrm{Tr}(J,\alpha)_{NK}$, if the angular momentum J is smaller than $J_{\max}$ allowed for a system of q particles, the freezing relation [13] can be used for removing from the string α a singlet-coupled pair of orbitals (i.e. a doubly-occupied orbital or two singly-occupied orbitals coupled to a singlet). Thus, if $q' = 2J < q$ are the remaining orbital labels after the freezing, and $n = q - q'$, then

$$\mathrm{Tr}(J,\alpha)_{NK} = \mathrm{Tr}(J,\alpha')_{N-2n,K-n} \tag{38}$$

where α' is a string of $2J$ orbital labels.

The trace $\mathrm{Tr}(J,\alpha')_{N-2n,K-n}$ in $\mathcal{H}^A(K,S,N)$ may be expressed as [14]

$$\mathrm{Tr}(J,\alpha')_{N-2n,K-n} = \sum_{i=0}^{J-\delta} m^J_i\ W_{2J-2i}(i+n) \tag{39}$$

where $\delta = 0$ if the number of labels ($2J$) is even and $\delta = 1$ if $2J$ is odd; $W_{2J-2i}(i+n)$ is defined according to (3); m^J_i are coefficients tabulated in [14]. These coefficients have been

determined by means of a recurrence procedure, that may be expressed by the following equation

$$m_i^J = \varepsilon(i) \sum_{j=0}^{i-1} f(J-i, 2J-2j)\, m_j^J \tag{40}$$

where $\varepsilon(i) = (-1)^i$, $m_0^J = 1$ and $f(x, y)$ is defined according to (9). From (40) we get

$$m_0^J = \binom{2J}{0} \tag{41}$$

$$m_1^J = -\binom{2J-1}{1} \tag{42}$$

and, by induction,

$$m_i^J = \varepsilon(i) \binom{2J-i}{i}. \tag{43}$$

As an illustration, let us calculate the trace $\mathrm{Tr}({}^{[2]}E^{123456[\mu]}_{\mathcal{P}(123456)[\nu]})$

$$\mathrm{Tr}({}^{[2]}E^{123456[\mu]}_{\mathcal{P}(123456)[\nu]}) = U_2^6(\mathcal{P})_{\nu\mu}\, \mathrm{Tr}(J=2; \alpha = 123456)_{NK}.$$

An application of the freezing theorem [13] yields

$$\mathrm{Tr}(J=2; \alpha = 123456)_{NK} = \mathrm{Tr}(J=2; \alpha = 1234)_{N-2,K-1}.$$

Now, owing to (39), we may transform the above trace into a linear combination of traces of the occupation number operators

$$\mathrm{Tr}(J=2; \alpha = 1234)_{N-2,K-1} = m_0^2\, W_4(0+1) + m_1^2 W_2(1+1) + m_2^2 W_0(2+1).$$

From (43) we get the coefficients:

$$m_0^2 = \binom{4}{0} = 1$$

$$m_1^2 = -\binom{3}{1} = -3$$

$$m_2^2 = \binom{2}{2} = 1$$

and finally

$$\mathrm{Tr}({}^{[2]}E^{123456[\mu]}_{\mathcal{P}(123456)[\nu]}) = U_2^6(\mathcal{P})_{\nu\mu}(W_4(1) - 3W_2(2) + W_0(3)).$$

7. Concluding remarks

Studies of an eigenvalue spectrum in which the individual eigenvalues are evaluated either by diagonalizing the Hamiltonian matrix or by using one of the approximate methods to estimate the locations of the eigenvalues, which is most useful when one is interested in a few eigenvalues, become prohibitively inefficient when the number of levels is very large (as in the case of a confined electron gas or in complex atomic or nuclear spectra). In such cases some global characteristics of the spectra are needed. They may be derived from a knowledge of the spectral density distribution moments, closely related to traces of powers of the Hamiltonian matrix [8]. The set of eigenvalues is treated here as a statistical ensemble and the resulting approach is often referred to as *statistical spectroscopy*. It is known (see e.g. [5]) that the spectral density distribution moments may be expressed

as linear combinations of products of *interaction factors* and *propagation coefficients*. The interaction factors depend upon the specific form of the interactions and upon the structure of the one-particle space. They depend neither on the number of particles nor on the quantum numbers describing the system under consideration. The information about the number of particles, the total spin and, if applicable, other quantum numbers, is contained in the propagation coefficients. The propagation coefficients are expressible in a simple way by traces of RDOs [5]. Therefore, from explicit formulae for the traces one can deduce how the specific information about the system, contained in the interaction factors is reshaped when the number of particles and the quantum numbers are changed.

Explicit formulae for traces of certain kinds of RDOs and of some related operators (in particular of products of the occupation number operators) have already been published [9, 12]. Traces of arbitrary RDOs have also been expressed as linear combinations of traces of products of the occupation number operators [13, 14]. However, in the earlier works the coefficients in these combinations have been determined through rather complicated recurrence relations. Equations (16), (19) and (43) of the present paper supply simple closed-form formulae for these coefficients. The formulae are useful for several reasons. First they supply a tool for studying the dependence of the spectra on the number of particles, on the total spin and on other quantum numbers. For example, the results of section 5 proved to be most useful in exploring the behaviour of spectra in the low-density limit, i.e. in the case of $K \gg N \gg 1$ [17]. This analysis, applicable in a case when the number of electrons is large and when the spectrum is discrete, may be extended, for example, to describing the spectrum of a spatially confined electron gas. Second, evaluation of moments given by explicit formulae may be technically easier. Finally, last but not least, the explicit formulae are appealing because of their unexpected simplicity.

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