ABSTRACT: New algebraic structure on electronic Fock space is studied in detail. This structure is defined in terms of a certain multiplication of many electron wave functions and has close interrelation with coupled cluster and similar approaches. Its study clarifies and simplifies the mathematical backgrounds of these approaches. And even more, it leads to many relations that would be very difficult to derive using conventional technique. Formulas for action of the creation-annihilation operators on products of state vectors are derived. Explicit expressions for action of simplest particle-conserving products of the creation-annihilation operators on powers of state vectors are given. General scheme of parametrization of representable density operators of arbitrary order is presented.

Key words: Fock space, commutative and skew-commutative algebras, configuration interaction, coupled cluster approach, density operators

Introduction

In our previous paper [1] new structure of associative and skew-commutative algebra (which is called superalgebra structure by physicists) on electronic Fock space was defined. This structure presupposes initial selection of some Hartree-Fock (HF) vacuum state and is actually introduced on the so-called pointed Fock space. Selection of HF vacuum states corresponding to different numbers of electrons results in different superalgebra structures. In particular, selection of the ‘absolute’ vacuum state (with no particles) leads to the standard Grassmann algebra with the classic wedge product. If some \( p \)-electron determinant is selected as the HF vacuum state then \( p \)-electron sector of the Fock space is closed with respect to the multiplication introduced and it turns out that this sector becomes a commutative and associative algebra. The structure of commutative algebra thus defined proves to be very closely related to the coupled cluster (CC) [2]-[7] and quadratic configuration interaction (QCI) approaches [8].
In present paper we continue our study of new algebraic structure introduced on the electronic Fock space. In Section I necessary basic definitions are given. In Section II the action of the creation-annihilation operators on arbitrary products of state vectors (not necessarily corresponding the the same number of electrons) is studied. Section III is dedicated to investigation of commutative algebra structure on the $p$–electron sector of the Fock space. In particular, general formulas obtained in Section II are applied to arbitrary powers of $p$–electron state vectors. General polynomial parametrization of $p$–electron states, embracing both CC and QCI parametrizations, is described. Compact expression for the first order CC density matrix is derived. In Section IV non-standard realizations of electronic Fock space suggested in [9, 10] and based on the notion of $(p,q)$–vector are discussed. It is demonstrated that these realizations are easily defined with the aid of the so-called Hodge isomorphism [11]. Since the notion of $(p,q)$–vector is rather unusual for quantum chemists, formal definitions are accompanied by a number of simple examples. Close relation of $(p,q)$–vectors and reduced density operators of order $q$ is discussed. It is shown that non-standard realizations of the Fock space give rare possibility to construct parametric representable density operators in uniform and general way.

**Basic Definitions**

Let $N = \{1, 2, \ldots, n\}$ be the molecular spin-orbital (MSO) index set. For arbitrary $K = k_1 < k_2 < \ldots < k_s \subset N$ let us put

$$\Delta_K = \{1, 2, \ldots, k_1\} \Delta \ldots \Delta \{1, 2, \ldots, k_s\}$$

where $\Delta$ is associative set-theoretical operation (symmetric difference) defined on the set $P(N)$ of all subsets of $N$ as

$$R \Delta S = (R \cup S) \setminus (R \cap S).$$

For example, if $K = \{2, 4, 7\}$ then

$$\Delta_K = \{1, 2\} \Delta \{1, 2, 3, 4\} \Delta \{1, 2, 3, 4, 5, 6, 7\} = \{1, 2, 5, 6, 7\}.$$
Among numerous relations involving operation $\Delta_K$ the equality

$$|K \cap \Delta_R| + |R \cap \Delta_K| \equiv |K||R| + |K \cap R| \ (mod\ 2) \quad (2)$$

that is an immediate consequence of definition (1), is of primary importance for further analysis.

Finite-dimensional Fock space $\mathcal{F}_N$ generated by some orthonormal set $\{\psi_i\}_{i \in N}$ of MSOs is constructed as follows. The basic space is the one-electron sector of the Fock space

$$\mathcal{F}_{N,1} = \bigoplus_{i \in N} \mathbb{C}\psi_i \quad (3)$$

The direct sum of exterior powers of $\mathcal{F}_{N,1}$ is, by definition, the electronic Fock space

$$\mathcal{F}_N = \bigoplus_{p=0}^n \bigwedge^p \mathcal{F}_{N,1} \quad (4)$$

where

$$\mathcal{F}_{N,0} = \bigwedge^0 \mathcal{F}_{N,1} = \mathbb{C}|\emptyset\rangle, \quad (5)$$

$\mathbb{C}$ is the field of complex numbers, $|\emptyset\rangle$ is the so-called 'absolute' vacuum vector being nothing more than a special notation for the unit of $\mathbb{C}$. Sector of the Fock space corresponding to $p-$electron system is just the $p-$th exterior power in the sum (4). It is spanned by \binom{n}{p} vectors

$$|R\rangle = \psi_{r_1} \wedge \ldots \wedge \psi_{r_p} \quad (6)$$

that are called 'determinants' by quantum chemists, and by factorable $p-$vectors by mathematicians. In Eq.(6) we assume that $R = r_1 < \ldots < r_p \subset N$.

Basis determinants (factorable multivectors) spanning the Fock space will be labelled by subsets of the index set $N$ and all sign conventions connected with their representation as the wedge products of ordered spin-orbitals will be included in the definition of the creation-annihilation operators. This representation is very close to the so-called space of occupation numbers where each factorable multivector is identified with a certain bit vector.

For any two determinants $|R\rangle, |S\rangle$ their exterior product is defined as

$$|R\rangle \wedge |S\rangle = \begin{cases} (-1)^{\varepsilon(R,S)}|R \cup S\rangle & \text{if } R \cap S = \emptyset \\ 0 & \text{if } R \cap S \neq \emptyset \end{cases} \quad (7)$$
where \( \varepsilon(R,S) \) is the number of pairs \( (r,s) \in R \times S \) such that \( r > s \). It is easy to show that

\[
\varepsilon(R,S) = |S \cap \Delta_R|
\]  

(8)

Fock space equipped with the multiplication (7) is associative and skew-commutative algebra that is called Grassmann or exterior algebra of the one-electron Fock space \( \mathcal{F}_{N,1} \). Skew-commutativity

\[
|R\rangle \wedge |S\rangle = (-1)^{|R||S|} |S\rangle \wedge |R\rangle
\]  

(9)

readily follows from Eqs.(2) and (8).

Creation-annihilation operators associated with spin-orbital index \( i \) are defined by the following relations

\[
a_i \dagger |R\rangle = (-1)^{|R|}(1 - \zeta_{i,R})(-1)^{|\{i\} \cap \Delta_R|} |R \cup \{i\}\rangle
\]  

(10a)

\[
a_i |R\rangle = (-1)^{|R|}\zeta_{i,R}(-1)^{|\{i\} \cap \Delta_R|} |R \setminus \{i\}\rangle
\]  

(10b)

where

\[
\zeta(I,R) = \begin{cases} 1 & \text{if } I \subset R \\ 0 & \text{if } I \not\subset R \end{cases}
\]  

(11)

is the well-known combinatorial \( \zeta \) function of partially ordered by inclusion set \( \mathcal{P}(N) \). Note that by an abuse of notation we use symbol \( \zeta(i,R) \) instead of \( \zeta(\{i\},R) \).

It is not difficult to ascertain that this definition of the creation-annihilation operators is identical to the commonly used one [1].

**Pointed Fock Space**

Let us consider pointed Fock space \( \mathcal{A}_R = (\mathcal{F}_N, |R\rangle) \), that is the Fock space where some factorable \( p \)-vector (determinant) \( |R\rangle \) is selected. It will be convenient to introduce the following notation for basis determinants of the pointed Fock space:

\[
e^I_j(R) = |(R \setminus J) \cup I\rangle
\]  

(12)

It is pertinent to emphasize that Eq.(12) is just a notation for \( 2^n \) basis determinants of the Fock space where some factorable multivector (determinant
$|R\rangle$) is selected. The selected point $|R\rangle$ is referred to as either the HF vacuum or the HF reference state.

Let us define the multiplication in $\mathcal{A}_R$ by putting

$$
e^I_j(R) \ast e^{I'}_{j'}(R) = \begin{cases} 
-1)^{|J \cup J' \cap \Delta(J \cup J')}e^{|J \cup J'|}_{J \cup J'}(R) & \text{if } J \cap J' = \emptyset \text{ and } I \cap I' = \emptyset \\
0 & \text{if } J \cap J' \neq \emptyset \text{ or } I \cap I' \neq \emptyset
\end{cases}.
$$

(13)

$\mathcal{A}_R$ with multiplication (13) becomes associative algebra with the identity $e_0^R(R)$. Associativity follows from the relation

$$\|(J_3 \cup I_3) \cap \Delta(J_2 \cup I_2\cup I_3)\| + |(J_2 \cup J_3 \cup I_2 \cup I_3) \cap \Delta(J_1 \cup I_1)\|
\equiv |(J_2 \cup I_2) \cap \Delta(J_1 \cup I_1)\| + |(J_3 \cup I_3) \cap \Delta(J_1 \cup I_1 \cup I_2)\|(mod 2).
$$

From Eq. (2) we readily obtain the equality

$$e^I_j(R) \ast e^{I'}_{j'}(R) = (-1)^{|J \cup J'|\cdot|J' \cup I'|}e^{|J \cup J'|}_{J \cup J'}(R) \ast e^I_j(R)
$$

(14)

which means that the multiplication (13) is skew-commutative.

$\mathcal{A}_R$ is a direct sum

$$\mathcal{A}_R = \mathcal{A}_R^+ \oplus \mathcal{A}_R^-$$

(15)

where subspaces $\mathcal{A}_R^+$ and $\mathcal{A}_R^-$ are spanned by basis vectors $e^I_j(R)$ with even and odd values of $|J \cup I|$, respectively.

From Eq. (14) it follows that

$$\mathcal{A}_R^+ \ast \mathcal{A}_R^+ \subset \mathcal{A}_R^+; \mathcal{A}_R^+ \ast \mathcal{A}_R^- \subset \mathcal{A}_R^-; \mathcal{A}_R^- \ast \mathcal{A}_R^+ \subset \mathcal{A}_R^+; \mathcal{A}_R^- \ast \mathcal{A}_R^- \subset \mathcal{A}_R^+,$$

(16)

which means that $\mathcal{A}_R$ is $\mathbb{Z}_2$-graded (super)algebra and that $\mathcal{A}_R^+$ is a subalgebra of $\mathcal{A}_R$.

Let us consider the pointed Fock space $\mathcal{A}_0$ that is the Fock space where the ‘absolute’ vacuum state $|R\rangle = |0\rangle$ is selected. In this case we have

$$e^I_0(\emptyset) \ast e^{I'}_{j'}(\emptyset) = \begin{cases} 
-1)^{|J \cup J' \cap \Delta(J \cup J')}e^{|J \cup J'|}_{j'}(\emptyset) & \text{if } I \cap I' = \emptyset \\
0 & \text{if } I \cap I' \neq \emptyset
\end{cases}.
$$

(17)

and, consequently, the multiplication (13) in this case is identical to the standard exterior product in the Fock space as follows from Eqs. (7) and (8).

There exists another multiplication in $\mathcal{A}_R$ defined by the relation

$$e^I_j(R) \circ e^{I'}_{j'}(R) = \begin{cases} 
-1)^{|J \cup J' \cap \Delta(J \cup J')}e^{|J \cup J'|}_{J \cup J'}(R) & \text{if } J \cap J' = \emptyset \text{ and } I \cap I' = \emptyset \\
0 & \text{if } J \cap J' \neq \emptyset \text{ or } I \cap I' \neq \emptyset
\end{cases}.
$$

(18)
With this multiplication $A_R$ is also $\mathbb{Z}_2$-graded (super)algebra. The pointed Fock space $A_{\emptyset}$ with bullet product (18) is, however, not identical to the Grassmann algebra. It is easy to show that for arbitrary $x, y \in A_R$

$$x \ast y = y \bullet x$$

(19)

that is star and bullet products are just mutually opposite composition laws.

Let us denote by the symbol $A^p_R$ the $p$-electron sector of the Fock space where some determinant $\langle R \rangle$ is selected. In other words, $A^p_R$ is a pointed exterior power of the one-electron Fock space. $A^p_R$ is spanned by basis elements $e^I_J(R)$ with $J \subset R, I \subset N \setminus R$, and $|J| = |I|$. It is easy to see that both the star product (13) and the bullet product (18) coincide on $A^p_R$ (see Eq.(19)) and define on $A^p_R$ the structure of associative and commutative algebra. This structure turned out to be closely related to the coupled cluster approach [2]-[7].

In the remainder part of this paper we will consider pointed Fock space as a superalgebra with the star product (13).

Let us examine the action of the creation-annihilation operators on star product of basis determinants. We start with two formulas that readily follows from Eqs.(10a) and (10b):

$$a_i^\dagger e^I_J(R) = (-1)^\gamma \left[ \zeta_{i,J}(R) e^I_J(R) + \zeta_{i,N\setminus R \setminus I}(R) \right]$$

(20a)

$$a_i e^I_J(R) = (-1)^\gamma \left[ \zeta_{i,J}(R) e^I_J(R) + \zeta_{i,I}(R) \right]$$

(20b)

where

$$\gamma = |(R \setminus J) \cup I| + |\{i\} \cap \Delta_{(R \setminus J) \cup I}|.$$  

(21)

Simple but somewhat tedious manipulations with phase prefactors lead to

$$a_i^\dagger [e^I_J(R) \ast e^I_{J'}(R)] = \zeta_{i,N\setminus R} \left[ a_i^\dagger e^I_J(R) \right] \ast e^I_{J'}(R)$$

$$+ \zeta_{i,R} \left[ a_i^\dagger e^I_J(R) \right] \ast e^I_{J'}(R) + (-1)^{|J\setminus I|} e^I_J(R) \ast \left[ a_i^\dagger e^I_{J'}(R) \right]$$

(22a)

$$a_i [e^I_J(R) \ast e^I_{J'}(R)] = \zeta_{i,R} \left[ a_i e^I_J(R) \right] \ast e^I_{J'}(R)$$

$$+ \zeta_{i,N\setminus R} \left[ a_i e^I_J(R) \right] \ast e^I_{J'}(R) + (-1)^{|J\setminus I|} e^I_J(R) \ast \left[ a_i e^I_{J'}(R) \right]$$

(22b)
\[
\[ a_i^\dagger e_j^f(R) \star e_{j'}^f(R) = (-1)^{|J\cup I|} e_j^f(R) \star [a_i^\dagger e_{j'}^f(R)] \], \quad \text{if } i \in N \setminus R \quad (22c)
\]

\[
[a_i e_j^f(R)] \star e_{j'}^f(R) = (-1)^{|J\cup I|} e_j^f(R) \star [a_i e_{j'}^f(R)] , \quad \text{if } i \in R \quad (22d)
\]

Combination of Eq.(22a)-(22d) gives

\[
a_i^\dagger \left[ e_j^f(R) \star e_{j'}^f(R) \right] = \frac{1}{1 + \zeta_{i,N \setminus R}} \left\{ \left[ a_i^\dagger e_j^f(R) \right] \star e_{j'}^f(R) + (-1)^{|J\cup I|} e_j^f(R) \star \left[ a_i^\dagger e_{j'}^f(R) \right] \right\} \quad (23a)
\]

and

\[
a_i \left[ e_j^f(R) \star e_{j'}^f(R) \right] = \frac{1}{1 + \zeta_{i,R}} \left\{ [a_i e_j^f(R)] \star e_{j'}^f(R) + (-1)^{|J\cup I|} e_j^f(R) \star [a_i e_{j'}^f(R)] \right\} \quad (23b)
\]

**Pointed p-Electron Sector of the Fock Space**

Let \( \mathcal{A}_R^p \) be the \( p \)-electron sector \( \mathcal{F}_{N,p} \) of the Fock space where some determinant \( |R\rangle \) is selected. As has already been mentioned, the vector space \( \mathcal{A}_R^p \) with star product (13) is a commutative algebra with \( e_0^f(R) = |R\rangle \) as its identity. \( \mathcal{A}_R^p \) is spanned by the basis vectors \( e_j^f(R) = |(R \setminus I) \cup J\rangle \) with \( |J| = |I| \).

We illustrate star multiplication in algebra \( \mathcal{A}_R^p \) on simple example. Let \( N = \{1, 2, 3, 4\}, p = 2, \) and \( R = \{1, 2\} \). There are six basis vectors and their multiplication rules are presented in Table I.

From Eqs.(23a)-(23b)) it follows that for arbitrary vectors \( x \in \mathcal{A}_R^p \) and \( y \in \mathcal{A}_R^p \)

\[
a_i^\dagger [x \star y] = \frac{1}{1 + \zeta_{i,N \setminus R}} \left\{ (a_i^\dagger x) \star y + x \star (a_i^\dagger y) \right\} \quad (24a)
\]

and

\[
a_i [x \star y] = \frac{1}{1 + \zeta_{i,R}} \left\{ (a_i x) \star y + x \star (a_i y) \right\} \quad (24b)
\]
TABLE I
Basis vectors multiplication table: N={1,2,3,4} and R={1,2}.

|      | $e_0^0(R)$ | $e_1^{[3]}(R)$ | $e_1^{[4]}(R)$ | $e_2^{[3]}(R)$ | $e_2^{[4]}(R)$ | $e_{1,2}^{[4]}(R)$ |
|------|------------|----------------|----------------|----------------|----------------|------------------|
| $e_0^0(R)$ | $e_0^0(R)$ | $e_1^{[3]}(R)$ | $e_1^{[4]}(R)$ | $0$            | $0$            | $0$              |
| $e_1^{[3]}(R)$ | $e_1^{[3]}(R)$ | $0$     | $0$           | $e_{1,2}^{[4]}(R)$ | $0$            | $0$              |
| $e_1^{[4]}(R)$ | $e_1^{[4]}(R)$ | $0$     | $0$           | $e_{1,2}^{[4]}(R)$ | $0$            | $0$              |
| $e_2^{[3]}(R)$ | $e_2^{[3]}(R)$ | $0$     | $e_{1,2}^{[4]}(R)$ | $0$            | $0$            | $0$              |
| $e_2^{[4]}(R)$ | $e_2^{[4]}(R)$ | $-e_{1,2}^{[4]}(R)$ | $0$ | $0$           | $0$            | $0$              |
| $e_{1,2}^{[4]}(R)$ | $e_{1,2}^{[4]}(R)$ | $0$     | $0$           | $0$            | $0$            | $0$              |

In view of Eqs. (22c) and (22d) we have

$$(a_i^\dagger x) \ast y = x \ast (a_i^\dagger y) \quad \text{if} \quad i \in N \setminus R \quad (25a)$$

and

$$(a_i x) \ast y = x \ast (a_i y) \quad \text{if} \quad i \in R \quad (25b)$$

It is pertinent to emphasize that Eqs. (24)-(25) are valid for arbitrary $y \in A_R$ not necessarily belonging to the $p$–electron sector of the Fock space.

The following relations are readily obtained from Eqs. (24a)-(24b):

$$a_i^\dagger x^\mu = \frac{\mu}{1 + (\mu - 1)\zeta_{i,N \setminus R}} \left[ x^{\mu - 1} \ast a_i^\dagger x \right] \quad (26a)$$

$$a_i x^\mu = \frac{\mu}{1 + (\mu - 1)\zeta_{i,R}} \left[ x^{\mu - 1} \ast a_i x \right] \quad (26b)$$

where $x$ is arbitrary vector from $A_R^p$. Here $x^\mu = \underbrace{x \ast \ldots \ast x}_\mu$.

$A_R^p$ is a Hermitean space with scalar product

$$\langle x | y \rangle = \sum_{\mu=0}^{p} \sum_{J \subset R}^{(\mu)} (x^I_J)^* y^I_J \quad (27a)$$

and norm

$$\| x \| = \langle x | x \rangle^{\frac{1}{2}} \quad (27b)$$
There exists an important question concerning interrelation of algebra structure on $A_R^p$ and its structure as a normed space with the norm (27b). This question may be formulated as: Is the multiplication (13) consistent with the norm (27b), or, in other words, does the inequality

$$\|x \ast y\| \leq \|x\| \cdot \|y\|$$

(28)

hold true for arbitrary $x, y \in A_R^p$? The following simple example shows, that in general the answer to this question is negative. If $n = 2$ and $p = 1$, then for $x = e^0_0 + e^2_{\{1\}}$ the inequality (28) is violated. Indeed, in this case $x \ast x = e^0_0 + 2e^2_{\{1\}}$ and $\|x \ast x\| = \sqrt{5}$ whereas $\|x\|^2 = 2$. Computer experiments show that for $n \leq 8$ the inequality (28) does not hold true, at least if $p = 1, n - 1$.

Till now no violation of this inequality has been detected for $n > 8$. We may suggest that for sufficiently large $n$ the inequality (28) holds true for all $x, y \in A_R^p$, or, in other words, that there exists $n_0$ such that for $n > n_0$ $A_R^p$ is a unital Banach algebra. Verification of this suggestion may be a rather complicated task.

For each pair $(k, l)$ with $k \leq l$ let us introduce subspace $W_R^{(k,l)}$ spanned by vectors $e^I_J(R)$ with $k \leq |J| = |I| \leq l$. It is clear that

$$A_R^p = \bigoplus_{k=0}^{p} W_R^{(k,k)}$$

(29)

and that

$$W_R^{(k_1,k_1)} \ast W_R^{(k_2,k_2)} \subset W_R^{(k_1+k_2,k_1+k_2)}$$

(30)

where $k_1 + k_2 \leq p$, which means that $A_R^p$ is a graded algebra. The subspace $W_R^{(1,p)}$ is its maximal nilpotent ideal and the algebra under discussion is just a direct sum of the field of complex numbers and this nilpotent ideal

$$A_R^p = \mathbb{C}e^0_0(R) \oplus W_R^{(1,p)}$$

(31)

Note also that $A_R^p$ is algebra with involution induced by the complex conjugation.

Spectral theory (see, e.g., [13]) in algebra $A_R^p$ is very simple. Indeed, let us write arbitrary element $x \in A_R^p$ as

$$x = x^0_0e^0_0 + \tau$$

(32)
where $\tau \in \mathcal{W}_R^{(1,p)}$. Its spectrum is defined as the set of all $\lambda \in \mathbb{C}$ such that $(\lambda e^\theta - x)$ is not invertible in $\mathcal{A}_R^p$. It is easy to see that

$$
(\lambda e^\theta - x)^{-1} = \sum_{k=0}^{p} \frac{\tau^k}{(\lambda - x^\theta)^{k+1}} = \mathcal{R}(x, \lambda)
$$

exists for all $\lambda \neq x^\theta$. Thus, any element $x \in \mathcal{A}_R^p$ has a single point spectrum

$$
Sp x = \{\langle x|e^\theta \rangle\}
$$

and resolvent $\mathbb{C}\\backslash\{x^\theta\} \to \mathcal{A}_R^p$ defined by Eq.(33). In particular, $Sp \tau = \{0\}$ for any element $\tau \in \mathcal{W}_R^{(1,p)}$.

It is well-known that in commutative algebras of the type of Eq.(31) it is easy to define algebraically both the exponential mapping and its inverse. Namely,

$$
\exp : \tau \to \sum_{\mu=0}^{p} \frac{\tau^\mu}{\mu!}
$$

is the exponential mapping $\mathcal{W}_R^{(1,p)} \to e^\theta(R) + \mathcal{W}_R^{(1,p)}$ and

$$
\log : e^\theta(R) + \tau \to \sum_{\mu=1}^{p} (-1)^{\mu-1} \frac{\tau^\mu}{\mu}
$$

is the logarithmic mapping $e^\theta(R) + \mathcal{W}_R^{(1,p)} \to \mathcal{W}_R^{(1,p)}$.

For mappings (35) and (36) all classic relations hold true:

$$
\exp(\tau_1) \ast \exp(\tau_2) = \exp(\tau_1 + \tau_2), \quad (37a)
$$

$$
[\exp(\tau)]^{-1} = \exp(-\tau), \quad (37b)
$$

$$
\exp(\log(e^\theta(R) + \tau)) = \tau, \quad (37c)
$$

and

$$
\log(\exp(\tau)) = \tau, \quad (37d)
$$

where $\tau, \tau_1, \tau_2$ are arbitrary elements from $\mathcal{W}_R^{(1,p)}$.

Using Eqs.(24)-(26), it is possible to calculate explicitly the action of particle number conserving products of the creation-annihilation operators
on powers of state vectors (elements of algebra $\mathcal{A}_R^p$). For the simplest product $a_i^\dagger a_j$ we have

$$a_i^\dagger a_j x^\mu = \begin{cases} 
-(\mu - 1) \delta_{ij} x^\mu + \mu x^{\mu - 1} \star a_i^\dagger a_j x 
& \text{if } i, j \in R \\
\mu x^{\mu - 2} \star \left[ (\mu - 1) a_i^\dagger x \star a_j x + x \star a_i^\dagger a_j x \right] 
& \text{if } i \in R, j \in N \setminus R \\
x^{\mu - 1} \star a_i^\dagger a_j x 
& \text{if } i \in N \setminus R, j \in R \\
\mu x^{\mu - 1} \star a_i^\dagger a_j x 
& \text{if } i, j \in N \setminus R
\end{cases}$$

Thus, the action of the operator $a_i^\dagger a_j$ on arbitrary power of vector $x \in \mathcal{A}_R^p$ is completely determined by the action of three operators $a_i^\dagger$, $a_j$, and $a_i^\dagger a_j$ on this vector. It is pertinent to note that the expression $a_i^\dagger x \star a_j x$ involved in the right-hand side of Eq.(38) is not reduced to $x \star a_i^\dagger a_j x$ (see restrictions on indices in Eqs.(25a)-(25b)).

Many methods of quantum chemistry are based on simple idea of parametrization of many electron wave functions with a relatively small number of free parameters with their subsequent optimization using one or other optimality criterium. In particular, in CC and related approaches subsets of $\mathcal{A}_R^p$ are parametrized with the aid of elements ('amplitudes') from $\mathcal{W}_R^{(1,l)}$ where $l$ is the maximal CC excitation level. General parametrization of such a type may be defined as a differentiable mapping

$$\pi : \mathcal{W}_R^{(1,l)} \rightarrow \mathcal{A}_R^p$$

satisfying two requirements:

(i) $\pi$ is an injective mapping;

(ii) $\pi(\tau)$ is invertible for any $\tau \in \mathcal{W}_R^{(1,l)}$.

The last requirement guarantees that $\langle \pi(\tau) | \epsilon_\emptyset \rangle \neq 0$, or, in other words, that the HF vacuum state $|R\rangle$ appears with nonzero coefficient in expansion of $\pi(\tau)$ for each $\tau$.

Polynomial mapping

$$P_a : \tau \rightarrow \sum_{\mu=0}^p a_\mu \tau^\mu,$$

where $a = (a_0, a_1, \ldots, a_p) \in \mathbb{C}^{p+1}$, is a parametrization if and only if $a_0 \cdot a_1 \neq 0$. Indeed, $a_0 \neq 0$ means that $P_a(\tau)$ is invertible for each $\tau$. The mapping inverse to $P_a$ may be written in the form

$$P_{a_0}^{-1} : a_0 \epsilon_\emptyset + \tau \rightarrow \sum_{\mu=1}^p (-1)^{\mu-1} b_\mu \tau^\mu,$$
where coefficients \( b_\mu \) are easily obtained from the recurrence relation

\[
b_\mu = \frac{(-1)^\mu}{a_1^\mu} \sum_{\nu=1}^{\mu-1} (-1)^{\nu-1} b_{\nu} \sum_{i_1+\cdots+i_\nu=\mu} a_{i_1} \cdots a_{i_\nu},
\]

(42a)

\[
b_1 = \frac{1}{a_1}.
\]

(42b)

For example, QCI parametrization \( \tau \to \mathcal{R}(\tau, 1) \) corresponds to the case \( a_0 = a_1 = \cdots = a_p = 1 \) and from Eqs. (42a)-(42b) we easily obtain \( b_1 = \cdots = b_p = 1 \). For the exponential parametrization these equations give \( b_\mu = \frac{1}{\mu} \) in full accordance with Eq. (35).

It is clear that without loss of generality we can put \( a_0 = a_1 = 1 \). Indeed, the condition \( a_0 = 1 \) means that the intermediate normalization condition \( \langle x|\epsilon_0^B\rangle = 1 \) for state vectors is used. Going from arbitrary nonzero \( a_1 \) to \( a_1 = 1 \) simply corresponds to scaling of vector \( \tau \) of CC amplitudes and such scaling is of no consequence if components of \( \tau \) vector and coefficients \( a_1, a_2, \ldots, a_p \) are considered as free parameters.

There exits as well standard integral representation for polynomial functions on \( \mathcal{W}_R^{(1,p)} \):

\[
P_a(\tau) = \frac{1}{2\pi i} \oint_{|\lambda|=1} P_a(\lambda) \mathcal{R}(\tau, \lambda) d\lambda
\]

(43)

where \( \lambda \) is complex variable. This integral representation, being trivial for polynomials, could be extended to certain algebras of analytic functions if our hypothesis that \( \mathcal{A}_R^{p} \) is a Banach algebra, turns out to be true.

Let us suppose that polynomial parametrization covers some eigenvector of the electronic Hamiltonian \( \mathcal{H} \), that is there exist coefficients \( a = (1, 1, a_2, \ldots, a_p) \) and vector \( \tau \in \mathcal{W}_R^{(1,l)} \) such that

\[
\mathcal{H}P_a(\tau) = EP_a(\tau).
\]

(44)

Let us put

\[
P_{a,E} : \tau \to E P_a(\tau)
\]

(45)

Its inverse is

\[
P_{a,E}^{-1} : E\epsilon_0^B + \tau \to \sum_{\mu=1}^{p} (-1)^{\mu-1} \frac{b_\mu}{E^\mu} \tau^D
\]

(46)
Application of this transformation to the both sides of Eq.(44) gives

$$
\sum_{\mu=1}^{p} (-1)^{\mu-1} \frac{b_{\mu}}{E_{\mu}} \left[ HP_{\alpha}(\tau) - E_{\mu}^{\emptyset} \right]^{\mu} = \tau
$$

This relation may serve as a base for iterative algorithms for solution of Eq.(44).

The polynomial derivative of $P_{\alpha}(\tau)$ in algebra $A_{R}^{p}$ is defined as

$$\frac{d}{d\tau} P_{\alpha}(\tau) = \sum_{k>0} k a_{k} \tau^{k-1}$$

Partial derivatives of $P_{\alpha}(\tau)$ with respect to components of vector $\tau$ are connected with its polynomial derivative by the relation

$$\frac{\partial}{\partial t_{I J}} P_{\alpha}(\tau) = \left[ \frac{d}{d\tau} P_{\alpha}(\tau) \right] * e_{I J}^{l}(R)$$

Note that $\tau^{p}$, if nonzero, is a linear combination of basis vectors $e_{R}^{I'}(R)$ where $I' \subset N \setminus R$ with $|I'| = p$. As a result, $\tau^{p} * e_{I J}^{l}(R) = 0$ for any basis vector $e_{I J}^{l}(R)$ with $J \neq \emptyset$ and

$$\frac{\partial}{\partial t_{I J}} \exp(\tau) = \exp(\tau) * e_{I J}^{l}(R)$$

If $\tau \in W_{R}^{(1,l)}$ is a vector of CC amplitudes then the coefficients in expansion of $\exp(\tau)$ in algebra $A_{R}^{p}$ with respect to the basis $e_{I J}^{l}(R)$ are just the CC configuration interaction (CI) coefficients:

$$\exp(\tau) = \sum_{\mu=0}^{p} \sum_{I \subset N \setminus R}^{(\mu)} T_{\mu}^{l}(J,I)e_{I J}^{l}(R),$$

where

$$T_{\mu}^{l}(J,I) = \langle \exp(\tau) | e_{I J}^{l}(R) \rangle.$$
With the aid of Eq.(26b) it is easy to get an expression for matrix elements

\[ \rho_{ij} = \langle \exp(\tau) | a_i^\dagger a_j \exp(\tau) \rangle = \langle a_i \exp(\tau) | a_j \exp(\tau) \rangle \]  

of (not normalized) CC 1-density operator. We have

\[ \rho_{ij} = \begin{cases} 
\langle s_1(\tau) \ast a_i \tau | s_1(\tau) \ast a_j \tau \rangle & \text{if } i, j \in R \\
\langle s_1(\tau) \ast a_i \tau | s_2(\tau) \ast a_j \tau \rangle & \text{if } i \in R, j \in N \setminus R \\
\langle s_2(\tau) \ast a_i \tau | s_1(\tau) \ast a_j \tau \rangle & \text{if } i \in N \setminus R, j \in R \\
\langle s_2(\tau) \ast a_i \tau | s_2(\tau) \ast a_j \tau \rangle & \text{if } i, j \in N \setminus R 
\end{cases} \]  

(53)

where

\[ s_1(\tau) = \sum_{\mu=0}^{p-1} \frac{\tau^\mu}{(\mu + 1)!} \]  

(54a)

and

\[ s_2(\tau) = \frac{d}{d\tau} \exp(\tau) \]  

(54b)

Note that the simplicity of Eq.(53) is somewhat misleading because in this equation two sectors of the Fock space are involved. If it is desirable to stay in \(p\)-electron sector then one should employ Eq.(38) with direct expansion of the product \(a_i^\dagger x \ast a_j x\) via basis \(p\)-electron vectors \(e_I^J(R)\).

**Non-Standard Realizations of \(p\)-Electron Sector of the Fock Space**

In this section we consider realizations of the \(p\)-electron sector of the Fock space suggested in \([9, 10]\). The main idea consists in replacing \(p\)-electron state vector by a certain family of \(q\)-electron vectors. If \(p+q = n\) then there exists a well-known isomorphism between \(q\)- and \(p\)-electron sectors of the Fock space that is called Hodge isomorphism and is denoted by the symbol \(*_N^I: N\) : 

\[ (*_N^I: N\) : (\psi_{i_1} \wedge \ldots \wedge \psi_{i_q}) = (-1)^{|J \cap \Delta N|} \psi_{j_1} \wedge \ldots \wedge \psi_{j_p} \]  

(55)

where \(I = i_1 < \ldots < i_q, J = j_1 < \ldots < j_p, \) and \(I \cup J = N\). Eq.(55) defines linear mapping

\[ * : \bigwedge^q \mathcal{F}_{N,1} \rightarrow \bigwedge^{n-q} \mathcal{F}_{N,1}. \]  

(56)

that does not depend on the choice of the (orthonormal) MSO basis set in the case when the one-electron sector of the Fock space is Euclidean and oriented.
one. For complex Fock space Eq.(55) certainly defines isomorphic mapping but this mapping may depend on the choice of MSO basis set. Note that in Eq.(55) we introduced the phase prefactor that differs from that in [11] by the constant factor \((-1)^{\left\lfloor \frac{p+1}{2} \right\rfloor}\). Note as well that the Hodge isomorphism is not an involution.

In general case we can consider a family \(\{x^Z_q\}_{Z \subset N}\) of \(q\)-electron vectors indexed by \((p + q)\)-element subsets of the index set \(N\) where \(x^Z_q \in \mathcal{F}_{Z,q}\) and apply Hodge isomorphism \(* : \mathcal{F}_{Z,q} \rightarrow \mathcal{F}_{Z,p}\) to each vector \(x^Z_q\) (by an abuse of notation we use the same symbol for Hodge isomorphisms defined on different subspaces):

\[
* \left( \sum_{S \subset Z} \langle S|x^Z_q| \rangle S \right) = \sum_{S \subset Z} (-1)^{|Z \setminus S| \cap \Delta Z} \langle S|x^Z_q| \rangle S \quad (57)
\]

If the family \(\{x^Z_q\}_{Z \subset N}\) satisfies the conditions

\[
(-1)^{|(Z \setminus S) \cap \Delta Z|} \langle S|x^Z_q\rangle = (-1)^{|(Z' \setminus S') \cap \Delta Z'|} \langle S'|x^Z_q'\rangle \quad (58)
\]

for all pairs \((Z, S), (Z', S')\) such that

\[
S \subset Z, \quad S' \subset Z', \quad \text{and} \quad Z \setminus S = Z' \setminus S'. \quad (59)
\]

then it is possible to assemble the unique \(p\)-electron vector

\[
x_p = \frac{1}{(n-p)^{q}} \sum_{Z \subset N} * (x^Z_q) \quad (60)
\]

Each family \(\{x^Z_q\}_{Z \subset N}\) of \(q\)-electron vectors satisfying the conditions (58) will be called \((p,q)\)-vector. Members \(x^Z_q\) of this family will be called its \(q\)-components. For the set of all \((p,q)\)-vectors the symbol \(\mathcal{S}_{N,p,q}\) will be used. The mapping

\[
s_{q \uparrow p} : \{x^Z_q\}_{Z \subset N} \rightarrow \{ * (x^Z_q) \}_{Z \subset N} \rightarrow \frac{1}{(n-p)^{q}} \sum_{Z \subset N} * (x^Z_q) \quad (61)
\]

of the set \(\mathcal{S}_{N,p,q}\) to the \(p\)-electron sector of the Fock space is called ‘the assembling mapping’. It is easy to ascertain that it is a bijection and its
Arbitrary family 

\[ s_{p,q} : x_p \rightarrow \left\{ \sum_{R \subseteq Z} (-1)^{|R \cap \Delta Z|} \langle R \mid x_p \rangle \mid Z \setminus R \right\} \quad (62) \]

Let us consider simple example. For \( N = \{1, 2, 3, 4\}, p = 2, \) and \( q = 1 \) there are four 3–element subsets of \( \Delta Z \):

\begin{align*}
Z_1 &= \{1, 2, 3\}, \quad Z_2 = \{1, 2, 4\}, \quad Z_3 = \{1, 3, 4\}, \quad Z_4 = \{2, 3, 4\}.
\end{align*}

The corresponding subsets \( \Delta_{Z_i} \) are:

\begin{align*}
\Delta_{Z_1} &= \{1, 3\}, \quad \Delta_{Z_2} = \{1, 3, 4\}, \quad \Delta_{Z_3} = \{1, 4\}, \quad \Delta_{Z_4} = \{1, 2, 4\}
\end{align*}

Arbitrary family \( \{x_{1i}^Z\}_{i=1}^4 \) is constituted by the vectors:

\begin{align*}
x_1^{Z_1} &= c_1^{123} |1\rangle + c_2^{123} |2\rangle + c_3^{123} |3\rangle \in F_{Z_1,1} \\
x_1^{Z_2} &= c_1^{124} |1\rangle + c_2^{124} |2\rangle + c_4^{124} |4\rangle \in F_{Z_2,1} \\
x_1^{Z_3} &= c_1^{134} |1\rangle + c_3^{134} |3\rangle + c_4^{134} |4\rangle \in F_{Z_3,1} \\
x_1^{Z_4} &= c_2^{234} |2\rangle + c_3^{234} |3\rangle + c_4^{234} |4\rangle \in F_{Z_4,1}
\end{align*}

In the case under consideration there are six relations of the type of Eq.(59):

\begin{align*}
Z_1 \setminus \{1\} &= Z_4 \setminus \{4\} = \{2, 3\}, \quad Z_1 \setminus \{2\} = Z_3 \setminus \{4\} = \{1, 3\}, \\
Z_1 \setminus \{3\} &= Z_2 \setminus \{4\} = \{1, 2\}, \quad Z_2 \setminus \{1\} = Z_4 \setminus \{3\} = \{2, 4\}, \\
Z_2 \setminus \{2\} &= Z_3 \setminus \{3\} = \{1, 4\}, \quad Z_3 \setminus \{1\} = Z_4 \setminus \{2\} = \{3, 4\}.
\end{align*}

Using Eq.(58), we obtain

\begin{align*}
c_1^{123} &= c_4^{234} = C_{23}, \quad c_2^{123} = -c_4^{134} = C_{13}, \\
c_3^{123} &= c_4^{124} = C_{12}, \quad c_1^{124} = -c_3^{234} = C_{24}, \\
c_2^{124} &= c_3^{134} = C_{14}, \quad c_1^{134} = c_2^{234} = C_{34},
\end{align*}

and family \( \{x_{1i}^Z\}_{i=1}^4 \) is (2, 1)–vector if and only if

\[ x_{1i}^Z = C_{23} |1\rangle + C_{13} |2\rangle + C_{12} |3\rangle \]
\[ x_1^Z = C_{24}|1⟩ + C_{14}|2⟩ + C_{12}|4⟩ \]
\[ x_1^Z = C_{34}|1⟩ + C_{14}|3⟩ - C_{13}|4⟩ \]
\[ x_1^Z = C_{34}|2⟩ - C_{24}|3⟩ + C_{23}|4⟩ \]

Application of Hodge isomorphism to each 1-component of this vector gives

\[ * (x_1^Z) = -C_{23}|23⟩ + C_{13}|13⟩ - C_{12}|12⟩ \]
\[ * (x_1^Z) = -C_{24}|24⟩ + C_{14}|14⟩ - C_{12}|12⟩ \]
\[ * (x_1^Z) = -C_{34}|34⟩ + C_{14}|14⟩ + C_{13}|13⟩ \]
\[ * (x_1^Z) = -C_{34}|34⟩ - C_{24}|24⟩ - C_{23}|23⟩ \]

The corresponding uniquely determined 2–electron vector is

\[ \frac{1}{2} \sum_{i=1}^{4} * (x_1^Z) = \]
\[ = -C_{12}|12⟩ + C_{13}|13⟩ + C_{14}|14⟩ - C_{23}|23⟩ - C_{24}|24⟩ - C_{34}|34⟩ \]

Let us put

\[ \lambda \{ x_q^Z \}_{Z \subset N} + \mu \{ y_q^Z \}_{Z \subset N} = \{ \lambda x_q^Z + \mu y_q^Z \}_{Z \subset N} \]  \hspace{1cm} (63)

where \( \lambda, \mu \in \mathbb{C} \).

Due to linearity of conditions (58) the right-hand side of Eq.(63) is a \((p, q)\)–vector and this equation defines vector space structure on the set \( S_{N,p,q} \). It is clear that the disassembling mapping is an isomorphism of vector spaces \( F_{N,p} \) and \( S_{N,p,q} \).

Scalar product in \( S_{N,p,q} \) consistent with that in \( F_{N,p} \) is

\[ \left\langle \{ x_q^Z \}_{Z \subset N} | \{ y_q^Z \}_{Z \subset N} \right\rangle = \frac{1}{\binom{n-p}{q}} \sum_{Z \subset N} \left\langle x_q^Z | y_q^Z \right\rangle \]  \hspace{1cm} (64)

Thus, for fixed \( N \) and \( p \) with vector space \( F_{N,p} \) it is possible to associate its (isomorphic) models \( S_{N,p,1}, S_{N,p,2}, \ldots \).

For each \((p + q)\)–element subset \( Z \subset N \) let us introduce the mapping

\[ \pi_{p,q}^Z : \{ x_q^Z' \}_{Z' \subset N} \rightarrow x_q^Z \]  \hspace{1cm} (65)
that is obviously a surjective homomorphism (projection) of $S_{N,p,q}$ on $F_{Z,q}$.

Application to $q$—electron vector $x_q^Z$ the Hodge isomorphism with subsequent disassembling of vector $*(x_q^Z)$ gives

$$s_{p\downarrow q} * (x_q^Z) = \left\{ \sum_{R \subset \Delta \cap Z} (-1)^{|R \Delta Z| + |R \Delta Z'|} \langle Z \setminus R | x_q^Z \rangle | Z' \setminus R \rangle \right\}_{Z' \subset N}$$

(66)

From this equation it readily follows that

$$\pi_{p,q}^{-1} s_{p \downarrow q} * (x_q^Z) = x_q^Z$$

(67)

or, in other words, the mapping $s_{p \downarrow q}$ is a right inverse of the projection $\pi_{p,q}$, being linear injective mapping. Note that for obvious reason we omit the composition symbol in writing composition of mappings.

Eq.(67) means that any $(p,q)$—vector of the type of Eq.(66) involves initial $q$—electron vector $x_q^Z$ as its $q$—component. We say that $(p,q)$—vector (66) is generated by its $q$—component $x_q^Z$. Of course, not each $(p,q)$—vector is generated by some of its $q$—component but those, that are generated, are so important that deserve special name.

**Definition.** $(p,q)$—vector is called simple if it is generated by one of its $q$—components, that is if there exists $(p+q)$—element subset $Z \subset N$ such that the following equality holds true:

$$s_{p\downarrow q} * \pi_{p,q}^{-1} \left\{ \left\{ x_q^Z \right\}_{Z' \subset N} \right\} = \left\{ x_q^Z \right\}_{Z' \subset N}$$

(68)

Returning to the example, discussed above, we have

$$s_{2\downarrow 1} * (x_1^{Z_1}) = \left( \begin{array}{c} c_1^{123} |1\rangle + c_2^{123} |2\rangle + c_3^{123} |3\rangle \\ c_3^{123} |4\rangle \\ -c_2^{123} |4\rangle \\ c_1^{123} |4\rangle \end{array} \right)$$

Here $(2,1)$—vector is represented as a column vector with entries indexed by subsets $Z_1, Z_2, Z_3, \text{ and } Z_4$.

Each non-zero $q$—component $x_q^Z$ of a given $(p,q)$—vector $\left\{ x_q^Z \right\}_{Z \subset N}$ generates some simple $(p,q)$—vector $s_{p\downarrow q} * (x_q^Z)$ and it is easy to ascertain that the initial $(p,q)$—vector belongs to the linear hull $V\left( \left\{ x_q^Z \right\}_{Z \subset N} \right)$ of these simple
\((p, q)\)-vectors:

\[
\{x^Z_q\}_{Z \subset N} \in V \left( \{x^Z_{q}\}_{Z \subset N} \right) = \sum_{Z \subset N} \mathbb{C}s_{p|q} * \pi^Z_{p,q} \left( \{x^Z_q\}_{Z \subset N} \right)
\]  

(69)

Since Hodge isomorphism in the case of Euclidean Fock space does not depend upon the choice of (orthonormal) MSO basis, the correspondence

\[
x_p \rightarrow V (s_{p|q}(x_p))
\]  

(70)
supplies us with a family of invariants associated with a given real \(p\)-electron vector \(x_p\).

There exist obvious isomorphisms between spaces with different \(q\):

\[
S_{N,p,q} \xrightarrow{s_{q|p}} F_{N,p} \xrightarrow{s_{p|q'}} S_{N,p,q'}
\]  

(71)

Disassembling of arbitrary factorable \(p\)-vector (determinant) \(|R\rangle\) gives

\[
s_{p|q}(|R\rangle) = \left\{ (-1)^{|R \cap \Delta Z|}|Z \setminus R\rangle \right\}_{Z \supset R}
\]  

(72)

It is clear that any nonzero \(q\)-component of the vector (72) generates it. It is easy to prove that it is a characteristic property of disassembled factorable \(p\)-vectors: \((p, q)\)-vector corresponds to some factorable \(p\)-vector (determinant) if and only if it is generated by any of its nonzero \(q\)-components.

Direct use of Eq. (64) shows that simple \((p, q)\)-vectors \(s_{p|q}(|R\rangle)\) constitute orthonormal (with respect to scalar product (64)) basis of the vector space \(S_{N,p,q}\) of all \((p, q)\)-vectors.

Now let us consider the pointed space \(S^{p,q}_R = (S_{N,p,q}, s_{p|q}(|R\rangle))\). It is easy to endow it with commutative algebra structure by direct transfer of the corresponding structure from \(A^p_R\):

\[
\{x^Z_q\}_{Z \subset N} * \{y^Z_q\}_{Z \subset N} = s_{p|q} \left( s_{q|p} \left( \{x^Z_q\}_{Z \subset N} \right) * s_{q|p} \left( \{y^Z_q\}_{Z \subset N} \right) \right)
\]  

(73)

It would be desirable, however, to give a definition for multiplication of \((p, q)\)-vectors that does not appeal explicitly to the assembling mapping. It is easy to see that such multiplication cannot be componentwise.

First let us select convenient basis in each \(q\)-electron subspace \(F_{Z,q}\). To this end we consider pairs of subsets \(J \subset R\) and \(I \subset N \setminus R\) such that

\[
R \setminus (R \cap Z) \subset J \subset R;
\]  

(74a)
\[ I \subset Z \backslash (R \cap Z); \quad |J| = |I|. \]  

(74b)

The total number of such pairs is equal to

\[ \sum_{k \geq 0} \binom{|R \cap Z|}{k} \binom{p + q - |R \cap Z|}{p + q} = \dim \mathcal{F}_{Z,q} \]  

(75)

Basis vectors in \( \mathcal{F}_{Z,q} \) may be written as

\[ e^I_J(Z,R) = (-1)^{|(R \setminus J) \cup I \setminus \Delta Z|} e_{R \setminus (Z \cap J)}^{Z \setminus R \setminus I}(R) \]  

(76)

Selection of this concrete form of basis vectors is motivated by the relation

\[ s_{p,q}(e^I_J(R)) = \{ e^I_J(Z,R) \}_{Z \supset (R \setminus J) \cup I} \]  

(77)

that holds true for arbitrary basis determinant \( e^I_J(R) \).

Let us return to the example discussed above and suppose that we selected \( R = \{1, 2\} \). Then

(1) In the vector space \( \mathcal{F}_{Z_1,1} \) basis vectors indexed by subsets

\[ J \subset R, \ I \subset \{3\} \]

are

\[ e^{\emptyset}_0(Z_1, R) = -e^{\{3\}}_R(R) = -|3| \]
\[ e^{\{1\}}_1(Z_1, R) = -e^{\{2\}}_R(R) = -|1| \]
\[ e^{\{3\}}_2(Z_1, R) = e^{\emptyset}_0(R) = |2| \]

(2) In the vector space \( \mathcal{F}_{Z_2,1} \) basis vectors indexed by subsets

\[ J \subset R, \ I \subset \{4\} \]

are

\[ e^{\emptyset}_0(Z_2, R) = -e^{\{4\}}_R(R) = -|4| \]
\[ e^{\{1\}}_1(Z_2, R) = -e^{\{2\}}_R(R) = -|1| \]
\[ e^{\{4\}}_2(Z_2, R) = e^{\emptyset}_0(R) = |2| \]

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(3) In the vector space $\mathcal{F}_{Z_3,1}$ basis vectors indexed by subsets

$$\{2\} \subset J \subset R, \ I \subset \{3,4\}$$

are

$$e^{[3]}_{\{2\}}(Z_3, R) = -e^{[4]}_{R}(R) = -|4|$$

$$e^{[4]}_{\{2\}}(Z_3, R) = e^{[3]}_{R}(R) = |3|$$

$$e^{[3,4]}_{\{1,2\}}(Z_3, R) = -e^{0}_{\{2\}}(R) = -|1|$$

(4) In the vector space $\mathcal{F}_{Z_4,1}$ basis vectors indexed by subsets

$$\{1\} \subset J \subset R, \ I \subset \{3,4\}$$

are

$$e^{[3]}_{\{1\}}(Z_4, R) = -e^{[4]}_{R}(R) = -|4|$$

$$e^{[4]}_{\{1\}}(Z_4, R) = e^{[3]}_{R}(R) = |3|$$

$$e^{[3,4]}_{\{1,2\}}(Z_4, R) = -e^{0}_{\{1\}}(R) = -|2|$$

Basis $(2,1)$—vectors (see Eq.(77)), presented as four-component column vectors with entries indexed by subsets $Z_i$, are

$$
\begin{pmatrix}
e^{0}_{\{1\}}(Z_1, R) \\
e^{0}_{\{2\}}(Z_2, R) \\
0 \\
0
\end{pmatrix}
\begin{pmatrix}
e^{[3]}_{\{1\}}(Z_1, R) \\
e^{[3]}_{\{2\}}(Z_2, R) \\
0 \\
0
\end{pmatrix}
\begin{pmatrix}
e^{0}_{\{1\}}(Z_1, R) \\
0 \\
e^{[3]}_{\{1\}}(Z_2, R) \\
e^{[4]}_{\{1\}}(Z_4, R)
\end{pmatrix}
\begin{pmatrix}
e^{[3]}_{\{1\}}(Z_1, R) \\
0 \\
e^{[3]}_{\{2\}}(Z_2, R) \\
e^{[3,4]}_{\{1,2\}}(Z_4, R)
\end{pmatrix}
$$

Each basis vector (77) corresponds to disassembled determinant, and, consequently, it is uniquely determined by any of its non-zero $q$—components. Let us suppose that $(p + q)$—element subsets $Z \subset N$ are listed in some fixed ordering (e.g., lexical) and let $Z^I_j$ be the subset of the minimal rank satisfying the condition $Z \supset (R\setminus J) \cup I$. Then the relation

$$e^{p''}_{j''}(Z^{j''}, R) * e^{p''}_{j''}(Z^{j''}, R) =$$
completely determines star product of any two basis \((p,q)\)-vectors.

For example, to get the product of the second and the fifth four-component vectors listed above, it is sufficient to calculate

\[
e^{(3)}_{\{1\}}(Z_1, R) \star e^{(4)}_{\{2\}}(Z_2, R) = -e^{(3,4)}_{\{1,2\}}(Z_3, R)
\]

and then in zero four-component vector insert \(-e^{(3,4)}_{\{1,2\}}(Z_i, R)\) in all positions corresponding to \(Z_i \supset \{3, 4\}\).

Thus, if some ordering of \((p + q)\)-element subsets of \(N\) is fixed and for each admissible \(J\) and \(I\) subset \(Z^I_J\) of minimal rank, satisfying the condition \(Z \supset (R \setminus J) \cup I\), is selected then we can consider the following model of the algebra \(S^q_R\): It is a vector space of formal linear combinations of \(q\)-electron vectors \(e^J_f(Z^I_J, R)\) with star product defined by Eq. (78). Note that this model requires additional structure of linear ordering of all \((p + q)\)-element subsets of \(N\).

For arbitrary \((p,q)\)-vector \(\{x^Z_\{p,q\}\}_{Z \subset N}\), its \(q\)-components may be written in the form

\[
x^Z_q = \sum_{R \setminus (R \cap Z) \subset J \subset R} \sum_{I \subset Z \setminus (R \cap Z)} x^I_J e^I_f(Z, R)
\]

where \(|J| = |I|\) and the coefficients \(x^I_J\) do not depend on \(Z\). If, on the other hand, we have arbitrary family constituted by vectors (79), then this family is a \((p,q)\)-vector because independence of coefficients in expansion (79) on \(Z\) is equivalent to the conditions (58).

For calculation of \(q\)-component of star product of two arbitrary \((p,q)\)-vectors the following formula may be used:

\[
\pi^Z_{p,q} \left( \left\{ x^Z_q \right\}_{Z' \subset N} \right) \star \left( \left\{ y^Z_q \right\}_{Z' \subset N} \right) = \sum_{R \setminus (R \cap Z) \subset J \subset R} \sum_{I \subset Z \setminus (R \cap Z)} \langle e^J_f(R) | x_p \ast y_p e^I_f(Z, R) \rangle.
\]

Here

\[
\langle e^J_f(R) | x_p \ast y_p \rangle = \sum_{k_1=0}^{k} \sum_{j_1 \subseteq J \setminus I} (-1)^{k_1 + |(J_1 \cup I_1) \cap \Delta(J \cup I)|} x^I_{j_1} y^I_{J_1} \delta_{J_1},
\]

(81a)
\[ x_p = s_{q\uparrow p}\left( \left\{ x_q^{Z'} \right\}_{Z' \subset N} \right), \quad y_p = s_{q\uparrow p}\left( \left\{ y_q^{Z'} \right\}_{Z' \subset N} \right), \quad (81b) \]

and \( k = |J| = |I| \).

In our previous paper [10] it was shown that \((p, q)\)-vectors and reduced density operators of order \( q \) are closely related as seen from the equality

\[ \rho_q = \frac{1}{(n-p) q} \sum_{Z \subset N} |x_q^Z\rangle \langle x_q^Z| \quad (82) \]

Thus, disassembling mapping may be interpreted as a certain \textit{pre-contraction operation} applied to \( p \)-electron state. Actual contraction is defined as

\[ x_p \rightarrow s_{p\downarrow q}(x_p) \rightarrow \frac{1}{(n-p) q} \sum_{Z \subset N} \left| \pi_{p,q}^Z s_{p\downarrow q}(x_p) \right\rangle \langle \pi_{p,q}^Z s_{p\downarrow q}(x_p) \right| \quad (83) \]

It is pertinent to mention that the representation of density operator in the form of Eq.(82) is connected with the commonly used one by a certain non-degenerate transformation described in detail in paper [13].

Eq.(82) means that any representable by pure \( p \)-electron state density operator of order \( q \) is a convex hull of pure normalized \( q \)-electron states \( v_q^Z \in F_{Z,q} \)

\[ \rho_q = \sum_{Z \subset N} \lambda_Z^2 |v_q^Z\rangle \langle v_q^Z| \quad (84) \]

such that the family \( \left\{ \lambda_Z^2 v_q^Z \right\}_{Z \subset N} \) is a \((p, q)\)-vector. This statement, being interesting by itself, may serve as a base for different parametrizations of density operators. For example, let us consider \((n)\) vectors constituting an orthonormal basis of \( F_{N,q} \):

\[ x_q(i) = \sum_{S \subset N}^{(q)} c_S |S\rangle \quad (85) \]

and by the symbol \( x_q^Z(i) \) let us denote its \( Z \)-component

\[ x_q^Z(i) = \sum_{S \subset Z}^{(q)} c_S |S\rangle \quad (86) \]
\[(p, q)\text{-vector}\]

\[
\{ q^z \}_{z \subset N} = s_{p \downarrow q} \left( C_R |R \rangle + \sum_{i=1}^{n_q} \mu_i \sum_{z' \subset N} \left( x^{z'}_q (i) \right) \right)
\]  

(87)

depending on \( \frac{1}{2} \binom{n}{q} \left( \binom{n}{q} + 1 \right) \) parameters can be used to parametrize representable by pure \( p \)-electron states density operators of order \( q \). Here \( |R \rangle \) is relevant HF reference state. Note that use of parametrized density operators associated with parametric \( (p, q) \)-vector (87) leads to genuine \( q \)-electron optimization problem but in a certain \( p \)-electron metric (see [10]).

**Conclusion**

Any new representation of the space of state vectors and especially any new algebraic structure on this space are of great interest by themselves and deserve thorough study even if perspectives of their immediate application are vague. In our opinion with new structure revealed on the Fock space the situation is different. Its study clarifies and simplifies the mathematical backgrounds of CC and related approaches. And even more, it leads to many relations that would be very difficult to derive using conventional technique. Eqs.(38), (47), and (53) supply us with convincing examples of validity of this statement.

The situation with models of the Fock space as vector spaces of \( (p, q) \)-vectors is not so unambiguous. These models originate from the representability theory and at first glance are very complicated. As an immediate application of these models we can point out possibility to construct parametric *representable* density operators of arbitrary order in a very general way. Of course, the crucial question arising is the following: what part of the set of all representable density operators is covered by such parametrizations? This question, which is probably of moderate mathematical interest, will has some sense for quantum chemists only if computer implementation of our approach will lead to perspective methods for electronic structure calculations. The work on implementation of computational methods based on relations of the type of Eq.(87) is in progress now.
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