Electronic Fock Spaces: Phase Prefactors and Hidden Symmetry

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ABSTRACT: Efficient technique of manipulation with phase prefactors in electronic Fock spaces is developed. Its power is demonstrated on example of both relatively simple classic configuration interaction matrix element evaluation and essentially more complicated coupled cluster case. Interpretation of coupled cluster theory in terms of a certain commutative algebra is given.

Key words: Configuration interaction, excitation operators, coupled cluster approach, density operators, commutative algebras

Introduction

Many years ago in paper [1] some special set-theoretical operation $\Delta_K$ was introduced. It was used to reduce manipulations with phase prefactors in the Fock space (Grassmann algebra) to pure set theoretical ones. More detailed discussion of this operation was given in [2], Appendix A. The main purpose of this paper is to show that the operation mentioned makes it easy to obtain very complicated analytic expressions in effective and uniform manner. In addition, this technique helps to reveal hidden symmetry of the electronic Fock space. Fock space equipped with new algebraic structure can be considered as a natural domain for a certain class of Post Hartree-Fock (HF) methods.

In Section I we discuss properties of the operation $\Delta_K$ both for the case of molecular spin orbital (MSO) basis and molecular orbital (MO) basis.

Section II is dedicated to classic configuration interaction (CI) matrix elements. It does not contain any new results and is included only as simple but important application of our technique of manipulations with phase prefactors.

In Section III excitation operators and coupled cluster (CC) approach [4] - [10] are discussed. General analytic expression for CI expansion of CC wave function is given. For the CC CI coefficients recurrence relations are derived. Analytic expressions for derivatives of CC CI coefficients with respect to CC
amplitudes are given. CC density operator of the first order necessary for calculation of molecular properties (see, e.g., [9]) is constructed.

Sections IV and V are dedicated to new algebraic structure on the finite-dimensional electronic Fock spaces.

In Section VI and Appendix some hints concerning computer implementation of our approach are given.

**Basic Definitions**

Let $N = \{1, 2, \ldots, n\}$ be the molecular spin-orbital (MSO) index set. On the set $\mathcal{P}(N)$ of all subsets of $N$ let us consider the operation (symmetric difference)

$$ R \Delta S = (R \cup S) \setminus (R \cap S) \quad (1) $$

where $R, S \in \mathcal{P}(N)$. This operation endows $\mathcal{P}(N)$ with Abelian group structure with empty set as its unit. Each element of this group is of order 2 ($R \Delta R = \emptyset$).

Let us define the operation $\Delta_K$ as

$$ \Delta_K = \Delta_{\{1, 2, \ldots, k\}} \quad (2) $$

where $K \subset N$. For example, if $K = \{2, 4, 5, 7\}$ then

$$ \Delta_K = \{1, 2\} \Delta\{1, 2, 3, 4\} \Delta\{1, 2, 3, 4, 5\} \Delta\{1, 2, 3, 4, 5, 6, 7\} = \{3, 4, 6, 7\} $$

The mapping

$$ \varphi : K \rightarrow \Delta_K \quad (3) $$

is a group homomorphism. Indeed, $\Delta_0 = \emptyset$ and $(\Delta_K) \Delta(\Delta_L) = \Delta_{K \Delta L}$.

In general case, for $K = k_1 < k_2 < \ldots < k_s$

$$ \Delta_K = \begin{cases} \bigcup_{i=1}^{[s/2]} \{k_{2i-1} + 1, \ldots, k_{2i}\} & \text{if } s \text{ is even} \\ \bigcup_{i=0}^{[s/2]} \{k_{2i} + 1, \ldots, k_{2i+1}\} & \text{if } s \text{ is odd} \end{cases} \quad (4) $$

Directly from the definition of operation (1) the following useful relation may be obtained

$$ |K \cap R| + |K \cap S| \equiv |K \cap (R \Delta S)| \ (mod \ 2) \quad (5) $$
For a fixed basis set of $n$ orthonormal spin-orbitals the corresponding finite-dimensional Fock space $\mathcal{F}_N$ is spanned by determinants $|R\rangle$ where $R$ runs over all subsets of the spin-orbital index set $N$. Its $p$–electron sector $\mathcal{F}_{N,p}$ is spanned by determinants $|R\rangle$ with $|R| = p$. Basis determinants will be labelled by subsets and all sign conventions connected with their representation as the Grassmann product of ordered spin-orbitals will be included in the definition of the creation-annihilation operators.

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

$$a_i^\dagger |R\rangle = (1 - \zeta_{i,R}) (-1)^\varepsilon |R \cup \{i\}\rangle$$

$$a_i |R\rangle = \zeta_{i,R} (-1)^\varepsilon |R \setminus \{i\}\rangle$$

where

$$\varepsilon = |\{1,2,\ldots, i-1\} \cap R|$$

is the sign counter and

$$\zeta(I,R) = \begin{cases} 1 & \text{if } I \subseteq R \\ 0 & \text{if } I \not\subseteq R \end{cases}$$

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 pertinent to mention as well that $|R| = |S|$ and $\zeta(R,S) = 1$ imply $R = S$.

The main purpose of this section is to get explicit and easily evaluated expression for the action of products of the creation-annihilation operators on arbitrary determinant wave function. We start with calculation of the sum $|K \cap \Delta_R| + |R \cap \Delta_K|$. From Eq.(5) it readily follows that for arbitrary $K, R \subseteq N$

$$|K \cap \Delta_R| + |R \cap \Delta_K| \equiv \sum_{(k,r) \in K \times R} |\{k\} \cap \Delta_{\{r\}}| + |\{r\} \cap \Delta_{\{k\}}| \pmod{2}$$

But

$$|\{k\} \cap \Delta_{\{r\}}| + |\{r\} \cap \Delta_{\{k\}}| = \begin{cases} 1 & \text{if } k \neq r \\ 2 & \text{if } k = r \end{cases}$$

As a result,

$$|K \cap \Delta_R| + |R \cap \Delta_K| \equiv |K||R| + |K \cap R| \pmod{2}$$
Let us return to the creation-annihilation operators and their products. If $i \not\in R$ then

$$\{1, 2, \ldots, i - 1\} \cap R \equiv |R \cap \Delta_i| \equiv |R| + |\{i\} \cap \Delta_R| \pmod{2} \quad (12a)$$

where Eq.(11) was used. If $i \in R$ then

$$\{1, 2, \ldots, i - 1\} \cap R \equiv |(R \setminus \{i\}) \cap \Delta_i| \pmod{2}$$

With the aid of Eq.(11) we can rewrite the last expression as

$$\{1, 2, \ldots, i - 1\} \cap R \equiv |R \setminus \{i\}| + |\{i\} \cap \Delta_{R \setminus \{i\}}| \equiv |R| + |\{i\} \cap \Delta_R| \pmod{2} \quad (12b)$$

Now formulas (6a) and (6b) may be recast as

$$a_i^\dagger |R\rangle = (-1)^{|R|}(1 - \zeta_{i,R})(-1)^{|\{i\} \cap \Delta_R|} |R \cup \{i\}\rangle \quad (13a)$$

$$a_i |R\rangle = (-1)^{|R|\zeta_{i,R}}(-1)^{|\{i\} \cap \Delta_R|} |R \setminus \{i\}\rangle \quad (13b)$$

Are Eqs.(13a) and (13b) more convenient than Eqs.(6a) and (6b)? In our opinion in general situation it is more a matter of taste than convenience. But if the reference determinant $|R\rangle$ is fixed and it is necessary to calculate the action of different creation-annihilation operators on this determinant, then it is possible to find at first the bit vector representing subset $\Delta_R$ and then each time check only one bit of this vector in contrast to multiple checks if Eq.(7) is used.

We are interested in expressions of the type $a_{i_k}^\dagger \ldots a_{i_1}^\dagger a_{j_k} \ldots a_{j_1} |R\rangle$ involving particle number preserving products of the creation-annihilation operators. Successive application of Eqs.(13b) and (13a) gives

$$a_{i_k}^\dagger \ldots a_{i_1}^\dagger a_{j_k} \ldots a_{j_1} |R\rangle =$$

$$= \prod_{l=1}^{k} (1 - \zeta_{i_l,(R \setminus J_k) \cup J_{l-1}}) \prod_{l=1}^{k} \zeta_{j_l,R \setminus J_{l-1}} \times (-1)^\varepsilon |(R \setminus J_k) \cup J_k\rangle \quad (14)$$

where

$$J_l = \bigcup_{\mu=1}^{t} \{j_\mu\}$$
\[ I_l = \bigcup_{\mu=1}^{l} \{i_\mu\} \]

and

\[
\varepsilon = \sum_{l=1}^{k} \left[ |R\setminus J_{l-1}| + |(R\setminus J_k) \cup I_{l-1}| + |\{j_l\} \cap \Delta_{R\setminus J_{l-1}}| + |\{i_l\} \cap \Delta_{(R\setminus J_k) \cup I_{l-1}}| \right]
\]

(15)

Let us try to simplify the expression for \( \varepsilon \). It is clear that the right-hand side of Eq.(14) is nonzero only if \( |J_l| = l \) and \( |I_l| = l \) for any \( l = 1, \ldots, k \). As a result,

\[
\sum_{l=1}^{k} \left[ |R\setminus J_{l-1}| + |(R\setminus J_k) \cup I_{l-1}| \right] \equiv k \mod 2
\]

and the expression for \( \varepsilon \) takes the form

\[
\varepsilon = k + \sum_{l=1}^{k} \sum_{r=1}^{l-1} |\{j_l\} \cap \Delta_{j_r}| + \sum_{l=1}^{k} \sum_{r=1}^{k} |\{i_l\} \cap \Delta_{j_r}|
\]

\[
+ \sum_{l=1}^{k} \sum_{r=1}^{l-1} |\{i_l\} \cap \Delta_{i_r}| + \sum_{l=1}^{k} |\{j_l\} \cap \Delta_R| + \sum_{l=1}^{k} |\{i_l\} \cap \Delta_R|
\]

(16)

Note that the \( R \)-dependent part of this formula is very easy to handle: it is sufficient to construct the set \( \Delta_R \) and then just to check if the indices \( j_1, \ldots, j_k \) and \( i_1, \ldots, i_k \) belong to this set. The remainder terms in this formula depend only on the order relation between indices of the creation-annihilation operators involved.

Expression (16) takes more simple and compact form if \( j_1 < \ldots < j_k \) and \( i_1 < \ldots < i_k \). Indeed, in this case, as easily follows from Eq.(4), subsets \( \{j_l\} \cap \Delta_{J_{l-1}} \) and \( \{i_l\} \cap \Delta_{I_{l-1}} \) are empty. As a result,

\[
\varepsilon = k + |I_k \cap \Delta_{J_k}| + |I_k \cap \Delta_R| + |J_k \cap \Delta_R|
\]

(17)

If \( k = 1 \) then

\[
a_i^\dagger a_j |R\rangle = (1 - \zeta_{i,R\setminus\{j\}}) \zeta_{j,R} (-1)^\varepsilon |(R\setminus\{j\}) \cup \{i\}\rangle
\]

(18)

where

\[
\varepsilon = 1 + |\{i\} \cap \Delta_{\{j\}}| + |\{i,j\} \cap \Delta_R|
\]

(19)
If \( k = 2 \) then
\[
\begin{align*}
    a_i^\dagger a_j^\dagger a_i a_j |R\rangle &= \\
    &= (1 - \zeta_i, R \backslash \{k, l\}) (1 - \zeta_j, R \backslash \{k, l\}) \zeta_k, R (-1)^\varepsilon |(R \backslash \{k, l\}) \cup \{i, j\}\rangle \tag{20}
\end{align*}
\]
where
\[
\varepsilon = |\{i\} \cap \Delta_{\{j\}}| + |\{i, j\} \cap \Delta_{\{k\}}| + |\{i, j\} \cap \Delta_{\{l\}}| + |\{i, j, k\} \cap \Delta_{\{l\}}| \quad \tag{21}
\]

In Handy orbital representation [3] each MSO index set is split in its \( \alpha \) and \( \beta \) components. In particular, in expression \( K \cap \Delta_R \) subsets \( K, R \) go to \( (K_\alpha, K_\beta) \) and \( (R_\alpha, R_\beta) \), respectively. Let us introduce the sets \( K_\beta = m + K_\beta \) and \( R_\beta = m + R_\beta \) where \( m \) is the number of molecular orbitals (MO). We have \( K = K_\alpha \Delta K_\beta \) and \( R = R_\alpha \Delta R_\beta \) and
\[
|K \cap \Delta_R| \equiv |K_\alpha \cap \Delta_{R_\alpha}| + |K_\alpha \cap \Delta_{R_\beta}| + |K_\beta \cap \Delta_{R_\alpha}| + |K_\beta \cap \Delta_{R_\beta}| \quad \text{mod} \ 2.
\]
It is clear that \( |K_\beta \cap \Delta_{R_\alpha}| = 0 \) and \( |K_\alpha \cap \Delta_{R_\beta}| \equiv |K_\alpha||R_\beta| \quad \text{mod} \ 2. \) As a result,
\[
|K \cap \Delta_R| \equiv |K_\alpha \cap \Delta_{R_\alpha}| + |K_\beta \cap \Delta_{R_\beta}| + |K_\alpha||R_\beta| \quad \text{mod} \ 2. \quad \tag{22}
\]

**Standard Matrix Elements**

One-electron operator is of the form
\[
h = \sum_{i, j \in N} \langle i | h | j \rangle a_i^\dagger a_j \tag{23}
\]
and its action on determinant \( |R\rangle \) may be presented as
\[
h | R \rangle = -\sum_{j \in R} \sum_{i \in (N \backslash R) \cup \{j\}} \langle i \cap \Delta_{\{j\}}| + |(i \cap \Delta_{\{j\}}) \cup \{i\}\rangle \langle i | h | j \rangle \langle (R \backslash \{j\}) \cup \{i\}\rangle \tag{24}
\]
For matrix element \( < S | h | R > \) we have the expression
\[
< S | h | R > = -\sum_{j \in R} \sum_{i \in (S \backslash R) \cup \{j\}} \langle i \cap \Delta_{\{j\}}| + |(i \cap \Delta_{\{j\}}) \cup \{i\}\rangle \langle i | h | j \rangle \zeta_{(R \backslash \{j\}) \cup \{i\}, S} \tag{24}
\]
Matrix element \( < i|h|j > \) is zero if MSO involved are of different spin. As a result, in MO basis only cases \( j \in R_\alpha, i \in S_\alpha \) and \( j \in R_\beta, i \in S_\beta \) are to be treated. Note that by an abuse of notation we use the same letters for indices of MSOs and MOs.

**Case ’\( \alpha\alpha \)’**. From Eq.(22) it follows that
\[
|(\{k_1\}, \emptyset) \cap \Delta_R| \equiv |\{k_1\} \cap \Delta_{R_\alpha}| + |R_\beta|(\text{mod } 2) \tag{25}
\]
and
\[
\varepsilon_{\alpha\alpha} = |\{i\} \cap \Delta_{\{j\}}| + |\{i, j\} \cap \Delta_{R_\alpha}|
\tag{26}
\]

**Case ’\( \beta\beta \)’**. We have
\[
|(\emptyset, \{k_1\}) \cap \Delta_R| \equiv |\{k_1\} \cap \Delta_{R_\beta}|(\text{mod } 2) \tag{27}
\]
and
\[
\varepsilon_{\beta\beta} = |\{i\} \cap \Delta_{\{j\}}| + |\{i, j\} \cap \Delta_{R_\beta}|
\tag{28}
\]

Thus, in MO basis Eq.(24) becomes
\[
< (S_\alpha, S_\beta)|h|(R_\alpha, R_\beta) > =
-\zeta_{\beta\beta,S_\beta} \sum_{j \in R_\beta} \sum_{i \in (S_\alpha \setminus R_\alpha) \cup \{ j \}} (-1)^{\varepsilon_{\beta\beta}} < i|h|j > \zeta_{(R_\beta \setminus \{j\}) \cup \{i\}, S_\beta}
-\zeta_{\alpha\alpha,S_\alpha} \sum_{j \in R_\alpha} \sum_{i \in (S_\beta \setminus R_\beta) \cup \{ j \}} (-1)^{\varepsilon_{\alpha\alpha}} < i|h|j > \zeta_{(R_\alpha \setminus \{j\}) \cup \{i\}, S_\alpha} \tag{29}
\]

Two-electron operator is of the form
\[
g = \sum_{i,j,k,l \in N} < ij|kl | a_i^\dagger a_j^\dagger a_l a_k \tag{30}
\]
and its matrix element \( < S|g|R > \) may be written as
\[
< S|g|R > = \sum_{k,l \in R \atop (k \neq l)} \sum_{i, j \in (S \setminus \{k,l\}) \cup \{ k,l \} \atop (i \neq j)} (-1)^\varepsilon < ij|kl > \zeta_{(R \setminus \{k,l\}) \cup \{i,j\}, S} \tag{31}
\]
where \( \varepsilon \) is given by Eq.(21).

Two-electron integrals \( < ij|kl > \) equal to zero if MSOs with indices \( i, k \) or with indices \( j, l \) are of different spins. In MO basis two-electron integrals are written as \( (ik|jl) \) and there are four cases to be analyzed.
Case 'αααα'. All orbitals are of the same spin α and in this case

\[ |\{(k_1, k_2), \emptyset\} \cap \Delta_R| \equiv |\{k_1, k_2\} \cap \Delta_{R_\alpha}| + 2|R_\beta|(\text{mod } 2) \] (32)

and

\[ \varepsilon_{\alpha\alpha\alpha\alpha} = |\{i\} \cap \Delta_{\{k\}}| + |\{j\} \cap \Delta_{\{k\}}| + |\{i\} \cap \Delta_{\{l\}}| + |\{j\} \cap \Delta_{\{l\}}| \]
\[ + |\{i\} \cap \Delta_{\{l\}}| + |\{i\} \cap \Delta_{\{j\}}| + |\{i, j\} \cap \Delta_{R_\alpha}| + |\{k, l\} \cap \Delta_{R_\alpha}| \] (33)

Case 'ααββ'. Orbitals with indices \(i, k\) are of α spin and with indices \(j, l\) are of β spin. We have

\[ |\{(k_1, k_2)\} \cap \Delta_R| \equiv |\{k_1\} \cap \Delta_{R_\alpha}| + |\{k_2\} \cap \Delta_{R_\beta}| + |R_\beta|(\text{mod } 2) \] (34)

and

\[ \varepsilon_{\alpha\alpha\beta\beta} = |\{i\} \cap \Delta_{\{k\}}| + |\{j\} \cap \Delta_{\{l\}}| + |\{i, k\} \cap \Delta_{R_\alpha}| + |\{j, l\} \cap \Delta_{R_\alpha}| \] (35)

Case 'ββαα'. Orbitals with indices \(i, k\) are of β spin and with indices \(j, l\) are of α spin. We have

\[ \varepsilon_{\beta\beta\alpha\alpha} = |\{i\} \cap \Delta_{\{k\}}| + |\{j\} \cap \Delta_{\{l\}}| + |\{i, k\} \cap \Delta_{R_\beta}| + |\{j, l\} \cap \Delta_{R_\alpha}| \] (36)

Case 'ββββ'. All orbitals are of the same spin β and in this case

\[ |\{(\emptyset, k_1, k_2)\} \cap \Delta_R| \equiv |\{k_1, k_2\} \cap \Delta_{R_\beta}|(\text{mod } 2) \] (37)

and

\[ \varepsilon_{\beta\beta\beta\beta} = |\{l\} \cap \Delta_{\{k\}}| + |\{j\} \cap \Delta_{\{l\}}| + |\{i\} \cap \Delta_{\{k\}}| + |\{j\} \cap \Delta_{\{l\}}| \]
\[ + |\{i\} \cap \Delta_{\{l\}}| + |\{i\} \cap \Delta_{\{j\}}| + |\{i, j\} \cap \Delta_{R_\beta}| + |\{k, l\} \cap \Delta_{R_\beta}| \] (38)

In MO basis the expression (31) takes the form

\[ < (S_\alpha, S_\beta)|g|(R_\alpha, R_\beta) > = \]
\[ \zeta_{R_\beta, S_\beta} \sum_{k \in R_\alpha} \sum_{l \in (S_\alpha \setminus R_\alpha) \cup \{k, l\}} (-1)^{\varepsilon_{\alpha\alpha\alpha\alpha}(ikjl)} \zeta(R_\alpha \setminus \{k, l\}) \cup \{i, j\}, S_\alpha \]
\[ + \sum_{k \in R_\alpha} \sum_{l \in (S_\alpha \setminus R_\alpha) \cup \{k\}} \sum_{j \in (S_\beta \setminus R_\beta) \cup \{l\}} (-1)^{\varepsilon_{\alpha\alpha\beta\beta}(ikjl)} \zeta(R_\alpha \setminus \{k\}) \cup \{i\}, S_\alpha \zeta(R_\beta \setminus \{l\}) \cup \{j\}, S_\beta \]
under consideration is presented in the form

\[ \sum_{k \in \mathcal{R}_\beta} \sum_{l \in \mathcal{R}_\alpha} (-1)^{\varepsilon_{\beta \alpha \alpha}} (ik|jl) \zeta_{(R_{\alpha}\{l\}) \cup (j), S_{\alpha}} \zeta_{(R_{\beta}\{k\}) \cup (i), S_{\beta}} \]

\[ + \zeta_{R_{\alpha}, S_{\alpha}} \sum_{k, i \in \mathcal{R}_\beta} \sum_{l, j \in (S_{\beta} \setminus R_{\alpha}) \cup (k, l)} (-1)^{\varepsilon_{\beta \beta \beta}} (ik|jl) \zeta_{(R_{\beta}\{l\}) \cup (i,j), S_{\beta}} \]  \hspace{1cm} (39)

To reduce the dimension of configuration interaction (CI) space one may turn to the notion of the active space. Let us suppose that each determinant under consideration is presented in the form

\[ (R_{\alpha}, R_{\beta}) = (I \cup R_{\alpha}^a, I \cup R_{\beta}^a) \]  \hspace{1cm} (40)

where \( I = \{1, 2, \ldots, n_i\} \) is the set of the so-called inactive MO indices that occur in each determinant with the occupancy 2.

From Eq.(29) it easily follows that either \( i, j \in I \) or \( i, j \notin I \). As a result,

\[ < (I \cup S_{\alpha}^a, I \cup S_{\beta}^a)|h|(I \cup R_{\alpha}^a, I \cup R_{\beta}^a) > = \]

\[ \zeta_{R_{\alpha}, S_{\alpha}} \zeta_{R_{\beta}, S_{\beta}} \sum_{i \in I} 2 < i|h|i > \]

\[ - \zeta_{R_{\alpha}, S_{\alpha}} \sum_{j \in R_{\alpha}^a} \sum_{i \in (S_{\alpha}^a \setminus R_{\alpha}^a) \cup \{j\}} (-1)^{\varepsilon_{\alpha}} < i|h|j > \zeta_{(R_{\alpha}^a \setminus \{j\}) \cup \{i\}, S_{\alpha}^a} \]

\[ - \zeta_{R_{\beta}, S_{\beta}} \sum_{j \in R_{\beta}^a} \sum_{i \in (S_{\beta}^a \setminus R_{\beta}^a) \cup \{j\}} (-1)^{\varepsilon_{\beta \beta}} < i|h|j > \zeta_{(R_{\beta}^a \setminus \{j\}) \cup \{i\}, S_{\beta}^a} \]  \hspace{1cm} (41)

In the same manner Eq.(39) may be treated. We have

\[ < (I \cup S_{\alpha}^a, I \cup S_{\beta}^a)|g|(I \cup R_{\alpha}^a, I \cup R_{\beta}^a) > = \]

\[ \zeta_{R_{\alpha}, S_{\alpha}} \zeta_{R_{\beta}, S_{\beta}} \sum_{i, j \in I} 2 [2(ii|jj) - (ij|ji)] \]

\[ + \zeta_{R_{\alpha}, S_{\alpha}} \sum_{k, l \in R_{\beta}^a} \sum_{j \in (S_{\beta}^a \setminus R_{\alpha}^a) \cup (k, l)} (-1)^{\varepsilon_{\alpha \alpha \alpha \alpha}} (ik|jl) \zeta_{(R_{\alpha}^a \setminus \{l\}) \cup \{i,j\}, S_{\alpha}^a} \]

\[ + \sum_{k \in R_{\alpha}^a} \sum_{l \in R_{\beta}^a} \sum_{j \in (S_{\beta}^a \setminus R_{\alpha}^a) \cup \{k\}} (-1)^{\varepsilon_{\alpha \alpha \beta \beta}} (ik|jl) \zeta_{(R_{\alpha}^a \setminus \{k\}) \cup \{i\}, S_{\alpha}^a} \zeta_{(R_{\beta}^a \setminus \{l\}) \cup \{j\}, S_{\beta}^a} \]  \hspace{1cm} (42)
\[ + \sum_{k \in R_\beta^a} \sum_{i \in (S_\beta^a \backslash R_\beta^a) \cup \{i \}} \sum_{j \in (S_\beta^a \backslash R_\beta^a) \cup \{j \}} (-1)^{\varepsilon_{\beta\alpha\alpha}} (ik | jl) \zeta_{(R_\beta^a \backslash \{i \}) \cup \{j \}, S_\alpha^a} \zeta_{(R_\beta^a \backslash \{k \}) \cup \{i \}, S_\beta^a} \]

\[ + \zeta_{R_\beta^a, S_\alpha^a} \sum_{k \in R_\beta^a} \sum_{i \in (S_\beta^a \backslash R_\beta^a) \cup \{i \}} \sum_{j \in (S_\beta^a \backslash R_\beta^a) \cup \{j \}} (-1)^{\varepsilon_{\beta\beta\beta}} (ik | jl) \zeta_{(R_\beta^a \backslash \{k \}) \cup \{i, j \}, S_\beta^a} \]

**Excitation Operators**

The operator performing \( k \)-fold excitation from some fixed single determinant reference state \( | R > \) is defined as

\[ a_{J_k}^I = a_{i_1}^+ \cdots a_{i_k}^+ a_{j_1} \cdots a_{j_k} \] (43)

where \( J_k = \{ j_1 < \ldots < j_k \} \subset R \) and \( I_k = \{ i_1 < \ldots < i_k \} \subset N \backslash R \). We have

\[ a_{J_k}^I | R > = (-1)^{k+|I_k \cap \Delta J_k| + |I_k \cap \Delta R| + |J_k \cap \Delta R|} (|R \backslash J_k) \cup I_k > \]

Product

\[ a_{I_{k_\mu} \ldots I_{k_1}} = a_{I_{k_\mu}} \cdots a_{I_{k_1}} \] (44)

gives non-vanishing result when applied to \( | R > \) if and only if families \( I_{k_1}, \ldots, I_{k_\mu} \) and \( J_{k_1}, \ldots, J_{k_\mu} \) include *mutually disjoint* subsets. After simple manipulations we get

\[ a_{J_{k_\mu} \ldots J_{k_1}} | R > = (-1)^\varepsilon (|R \backslash J) \cup I > \] (45)

where

\[ \varepsilon = \sum_{i=1}^{\mu} k_i + \sum_{i=1}^{\mu} |I_{k_i} \cap \Delta J_{k_i}| + |I \cap \Delta R| + |J \cap \Delta R| + \sum_{i>j} |(I_{k_i} \cup J_{k_i}) \cap \Delta (I_{k_j} \cup J_{k_j})| \]

(46)

and \( I = \bigcup_{i=1}^{\mu} I_{k_i}, J = \bigcup_{i=1}^{\mu} J_{k_i} \).

The expression for \( \varepsilon \) can be simplified if we suppose that the reference determinant \( | R > \) is built on the first \( p \) spin-orbitals that is \( | R > = | \{1, 2, \ldots, p\} \rangle \).

We, however, do not presuppose any special choice of indices of occupied HF MSOs in our further discussion.
Definition 1. Family \( \{ J_i \}_{i=1}^{\mu} \) is a set partition of \( J \) into \( \mu \) blocks if
(1) \( J_i \neq \emptyset \) for all \( i = 1, 2, \ldots, \mu \);
(2) \( J_i \cap J_j = \emptyset \) for all \( i \neq j \);
(3) \( J = \bigcup_{i=1}^{\mu} J_i \).

Normally set partition has its blocks listed in increasing order of smallest element in each block. We will call such partitions block ordered ones, reserving the term 'set partitions' for arbitrary families with properties (1) - (3) of Definition 1.

If \( |J| = k \) then the number of all possible block ordered set partitions of \( J \) is equal to the \( k \)th Bell number \( B_k \) (see, e.g., [11]).

Definition 2. Family \( \{(J_i, I_i)\}_{i=1}^{\mu} \) is a consistent set partition of a pair of subsets \( (J, I) \) if
(1) \( \{J_i\}_{i=1}^{\mu} \) is a block ordered set partition of \( J \);
(2) \( \{I_i\}_{i=1}^{\mu} \) is a set partition of \( I \);
(3) \( |J_i| = |I_i| \) for all \( i = 1, 2, \ldots, \mu \).

Excitation operators appear explicitly in coupled cluster theory [4] - [10] where the exponential ansatz of wave function is used:

\[ |\Psi> = e^X |R> . \]  

Here

\[ X = \sum_{k=1}^{l} \sum_{k \in R \setminus R} \left( \prod_{j=1}^{(k_j)} \right) t_{J_j}^{I_k} a_{J_k}^{I_k}, \]  

is the excitation operator associated with chosen reference determinant \( |R> \), and \( l \leq p \) is the maximal excitation order.

Let us consider the standard expansion

\[ e^X = \sum_{\mu \geq 0} \frac{1}{\mu!} X^\mu \]  

and try to present the expression for the restriction of \( X^\mu \) on one-dimensional reference subspace \( \mathbb{C}|R> \) in a form convenient for further analysis. We have

\[ X^\mu |R> = \sum_{k=\mu}^{\min(p,\mu)} \sum_{J \subset R} \sum_{\prod_{j=1}^{(k_1+\ldots+k_\mu)} t_{J_{k_j}}^{I_{k_j}} \ldots t_{J_{k_1}}^{I_{k_1}} a_{I_{k_\mu}}^{I_{k_\mu}} |R> \]  

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where the inner sum goes over families that determine consistent set partitions of subsets \( J \) and \( I \) with \( 1 \leq k_i \leq l \). Summation of both sides of the last equality over \( \mu \) gives

\[
e^{X|R >} = |R > + \sum_{\mu=1}^{p} \mu \left( \min(p, \mu) \right) \sum_{k=\mu}^{(k)} \frac{1}{\mu!} \sum_{\sum_{i \subseteq N \setminus R}^{(k)}} \sum_{i<k} \sum_{J \subseteq R} \sum_{I \subseteq N \setminus R}^{(k)} \sum_{J \subseteq R} \sum_{I \subseteq N \setminus R}^{(k)} t^{I_{k_{\mu} \ldots t_{k_{1}}} a_{I_{k_{\mu} \ldots t_{k_{1}}}} |R >}
\]

(51)

The right-hand side of Eq.(51) contains similar terms. Indeed, if \( \mu \) is fixed and some family \( \{J_{k_{\mu i}}\}^{\mu}_{i=1}, \{I_{k_{\mu i}}\}^{\mu}_{i=1} \) is selected then any permutation \( \sigma \in S_{\mu} \) generates new family \( \{J_{k_{\sigma i}}\}^{\mu}_{i=1}, \{I_{k_{\sigma i}}\}^{\mu}_{i=1} \). Of \( \mu! \) families thus obtained let us choose one and put

\[
\varepsilon = \sum_{i>j} \left| (I_{k_{\sigma i}} \cup J_{k_{\sigma j}}) \cap \Delta (I_{k_{\sigma j}} \cup J_{k_{\sigma j}}) \right|
\]

(52)

Then the summation over \( \mu! \) families on the right-hand side of Eq.(51) is reduced to calculation of the following sum

\[
s_{\mu}(\{J_{k_{\mu i}}\}^{\mu}_{i=1}, \{I_{k_{\mu i}}\}^{\mu}_{i=1}) = \frac{(-1)^{\varepsilon}}{\mu!} \sum_{\sigma \in S_{\mu}} (-1)^{\varepsilon_{\sigma}}
\]

(53)

where

\[
\varepsilon = \sum_{i=1}^{\mu} k_{i} + \sum_{i=1}^{\mu} |I_{k_{i}} \cap \Delta J_{k_{i}}| + |I \cap \Delta R| + |J \cap \Delta R|
\]

(54)

But from Eq.(11) it easily follows that

\[
|(I_{k_{i}} \cup J_{k_{j}}) \cap \Delta (I_{k_{j}} \cup J_{k_{j}})| + |(I_{k_{j}} \cup J_{k_{j}}) \cap \Delta (I_{k_{i}} \cup J_{k_{i}})| \equiv 0 (mod 2).
\]

As a result, \( s_{\mu}(\{J_{k_{i}}\}^{\mu}_{i=1}, \{I_{k_{i}}\}^{\mu}_{i=1}) = (-1)^{\varepsilon} \) and final expression for \( e^{X|R >} \) is

\[
e^{X|R >} = \sum_{k=0}^{p} \sum_{\sum_{i \subseteq N \setminus R}^{(k)}} \sum_{J \subseteq R} T_{k}^{\mu}(J, I)(R \setminus J) \cup I >,
\]

(55)

where

\[
T_{k}^{\mu}(J, I) = \sum_{\mu \in M_{k}} \left( \frac{1}{\mu!} \sum_{\sum_{i \subseteq N \setminus R}^{(k)}} \sum_{J \subseteq R} \sum_{I \subseteq N \setminus R}^{(k)} \sum_{J \subseteq R} \sum_{I \subseteq N \setminus R}^{(k)} t^{I_{k_{\mu} \ldots t_{k_{1}}} a_{I_{k_{\mu} \ldots t_{k_{1}}}} |R >}
\]

(56a)
and
\[ T_0^0(\emptyset, \emptyset) = 1 \quad (56b) \]

In Eq.(56) the index set \( M_k \) is defined as
\[ M_k = \{ \mu : [\mu, \min(p, \mu l)] \ni k \} \]

It is easy to see that \( k \) is the maximal element of \( M_k \). Its minimal element may be found from the inequality
\[ k = l \cdot \left[ \frac{k}{l} \right] + r \leq \mu \cdot l \]
where \( 0 \leq r < l \), and is given by the following relation
\[ \mu_{\text{min}} = \begin{cases} \left[ \frac{k}{l} \right] & \text{if } k \equiv 0 (\text{mod } l) \\ \left[ \frac{k}{l} \right] + 1 & \text{if } k \not\equiv 0 (\text{mod } l) \end{cases} \quad (57) \]

This \( \mu_{\text{min}} \) corresponds to the minimal possible number of blocks of sizes not greater than \( l \) (see Appendix). Thus, the summation in Eq.(56a) goes actually over all consistent set partitions of the pair \((J, I)\) such that each block size does not exceed \( l \), and \( \varepsilon \) is defined by Eq.(46).

At this stage it seems reasonable to introduce new CC amplitudes that differ from the initial ones defined by Eq.(48), only by phase prefactors:
\[ t^I_J \to (-1)^{|J|+|I \cap \Delta_J|+|I \cap \Delta_R|+|J \cap \Delta_R|} t^I_J \quad (58) \]

By an abuse of notation for phase modified CC amplitudes we will use the same symbols as for the initial ones. With new definition of CC amplitudes Eqs.(55) and (56) stay unchanged except for \( \varepsilon \) in Eq.(56) that becomes
\[ \varepsilon = \sum_{i>j} \left| (I_{k_i} \cup J_{k_i}) \cap \Delta_{(I_{k_j} \cup J_{k_j})} \right| \quad (59) \]

The expression (55) establishes a connection between CC and CI expansions in most general case. It is pertinent to mention that in CC expansion all determinants are involved, even if the CC operator (48) is of low excitation order.

Now we are ready to get the expression for the first order density operator
\[ \rho^{CC}_R = \frac{1}{p!} e^{p-1} \left[ e^X |R><R| e^X \right], \quad (60) \]
where the contraction operator is defined by
\[
\frac{1}{p!} |^p R \rangle \langle S | = \frac{1}{p} \begin{cases} 
\sum_{j \in R} |j \rangle \langle j | & \text{if } S = R \\
-(-1)^d |j \rangle \langle i | & \text{if } S = (R \setminus \{j\}) \cup \{i\} \\
0 & \text{if } |S \cap R| < p - 1
\end{cases}
\] (61)

with

\[ \delta = |\{i\} \cap \Delta_{\{j\}}| + |\{i, j\} \cap \Delta_R| \]

and \(i \neq j\).

After simple manipulations we come to the following expression:

\[
\rho^{CC}_{R} = \sum_{k=0}^{p} \sum_{\substack{J \subset R \\ I \subset N \setminus R}} \left[ T^l_k(J, I) \right]^2 \sum_{j \in R \setminus J, I} |j \rangle \langle j |
\]

\[
- \sum_{k=1}^{p} \sum_{\substack{J \subset R \\ I \subset N \setminus R}} T^l_k(J, I) \sum_{j \in R \setminus \{j\}, i \in J} (-1)^{\gamma_1 + \gamma_2} T^l_{k+1}((J \setminus \{i\}) \cup \{j\}, I) |j \rangle \langle i |
\]

\[
- \sum_{k=0}^{p-1} \sum_{\substack{J \subset R \\ I \subset N \setminus R}} T^l_k(J, I) \sum_{j \in R \setminus \{j\}, i \in J} (-1)^{\gamma_1 + \gamma_2} T^l_{k+1}(J \cup \{i\}, I \cup \{j\}) |j \rangle \langle i |
\]

\[
- \sum_{k=1}^{p} \sum_{\substack{J \subset R \\ I \subset N \setminus R}} T^l_k(J, I) \sum_{j \in I \setminus R, i \in J} (-1)^{\gamma_1 + \gamma_2} T^l_{k-1}(J \setminus \{i\}, I \setminus \{j\}) |j \rangle \langle i |
\]

\[
- \sum_{k=1}^{p} \sum_{\substack{J \subset R \\ I \subset N \setminus R}} T^l_k(J, I) \sum_{j \in I \setminus R, i \in J} (-1)^{\gamma_1 + \gamma_2} T^l_k(J, (I \setminus \{j\}) \cup \{i\}) |j \rangle \langle i |
\] (62a)

where

\[ \gamma_1 = |\{i\} \cap \Delta_{\{j\}}|, \gamma_2 = |\{i, j\} \cap \Delta_{(R \setminus \{j\}) \setminus I}| \] (62b)

or, after collecting similar terms,

\[
\rho^{CC}_{R} = \sum_{j \in R} |j \rangle \langle j | \sum_{k=0}^{p} \sum_{\substack{J \subset R \setminus \{j\} \\ I \subset N \setminus R}} \left[ T^l_k(J, I) \right]^2
\]

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operator may be obtained.

\[ \mu \]

It is clear that

\[ \text{in the analogous manner the expression for the second order CC density operator may be obtained.} \]

For further analysis it is convenient to introduce the coefficients

\[ [T_{k,0}^l(\tau)]_{JI} = T_k^l(J,I), \text{ and that } [T_{0,q}^l(\tau)]_{JI} = \frac{q}{l}. \]

Let us present the coefficient \([T_{k,0}^l(\tau)]_{JI}\) in the form

\[ [T_{k,0}^l(\tau)]_{JI} = \int_0^1 \frac{d\lambda}{d\lambda} [T_{k,0}^l(\lambda\tau)]_{JI} d\lambda = \]

\[ = \sum_{k_s=1}^{\min(k,l)} \sum_{J_s \subset R} \int_0^{1/2} \frac{\partial}{\partial(\lambda l_{J_s}^l)} [T_{k,s}^l(\lambda\tau)]_{JI} t_{J_s}^l d\lambda \]

\[ (63) \]
Calculation of the derivatives of \([T_{k,q}^I(\tau)]_{JI}\) with respect to (phase modified) CC amplitudes we start with the analysis of phase prefactor. To this end let us recast Eq.(59), using Eq.(11), as

\[
\varepsilon = \sum_{i>j \ (i,j \neq i*)} | (I_{ki} \cup J_{ki}) \cap \Delta_{(I_{kj} \cup J_{kj})} | + \mu \sum_i | (I_{ki} \cup J_{ki}) \cap \Delta_{(I_{ki} \cup J_{ki})} | + | (I_{ki*} \cup J_{ki*}) \cap \Delta_{(I_{ki*} \cup J_{ki*})} | .
\]

Taking into account that

\[
| (I_{ki*} \cup J_{ki*}) \cap \Delta_{(I_{ki*} \cup J_{ki*})} | \equiv \left[ \frac{2k_{i*} + 1}{2} \right] \equiv k_{i*} \pmod{2}
\]

we can write the following elegant expression

\[
\int_0^1 \frac{\partial}{\partial (\lambda T_{k,q}^I(\tau))} [T_{k,q}^I(\lambda \tau)]_{JI} d\lambda = \left\{ \begin{array}{ll}
(-1)^{\eta(J_*,I_*)} [T_{k-k_*,q+1}^I(\tau)]_{J \setminus J_* \setminus I_*} & \text{if } J \supset J_* \text{ and } I \supset I_* \\
0 & \text{if } J \not\supset J_* \text{ or } I \not\supset I_*
\end{array} \right. (66)
\]

where

\[
\eta(J_*,I_*) = k_* + | (J_* \cup I_*) \cap \Delta_{(J \cup I)} |.
\]

Now Eq.(65) may be recast in the form of the recurrence relation:

\[
[T_{k,q}^I(\tau)]_{JI} = \sum_{k_*=1}^{\min(k,l)} \sum_{J_* \subset J \atop I_* \subset I} (-1)^{\eta(J_*,I_*)} [T_{k-k_*,q+1}^I(\tau)]_{J \setminus J_* \setminus I_*} t_{J_*}^I (68)
\]

CC CI coefficients correspond to the case \(q = 0\) in this equation. The recursion can go either to the vacuum \((k - k_* = 0)\) or to small values of \(k - k_*\) for which the required CC CI coefficients can be evaluated directly.
Structure of Commutative Algebra on p - Electron Sector of the Fock Space

Let us denote by the symbol $A^p_R$ the $p$-electron sector $F_{N,p}$ of the Fock space where some determinant $|R\rangle$ is selected. In more formal terms $A^p_R$ is a pointed space that is the pair $(F_{N,p}, |R\rangle)$. The selected point $|R\rangle$ is referred to as either the HF vacuum or the HF reference state. $A^p_R$ is spanned by the basis vectors $e^I_J(R) = |(R\setminus J) \cup I\rangle$ (69)

labelled by subsets $J \subset R$, $I \subset N\setminus R$ with $|J| = |I|$. Note that $e^I_J(R)$ is nothing more than a special convenient notation for the basis determinant in $F_{N,p}$.

If $S = (R\setminus J) \cup I$ then it is easy to ascertain that

$$e^I'_J(S) = e^{(I\setminus J') \cup J'_2}(R)$$ (70)

where

$$J'_1 = J' \cap (R\setminus J), \quad J'_2 = J' \cap I$$ (71a)

and

$$I'_1 = I' \cap J, \quad I'_2 = I' \cap (N\setminus R\setminus I).$$ (71b)

In particular, $e^\emptyset_{\emptyset}(S) = e^I_J(R)$ and $e^I_J(S) = e^\emptyset_{\emptyset}(R)$. Therefore, arbitrary finite linear combinations of vectors corresponding to different vacuum states are allowed since with the aid of Eqs. (70) - (71) such combinations are easily reduced to some common vacuum state.

We furthermore assume that the vacuum vector $|R\rangle$ is fixed and, by an abuse of notation, for basis vectors (69) we will use the symbol $e^I_J$.

$A^p_R$ is Hermitean space with scalar product

$$\langle x|y \rangle = \sum_{k=0}^{p} \sum_{\substack{J \subset R \setminus I, \quad I \subset N\setminus R}}^{(k)} (x^I_J)^* y^I_J$$ (72a)

and norm

$$\|x\| = \left[ \sum_{k=0}^{p} \sum_{\substack{J \subset R \setminus I, \quad I \subset N\setminus R}}^{(k)} |x^I_J|^2 \right]^{\frac{1}{2}}.$$ (72b)
Subspaces $\mathcal{A}_R^l$ of the dimension

$$\dim \mathcal{A}_R^l = \sum_{k=0}^{l} \binom{n}{k} \binom{n-p}{k},$$

spanned by the basis vectors $e_J^l$ with $1 \leq |J| = |I| \leq l$, form the following chain

$$\mathcal{A}_R^0 \subset \mathcal{A}_R^1 \subset \ldots \subset \mathcal{A}_R^p \quad (74a)$$

where

$$\mathcal{A}_R^0 = \mathbb{C} e_\emptyset. \quad (74b)$$

For each pair $(k, l)$ with $k \leq l$ we introduce subspace $\mathcal{W}_R^{(k,l)}$ spanned by vectors $e_J^l$ with $k \leq |J| = |I| \leq l$. It is clear that $\mathcal{W}_R^{(k,l)}$ is the orthogonal complement to $\mathcal{A}_R^{k-1}$ in $\mathcal{A}_R^l$ and

$$\mathcal{A}_R^p = \bigoplus_{k=0}^{p} \mathcal{W}_R^{(k,k)} \quad (75)$$

For a fixed CC excitation level $l$ the subspace $\mathcal{W}_R^{(1,l)}$ is ‘the subspace of CC amplitudes’.

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

$$e_J^l \ast e_{J'}^{l'} = \begin{cases} (-1)^{|(J \cup J') \cap \Delta(J' \cup J')|} e_{J \cup J'}^{l + l'} & \text{if } J \cap J' = \emptyset \text{ and } I \cap I' = \emptyset, \\ 0 & \text{if } J \cap J' \neq \emptyset \text{ or } I \cap I' \neq \emptyset. \end{cases} \quad (76)$$

It is easy to see that with such a multiplication the vector space $\mathcal{A}_R^p$ becomes a commutative and associative algebra with $e_\emptyset^0$ as its identity (compare with algebras studied by Paldus [6]). Commutativity follows directly from Eq.(11), associativity from the relation

$$|(J_1 \cup I_1) \cap \Delta(J_2 \cup I_2)| + |(J_1 \cup J_2 \cup I_1 \cup I_2) \cap \Delta(J_3 \cup I_3)|$$

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

The structure introduced depends on the choice of the HF vacuum vector and for a fixed MSO basis set there are exactly $\binom{n}{p}$ such (isomorphic) structures.

As has already been mentioned, for vector space structure on $\mathcal{A}_R^p$ the change of vacuum vector simply means change of notation for the same basis.
determinants (see Eqs.(70) - (71)). In contrast, the algebra structure defined by Eq.(76), is deeply connected with the basic vacuum vector. For example, \( e_\emptyset^\emptyset(S) = |S\rangle \) is the idempotent of algebra \( \mathcal{A}_S^p \) whereas the same determinant \( |S\rangle = e_J^J(R) \) in algebra \( \mathcal{A}_R^p \) is its nilpotent basis element. Isomorphism between \( \mathcal{A}_S^p \) and \( \mathcal{A}_R^p \) is induced, for example, by a permutation \( \sigma \) of the MSO index set \( N \) such that \( \sigma(S) = R \).

The relation

\[
\mathcal{W}_R^{(k_1,k_1)} \star \mathcal{W}_R^{(k_2,k_2)} \subset \mathcal{W}_R^{(k_1+k_2,k_1+k_2)}
\]  

(77)

where \( k_1 + k_2 \leq p \), shows that \( \mathcal{A}_R^p \) is a graded algebra. The subspace \( \mathcal{W}_R^{(1,p)} \) 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

\[
\mathcal{A}_R^p = \mathbb{C}e_\emptyset^\emptyset \oplus \mathcal{W}_R^{(1,p)}
\]  

(78)

Note also that \( \mathcal{A}_R^p \) is algebra with involution induced by the complex conjugation.

It is well-known [12] that in algebras of such type it is easy to define algebraically both the exponential mapping and its inverse. Namely,

\[
\exp : \tau \rightarrow \sum_{k=0}^{p} \frac{\tau^k}{k!}
\]  

(79)

is the exponential mapping \( \mathcal{W}_R^{(1,p)} \rightarrow e_\emptyset^\emptyset + \mathcal{W}_R^{(1,p)} \) and

\[
\log : e_\emptyset^\emptyset + \tau \rightarrow \sum_{k=1}^{p} (-1)^{k-1} \frac{\tau^k}{k}
\]  

(80)

is the logarithmic mapping \( e_\emptyset^\emptyset + \mathcal{W}_R^{(1,p)} \rightarrow \mathcal{W}_R^{(1,p)} \). Here

\[
\tau^k = \tau \cdot \ldots \cdot \tau \quad \text{for } k \geq 1.
\]  

(81)

For mappings (79) and (80) all classic relations hold true:

\[
\exp(\tau_1) \star \exp(\tau_2) = \exp(\tau_1 + \tau_2),
\]  

(82a)

\[
[\exp(\tau)]^{-1} = \exp(-\tau),
\]  

(82b)

\[
\exp(\log(e_\emptyset^\emptyset + \tau)) = \tau,
\]  

(82c)
and
\[ \log(\exp(\tau)) = \tau, \quad (82d) \]
where \( \tau, \tau_1, \tau_2 \) are arbitrary elements from \( W_R^{(1,p)} \).

If \( \tau \in W_R^{(1,l)} \) is a vector of CC amplitudes then it is easy to show that the CI coefficients (56) are just the components of the vector \( \exp(\tau) \) in algebra \( A_R^p \):
\[ \exp(\tau) = \sum_{k=0}^{p} \sum_{I \subset N \setminus R}^{(k)} T_k^I(J,I)e_I^J, \quad (83a) \]
where
\[ T_k^I(J,I) = \langle \exp(\tau)|e_I^J \rangle. \quad (83b) \]

In fact, \( \exp(\tau) \) in the last equation for each fixed \( k \) may be replaced by the sum of the first \( k \) terms in its expansion. Eqs.(82) - (83) may be considered as a source of different relations involving CC CI coefficients.

Thus, the Fock space equipped with the non-trivial structure of commutative algebra, defined by Eq.(76), can be considered as a natural domain for the CC and related approaches.

Spectral theory in algebra \( A_R^p \) is very simple. Indeed, let us write arbitrary element \( x \in A_R^p \) as
\[ x = x_0^\emptyset e_0^\emptyset + \tau \]
where \( \tau \in W_R^{(1,p)} \). Its spectrum is defined as the set of all \( \lambda \in \mathbb{C} \) such that \( (\lambda e_0^\emptyset - x) \) is not invertible in \( A_R^p \). It is easy to see that
\[ (\lambda e_0^\emptyset - x)^{-1} = \sum_{k=0}^{p} \frac{\tau^k}{(\lambda - x_0^\emptyset)^{k+1}} = \mathcal{R}(x, \lambda) \quad (84) \]
exists for all \( \lambda \neq x_0^\emptyset \). Thus, spectrum of element \( x \in A_R^p \) is
\[ Sp x = \{ \langle x|e_0^\emptyset \rangle \} \quad (85) \]
The mapping \( \mathbb{C}\{x_0^\emptyset\} \rightarrow A_R^p \) defined by Eq.(84) is called the resolvent of element \( x \in A_R^p \).

From Eq.(85) it follows that if element \( x \in A_R^p \) corresponds to normalized \( p \)-electron wave functions then its spectrum belongs to the unit disk of the complex plane:
\[ Sp x \subset \mathbb{D} = \{ z \in \mathbb{C} : |z| \leq 1 \} \]
In general case the structure of normed space on $\mathcal{A}_R^p$ is not compatible with the algebra structure defined by Eq.(76), that is the inequality
\[
\|x \star y\| \leq \|x\| \cdot \|y\|
\] (86)
not necessarily holds true. For example, if $n = 2$ and $p = 1$, then for $x = e_0^0 + e_{\{2\}}^1$ the inequality (86) is violated. Indeed, in this case $x \star x = e_0^0 + 2e_{\{2\}}^1$ and $\|x \star x\| = \sqrt{5}$ whereas $\|x\|^2 = 2$. Our hypothesis is

**Hypothesis.** For sufficiently large $n$ inequality (86) is satisfied for any $x, y \in \mathcal{A}_R^p$.

If this hypothesis is true then for values of $n$ of actual interest $\mathcal{A}_R^p$ is a commutative unital Banach algebra(see, e.g., [14, 15]). In this case differential calculus of full value could be developed on $\mathcal{A}_R^p$. It would be too restrictive to consider only finite expansions of the type of Eqs.(79) - (80) and it would be possible to define the exponential and logarithmic mappings by their series and prove classic relations (82a) - (82b) for arbitrary $x \in \mathcal{A}_R^p$. And even more, Banach algebras are very closely related to algebras of analytic functions of complex variables [14, 15] and this also could be of interest for applications.

The basic idea of CC and related methods is to parametrize subsets of $\mathcal{A}_R^p$ using elements('amplitudes') from $\mathcal{W}_R^{(1, l)}$ where $l$ is the maximal excitation level. General parametrization of such a type may be defined as an injective mapping
\[
\pi : \mathcal{W}_R^{(1, l)} \rightarrow \mathcal{A}_R^p
\] (87)
such that element $\pi(\tau)$ is invertible for any $\tau \in \mathcal{W}_R^{(1, l)}$. The last requirement guarantees that $\langle \pi(\tau) | e_0^0 \rangle \neq 0$, or, in other words, that the HF reference state appears with nonzero coefficient in expansion of $\pi(\tau)$ for each $\tau$. It is clear that the exponential mapping (79) is a parametrization (see Eq.(82b)). It possesses the following characteristic property: for any excitation level $l$ the set $\exp(\mathcal{W}_R^{(1, l)})$ is a multiplicative Abelian group. This property is referred to as 'size consistency' and is usually considered as essential advantage of the exponential parametrization over other ones.

Another parametrization used in the quadratic configuration interaction method (QCI) [13] is given by
\[
\mathcal{R}(\tau, 1) = \sum_{k=0}^{p} \tau^k = (e_0^0 - \tau)^{-1}
\] (88a)
where
\[ Q^l_k(J, I) = \langle \mathcal{R}(\tau, 1)|e^I_J \rangle. \] (88b)
are the corresponding CI coefficients. The mapping inverse to \( \mathcal{R}(\tau, 1) \) is
\[ \mathcal{R}^{-1} : e^0_0 + \tau \to \sum_{k=1}^{p} (-1)^{k-1}\tau^k \] (89)
The exponential and QCI parametizations are just special cases of general polynomial parametrization
\[ P_a : \tau \to \sum_{k=0}^{p} a_k \tau^k, \] (90)
where \( a = (a_0, a_1, \ldots, a_p) \in \mathbb{C}^{p+1} \). Element \( P_a(\tau) \) is invertible for any \( \tau \) and the mapping (90) is injective if and only if \( a_0 \cdot a_1 \neq 0 \). The inverse to \( P_a \) may be written in the form
\[ P_a^{-1} : a_0e^0_0 + \tau \to \sum_{k=1}^{p} (-1)^{k-1}b_k \tau^k, \] (91)
where coefficients \( b_k \) are easily obtained from the relation
\[ \sum_{k=1}^{p} (-1)^{k-1}b_k \left[ P_a(\tau) - a_0e^0_0 \right]^k = \tau. \] (92)
We have \( b_1 = \frac{1}{a_1}, b_2 = \frac{a_2}{a_1^2}, \) etc.
It is pertinent to mention that if the excitation level \( l \) is less than the number of electrons \( p \) then any parametrization covers only a part of the full CI space. If \( x \) is some CI vector and \( \langle \pi^{-1}(x)|e^I_J \rangle = 0 \) for all \( J, I \) with \( |J| = |I| > l \) then \( \pi^{-1}(x) \in \mathcal{W}_R^{1(l)} \), that is this CI vector \( x \) is covered by the parametrization used.
The main attractive feature of any polynomial parametrization consists in possibility to get approximation to the lowest eigenvector of Hamiltonian by iterative solution of non-linear system of relatively small order
\[ \langle e^I_J|H|P_a(\tau) \rangle = E\langle e^I_J|P_a(\tau) \rangle, \] (93)
where \( 1 \leq |J| = |I| \leq l \).
In algebra $A^p_R$, it is easy to derive relations involving vector $\tau$ and energy value $E$ and different from the standard CC type equations. For example, let us suppose that QCI parametrization (88) covers some eigenvector of the Hamiltonian $H$, that is there exists $\tau \in W_{R}^{(1,j)}$ such that

$$H\mathcal{R}(\tau, 1) = E\mathcal{R}(\tau, 1)$$

(94)

It is easy to ascertain that the mapping

$$\mathcal{R}_E^{-1}: Ee^0 + \tau \to \sum_{k=1}^{p} (-1)^{k-1} \frac{\tau_k}{E^k}$$

(95)

is inverse to the mapping $\tau \to E\mathcal{R}(\tau, 1)$. Since, by assumption, Eq.(94) holds true, we can apply the transformation (95) to both sides of Eq.(94) to get

$$\sum_{k=1}^{p} (-1)^{k-1} \left[ \frac{H\mathcal{R}(\tau, 1) - E^0}{E^k} \right]^k = \tau.$$  

(96)

This relation may serve as a base for Newton-Raphson type iterative algorithms for solution of Eq.(94).

In algebra $A^p_R$, the expression for the first order density operator for arbitrary polynomial parametrization takes the form:

$$p\rho_{R}^{CC} = \sum_{j \in R} \langle P_a(\tau) \left[ \sum_{k=0}^{p} \sum_{J \subseteq R, I \subseteq N \cap R} \langle e_j^I \rangle \langle e_j^I \rangle \right] |P_a(\tau)\rangle \langle j|$$

$$+ \sum_{j \in N \cap R} \langle P_a(\tau) \left[ \sum_{k=1}^{p} \sum_{J \subseteq R, I \subseteq N \cap R} \langle e_j^I \rangle \langle e_j^I \rangle \right] |P_a(\tau)\rangle \langle j|$$

$$- \sum_{j \in R \{i \neq j\}} \langle P_a(\tau) \left[ \sum_{k=1}^{p} \sum_{J \subseteq R \{i\}, I \subseteq N \cap R} (-1)^{\gamma_2} |e_j^I \rangle \langle e_j^I \rangle \right] |P_a(\tau)\rangle \langle j|$$

$$- \sum_{j \in R \{i \neq j\}} \langle P_a(\tau) \left[ \sum_{k=0}^{p} \sum_{J \subseteq R \{i\}, I \subseteq N \cap R} (-1)^{\gamma_1 + \gamma_2} |e_j^I \rangle \langle e_j^I \rangle \right] |P_a(\tau)\rangle \langle j|$$

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\[
+ \sum_{j \in N \setminus R \atop j \in R} \langle P_a(\tau) \rangle \left[ \sum_{k=1}^{p} \sum_{J \subset R \setminus \{i\}} (-1)^{\gamma_1 + \gamma_2} \langle e_{J \cup \{j\}} \rangle \langle e_j \rangle \right] |P_a(\tau)\rangle |j\rangle \langle i| \\
+ \sum_{i,j \in N \setminus R \atop (i \neq j)} \langle P_a(\tau) \rangle \left[ \sum_{k=1}^{p} \sum_{J \subset R \setminus \{i\}} (-1)^{\gamma_2} \langle e_{J \cup \{j\}} \rangle \langle e_j \rangle \right] |P_a(\tau)\rangle |j\rangle \langle i|,
\]

(97)

where the expressions for \(\gamma_1\) and \(\gamma_2\) are given by Eq.(62a).

If \(f\) and \(g\) are differentiable mappings \(\mathbb{R} \to \mathcal{A}_{R}^p\) then it is easy to see that

\[
\frac{d}{d\lambda} [f(\lambda) \ast g(\lambda)] = \left[ \frac{d}{d\lambda} f(\lambda) \right] \ast g(\lambda) + f(\lambda) \ast \left[ \frac{d}{d\lambda} g(\lambda) \right].
\]

(98)

In particular, for real vector \(\tau\) of CC amplitudes the following relations hold true

\[
\frac{\partial}{\partial t^k} = k\tau^{k-1} \ast e_j^I,
\]

(99a)

\[
\frac{\partial}{\partial t^k} \exp(\tau) = \exp(\tau) \ast e_j^I,
\]

(99b)

\[
\frac{d}{d\lambda} \exp(\lambda \tau) = \exp(\lambda \tau) \ast \tau,
\]

(99c)

and

\[
\frac{d}{d\lambda} \log(e_\emptyset^I + \lambda \tau) = \frac{\mathcal{R}^{-1}(\lambda \tau, 1)}{\lambda}.
\]

(99d)

In concluding this section let us note that it is easy to define algebra \(\mathcal{A}_{(R_\alpha, R_\beta)}^{(p_\alpha, p_\beta)}\) corresponding to orbital representation of \(p\)-electron sector of the Fock space spanned by determinants with fixed spin projection \(M_S = \frac{1}{2}(p_\alpha - p_\beta)\). The multiplication in \(\mathcal{A}_{(R_\alpha, R_\beta)}^{(p_\alpha, p_\beta)}\) is

\[
\langle I_\alpha, J_\beta \rangle \ast e_{(I'_\alpha, J'_\beta)} =
\]

\[
\begin{cases} 
(\frac{1}{1}) \sum \langle e_{I_\sigma \cup I'_\beta} \rangle \langle e_{J_\sigma \cup J'_\beta} \rangle & \text{if } I_\sigma \cap J'_\beta = \emptyset \text{ and } I'_\sigma \cap J_\beta = \emptyset \\
0 & \text{if } I_\sigma \cap J'_\beta \neq \emptyset \text{ or } I'_\sigma \cap J_\beta \neq \emptyset
\end{cases}
\]

(100)

where \(\sigma = \alpha, \beta\).
**Pointed Fock Spaces as Associative Superalgebras**

Let us describe possible extension of the multiplication rule (76) to the full Fock space. To this end we consider a pointed Fock space \( \mathcal{F}_R = (\mathcal{F}_N, |R\rangle) \) with the basis \( e_I^j(R) = (R \setminus J) \cup I \) where \( J \subset R \) and \( I \subset N \setminus R \) (on the whole \( 2^p \cdot 2^{n-p} = 2^n \) basis vectors) and present \( \mathcal{A}_R \) as a direct sum

\[
\mathcal{A}_R = \mathcal{A}^+_R \oplus \mathcal{A}^-_R
\]

(101)

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. Using the same definition (76) for the product of arbitrary basis vectors, we come to associative algebra with identity. From Eq.(11) it follows that \( \mathcal{A}_R \) is a skew-commutative (or supercommutative) algebra:

\[
e_I^j(R) \star e_{I'}^j(R) = (-1)^{|J \cup I||J' \cup I'|} e_I^j(R) \star e_{I'}^j(R).
\]

(102)

We have

\[
\mathcal{A}^+_R \star \mathcal{A}^+_R \subset \mathcal{A}^+_R, \quad \mathcal{A}^-_R \star \mathcal{A}^-_R \subset \mathcal{A}^-_R, \quad \mathcal{A}^+_R \star \mathcal{A}^-_R \subset \mathcal{A}^-_R, \quad \mathcal{A}^-_R \star \mathcal{A}^+_R \subset \mathcal{A}^+_R,
\]

(103)

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 \( \mathcal{A}_\emptyset \) that is the Fock space where the 'absolute' vacuum state \(|\emptyset\rangle = |\emptyset\rangle\) is selected. In this case we have

\[
e_\emptyset^I(\emptyset) \star e_\emptyset^{I'}(\emptyset) = \begin{cases} (-1)^{|I \cap \Delta_{I'}|} e_\emptyset^{I \cup I'}(\emptyset) & \text{if } I \cap I' = \emptyset \\ 0 & \text{if } I \cap I' \neq \emptyset \end{cases}
\]

(104)

It is interesting to compare the star product in \( \mathcal{A}_\emptyset \) with the standard exterior (wedge) product in the Grassmann algebra \( \mathcal{F}_N \). We have

\[
|I\rangle \wedge |I'| = \begin{cases} (-1)^{\varepsilon(I, I')} |I \cup I'| & \text{if } I \cap I' = \emptyset \\ 0 & \text{if } I \cap I' \neq \emptyset \end{cases}
\]

(105)

where \( \varepsilon(I, I') \) is the number of pairs \((i, i') \in I \times I' \) such that \( i > i' \). It is easy to show (see Eq.(11)) that

\[
\varepsilon(I, I') = |I' \cap \Delta_I| \equiv |I \cap \Delta_{I'}| + |I| \cdot |I'| \text{(mod 2)}
\]
and this means that even in the case of algebra $\mathcal{A}_\emptyset$ the star product is different from the standard exterior product in the Grassmann algebra $\mathcal{F}_N$. For example, if $I = \{1, 2, 7\}$ and $I' = \{4, 5, 6\}$ then $\Delta_{I'} = \{1, 2, 3, 4, 6\}$. We have $|I \cap \Delta_{I'}| = 2$

whereas

$$\varepsilon(I, I') = |\{(7, 4), (7, 5), (7, 6)\}| = 3.$$  

Another possible extension of the multiplication rule (76) is given by the relation

$$e_I \star e_{I'} = \begin{cases} (-1)^{|(J' \cup I') \cap \Delta_{(J \cup I)}|} e_{J' \cup I'} & \text{if } J \cap J' = \emptyset \text{ and } I \cap I' = \emptyset \\ 0 & \text{if } J \cap J' \neq \emptyset \text{ or } I \cap I' \neq \emptyset \end{cases} \quad (106)$$

Both definition (76) and definition (106) lead to the same structure on the $p-$electron sector of the Fock space. Their extension to the full Fock space gives, however, different results. In particular, with the definition (106) algebra $\mathcal{A}_\emptyset$ is identical to the Grassmann algebra.

**Computer Implementation of Star Product**

For two arbitrary vectors $x, y \in \mathcal{A}_p^R$ we have

$$x \star y = x_0^\emptyset y_0^\emptyset + \sum_{k=1}^{p} \sum_{J \subset R, I \subset N \setminus R} \left[ \sum_{k_1=1}^{k-1} \sum_{J \subset J_1, I \subset I_1} \sum_{J \subset J_1} (-1)^{k_1 + |(J_1 \cup J_1) \cap \Delta_{(J_1 \cup J_1)}|} e_{J_1 \cup J_1} \right] e_I.$$  

(107)

Methods of calculation of this rather complicated product are based on two fundamental combinatorial notions: listing and ranking. Listing means generation of combinatorial objects (subsets of a given index set in our case) in some fixed ordering. Ranking algorithms allow to set up arrays indexed by subsets (vectors of algebra $\mathcal{A}_p^R$ in our case). In other words, rank of a subset is the position this subset occupies in a given ordering.

There exists simple formula for calculation of subset rank under lexicographic ordering of the set of all $k-$element subsets of the index set $N$ (see, e.g., [19]):

$$\text{lex}_N(J) = \binom{n}{k} \sum_{j=1}^{n} \zeta_{j, J} \left( k - |J \cap \Delta_{\{j\}}| + 1 \right). \quad (108)$$

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In algebra $A^p_R$, components of arbitrary vector $x$ are indexed by pairs of subsets $(J, I)$ with $J \subset R$ and $I \subset N \setminus R$. Let us put
\[
lex_R(J) = lex_{r^{-1}(R)}(r^{-1}(J))
\]
and
\[
lex_{N \setminus R}(I) = lex_{s^{-1}(N \setminus R)}(s^{-1}(I))
\]
where $R = r_1 < \ldots < r_p$ and $N \setminus R = s_1 < \ldots < s_{n-p}$. Vector $x \in A^p_R$ has its components indexed as
\[
(J, I) \rightarrow (lex_R(J) - 1) \binom{n-p}{k} + lex_{N \setminus R}(I).
\]

In our opinion ranking and listing algorithms required for evaluation of products $x \star y$ should not necessarily be closely related. For example, we can use Gray codes generation algorithms [16, 17] and lexical indices (110).

**Conclusion**

Advanced technique of manipulations with phase prefactors arising in many problems of quantum chemistry is demonstrated. On the base of this technique three methods of evaluation of CC CI coefficients and CC density matrices are suggested.

The first method (see Eq.(56)) requires rather complicated combinatorial algorithms for set partitions generation and permutations of multisets (see Appendix). The success of its implementation strongly depends on the program code efficiency.

The second method (see Eq.(68)) is based on the recurrence relations for CC CI coefficients and its efficiency is closely related both to the efficiency of recursive algorithms in programming language used and available hardware.

The third method employs new algebraic structure revealed on the Fock space. The efficiency of implementation of a rather special product of two vectors determines the overall efficiency of any algorithms using this multiplication rule.

The first two methods do not require full size CC CI vector to be kept in fast memory but they may be rather time consuming. The third method can be programmed in a very efficient way but at least two CC CI vectors should be stored.
Appendix: RG strings and set partitions

All information contained in this Appendix is well-known and is given here only to show how direct evaluation of expressions of the type of Eq.(56) can be performed in non-recursive way. Standard references are [16, 17]. A lot of interesting information may also be found on Frank Ruskey site [18].

Let \( \{J_i\}_{i=1}^\mu \) be a set partition of the set \( N = \{1, 2, \ldots, n\} \) having its blocks listed in accordance to the following rule: block \( J_i \) contains the minimal element of the set \( N \setminus (\bigcup_{j=1}^{i-1} J_j) \). In particular, \( J_1 \ni 1 \). In this Appendix the term ‘set partition’ means ‘block ordered set partition’ unless otherwise stated.

**Definition.** Restricted Growth (RG) string of length \( n \) is an integral vector \( a = (a_1, a_2, \ldots, a_n) \) such that
\[
a_1 \leq a_i \leq \max_{1 \leq j < i} \{a_j\} + 1
\]
where \( a_1 = 1 \).

With each RG string it is convenient to associate the following vector
\[
\nu = (\nu_1, \ldots, \nu_n)
\]
where \( \nu_i = \max\{a_1, \ldots, a_i\} \).

**Lemma.** There exists a bijection between the set of all RG strings of length \( n \) and the set of all set partitions of \( N \).

**Proof.** See [16, 17].

Non-recursive generation of all RG strings in *lexical* order can be described as follows. We start with the minimal RG string
\[
a_{\text{min}} = (1, 1, \ldots, 1)
\]
(3)

Let us suppose that on some step we have current RG string
\[
(1, \ldots, a_m, a_{m+1}, \ldots, a_n)
\]
(4)
where \( |J_{a_m}| > 1 \) and \( |J_{a_{m+1}}| = \ldots = |J_{a_n}| = 1 \). It is easy to see that in RG string (4) \( a_{m+1} > \nu_m \). Indeed, in the opposite case the smallest element of \( J_{a_{m+1}} \) would be not greater than \( m \) but this is in contradiction with the assumption that \( J_{a_{m+1}} \) is a block of size 1 containing index \( m + 1 \). As a result, the current RG string (4) takes actually the form
\[
(1, \ldots, a_m, \nu_m + 1, \ldots, \nu_m + n - m)
\]
(5)
The corresponding set partition with $\nu_m + n - m$ blocks is
\[ \{J_1, \ldots, J_{a_m}, \ldots, J_{\nu_m}, \{m+1\}, \ldots, \{n\} \} \]

The next (in lexical order) RG string is
\[ (1, \ldots, a_m + 1, 1, \ldots, 1) \] (6)

In going from RG string (5) to RG string (6) the size of the block $J_1$ increases by $n - m$ and the current number of blocks decreases by the same value and becomes equal to $\nu_m$ if $a_m \neq \nu_m$. If $a_m = \nu_m$ then RG string (6) corresponds to the set partition with $\nu_m + 1$ blocks.

Generation of RG strings should be terminated when the number of current blocks becomes equal to $n$ that corresponds to the maximal RG string
\[ a_{\text{max}} = (1, 2, \ldots, n) \] (7)
and the set partition with exactly $n$ blocks $J_i = \{i\}$.

We are interested in generation of set partitions with the additional restriction on block sizes. Namely, for any partition of $N$ the size of each its block should not be greater than the maximal excitation order $l$. This implies, in particular, that with such a restriction the number of blocks can not be less than
\[ k = \begin{cases} \left\lceil \frac{n}{l} \right\rceil & \text{if } n \equiv 0(\mod l) \\ \left\lceil \frac{n}{l} \right\rceil + 1 & \text{if } n \not\equiv 0(\mod l) \end{cases} \] (8)

With *lexical* ordering of admissible RG strings the minimal one is
\[ a_{\text{min}} = \begin{cases} (1, \ldots, 1, 2, \ldots, 2, \ldots, k, \ldots, k) & \text{if } n \equiv 0(\mod l) \\ (1, \ldots, 1, 2, \ldots, 2, \ldots, k, \ldots, k) & \text{if } n \not\equiv 0(\mod l) \end{cases} \] (9)

and the maximal one is given by Eq.(7).

Let us suppose that the current RG string is of the form of Eq.(5) and that the corresponding vector of block sizes is
\[ s = (|J_1|, \ldots, |J_{a_m}|, \ldots, |J_{\nu_m}|, 1, \ldots, 1). \] (10)

Since each block size should not exceed $l$, it is necessary to scan vector (10) from the position $a_m + 1$ till $\nu_m$ to find the smallest index $\bar{a}_m$ such that
\(|J_{a_m}| < l\). If such an index is not found then we put \(a_m = \nu_m + 1\). The next string is

\((1, \ldots, a_m, 1, 1, \ldots, 2, 2, \ldots, \ldots)\)

where \(\kappa_1 = \min\{l - |J_1|, n - m\}\), \(\kappa_2 = \min\{l - |J_2|, n - m - \kappa_1\}\), etc. If after sorting blocks \(J_1, \ldots, J_{\nu_m}(J_{\nu_m+1})\) there are still \(\kappa = n - m - \sum_{i=1}^{\nu_m} \kappa_i > 0\) unfilled positions in the string under consideration, then we should fill them by \(\delta_1 = \min\{l, \kappa\}\) integers \(\nu_m + 1(\nu_m + 2)\), etc.

The next algorithm required is the algorithm of generation of all set partitions (not necessarily block ordered ones) corresponding to a given vector \(s = (s_1, \ldots, s_\mu)\) of block sizes. But this problem is equivalent to the problem of generation of multiset permutations and the corresponding non-recursive lexical algorithm is easily obtained by modification of, say, algorithm 5.1 from the book [19].

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