(p,q)-Sheaves and the Representability Problem
A. I. Panin

Chemistry Department, St.-Petersburg State University,
University prospect 26, St.-Petersburg 198504, Russia
e-mail: andrej@AP2707.spb.edu

ABSTRACT: General properties of new models of the electronic Fock spaces based on the notion of (p, q)-sheaves are studied. Interrelation between simple sheaves and density operators is established. Explicit expressions for the transformed reduced Hamiltonians in terms of the standard creation-annihilation operators are presented. General scheme of parametrization of p-electron states by \( \kappa \)-electron means (\( \kappa = 2, 3, \ldots \)) is described and studied in detail for the case of sheaves induced by \( \kappa \)-electron wavefunctions. It is demonstrated that under certain conditions p-electron problem may be reformulated as the eigenvalue problem in \( \kappa \)-electron space equipped with certain p-electron metric. Simple numerical examples are given to illustrate our approach.

Key words: representability problem; density operators; CI method; electron correlation.

Introduction

In present work we continue study of properties of new models of p-electron sections of the Fock spaces introduced in our previous work \([1]\). These models are based on the notion of (p, q)-sheaves that can be considered as q-electron representation of p-electron states (q \( \leq \) p). Figuratively speaking, the space of all (p, q)-sheaves is a model of p-electron space ‘ready for q-electron interactions’. This means that no contraction is required for calculation of matrix elements of arbitrary q-electron operators. The contraction is replaced by the summation over q-electron functions (germs) constituting the sheaf.

In the second section necessary basic definitions are given.

In the third section general properties of simple (p, q)-sheaves are studied. Important notion of vector Z-cell is introduced. Explicit characterization of images of simple sheaves with respect to different compositions of the assembling-disassembling mappings is given.

In the fourth section it is shown that there exists a one-to-one correspondence (up to arbitrary overall phase prefactor) between simple sheaves and a certain class of density operators.
In the fifth section the explicit expression for the transformed reduced Hamiltonian in terms of the creation-annihilation operators is obtained.

In the sixth section the notion of \( p \)-electron metric in \( \kappa \)-electron space \((\kappa = 1, 2, 3, \ldots)\) is introduced and it is demonstrated that under certain conditions \( p \)-electron problem reduces to the eigenvalue problem in \( \kappa \)-electron space equipped with \( p \)-electron metric.

In the seventh section orbital representation of \((p, q)\)-sheaves is discussed and relevant formulas for metrics and Hamiltonians are derived in terms of molecular orbitals.

The eighth section is dedicated to numerical testings.

---

**Basic Definitions.**

For 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. Basis determinants will be labelled by *subsets* and all sign conventions connected with their representation as the Grassman product of *ordered* spin-orbitals will be included in the definition of the creation-annihilation operators and in the definition of specific set-theoretical operation \( \Delta_K, K \subset N \) that was introduced in [2] and studied in detail in [3]. Here \( N \) is the spin-orbital index set.

For any \((p + q)\)-element subset \( Z \) of the index set \( N \) let us denote by the symbol \( \mathcal{F}_{n,q}(Z) \) the following subspace of the \( q \)-electron sector of the Fock space:

\[
\mathcal{F}_{n,q}(Z) = \bigoplus_{S \subset Z} \mathbb{C}|S\rangle
\]

where \( \mathbb{C} \) is the field of complex numbers. Let us define the set

\[
B_{n,p,q} = \{(Z, S) \subset N \times N : |Z| = p + q \& |S| = q \& S \subset Z\},
\]

and the equivalence relation on this set

\[
(Z, S) \sim (Z', S') \iff Z \setminus S = Z' \setminus S'.
\]

The set of the corresponding equivalence classes contains \( \binom{n}{p} \) elements and in each equivalence class there are \( \binom{n-p}{q} \) elements.
Definition. Family \( \{ \psi_Z \}_{Z \subseteq N} \) of \( q \)-electron functions, \( \psi_Z \in \mathcal{F}_{n,q}(Z) \), is called a sheaf of \( q \)-electron germs of \( p \)-electron wavefunction, or just a \( (p,q) \)-sheaf, if the mapping

\[
(Z, S) \rightarrow (-1)^{|(Z \setminus S) \cap \Delta_Z|} \langle S | \psi_Z \rangle, |Z| = p + q, |S| = q, S \subseteq Z
\]

is constant on the equivalence classes of the set \( B_{n,p,q} \) modulo the equivalence relation (3). Here \( \Delta_Z \) is the mentioned above set-theoretical operation that is used to reduce manipulations with sign prefactors in Grassman algebra to pure set-theoretical ones.

The set of all \( (p,q) \)-sheaves is denoted as \( \mathcal{S}_{n,p,q} \).

In paper [1] it was demonstrated that there exists a one-to-one correspondence between the set of all \( (p,q) \)-sheaves and vectors of the \( p \)-electron sector of the Fock space. The mapping

\[
s_{n,p,q} : (p) \sum_{R \subseteq N} C_R |R \rangle \rightarrow \{ \psi_Z \}_{Z \subseteq N}
\]

where

\[
|\psi_Z\rangle = (q) \sum_{S \subseteq Z} (-1)^{|(Z \setminus S) \cap \Delta_Z|} C_{Z \setminus S} |S \rangle.
\]

is called the disassembling mapping and is used to transfer all relevant structures from the \( p \)-electron sector of the Fock space on the set of all \( (p,q) \)-sheaves. The linear structure is transferred as

\[
s_{n,p,q} \left( \sum_i \lambda_i \Psi^{(i)} \right) = \left\{ \sum_i \lambda_i \Psi^{(i)} \right\}_Z \left| \sum_i \lambda_i \psi_Z \right|_{Z \subseteq N}.
\]

This equality just expresses the fact due to the linear character of the gluing conditions (4) arbitrary linear combination of \( (p,q) \)-sheaves is a \( (p,q) \)-sheaf.

The inner product (Euclidean structure) is defined as

\[
\langle \{ \psi_Z \}_{Z \subseteq N} | \{ \phi_Z \}_{Z \subseteq N} \rangle = \frac{1}{n-p-q} \sum_{Z \subseteq N} \langle \psi_Z | \phi_Z \rangle
\]

and it is consistent with the inner product of the corresponding \( p \)-electron wavefunctions.
The inverse to $s_{n,p,q}$ is called the assembling mapping and is used to restore $p$-electron vectors from $(p,q)$-sheafs with the aid of the gluing conditions (4).

In paper [1] it was mentioned that from the very beginning it seems reasonable to associate with each $p$-electron wavefunction $\Psi$ its sheaf $s_{n,p,q}(\Psi)$ and co-sheaf $s_{n,n-p,q}(\mathbb{1}\Psi)$ where $\mathbb{1} : |R\rangle \rightarrow |N\setminus R\rangle$ is the particle-hole involution. However, since general properties of sheaves and co-sheaves are identical, and actual difference appears only on the level of evaluation of reduced Hamiltonian matrix elements, we study properties of sheaves, keeping in mind that the analogous properties are valid also for co-sheaves.

The family
\[
\{\pi_{n,p,q}(Z) : \{\psi_Z\}^\epsilon_{Z' \subset N} \rightarrow \psi_Z\}^\epsilon_{Z \subset N}
\] (9)

involves linear mappings that perform projections of the vector space $S_{n,p,q}$ on the vector spaces $F_{n,q}(Z)$.

Let us suppose that some $q$-electron wavefunction $\psi_Z \in F_{n,q}(Z)$ is chosen:
\[
\psi_Z = \sum_{S \subset Z}^q c_S |S\rangle = \sum_{R \subset Z}^p (-1)^{|R \cap \Delta Z|} \bar{C}_R |Z\setminus R\rangle
\] (10)

where $R = Z \setminus S$ and
\[
\bar{C}_R = (-1)^{|R \cap \Delta Z|} c_S
\] (11)

Since $F_{n,q}(Z)$ is isomorphic to $F_{n,p}(Z)$, we can easily lift $q$-electron wavefunction to the level $p$ using, for example, the linear mapping:
\[
u_q^p(Z) : \sum_{R \subset Z}^p (-1)^{|R \cap \Delta Z|} C_R |Z\setminus R\rangle \rightarrow \sum_{R \subset Z}^p C_R |R\rangle
\] (12)

Subsequent disassembling of $p$-electron wavefunction $\nu_q^p(Z)\psi_Z$ gives us $(p,q)$-sheaf that may be considered as generated by $q$-electron wavefunction $\psi_Z$. Compositions $s_{n,p,q} \circ \nu_q^p(Z) = j_{n,p,q}(Z)$ constitute the family of linear injective mappings
\[
j_{n,p,q}(Z) : F_{n,q}(Z) \rightarrow S_{n,p,q}
\] (13)

that are right inverses (sections) of the projections (9).

**Definition.** $(p,q)$-sheaf generated by $q$-electron wavefunction $\psi_Z$ is called simple and is denoted as $\{\psi_Z\}^\epsilon_{Z' \subset N}$.

It is to be noted that the same simple $(p,q)$-sheaf may be generated by different $q$-electron wavefunctions.


\((p, q)\)-sheaves corresponding to single determinant \(p\)-electron wavefunctions are called determinant sheaves. The characteristic property of determinant sheaves is: simple \((p, q)\)-sheaf is the determinant one if and only if it is generated by any of its nonzero germ (see\([2]\)).

It is clear that the assembling and disassembling mappings may be used to establish isomorphism between operator spaces over \(F_{n,p}\) and over \(S_{n,p,q}\). Indeed, if \(h \in \text{End}_C(F_{n,p})\) then the mapping

\[
h \rightarrow s_{n,p,q} \circ h \circ s^{-1}_{n,p,q}
\]

is the required isomorphism. For physically relevant operators it is usually possible to express their matrix elements between two \((p, q)\)-sheaves as a sum of matrix elements of certain \(q\)-electron operators between germs of these sheaves. In our previous paper [1] the electronic Hamiltonian \(H\) was handled in such a way. Namely, due to the specific form of \(H\), its matrix element between two \((p, q)\)-sheaves may be written as

\[
\langle \{\phi_Z\}_{Z \in N} | H | \{\psi_Z\}_{Z \in N} \rangle = \frac{1}{(n-p)q} \sum_{Z \subseteq N} \langle \phi_Z | A^{-1}(n, p, q)H_{p \rightarrow q} | \psi_Z \rangle,
\]

where

\[
H_{p \rightarrow q} = \left( \frac{p}{q} \right) \left[ \frac{q-1}{p-1} \sum_{i,j} \langle i|h|j \rangle a_i^\dagger a_j + \frac{1}{2} \sum_{i,j,k,l} \langle ij | kl \rangle \frac{1}{r_{12}} a_i^\dagger a_j^\dagger a_k a_l \right]
\]

is the so-called reduced Hamiltonian and \(A(n, p, q)\) is introduced in [3] operator acting on the operator space \(F_{n,q} \otimes F_{n,q}^*\).

---

**Properties of Simple Sheaves.**

With each function \(\psi_Z \in F_{n,q}(Z)\) written in the form of Eq.(10) let us associate two sets:

\[
I_p(\psi_Z) = \{R \subset Z : |R| = p \& \bar{C}_R \neq 0\}
\]

\[
L(\psi_Z) = \bigcup_{R \in I_p(\psi_Z)} R
\]

Let \(\{\psi_{Z'Z}\}_{Z' \subset N}\) be some simple \((p, q)\)-sheaf generated by \(q\)-electron wavefunction \(\psi_Z\). Then any germ of this sheaf may be written as

---
\[ \psi_{ZZ'} = \sum_{R' \subset Z' \cap Z} (-1)^{|R' \cap \Delta Z'|} \tilde{C}_{R'} |Z' \setminus R'|, \]  
\tag{19} \]

where the coefficients \( \tilde{C}_{R'} \) are given by Eq.\( (11) \).

**Proposition 1.** \( q \)-electron wavefunction generating simple \((p, q)\)-sheaf is necessarily a germ of this sheaf.

**Proof.** Follows directly from the relation \( \pi_{n,p,q}(Z) \circ j_{n,p,q}(Z) = id_{\mathcal{F}_{n,q}(Z)} \)

**Proposition 2.** \( q \)-electron functions \( \psi_{Z_1} \) and \( \psi_{Z_2} \) generate the same simple \((p, q)\)-sheaf if and only if

(i) \( I_p(\psi_{Z_1}) = I_p(\psi_{Z_2}) \);

(ii) For any \( R \in I_p(\psi_{Z_1}) \) functions \( \psi_{Z_1} \) and \( \psi_{Z_2} \) are subject to the following "gluing" conditions

\[-1)^{|R \cap \Delta Z_1|} \langle Z_1 \setminus R | \psi_{Z_1} \rangle = (1)^{|R \cap \Delta Z_2|} \langle Z_2 \setminus R | \psi_{Z_2} \rangle. \]

**Proof.** Let us write down \( q \)-electron functions \( \psi_{Z_1} \) and \( \psi_{Z_2} \) in the form of Eq.\( (10) \)

\[ \psi_{Z_i} = \sum_{R \subset Z_i} (p) (-1)^{|R \cap \Delta Z_i|} C_R^{(i)} |Z_i \setminus R| \]  
\( (i = 1, 2) \)

From the equality \( \{ \psi_{Z_1 Z'} \}_{Z' \subset N} = \{ \psi_{Z_2 Z'} \}_{Z' \subset N} \) it follows that \( \psi_{Z_1} = \psi_{Z_2 Z_1} \) and \( \psi_{Z_2} = \psi_{Z_1 Z_2} \). These equalities together with Eq.\( (19) \) imply that \( \tilde{C}_R^{(1)} = \tilde{C}_R^{(2)} \), and, consequently, condition (i) and (ii) are fulfilled.

Now let us suppose that for given functions \( \psi_{Z_1} \) and \( \psi_{Z_2} \) the conditions (i) and (ii) hold true. Then from (i) it follows that for arbitrary \( Z' \subset N \)

\[ \psi_{Z_i Z'} = \sum_{R \subset Z' \cap Z_1 \cap Z_2} (p) (-1)^{|R \cap \Delta Z'|} \tilde{C}_R^{(i)} |Z' \setminus R|, \]  
where \( i=1,2 \). Use of conditions (ii) immediately leads to the equality

\( \{ \psi_{Z_1 Z'} \}_{Z' \subset N} = \{ \psi_{Z_2 Z'} \}_{Z' \subset N} \)

**Proposition 3.** The number of \( q \)-germs generating simple \((p, q)\)-sheaf \( \{ \psi_{Z Z'} \}_{Z' \subset N} \) is equal to

\[
\left( \begin{array}{c} n - |L(\psi_Z)| \\ p + q - |L(\psi_Z)| \end{array} \right)
\]
Proof. By definition, $L(\psi_Z) \subset Z$. For any $Z_1 \supset L(\psi_Z)$ the germs $\psi_Z$ and $\psi_{Z_1}$ obviously satisfy the conditions of proposition 2. □

Corollary 1. For any determinant sheaf $|L(\psi_Z)| = p$ and it is generated by any of its $\binom{n-p}{q}$ germs.

Corollary 2. Non-determinant $(p,1)$-sheaf has only one generator.

Proof. For non-determinant sheaves $|L(\psi_Z)|$ should necessarily be equal to $p + 1$. □

Definition. $q$-electron functions $\psi_{Z_1}$ and $\psi_{Z_2}$ are called $p$-equivalent ($\psi_{Z_1} \sim \psi_{Z_2}$) if they generate the same simple $(p,q)$-sheaf.

Proposition 4. Let $\{\psi_{Z_1(Z')}\}_{Z' \subset N}$ be simple $(p,q)$-sheaf generated by $q$-electron wavefunction $\psi_Z$. Then any $q$-electron function from $F_{n,q}(Z)$ is orthogonal to all $\psi_{Z(Z')}$ with $Z' \neq Z$.

Proof. Expansion of arbitrary $q$-electron function from $F_{n,q}(Z)$ (see Eq.(10)) involves $q$-electron determinants $|Z \setminus R\rangle$. From Eq.(19) it follows that each $q$-germ $\psi_{Z(Z')}$ of the sheaf under consideration is expanded via $q$-electron determinants $|Z' \setminus R'\rangle$. It is easy to see that $Z' \neq Z$ and $R' \subset Z' \cap Z$ implies $Z' \setminus R' \subset Z$. □

Corollary. $q$-germs generating simple $(p,q)$-sheaf are mutually orthogonal.

Let us consider a family of $k$ simple $(p,q)$-sheaves $\{\psi_{Z_1(Z')}}_{Z' \subset N}$, $i = 1, 2, \ldots, k$ and sort out this family in the following manner:

Select some subset $Z_1$ from the family $Z_1', Z_2', \ldots, Z_k'$ and collect all $(p,q)$-sheaves such that $\psi_{Z_1(Z')} \sim \psi_{Z_1'}$. The resulting subfamily will be denoted as $\{\psi_{Z_1(Z')_{i_1}}\}_{Z' \subset N}$, $i_1 = 1, 2, \ldots, k_1$.

From the rest of the initial family select subset $Z_2$ and collect all $(p,q)$-sheaves such that $\psi_{Z_2(Z')} \sim \psi_{Z_2'}$. The resulting subfamily will be denoted as $\{\psi_{Z_2(Z')_{i_2}}\}_{Z' \subset N}$, $i_2 = 1, 2, \ldots, k_2$.

Repeating the last step till the initial family is exhausted, we arrive finally at the family $\{\psi_{Z_i(Z')}\}_{Z' \subset N}$, $i_t = 1, 2, \ldots, k_l, l = 1, 2, \ldots$. By construction, each subfamily of this family corresponding to some fixed index $l$ involves simple $(p,q)$-sheaves generated by $q$-germs from the vector space $F_{n,q}(Z_l)$. As a result, the problem of orthogonalization of simple sheaves within this subfamily seems to be not very complicated, especially if one takes into account the following assertion.

Proposition 5. Let $\psi^{(1)}_{Z(Z')}_{Z' \subset N}$ and $\psi^{(2)}_{Z(Z')}_{Z' \subset N}$ be simple $(p,q)$-sheaves...
generated by \( q \)-electron functions \( \psi_Z^{(1)}, \psi_Z^{(2)} \in \mathcal{F}_{n,q}(Z) \). Then

\[
\langle \{ \psi_{ZZ'}^{(1)} \} _{Z' \subset N} | \{ \psi_{ZZ'}^{(2)} \} _{Z' \subset N} \rangle = \langle \psi_Z^{(1)} | \psi_Z^{(2)} \rangle.
\]  
(20)

**Proof.** Direct calculation based on the definition (8) of the inner product leads readily to the equality required ■

The question when linear combination of simple sheaves is simple is of a certain interest in connection with the problem of selection of linearly independent simple sheaves. The answer to this question is given by the following assertion.

**Proposition 6.** Linear combination

\[
\sum_{i=1}^{k} \lambda_i \{ \psi_{Z,Z'} \} _{Z' \subset N}
\]

of simple \((p,q)\)-sheaves is simple if and only if there exists \((p+q)\)-element subset \( Z \subset N \) such that

\[
R \not\subset Z \Rightarrow \sum_{i \in I_{Z_1 \ldots Z_k}^R} \lambda_i \bar{C}_i^R = 0,
\]

where

\[
I_{Z_1 \ldots Z_k}^R = \{ 1 \leq i \leq k : Z_i \supset R \}.
\]

**Proof.** Arbitrary linear combination of simple sheaves may be written in the form

\[
\sum_{i=1}^{k} \lambda_i \{ \psi_{Z,Z'} \} _{Z' \subset N} = \left\{ \sum_{R' \subset Z'} |Z' \setminus R'| (1)^{|R' \cap \Delta_{Z'}} \left( \sum_{i \in I_{Z_1 \ldots Z_k}^R} \lambda_i \bar{C}_i^R \right) \right\} _{Z' \subset N}.
\]

If we suppose that this sheaf is simple then there should exist index set \( Z \subset N \) such that the \( q \)-germ

\[
\sum_{R \subset Z} \binom{(p)}{|Z \setminus R|} (1)^{|R' \cap \Delta_{Z'}} \left( \sum_{i \in I_{Z_1 \ldots Z_k}^R} \lambda_i \bar{C}_i^R \right)
\]

generates this sheaf. It can, however, be true if and only if the coefficients by the basis determinants \( |Z' \setminus R'| \) in expansion of \( q \)-germs are equal to zero for all \( R' \not\subset Z \) ■

8
**Corollary.** Arbitrary linear combination of determinant \((p, q)\)-sheaves generated by \(q\)-germs

\[
\psi_{Z_i} = (-1)^{|R_i \cap \Delta_z|} \overline{C}_{R_i}^{(i)} |Z_i \setminus R_i|
\]

is simple if and only if there exists index set \(Z \subset N\) such that \(Z \supset \bigcup_{i=1}^{k} R_i\), or, in other words, \(|\bigcup_{i=1}^{k} R_i| \leq p + q\).

**Proof.** Without loss of generality we may assume that the coefficients \(\lambda_i\) of linear combination of determinant sheaves are non-zero. Let us suppose that for any subset \(Z \subset N\) there exists \(R_j \not\subset Z\). In this case

\[
\sum_{i \in I^{p+q}_{R_j}} \lambda_i \overline{C}^{(i)}_{R_j} = \lambda_j \overline{C}^{(j)}_{R_j} \neq 0
\]

and, consequently, the linear combination under consideration can not be simple.

**Definition.** The image of \(F_{n,q}(Z)\) with respect to the monomorphism \(j_{n,p,q}(Z)\) is called the vector \(Z\)-cell of the vector space of all \((p,q)\)-sheaves and is denoted as \(J_{n,p,q}(Z)\).

It is pertinent to note that \(Z\)-cells depend on the MSO basis chosen. Each vector \(Z\)-cell is a \((p+q)\)-dimensional subspace of \(S_{n,p,q}\). The set of all simple \((p,q)\)-sheaves in \(S_{n,p,q}\) is a union of its vector \(Z\)-cells:

\[
J_{n,p,q} = \bigcup_{Z \subset N} J_{n,p,q}(Z).
\]  

(21)

It is easy to show that the set \(J_{n,p,q}\) generates the vector space of all \((p,q)\)-sheaves (see [1]).

The set of simple \((p,q)\)-sheaves \(\{\psi_{ZZ'}\}_{Z' \subset N} \in J_{n,p,q}(Z)\) such that

\[
|L(\psi_Z)| \leq k
\]

where \(k = p + q, p + q - 1, \ldots, p\), will be denoted as \(J_{n,p,q}^{(k)}(Z)\). It is clear that each \(Z\)-cell admits the following filtration

\[
J_{n,p,q}(Z) = J_{n,p,q}^{(p+q)}(Z) \supset J_{n,p,q}^{(p+q-1)}(Z) \supset \ldots \supset J_{n,p,q}^{(p)}(Z)
\]  

(22)
Topological dimension of $J_{n,p,q}^{(k)}(Z)$ is equal to $\binom{k}{p}$. Thus, each $Z$-cell possesses $k$-faces (borders) where simple $(p,q)$-sheaves from different cells are situated. It is likely that filtration (21) may serve as a starting point for further more advanced analysis of geometry of the set $J_{n,p,q}$.

Now let us consider the connection between spaces $S_{n,p,q}$ with different $q$. There exist obvious isomorphisms

$$S_{n,p,q} \xrightarrow{s_{n,p,q}^{-1}} F_{n,p} \xrightarrow{s_{n,p,q}^{-1}} S_{n,p,q \pm 1}. \quad (23)$$

Proposition 7. The image of any simple $(p,q)$-sheaf from $J_{n,p,q}$ with respect to the isomorphism $s_{n,p,q}^{-1} \circ s_{n,p,q}^{-1}$ is simple $(p,q+1)$-sheaf, and for $k = p + q, p + q - 1, \ldots, p$

$$s_{n,p,q}^{-1} \circ s_{n,p,q}^{-1} (J_{n,p,q}^{(k)}) \subset J_{n,p,q}^{(k+1)}, \quad (24)$$

that is the image of $J_{n,p,q}$ belongs to the border of $J_{n,p,q+1}$.

**Proof.** Let $\psi_Z \in F_{n,q}(Z)$ generate simple $(p,q)$-sheaf \{\psi_{ZZ'}\} \subset N$ and $w_q^p(Z)\psi_Z = \sum_{R \subset Z} \bar{C}_R|R| = \sum_{R \subset Z} \bar{C}_R|R|$.

For any index $i \in N \setminus Z$ the $p$-electron wavefunction

$$\Psi_{Z \cup \{i\}} = \sum_{\substack{R \subset Z \cup i \\ (R \ni i) \cup i}} \bar{C}_R|R| = \Psi_Z$$

can be disassembled to give simple $(p,q+1)$-sheaf with germs

$$\Psi_{Z \cup \{i\}}Z' = \sum_{R \subset Z' \cap Z} (-1)^{|R \cap Z'|} \bar{C}_R|R'|$$

where $|Z'| = p + q + 1$. It is clear as well that the choice of concrete index $i$ is irrelevant. Indeed, for any index $j \in N \setminus Z$, $(q+1)$-germ $\Psi_{Z \cup \{i\}Z \cup \{j\}}$ is $p$-equivalent to $\Psi_{Z \cup \{i\}}$.

Lowering of simple $(p,q)$-sheaf to the level $q-1$ leads, in general, to linear combinations of simple $(p,q-1)$-sheaves.

Proposition 8. Let \{\psi_{ZZ'}\} \subset N be simple $(p,q)$-sheaf generated by $q$-germ $\psi_Z$. Then

$$s_{n,p,q-1} \circ s_{n,p,q}^{-1} (\{\psi_{ZZ'}\} \subset N) = \frac{1}{q} \sum_{k \in Z} \{\psi_{Z \setminus \{k\}Z'}\} \subset N. \quad (25)$$
Proof. Disassembling of $p$-electron function $\Psi_Z = u_q^p(Z)\psi_Z$, $|Z| = p + q$, gives $(p, q - 1)$-sheaf with germs (see Eq. (6))

$$\psi_{Z''} = \sum_{R \subset Z'' \cap Z} (-1)^{|R \cap \Delta Z''|} C_R |Z'' \setminus R|,$$  \hspace{1cm} (26)

where $|Z''| = p + q - 1$.

On the other hand, let us consider the sum

$$\sum_{k \in Z} \{\psi_{Z \setminus \{k\}Z''}\}z'' \subset N = \left\{ \sum_{k \in Z} \psi_{Z \setminus \{k\}Z''} \right\}_{z'' \subset N},$$ \hspace{1cm} (27)

where simple $(p, q - 1)$-sheaf $\{\psi_{Z \setminus \{k\}Z''}\}z'' \subset N$ involves $(q - 1)$-germs

$$\psi_{Z \setminus \{k\}Z''} = \sum_{R \subset [Z'' \cap (Z \setminus \{k\})]} (-1)^{|R \cap \Delta Z''|} C_R |Z'' \setminus R|.$$

Thus, $(p, q - 1)$-sheaf on the right-hand side of Eq. (27) involves $(q - 1)$-germs

$$\sum_{k \in Z} \sum_{R \subset [Z'' \cap (Z \setminus \{k\})]} (-1)^{|R \cap \Delta Z''|} C_R |Z'' \setminus R|.$$  

The contribution to this sum from $k \not\in Z'' \cap Z$ is equal to $(p + q - |Z'' \cap Z|)\psi_{Z''}$ where $\psi_{Z''}$ is given by Eq. (26). On the other hand, for each fixed $R \subset Z'' \cap (Z \setminus \{k\})$ there exist $|Z'' \cap Z| - p$ different $k \in Z'' \cap Z$. As a result,

$$\sum_{k \in Z} \{\psi_{Z \setminus \{k\}Z''}\}z'' \subset N = q \{\psi_{Z''}\}z'' \subset N.$$  \hspace{1cm} ■

It is to be noted that if $L(\psi_Z)$ is a proper subset of $Z$ then for any $k \in Z \setminus L(\psi_Z)$ (the choice of $k$ is irrelevant), $s_{n,p,q-1}(\Psi_Z) = s_{n,p,q-1}(\Psi_{Z \setminus \{k\}})$ is simple $(p, q - 1)$-sheaf.

Corollary. For any admissible $q$ and any $\kappa < q$

$$s_{n,p,\kappa} \circ s_{n,p,q}^{-1}(\{\psi_{Z'Z''}\}z'' \subset N) = \frac{\kappa!}{q!} \sum_{K \subset Z} \{\psi_{Z \setminus KZ''}\}z'' \subset N.$$  \hspace{1cm} (28)

Very important is the following statement that is contrary in a certain sense to the Proposition 8.
Proposition 9. If $Z \subset N, |Z| = p + q$, and for each $(q - \kappa)$-element subset $K \subset Z$

$$\psi_{Z \setminus K} = \sum_{R \subset Z \setminus K}^{(p)} (-1)^{|R \cap \Delta Z \setminus K|} \tilde{C}^{(K)}_R |Z \setminus K \setminus R\rangle,$$

then the image of the sum

$$\sum_{K \subset Z}^{(q - \kappa)} \{\psi_{Z \setminus KZ'}\}_{Z' \subset N}$$

with respect to the assembling mapping $s_{n,p,q}^{-1}$ is $p$-electron wavefunction

$$\Psi_Z = \sum_{R \subset Z}^{(p)} \left( \sum_{K \subset Z \setminus R}^{(q - \kappa)} \tilde{C}^{(K)}_R \right) |R\rangle,$$

and its disassembling with the aid of $s_{n,p,q}$ gives simple $(p,q)$-sheaf generated by the $q$-germ

$$\sum_{R \subset Z}^{(p)} (-1)^{|R \cap \Delta Z|} \left( \sum_{K \subset Z \setminus R}^{(q - \kappa)} \tilde{C}^{(K)}_R \right) |Z \setminus R\rangle.$$

Proof. By direct calculation.

This Proposition can be used to parametrize subsets of the sets $J_{n,p,q}(Z)$ using $\kappa$-electron means ($\kappa < q$).

Simple Sheaves and Density Operators

Definition. The quadratic mapping $d_q : S_{n,p,q} \to F_{n,q} \otimes F^*_{n,q}$ defined by

$$d_q (\{|\psi_Z\}_{Z \subset N}) = \frac{1}{(n-p)} \sum_{Z \subset N}^{(p+q)} |\psi_Z\rangle \langle \psi_Z|$$

is called the density mapping of order $q$. The value of this mapping at some $(p,q)$-sheaf is called the $q$-density operator associated with this sheaf.

The problem of description of the set $d_q (S_{n,p,q})$ is called the pure representability problem and in slightly different form was formulated in the very
first papers by Coleman [4, 5, 6, 7]. By an abuse of notation the same symbol \(d_q\) will be used for the density mapping defined by Eq.(32) and for elements of the set \(d_q(S_{n,p,q})\).

Let us consider density operators corresponding to simple sheaves. From Eq.(19) it follows that

\[
d_q\left(\{\psi_{ZZ'}\}_{Z' \subset N}\right) = \frac{1}{(n-p)} \left[ |\psi_Z\rangle\langle \psi_Z| + \sum_{\begin{smallmatrix} Z' \subset N \\ (p<|Z' \cap Z|<p+q) \end{smallmatrix}} |\psi_{ZZ'}\rangle\langle \psi_{ZZ'}| + ||\psi_Z||^2 P_{N \setminus Z}^{(q)} \right],
\]

(33)

where

\[
P_X^{(q)} = \sum_{S \subset X} |S\rangle\langle S|
\]

(34)
is the projector associated with the index set \(X \subset N\). Note that the representation (33) of the density operator associated with some given simple sheaf is not unique (see Proposition 3).

Complete characterization of \(q\)-density operators corresponding to simple \((p,q)\)-sheaves is given by the assertion that readily follows from Eq.(33) and Proposition 4.

**Proposition 10.** \(q\)-electron operator \(d_q\) is associated with simple \((p,q)\)-sheaf if and only if there exists \((p+q)\)-element subset \(Z \subset N\) such that

(i) the operator \(P_{Z}^{(q)} d_q P_{Z}^{(q)}\) corresponds to some (not necessarily normalized) pure \(q\)-electron state, that is \(P_{Z}^{(q)} d_q P_{Z}^{(q)} = |\psi_Z\rangle\langle \psi_Z|\);

(ii) \(\left(I - P_{Z}^{(q)}\right) d_q \left(I - P_{Z}^{(q)}\right) = \sum_{\begin{smallmatrix} Z' \subset N \\ (p<|Z' \cap Z|<p+q) \end{smallmatrix}} |\psi_{ZZ'}\rangle\langle \psi_{ZZ'}|\),

where wavefunctions \(\psi_{ZZ'}\) are uniquely determined by the eigenfunction \(\psi_Z\) of the operator \(P_{Z}^{(q)} d_q P_{Z}^{(q)}\) corresponding to its non-zero eigenvalue.

Thus, for any fixed \((p+q)\)-element subset \(Z \subset N\) there exists one-to-one correspondence (up to arbitrary overall phase prefactor) between elements from the vector \(Z\)-cell \(J_{n,p,q}(Z)\) and representable density operators of the form of Eq.(33). Reservation ‘up to arbitrary overall phase prefactor’ may be removed by turning to the quotient of \(J_{n,p,q}(Z)\) obtained by identification of sheaves that differ by overall phase prefactor, or to the projective \(Z\)-cells if only normalized sheaves are of interest. We, however, prefer to use vector \(Z\)-cells saying that simple sheaves parametrize density operators of the form of Eq.(33) even if this statement is not quite correct.
The simplest density mapping corresponds to the case $q = 1$ and its value at some simple $(p,1)$-sheaf is equal to

$$d_1(\{\psi_{ZZ'}\}_{Z'\subset N}) = \frac{1}{n-p} \left[ |\psi_Z\rangle\langle \psi_Z| + P^{(1)}_{N\setminus Z} \right],$$

(35)

where $|Z| = p + 1$. The kernel of the operator on the right-hand side of this equation is $p$-dimensional subspace of occupied one-electron particle states (occupied molecular spin orbitals).

Using proposition 7 and Eq.(33), it is possible to lift one-density operators from $d_1(J_{n,p,1})$ to the level $q = 2$:

$$d_2(\{\psi_{Z\cup\{i\}}Z'\}_{Z'\subset N}) = \frac{1}{(n-p)^2} \left[ |\psi_{Z\cup\{i\}}\rangle\langle \psi_{Z\cup\{i\}}| ight.$$

$$+ \sum_{Z'\subset N \atop (Z'\cap Z = p+1)} |\psi_{Z\cup\{i\}}Z'\rangle\langle \psi_{Z\cup\{i\}}Z'| + P^{(2)}_{N\setminus (Z\cup\{i\})} \right].$$

(36)

Non-zero contributions to the sum on the right-hand side of Eq.(36) may appear in two cases: $Z' = Z \cup \{j\}, j \in N \setminus Z, j \neq i$ and $Z' = Z \setminus k \cup \{i,j\}, k \in Z, i, j \in N \setminus Z$. Analysis of these cases leads to the following final expression:

$$d_2(\{\psi_{Z\cup\{i\}}Z'\}_{Z'\subset N}) = \frac{1}{(n-p)} \left[ \sum_{k,k' \in Z} c_k c_{k'}^* \sum_{j \in N \setminus Z} (-1)^{\epsilon} |\{j,k\}\rangle\langle \{j,k'\}| + P^{(2)}_{N\setminus (Z\cup\{i\})} \right],$$

(37)

where

$$\epsilon = |(Z\setminus\{k\}) \Delta (Z\setminus\{k'\})| \cap \Delta_{\{j\}}| = \begin{cases} 0, & \text{if } k = k' \text{ or } k, k' > j; \\ 1, & \text{if } k \leq j \text{ & } k' > j \text{ or } k' \leq j \text{ & } k > j; \\ 2, & \text{if } k, k' \leq j. \end{cases}$$

By the symbol $\{j,k\}$ on the right-hand side of Eq.(37) non-ordered pairs of spin-orbital indices (two-element subsets) are denoted. It is pertinent to emphasize once again that the right-hand side of Eq.(37) does not depend on the choice of index $i \in N \setminus Z$ that appears explicitly on the left-hand side of this equality (see Proposition 7).
It is possible, following Coleman, to replace the requirement of pure representability by more simple requirement of representability by an ensemble of pure states. Instead of the quadratic \( q \)-density mapping (32) let us introduce the mapping
\[
d_q : \mathcal{S}_{n,p,q} \otimes \mathcal{S}^*_{n,p,q} \rightarrow \mathcal{F}_{n,q} \otimes \mathcal{F}^*_{n,q}
\]
that is defined on generators \(|\{\psi_Z\}_{Z \subset N}\rangle \langle\{\phi_Z\}_{Z \subset N}|\) as
\[
d_q(|\{\psi_Z\}_{Z \subset N}\rangle \langle\{\phi_Z\}_{Z \subset N}|) = \frac{1}{(n-p)^{(p+q)}} \sum_{Z \subset N} |\psi_Z\rangle \langle\phi_Z|
\]
and is continued to \( \mathcal{S}_{n,p,q} \otimes \mathcal{S}^*_{n,p,q} \) by linearity.

The set of all finite convex combinations of the type
\[
\sum_i \lambda_i |\{\psi_Z^{(i)}\}_{Z \subset N}\rangle \langle\{\psi_Z^{(i)}\}_{Z \subset N}|
\]
where \( \lambda_i \geq 0, \sum_i \lambda_i = 1, \) and \( ||\{\psi_Z^{(i)}\}_{Z \subset N}|| = 1 \) will be denoted as \( \text{Ens}(\mathcal{S}_{n,p,q}) \).
Its image with respect to \( d_q \) is the set of all ensemble representable \( q \)-density operators and the problem of its analytic description is known as the ensemble representability problem. For \( q = 1 \) its constructive solution was found by Coleman [4].

**Explicit Expressions for the Transformed Reduced Hamiltonians**

From Eq.(15) it follows that in the vector space of all \((p,q)\)-sheaves the usual \( p \)-electron Hamiltonian should be replaced by the reduced Hamiltonian transformed with the aid of the automorphism \( A^{-1}(n,p,q) \) introduced in [3]. For \( q = 2 \) it is not difficult to perform direct numerical transformation to construct the required operator. For \( q > 2 \), however, such an approach may appear to be complicated because the transforming operator is of huge dimension. Fortunately, it is possible to obtain simple explicit expression for \( A^{-1}(n,p,q)H_{p,q} \). We start with more general task of calculation of \( A(n,p,q) \) action on products of the creation-annihilation operators.
Operator $A(n, p, q)$ was defined in [3] via its matrix representation with respect to specially selected basis closely related to the basis of determinant generators:

$$A(n, p, q)e^{IJ}_K = (-1)^s \frac{p}{q} \left(\frac{p-s}{q-p}\right) \sum_{K' \subset N \setminus (I \cup J)} (-1)^{|K \cap K' - q|} \frac{1}{|q-K'\rangle} e^{IJ}_{K'} e^{00}_{K \cup \{i\}},$$

where $e^{IJ}_K = (-1)^{(I \cup J) \cap \Delta_K |I \cup K \rangle \langle J \cup K|}$ and $I \cap J = \emptyset, s = |I| = |J|$. 

Therefore, as the first step, it is necessary to expand the restrictions of products of the creation-annihilation operators on $q$-electron sector of the Fock space via the basis operators $e^{IJ}_K$. Using technique of manipulations with phase prefactors developed in [3], it is easy to derive the following formulas:

$$a^\dagger_i a_j = \sum_{K \subset N \setminus \{i\}} e^{00}_{K \cup \{i\}},$$

$$a^\dagger_i a_j = \sum_{K \subset N \setminus \{i, j\}} e^{ij}_{K}, \quad i \neq j,$$  

$$a^\dagger_i a^\dagger_j a_j a_i = \sum_{K \subset N \setminus \{i, j\}} e^{00}_{K \cup \{i, j\}}, \quad i \neq j,$$  

$$a^\dagger_i a^\dagger_j a_l a_i = \sum_{K \subset N \setminus \{i, j, l\}} e^{ij}_{K \cup \{i\}}, \quad i \neq j \neq l,$$  

$$a^\dagger_i a^\dagger_j a_l a_k = \sum_{K \subset N \setminus \{i, j, k, l\}} (-1)^{(i \cap \Delta_{\{i\}} + l \cap \Delta_{\{i\}})} e^{ij}_{K} e^{kl}_{K}, \quad i \neq j \neq k \neq l.$$

The second step is straightforward. One should apply the operator $A(n, p, q)$ to the right-hand sides of Eqs.(40a)-(40e). Simple but somewhat tiresome set-theoretical and combinatorial manipulations with extensive use of two classic relations (see, e.g., [3])

$$\sum_{k} (-1)^k \binom{r-k}{m} \binom{s}{k} = \binom{r-s}{r-m}.$$
and
\[
\binom{-r}{k} = (-1)^k \binom{r + k - 1}{k}
\]
lead to the following equalities:
\[
A(n, p, q)a_i^\dagger a_j = -\frac{p}{n - p}a_i^\dagger a_j + \frac{q}{n - p}I_q,
\]
\[
A(n, p, q)a_i^\dagger a_j^\dagger a_k = \binom{q}{2} \left( \binom{q}{2} a_i^\dagger a_j^\dagger a_l a_k - \frac{p}{q} \left( \delta_{i l} a_j^\dagger a_k + \delta_{j l} a_i^\dagger a_k \right) + \frac{p}{q} \left( \delta_{i k} a_j^\dagger a_l + \delta_{j k} a_i^\dagger a_l \right) \right)
\]
where \(I_q\) is the \(q\)-electron identity operator. Now, taking into account the equality \(A^{-1}(n, p, q) = A(n, n - p, q)\) (see [3]), we can write down the explicit expression for the transformed reduced Hamiltonian:
\[
A^{-1}(n, p, q)H_{p \rightarrow q} = \frac{1}{2} \left[ Tr( h + F_N) \right] I_q - \frac{1}{q} \frac{(n-p)}{1} \sum_{i,j} \langle i | F_N | j \rangle a_i^\dagger a_j
\]
\[
+ \frac{1}{2} \binom{n-p}{2} \sum_{i,j,k,l} \langle i j | k l \rangle a_i^\dagger a_j^\dagger a_k a_l,
\]
where the Fock operator associated with some MSO index set \(X \subset N\) is defined as
\[
F_X = h + \sum_{k \in X} (J_k - K_k).
\]
The first term on the right-hand side of Eq.(42) is the Hartree-Fock (HF) energy of the \(n\)-electron state \(|N\rangle\). It is pertinent to emphasize that the operator (42) should be applied to wavefunctions from the \(q\)-electron sector of the Fock space. Note also that with the aid of Eqs.(41a-41e) it is possible to expand any physically relevant operator via orthonormal basis of generators \(e^{ij}_K\), thus reducing the matrix element evaluation problem to the calculation of standard scalar products.

The energy of the vector \(Z\)-cell in fixed MSO basis for \(q > 1\) is obviously defined as
\[
E(J_{n,p,q}(Z)) = \min_{||\psi_Z||=1} Tr \left[ A^{-1}(n, p, q)H_{p \rightarrow q}d_q(\{|\psi_Z\rangle_{Z' \subset N}\}) \right].
\]
For $q = 1$ it is necessary to lift one-density operator to the level $q = 2$ and then define the energy of $Z$-cell $J_{n,p,q}(Z)$ as

$$E(J_{n,p,q}(Z)) = \min_{||\psi_Z||=1} Tr \left[ A^{-1}(n,p,2) H_{p\to 2} d_2(\{\psi_Z \cup \{i\}Z'\} \subset Z) \right], \quad (45)$$

where $i$ is an arbitrary index from $N \backslash Z$.

**Parametrizations and Induced Sheaves**

Arbitrary vector $Z$-cell $J_{n,p,q}(Z)$ is a subspace of the vector space $S_{n,p,q}$ of the dimension $(p+q)$. Its image with respect to the isomorphism $s_{n,p,\kappa} \circ s_{n,p,q}^{-1}$ is a sum of vector $Z \backslash K$-cells

$$s_{n,p,\kappa} \circ s_{n,p,q}^{-1} (J_{n,p,q}(Z)) = \sum_{K \subset Z} J_{n,p,\kappa}(Z \backslash K), \quad (46)$$

(see Proposition 8) being a subspace of the vector space $S_{n,p,\kappa}$ of the same dimension $(p+q)$. From Proposition 9 it follows that different choice of $\kappa$-electron functions of the type of Eq.(29) can be used to parametrize different subsets of the vector $Z$-cell $J_{n,p,q}(Z)$. General scheme of such parametrizations may be described as follows:

1. Select a certain family of $\kappa$-electron functions

$$\psi_{Z \backslash K} = \sum_{S \subset Z \backslash K} c^{(K)}_S |S\rangle \quad (47)$$

with a reasonable number of free parameters;

2. To each selected nonzero $\kappa$-electron function put into correspondence simple $(p,\kappa)$-sheaf generated by this function;

3. Construct $(p,\kappa)$-sheaf

$$\{\psi'_Z\} \subset N = \sum_{K \subset Z} \{\psi_{Z \backslash K'\cap Z}\} \subset N, \quad (48)$$

that, due to Proposition 9, corresponds to a certain simple $(p,q)$-sheaf from $Z$-cell $J_{n,p,q}(Z)$.
For example, functions
\[
ψ_{Z\setminus K} = \begin{cases} 
(-1)^{|R\cap ΔZ\setminus K|} C_R |Z\setminus R \setminus K⟩, & K \subseteq Z\setminus R \\
0, & K \not\subseteq Z\setminus R
\end{cases}
\]
correspond to HF determinant \(|R⟩\) and single parameter \(C_R\) is used to ensure its proper normalization.

It is pertinent to note that in the frameworks of this scheme families of \(\kappa\)-electrons functions are used to perform local parametrization of subsets from \(J_{n,p,q}(Z)\). Of course, the cases of small \(\kappa\) and \(q = n - p\) are of primary interest. The equality \(q = n - p\) means that \(Z = N\) on the level \(q\), \(S_{n,p,q} \sim \mathcal{F}_{n,p}\) and, consequently, the above scheme is applied, in fact, for parametrization of \(p\)-electron states. If \(n - p > p\) then it is necessary to turn to the hole representation of wavefunctions and operators and work with co-sheaves ((\(\bar{p}, q\))-sheaves with \(\bar{p} = n - p\)). Since \(n - p > p\) implies \(\bar{p} > n - \bar{p}\), for co-sheaves the equality \(q = n - \bar{p}\) can certainly be reached.

We illustrate our approach with one relatively simple but somewhat formal example. Let
\[
ψ_{Z} = \left(\frac{p + q - \kappa}{p}\right)^{(\kappa)} \sum_{S \subseteq Z} c_S |S⟩
\]  
be some trial \(\kappa\)-electron function expanded over \(\kappa\)-electron determinants with indices from the index set \(Z, |Z| = p + q\). Rewriting it in the form
\[
ψ_{Z} = \sum_{K \subseteq Z} \sum_{S \subseteq Z\setminus K} (q - \kappa)^{(\kappa)} c_S |S⟩ =
\]
\[
= \sum_{K \subseteq Z} \sum_{R \subseteq Z\setminus K} (p)^{(p)} (-1)^{|R\cap ΔZ\setminus K|} \bar{C}_R^{(K)} |Z\setminus K\setminus R⟩,
\]
where \(\bar{C}_R^{(K)} = (-1)^{|R\cap ΔZ\setminus K|} C_{Z\setminus K\setminus R}\), and replacing each \(K\)-component in expansion (50) by the corresponding simple sheaf, we arrive at the \((p, \kappa)\)-sheaf of the form of Eq.(48) depending on \((p + q)\) free \(\kappa\)-electron parameters. *Sheaf thus constructed will be called \((p, \kappa)\)-sheaf induced by \(\kappa\)-electron wavefunction (49) and will be denoted as \([ψ_Z]_{p,\kappa}^\dagger\).* It is easy to see that arbitrary linear combination of induced sheaves is induced sheaf.
The next step is to derive the explicit formulas for the matrix elements of the \( \kappa \)-electron Hamiltonian \( H_{p,q,\kappa}(Z) \) corresponding to the energy expression

\[
E_Z = \frac{1}{(n-p)} \sum_{K,K' \subset Z} \sum_{Z' \subset N} \langle \psi_{Z \setminus KZ'} | A^{-1}(n,p,\kappa) H_{p,q,\kappa} | \psi_{Z \setminus K'Z'} \rangle.
\]

(51)

This complicated and somewhat tiresome procedure is described in Appendix A.

Since the inner product of \((p,\kappa)\)-sheaves (see Eq.(8)) is consistent with the inner product of the corresponding \(p\)-electron wavefunctions, it comes as no surprise that the eigenvalue problem for the \( \kappa \)-electron Hamiltonian obtained from Eq.(51) should be solved in a certain \( p \)-electron metric.

With our choice of \( \kappa \)-electron functions \( \psi_{Z \setminus K} \) (see Eq.(50)) the coefficients in expansion of the corresponding \( p \)-electron wavefunction (30) are

\[
\sum_{K \subset Z \setminus R} \tilde{C}^{(K)}_R = (-1)^{|R \cap \Delta_R|} \sum_{S \subset Z \setminus R} (-1)^{|R \cap \Delta_S|} c_S,
\]

and the normalization condition for \( \kappa \)-electron coefficients \( c_S \) takes the form

\[
\sum_{S,S' \subset Z} \left( \sum_{R \subset Z \setminus (S \cup S')} (-1)^{|R \cap \Delta_{SS'}|} \right) c^*_S c_{S'} = 1,
\]

where the comparison \(|R \cap \Delta_S| + |R \cap \Delta_{S'}| \equiv |R \cap \Delta_{SS'}| \pmod{2}\) was taken into account (see Appendix A of [3]).

Let us introduce the metric matrix

\[
[G_{p,q,\kappa}(Z)]_{SS'} = \sum_{R \subset Z \setminus (S \cup S')} (-1)^{|R \cap \Delta_{SS'}|}.
\]

(52)

It is easy to show that the matrix (52) is nonnegative. However, it is not necessarily strictly positive. In Appendix B it is demonstrated how to derive the expression for the matrix elements of \( G_{p,q,\kappa}(Z) \) as a sum of binomials.

Matrices \( G_{p,q,\kappa}(Z) \) are of purely combinatorial nature (see Appendix B) and to study their properties methods of modern enumerative combinatorics should most likely be used. The explicit description of kernels of these matrices is of primary interest. It seems to be an interesting combinatorial
problem with unexpectedly simple and elegant solution. Indeed, numerical experiments led us to the following two hypothesis concerning the properties of these matrices.

**Hypothesis 1.**

\[
\dim \ker [G_{p,q,\kappa}(Z)] = \begin{cases} 
\binom{p+q-1}{\kappa-1} & \text{if } q - \kappa \equiv 1(\text{mod } 2), \\
0 & \text{if } q - \kappa \equiv 0(\text{mod } 2).
\end{cases}
\]

**Hypothesis 2.** If \( q \equiv 0(\text{mod } 2) \) then

\[
\ker [G_{p,q,1}(Z)] = C \sum_{s \in Z} (-1)^s |\{s\} \rangle.
\]

If the Hypothesis 1 is true, then for \( q - \kappa \equiv 0(\text{mod } 2) \) matrices \( G_{p,q,\kappa}(Z) \) are strictly positive and, consequently, in this case the minimization of energy (51) reduces to the solution of the standard generalized eigenvalue problem in the \( \kappa \)-electron space equipped with \( p \)-electron metric:

\[
H_{p,q,\kappa}(Z)\psi = E_Z G_{p,q,\kappa}(Z)\psi,
\]

Explicit expressions for \( \kappa \)-electron Hamiltonian \( H_{p,q,\kappa}(Z) \) both in the particle and hole representations are given in Appendix A.

When trial function (49) is chosen to be one-electron one (just a molecular spin orbital) then it is necessary at first to lift its \( K \)-components to a higher level \( \kappa \). In contrast to the situation described in Proposition 7, in the case under discussion the index set \( Z \) should stay unchanged. One of the ways to do it consists in construction of the functions

\[
\psi_{Z\setminus K'} = \left( \sum_{R \subset Z \setminus K'} \left( \sum_{K' \subset K \subset Z} (-1)^{|R \setminus \Delta Z \setminus K|} c^{(K)}_R \right) |Z\setminus K'\setminus R\rangle \right),
\]

where \( |K'| = q - \kappa \). With such choice of \( K' \)-components at the level \( \kappa \) the normalization condition for one-electron coefficients takes the form

\[
\sum_{i,j \in Z} c^*_i c_j \sum_{S' \subset Z \setminus \{i,j\}} [G_{p,q-2,\kappa-1}(Z \setminus \{i,j\})]_{S'S'} = 1,
\]

and, consequently, at the one-electron level we are faced with the generalized eigenvalue problem with respect to some contracted metric. We leave this aspect of theory to future study.
It is clear that for fixed $Z$ the number of linearly independent induced $(p, \kappa)$-sheaves is equal to $\binom{p+q}{\kappa} - \dim \ker [G_{p,q,\kappa}(Z)]$. One can hardly hope that linear combinations of induced $(p, \kappa)$-sheaves may be used directly in molecular calculations. First, the total number of free parameters is too small. Second, the scheme of construction of induced sheaves does not have any robust physical idea behind it. The situation may be partially improved by turning to $(p, \kappa)$-sheaf

$$\lambda s_{n,p,\kappa}(R) + [\psi Z]_{p,\kappa},$$

where

$$s_{n,p,\kappa}(R) = \{(-1)^{|R \cap \Delta Z'|}|Z' \setminus R\} \quad (R \subset Z \subset N)$$

is the determinant sheaf corresponding to HF $p$-electron wavefunction $|R\rangle$, and $\lambda$ is the additional parameter to be optimized. It is easy to demonstrate that the problem of determination of optimal parameters $\lambda$ and $c_S, S \subset Z$ in expression (54) may be reduced to the eigenvalue problem involving augmented Hamiltonian and augmented metric:

$$\begin{pmatrix} E_R & b_{p,q,\kappa}(Z) \\ b_{p,q,\kappa}^\dagger(Z) & H_{p,q,\kappa}(Z) \end{pmatrix} \begin{pmatrix} \lambda \\ c \end{pmatrix} = E_Z \begin{pmatrix} 1 & a_{p,q,\kappa}^\dagger(Z) \\ a_{p,q,\kappa}(Z) & G_{p,q,\kappa}(Z) \end{pmatrix} \begin{pmatrix} \lambda \\ c \end{pmatrix},$$

where

$$a_{p,q,\kappa}(Z) = \frac{\partial}{\partial c} \langle s_{n,p,\kappa}(R)|[\psi Z]_{p,\kappa}\rangle,$$

$$b_{p,q,\kappa}(Z) = \frac{\partial}{\partial c} \langle s_{n,p,\kappa}(R)|A^{-1}(n,p,\kappa)[\psi Z]_{p,\kappa}\rangle,$$

and $E_R$ is the HF energy of the determinant state $|R\rangle$. HF sheaf in expression (54) may be replaced by any available sheaf with subsequent obvious modifications of Eqs.(56)-(58).

Use of more general parametrizations in accordance to the scheme described at the beginning of this section is more complicated because it requires development of a certain strategy for systematic selection of reasonable number of free parameters $c_S^{(K)}$. Dependence of coefficients in expansion (47) on $K$ results in appearance of normalization conditions of the following general type

$$\sum_{S,S' \subset Z} \sum_{R \subset Z \setminus (S \cup S')} (-1)^{|R \cap \Delta S \setminus S'|} \left(c_S^{(Z \setminus R \setminus S')^*} c_S^{(Z \setminus R \setminus S')^*} \right) = 1.$$
If no additional restrictions on coefficients \( c_S^{(K)} \) are imposed then the corresponding metric matrix is of the form

\[
\left[ G_{p,q}^{(KK')}(Z) \right]_{SS'} = \sum_{R \subset Z \setminus (S \cup S')}^{(p)} (-1)^{|R \cap \Delta_S \Delta S'|} \zeta_{Z \setminus R, S,K} \zeta_{Z \setminus R, S',K'}, \tag{59}
\]

where \( \zeta \) is combinatorial zeta-function (see Appendix A). In fact, the sum on the right-hand side of Eq.(59) may be equal either to 0, or to \( \pm 1 \).

As an example one can consider parametrization that is a direct generalization of the HF case:

\[
\psi_{Z \setminus K} = \begin{cases} 
\sum_{S \subset Z \setminus K}^{(\kappa)} c_S^{(K)} |S\rangle & K \subset Z \setminus R, \\
0, & K \not\subset Z \setminus R 
\end{cases}
\]

The number of free parameters here is \( \left( ^{p+\kappa}_{\kappa} \right) \left( ^{q}_{\kappa} \right) \).

Parametrizations with the total number of free parameters equal to the dimension of the set \( \text{Ens}(S_{n,p,2}(Z)) \) are of primary interest. On this route we may hope to approach the exact solution of \( p \)-electron problem by \( \kappa \)-electron means that is the primary goal of the representability theory.

It seems pertinent to emphasize once again that equations of the type of Eq.(53) and Eq.(56) are \( \kappa \)-electron equations and in contrast to the standard configuration interaction method no expansions over \( p \)-electron determinants (states) appear in the frameworks of such an approach.

---

**Orbital Representation**

Molecular calculations are normally performed in orthonormal one-electron bases of molecular orbitals (MO). Turning from MSO to MO basis leads to somewhat cumbersome formulas but simplifies concrete calculations. Following Handy [9], we replace spin-orbital index set \( N \) by a pair of orbital index sets \( (M, M) \) of \( \alpha \) and \( \beta \) spins assuming that the spatial parts of molecular spin-orbitals with the same orbital index are identical. This corresponds to the so-called 'restricted' theories whereas general MSO basis embraces in addition 'unrestricted' theories. With such an approach each \( (p + q) \)-element subset \( Z \subset N \) should be replaced by the pair \( (Z_\alpha, Z_\beta) \subset M \times M \) with \( |Z_\alpha| + |Z_\beta| = p + q \).
If the total number $p$ of electrons is fixed and no other restrictions are imposed, then there is no essential difference between MSO and MO representations. For example, the expression for the metric matrix in terms of molecular orbitals may be easily derived from Eq.(52) and Eq.(C.1):

$$
G_{p,q}(Z_{\alpha}, Z_{\beta}) = \sum_{p_{\alpha}, p_{\beta}} (-1)^{p_{\alpha}(\kappa_{\beta} + \kappa'_{\beta})} \left[ G_{p_{\alpha}, q_{\alpha}, \kappa_{\alpha}}(Z_{\alpha}) S_{\alpha} S'_{\alpha} [G_{p_{\beta}, q_{\beta}, \kappa_{\beta}, q'_{\beta}}(Z_{\beta}) S_{\beta} S'_{\beta} \right], \quad (60)
$$

where

$$
\kappa_{\alpha} = |S_{\alpha}|, \kappa_{\beta} = |S_{\beta}|, \kappa_{\alpha} + \kappa_{\beta} = \kappa,
$$
$$
\kappa'_{\alpha} = |S'_{\alpha}|, \kappa'_{\beta} = |S'_{\beta}|, \kappa'_{\alpha} + \kappa'_{\beta} = \kappa,
$$
$$
q_{\alpha} = |Z_{\alpha}| - p_{\alpha}, q_{\beta} = |Z_{\beta}| - p_{\beta},
$$
$$
|Z_{\alpha}| + |Z_{\beta}| = p + q.
$$

If, in addition, the projection $M_S$ of the total spin is fixed, then the numbers $p_{\alpha}$ of $\alpha$ and $p_{\beta}$ of $\beta$ electrons are also fixed for each split basis determinant $|R_{\alpha}, R_{\beta}\rangle$. Moreover, the $q$ value for a given pair $(Z_{\alpha}, Z_{\beta}) \subset M \times M$ can be uniquely presented as a sum of its $\alpha$ and $\beta$ components:

$$
q = |Z_{\alpha}\rangle - R_{\alpha} + |Z_{\beta}\rangle - R_{\beta} = q_{\alpha} + q_{\beta}.
$$

**Definition.** Pair $(Z_{\alpha}, Z_{\beta})$ is called a pair of index $(q_{\alpha}, q_{\beta})$ if $|Z_{\alpha}| = p_{\alpha} + q_{\alpha}$ and $|Z_{\beta}| = p_{\beta} + q_{\beta}$.

Thus, in the orbital representation for the fixed value of the total spin projection there are $q + 1$ different types of pairs $(Z_{\alpha}, Z_{\beta})$ and arbitrary $(p, q)$-sheaf $\{\psi_{(Z_{\alpha}, Z_{\beta})}\}_{(Z_{\alpha}, Z_{\beta})\subset M \times M}$ involves, in general, $q$-germs with labels $(Z_{\alpha}, Z_{\beta})$ of different index.

In MO basis the expressions for $(p, q)$-sheaves become rather complicated (see Appendix C). Here we discuss only MO representation of the metric matrix and the Hamiltonian involved in Eqs.(53) and (56).

Simple combinatorial arguments lead to the conclusion that $(K_{\alpha}, K_{\beta})$ component of arbitrary $\kappa$-electron wavefunction $\psi_{(Z_{\alpha}, Z_{\beta})}$ corresponding to some given $M_S$ value is expanded over determinants $|S_{\alpha}, S_{\beta}\rangle$ with fixed $|S_{\alpha}| =
$\kappa_\alpha = q_\alpha - |K_\alpha|$ and $|S_\beta| = \kappa_\beta = q_\beta - |K_\beta|$. As a result, trial $\kappa$-electron wavefunction (see Eq.(49)) should be taken in the form

$$
\psi_{MS}^{(Z_\alpha, Z_\beta)} = \sum_{\kappa_\alpha = \max(0, \kappa_\alpha)}^{\min(\kappa_\alpha, q_\alpha)} \times \sum_{S_\alpha \in Z_\alpha} \sum_{S_\beta \in Z_\beta} \left( \frac{p_\alpha + q_\alpha - \kappa_\alpha}{p_\alpha} \right) \left( \frac{p_\beta + q_\beta - \kappa_\beta}{p_\beta} \right) c_{(S_\alpha, S_\beta)} |S_\alpha, S_\beta\rangle, \tag{61}
$$

where $\kappa_\beta = \kappa - \kappa_\alpha$.

The metric matrix corresponding to such choice of trial $\kappa$-electron wavefunction is

$$
[G_{p,q,x}(Z_\alpha, Z_\beta)]_{(S_\alpha, S_\beta)} = \sum_{\kappa_\alpha = \max(0, \kappa_\alpha)}^{\min(\kappa_\alpha, q_\alpha)} \times \sum_{S_\alpha \in Z_\alpha} \sum_{S_\beta \in Z_\beta} \left( \frac{p_\alpha + q_\alpha - \kappa_\alpha}{p_\alpha} \right) \left( \frac{p_\beta + q_\beta - \kappa_\beta}{p_\beta} \right) c_{(S_\alpha, S_\beta)} [G_{p_\alpha, q_\alpha, \kappa_\alpha, \kappa_\beta}'(Z_\alpha)]_{S_\alpha S_\alpha'} \times [G_{p_\beta, q_\beta, \kappa_\beta, \kappa_\beta}'(Z_\beta)]_{S_\beta S_\beta'}, \tag{62}
$$

where $p_\alpha = \frac{1}{2}(p + 2M_S)$ and $p_\beta = \frac{1}{2}(p - 2M_S)$.

In contrast to general metric matrix (60) its $M_S$ components (62) turn out to be always degenerate.

$M_S$ component of $\kappa$-electron Hamiltonian $H_{p,q,x}(Z)$ in the orbital representation is easily obtained from Eq.(A.12) with the aid of the relation (C.1):

$$
(-1)^{p_\alpha(\kappa_\beta + \kappa_\beta')}[H_{p,q,x}^{MS}(Z_\alpha, Z_\beta)]_{(S_\alpha, S_\beta)}(S_\alpha, S_\beta') =
$$

\begin{align*}
&= \left\{ \sum_{j \in Z_\alpha \setminus S_\alpha} (-1)^{|j\cap S_\alpha| + |i\cap S_\alpha'|} \langle i|h|j \rangle [G_{p_\alpha - 1.q_\alpha + 1, \kappa_\alpha + 1, \kappa_\beta}'(Z_\alpha)]_{S_\alpha \cup \{j\} S_\alpha' \cup \{i\}} \right. \\
&\quad \times [G_{p_\beta, q_\beta, \kappa_\beta} Z_\beta)]_{S_\beta S_\beta'} \\
&\quad + \left\{ \sum_{i \in Z_\beta \setminus S_\beta} (-1)^{|j\cap S_\beta| + |i\cap S_\beta'|} \langle i|h|j \rangle [G_{p_\beta - 1.q_\beta + 1, \kappa_\beta + 1, \kappa_\beta}'(Z_\beta)]_{S_\beta \cup \{j\} S_\beta' \cup \{i\}} \right. \\
&\quad \times [G_{p_\alpha, q_\alpha, \kappa_\alpha} Z_\alpha)]_{S_\alpha S_\alpha'} \\
&\end{align*}

25
\[ + \frac{1}{2} \left\{ \sum_{k,l \in Z_\alpha \setminus S_\alpha} (-1)^{||j\cap\Delta_{(i)}|+||l\cap\Delta_{(k)}|+||(k,l)\cap\Delta_{s_\alpha}|+||i,j\cap\Delta_{s'_\alpha}|} (ikjl) \right\} \]

\[ \times [G_{p_{\beta},q_{\beta}+1,\alpha,\kappa_{\beta}+1}(Z_{\alpha})]_{S_\alpha \cup \{k,l\}S'_{\alpha} \cup \{i,j\}} \]

\[ + \frac{1}{2} \left\{ \sum_{k \in Z_\beta \setminus S_\beta \atop i \in Z_\alpha \setminus S'_{\alpha} \atop j \in Z_\beta \setminus S'_{\beta}} (-1)^{||k\cap\Delta_{s_\beta}|+||l\cap\Delta_{s_\alpha}|+||i\cap\Delta_{s'_\alpha}|+||j\cap\Delta_{s'_\beta}|} (ikjl) \right\} \]

\[ \times [G_{p_{\beta},q_{\beta}+1,\alpha,\kappa_{\beta}+1}(Z_{\alpha})]_{S_\beta \cup \{k\}S'_{\beta} \cup \{i\}} \]

\[ \times [G_{p_{\beta},q_{\beta}+1,\alpha,\kappa_{\beta}+1}(Z_{\alpha})]_{S_\alpha \cup \{l\}S'_{\alpha} \cup \{j\}} \]

\[ + \frac{1}{2} \left\{ \sum_{k,l \in Z_\beta \setminus S_\beta} (-1)^{||j\cap\Delta_{(i)}|+||l\cap\Delta_{(k)}|+||(k,l)\cap\Delta_{s_\beta}|+||i,j\cap\Delta_{s'_\beta}|} (ikjl) \right\} \]

\[ \times [G_{p_{\beta},q_{\beta}+1,\alpha,\kappa_{\beta}+1}(Z_{\alpha})]_{S_\beta \cup \{k,l\}S'_{\beta} \cup \{i,j\}} \]

\[ \left\{ [G_{p_{\alpha},q_{\alpha}+1,\alpha_{\alpha}+1}(Z_{\alpha})]_{S_\alpha S'_{\alpha}} \right\}, \quad (63) \]

The analogous expression for this Hamiltonian in the hole representation may easily be obtained from Eq.(A.16).
Numerical Examples

To test numerous complicated formulas obtained in the preceding sections and to illustrate our approach, we performed several ground state calculations for small atomic and molecular systems using Eqs.(56)-(58). All HF calculations to generate MO basis and list of transformed molecular integrals were carried out with the aid of the GAMESS program [10].

Modification of the Davidson diagonalization routine [11] to handle eigenvalue problem in arbitrary non-degenerate metric (generalized eigenvalue problem) is not complicated and straightforward. We had certain doubts about possibility to use this routine for the case of degenerate metrics. To our surprise, after incorporation in Gram-Schmidt orthogonalization routine outflow for kernal vectors of the current metric we obtained stable working diagonalization procedure. It comes as no surprise that its convergence properties are worse than that of the original Davidson method for the standard Euclidean metric but it normally manifests itself only in the number of iterations that are necessary to reach the solution.

In Table I the results of calculations of few simple systems in STO-3G basis are presented. For $B, H_2O, NH_2$, and $NH_3$ the particle representation was used ($p \geq 2m - p$) whereas for $Be, and LiH$ transformation to the hole representation was required ($p < 2m - p$). In all calculations $q$ value was taken equal to $2m - p$ and, consequently, only the case $(Z_\alpha, Z_\beta) = (M, M)$ was under consideration.

In the basis of two-electron induced sheaves ($\kappa = 2$) only small percent of correlation energy is accounted (see Table II). This percent normally rises when $\kappa$ increases, and FCI limit corresponds to $\kappa = q$ in full accordance with general theory. It is interesting to note that for boron atom the energy corresponding to $\kappa = 4$ is greater than that for $\kappa = 3$. It is most probably connected with high degeneracy of the metric matrix for $\kappa = 4$ (its kernal dimension is equal to 35 for $\kappa = 3$ and 75 for $\kappa = 4$). As a result, in small basis used, the actual number of free parameters in energy turns out to be essentially less for $\kappa = 4$ in compare with the case $\kappa = 3$.

We did not try to calculate more extensive systems or use better bases because the parametric induced sheaves even if they are centered at the HF origin (see Eq.(54)) will hardly become a working tool of the computational quantum chemistry. In spite of mathematical beauty of metric matrices given by Eq.(B.6) and (B.7) the induced sheaves have no reasonable physical interpretation and for small $\kappa$ include too small number of parameters to be
adjusted. We used them just to illustrate the principal possibility to solve \( p \)-electron problems by diagonalization of \( \kappa \)-electron Hamiltonians in specially selected \( p \)-electron metrics.

**Conclusion**

We have presented a new way to approach many electron problems using \( \kappa \)-electron means (\( \kappa = 2, 3, \ldots \)). With the aid of special parametrizations it is possible to reduce \( p \)-electron optimization problem to generalized eigenvalue problem for Hamiltonians in spaces corresponding to numbers of electrons less than \( p \). These Hamiltonians and related metric matrices are uniquely determined by the parametrization selected. Systematic study of different parametrizations and their usefulness for concrete calculations is still an opened field for investigation. We have suggested two relatively simple parametrization schemes and studied in detail one of these schemes based on the notion of the induced sheaves. In spite of the fact that the induced sheaves are introduced in a very formal way and do not have any physical idea behind their definition, they may be used to analyze \( \kappa \)-electron contributions (\( \kappa = 2, 3, \ldots, q \)) to correlation energy.

There exists an opinion shared by a number of notable scientists that the romantic period of quantum chemistry came to its end with the appearance of universal computer programs such as GAUSSIAN, MOLCAS, GAMESS, etc. As we hope, the present paper demonstrates that it is fortunately not yet true.

**Appendix A**

Here we describe a general scheme of evaluation of matrix elements of products of the creation-annihilation operators involved in the energy expressions of the type of Eq.(51).

Let \( \psi_Z \) be \( \kappa \)-electron trial wave function expanded over determinants with indices from MSO index set \( Z, |Z| = p + q \). Rewriting this function as a sum of its \( K \)-components (see Eq.(50))

\[
\psi_Z = \sum_{K \subset Z}^{(q-\kappa)} \psi_{Z\backslash K}
\]
and replacing each component in this sum by the corresponding simple \((p, \kappa)\)-sheaf \(\{\psi_{Z|KZ'}\}_{Z \subset N}\) with germs
\[
\psi_{Z|KZ'} = \sum_{R \subset Z' \cap (Z \setminus K)} (-1)^{|R \cap Z'|} \tilde{C}_R^{(K)}|Z' \setminus R),
\]
where \(\tilde{C}_R^{(K)} = (-1)^{|R \cap Z'|} c_{Z|K} R\), we come to the problem of evaluation of matrix elements
\[
\langle \psi_Z | a | \psi_Z \rangle_G = \frac{1}{n-p}
\]
\[
\times \sum_{K,K' \subset Z} \sum_{Z' \subset N} \sum_{R \subset Z' \cap (Z \setminus K)} (-1)^{|R \cap Z'|} \left| \tilde{C}_R^{(K)} \right|^* \tilde{C}_R^{(K')}(Z' \setminus R)\langle a | Z' \setminus R' \rangle .
\]
Eq. (A.1)

where \(a\) stands for some relevant product of the creation-annihilation operators and subscript \(G\) means that the inner product is taken in the metric determined by the matrix \(G_{p,q,\kappa}(Z)\) (see Eq.(52)).

Changing the order of summations on the right-hand side of Eq.(A.1) and using technique of manipulations with phase prefactors developed in \([3]\), we can recast Eq.(A.1) as
\[
\langle \psi_Z | a | \psi_Z \rangle_G = \frac{1}{n-p} \sum_{S,S' \subset Z} \left( \frac{p+\kappa}{p} \right)^* \sum_{R \subset Z \setminus S} \sum_{R' \subset Z \setminus S'} (-1)^{|R \cap S'| + |R' \cap S'|} \left( \tilde{C}_R^{(K)} \right)^* \tilde{C}_R^{(K')} (Z' \setminus R) \langle a | Z' \setminus R' \rangle
\]
\[
\times \sum_{Z' \supset R \cup R'} (-1)^{|R \cap Z'| + |R' \cap Z'|} \langle \langle Z' \setminus R \setminus a | Z' \setminus R' \rangle \right\}. \quad \text{(A.2)}
\]

There are five cases to be analyzed (see Eqs.(40a)-(40e)).

Case 1: \(a = a_1^i a_i\).

In this case the inner sum on the right-hand size of Eq.(A.2) is equal to
\[
(1 - \zeta_{(i),R}) \sum_{Z' \supset R} (-1)^{|R \cap Z'|} \xi_{(i),Z'} = (1 - \zeta_{(i),R}) \left( \frac{n - p - 1}{p - 1} \right),
\]
where
\[
\zeta_{I,R} = \begin{cases} 1 & \text{if } I \subset R, \\ 0 & \text{if } I \not\subset R \end{cases}
\]

29
is the well-known in combinatorics zeta-function of partially ordered by inclusion set of all subsets of N \[\text{[12]}\). By an abuse of notation, we agree to use $\zeta_{i,R}$ instead of $\zeta_{\{i\},R}$ for one-element subsets of N. In this case this function is identical to the characteristic function of subset $R$ accepting the value 1 if $i \in R$ and 0 if $i \notin R$.

If $i \in S \cup S'$ or $i \in N \setminus Z$ then the sum over $R \subset Z \setminus (S \cup S')$ is just proportional to the matrix element $[G_{p,q,\kappa}]_{SS'}$. If $i \in Z \setminus (S \cup S')$ then this sum is proportional to the matrix element $[G_{p,q-1,\kappa}(Z \setminus \{i\})]_{SS'}$. The final expression for the desired matrix element is obtained with the aid of the recurrence relation (B.9):

$$\langle \psi_Z | a_i^\dagger a_j | \psi_Z \rangle_G = \left( \frac{\kappa - 1}{n-p} \right) \left\{ \langle \psi_Z | G_{p,q,\kappa}(Z) | \psi_Z \rangle - \sum_{S,S' \in Z} c_S^* c_{S'} (-1)^{|\{i\} \cap S \Delta S'|} \zeta_{i,Z \setminus (S \cup S')} [G_{p-1,q+1,\kappa+1}(Z)]_{S \cup \{i\} S' \cup \{i\}} \right\} \quad (A.3)$$

Case 2: $a = a_i^\dagger a_j$, $i \neq j$.

The sum over $Z'$ on the right-hand side of Eq.(A.2) is non-zero only for $R = R_1 \cup \{j\}$ and $R' = R_1 \cup \{i\}$. Substitution of expansion (40b) for the operator $a_i^\dagger a_j$ in matrix elements $\langle Z' \setminus R | a_i^\dagger a_j | Z' \setminus R' \rangle$ makes it easy to get the following expression for the sum under consideration:

$$(-1)^{|R_1 \cap \Delta \{i,j\}| + |\{i\} \cap \Delta \{j\}| + |\{j\} \cap \Delta \{i\}|} \left( \frac{n-p-1}{\kappa - 1} \right).$$

Since $|\{i\} \cap \Delta \{j\}| + |\{j\} \cap \Delta \{i\}| \equiv 1 (\mod 2)$ for $i \neq j$, the required matrix element takes the form

$$\langle \psi_Z | a_i^\dagger a_j | \psi_Z \rangle_G = -\left( \frac{\kappa - 1}{n-p} \right) \sum_{S,S' \in Z} c_S^* c_{S'} \times \sum_{R_1 \cup \{i\} \subset Z \setminus S \atop R_1 \cup \{j\} \subset Z \setminus S'} (-1)^{|R_1 \cup \{j\} \cap \Delta S| + |R_1 \cup \{i\} \cap \Delta S'| + |R_1 \cap \Delta \{i,j\}|}.$$
Taking into account that \( R_1 \cup \{ j \} \subset Z \setminus S \) implies \( j \notin S \), and \( R_1 \cup \{ i \} \subset Z \setminus S' \) implies \( i \notin S' \), we can write down the final expression:

\[
\langle \psi_Z | a_i^\dagger a_j | \psi_Z \rangle_G = \frac{(\gamma)}{(n-p)} \sum_{S,S' \in Z} \left( \sum_{R \subseteq Z \setminus (S \cup S')} c_S^* c_{S'} \left( -1 \right)^{\left| \{ i \} \cap \Delta_S \right| + \left| \{ j \} \cap \Delta_{S'} \right|} \times \zeta_{j,Z \setminus S} \zeta_{i,Z \setminus S'} \left[ G_{p-1,q+1,\kappa+1}(Z) \right]_{S \cup \{j\}, S' \cup \{i\}} \right).
\]  

(A.4)

Case 3: \( a = a_i^\dagger a_j a_j a_i, i \neq j \).

Substitution of expansion (40c) in matrix element \( \langle Z' \setminus R | a_i^\dagger a_j a_j a_i | Z' \setminus R' \rangle \) immediately shows that non-zero contributions correspond to the case \( R = R' \) and \( R \ni i, j \):

\[
\langle \psi_Z | a_i^\dagger a_j a_j a_i | \psi_Z \rangle_G = \frac{(\gamma)}{(n-p)} \sum_{S,S' \in Z} \left( \sum_{R \subseteq Z \setminus (S \cup S')} c_S^* c_{S'} \left( -1 \right)^{\left| R \cap \Delta_S \Delta_{S'} \right|} \right).
\]

Thorough analysis of mutual layout of indices \( i, j \) and relevant subsets of the MSO index set with subsequent use of the recurrence relations (B.9)-(B.10) leads to the following somewhat cumbersome expression:

\[
\langle \psi_Z | a_i^\dagger a_j a_j a_i | \psi_Z \rangle_G = \frac{(\gamma)}{(n-p)} \left[ \langle \psi_Z | G_{p,q,\kappa}(Z) | \psi_Z \rangle - \sum_{S,S' \in Z} \left( \sum_{R \subseteq Z \setminus (S \cup S')} c_S^* c_{S'} \left( -1 \right)^{\left| \{ i \} \cap \Delta_S \right| + \left| \{ j \} \cap \Delta_{S'} \right|} \times \zeta_{i,Z \setminus S} \zeta_{j,Z \setminus S'} \left[ G_{p-1,q+1,\kappa+1}(Z) \right]_{S \cup \{i\}, S' \cup \{j\}} \right) + \left( -1 \right)^{\left| \{ i \} \cap \Delta_S \Delta_{S'} \right|} \zeta_{j,Z \setminus S} \zeta_{i,Z \setminus S'} \left[ G_{p-1,q+1,\kappa+1}(Z) \right]_{S \cup \{j\}, S' \cup \{i\}} \right) - \left( -1 \right)^{\left| \{ i \} \cap \Delta_S \Delta_{S'} \right|} \zeta_{(i,j),Z \setminus (S \cup S')} \left[ G_{p-2,q+2,\kappa+2}(Z) \right]_{S \cup \{i,j\}, S' \cup \{i,j\}} \right) \right].
\]  

(A.5)

Case 4: \( a = a_i^\dagger a_j a_j a_i, i \neq j \neq l \).

Substitution of expansion (40d) in matrix element \( \langle Z' \setminus R | a_i^\dagger a_j a_j a_i | Z' \setminus R' \rangle \) readily leads to the conclusion that this matrix element is non-zero if \( R = R_1 \cup \{ l \}, R' = R_1 \cup \{ j \}, \) and \( R_1 \nsubseteq i \). The final expression is

\[
\langle \psi_Z | a_i^\dagger a_j a_j a_i | \psi_Z \rangle_G = \frac{(\gamma)}{(n-p)} \sum_{S,S' \in Z} \left( \sum_{R \subseteq Z \setminus (S \cup S')} c_S^* c_{S'} \zeta_{i,Z \setminus S} \zeta_{j,Z \setminus S'} \right).
\]
\( \times \left\{ (-1)^{|\{i\}\cap S|+|\{j\}\cap S'|} [G_{p-1,q+1,x+1}(Z)]_{S\cup\{i\}S'|\{j\}} \right. \\
\left. -(-1)^{|\{i\}\cap S|+|\{i,j\}\cap S'|+|\{i\}\cap S'|} \zeta_\{i,Z\}(S\cup S') [G_{p-2,q+2,x+2}(Z)]_{S\cup\{i,j\}S'|\{i,j\}} \right\} \) 

(A.6)

Case 5: \( a = a_i^\dagger a_j^\dagger a_k a_l, i \neq j \neq k \neq l \).

Matrix element \( \langle Z'|R|a_i^\dagger a_j^\dagger a_k a_l|Z\rangle \) is nonzero only if \( R = R_1 \cup \{k, l\} \), \( R' = R_1 \cup \{i, j\} \). We have

\[
\langle \psi_Z|a_i^\dagger a_j^\dagger a_k a_l|\psi_Z \rangle_G \\
= (-1)^{|\{j\}\cap S|+|\{k\}\cap S'|} \sum_{S,S' \in Z} c_{s}c_{s'} \left\{ (-1)^{|\{i,j\}\cap S'|} \zeta_{i,J}(S\cup S') \right. \\
\left. \times \zeta_k,Z_s \zeta_l,Z_s' \zeta_j,Z_s' \zeta_i,Z_s \zeta_i,Z_s' \right\} \] 

(A.7)

Now it is easy to derive the expression for the matrix elements of general one- and two-electron operators:

\[
h = \sum_{i,j=1}^{n} \langle i|a_j a_j^\dagger |j \rangle a_i^\dagger a_j, \quad (A.8) \]

\[
g = \sum_{i,j,k,l=1}^{n} \langle i|a_k a_l a_i^\dagger a_j^\dagger |j \rangle a_i^\dagger a_j a_k. \quad (A.9) \]

We have

\[
\langle \psi_Z|h|\psi_Z \rangle_G = \binom{n}{1} \left\{ Tr(h) \langle \psi_Z|G_{p,q,x}(Z)|\psi_Z \rangle \right. \\
\left. - \sum_{S,S' \in Z} c_{s}c_{s'} \sum_{j \in Z \setminus S \cup S'} (-1)^{|\{j\}\cap S|+|\{i\}\cap S'|} \langle i|a_j a_j^\dagger \right|G_{p-1,q+1,x+1}(Z)|S\cup\{i\}S'|\{j\} \rangle \right\}, \quad (A.10) \]
The Hamiltonian associated with the energy expression (51) is

\[
[H_{p,q,\kappa}(Z)]_{SS'} = \sum_{j \in Z \setminus S} (-1)^{|j \cap \Delta_s| + |j \cap \Delta_{s'}|} \times \langle i | h | j \rangle [G_{p-1,q+1,\kappa+1}(Z)]_{S \cup \{j\} \cup \{i\}} + \frac{1}{2} \sum_{k,l \in Z \setminus S \setminus S'} (-1)^{|j \cap \Delta_{\{i\}}| + |l \cap \Delta_{\{k\}}| + |k,l \cap \Delta_s| + |l \cap \Delta_{s'}|} \times \langle ij | kl \rangle [G_{p-2,q+2,\kappa+2}(Z)]_{S \cup \{k,l\} \cup \{i,j\}} \tag{A.12}
\]

As has already been mentioned, for \( p < n - p \) it is reasonable to turn to sheaves in hole representation (co-sheaves). Reduced hole Hamiltonian (see Appendix B of [3]) after its transformation with the aid of \( A^{-1}(n, \bar{p}, \kappa) = A(n, p, \kappa) \) may be written as

\[
A^{-1}(n, \bar{p}, \kappa) H_{\bar{p} \to \kappa}^\circ = \frac{(p \choose \bar{p}) \kappa}{(1 \choose 1) \kappa} \sum_{i,j=1}^{n} \langle i | h | j \rangle a_i^\dagger a_j
\]
\[ + \frac{1}{2} \binom{\tilde{p}}{2} \sum_{i,j,k,l=1}^{n} \langle ij|kl \rangle a_i^\dagger a_j^\dagger a_l a_k, \]  
\tag{A.13}

where

\[ \langle ij|hl \rangle = (-1)^{i+j} \langle j|h|i \rangle, \]  
\tag{A.14}
\[ \langle ij|kl \rangle = (-1)^{i+j+k+l} \langle kl|i j \rangle, \]  
\tag{A.15}

and \( \tilde{p} = n - p \). Using Eqs.\((A.10)-(A.11)\) it is easy to derive the expression for the Hamiltonian corresponding to the energy \((51)\) in the hole representation:

\[
\left[ H_{p,q,x}^o (Z) \right]_{SS'} = \frac{1}{2} [Tr(h + F_N)] G_{\tilde{p},q,x}(Z)_{SS'} \\
- \sum_{j \in Z \setminus S \atop R \subset Z \setminus (S \cup S')} (-1)^{\left| R \cap \Delta_{S} \right| + \left| R \cap \Delta_{S'} \right|} \left[ \frac{1}{2} I |F_N| j \right] G_{\tilde{p}-1,q-1,x+1}(Z)_{S \cup \{j\} \cup \{i\}} \\
+ \frac{1}{2} \sum_{k,l \in Z \setminus S \atop i,j \in Z \setminus S'} (-1)^{\left| \{j\} \cap \Delta_{\{i\}} \right| + \left| \{l\} \cap \Delta_{\{k\}} \right| + \left| \{k,l\} \cap \Delta_{S} \right| + \left| \{i,j\} \cap \Delta_{S'} \right|} \\
\times \langle ij|kl \rangle G_{\tilde{p}-2,q+2,x+2}(Z)_{S \cup \{k,l\} \cup \{i,j\}}, \]  
\tag{A.16}

where \( |Z| = \tilde{p} + q \) and \( F_N \) is the Fock operator defined by Eq.\((43)\).

---

**Appendix B**

With each subset \( Z \subset N, |Z| = p + q \) let us associate the linear mapping

\[
g_{p,q}(Z) : \bigoplus_{x=1}^{q} \mathcal{F}_{n,x}(Z) \to \bigoplus_{x=1}^{q} \mathcal{F}_{n,x}(Z), \]  
\tag{B.1}

defined by its matrix representation

\[
\left[ G_{p,q,x,x'}(Z) \right]_{SS'} = \sum_{R \subset Z \setminus (S \cup S')} (-1)^{|R \cap \Delta_{S} \Delta_{S'}|}. \]  
\tag{B.2}

with respect to the determinant basis set. Here \( |S| = x \), and \( |S'| = x' \). Diagonal (with respect to \( x \)) blocks of this matrix are identical to the \( p \)-electron metric matrices given by Eq.\((52)\). We agree to omit repeating index.
\( \kappa \) in writing diagonal (with respect to \( \kappa \)) matrix elements. Off-diagonal \((\kappa \neq \kappa')\) blocks appear in going from molecular spin-orbitals to molecular orbitals.

Let \( S \) and \( S' \) be \( \kappa \) and \( \kappa' \)-element subsets of the index set \( Z \subset N, |Z| = p + q \), respectively. Let us suppose that

\[
S \Delta S' = s_1 < s_2 < \ldots < s_l,
\]

\[
Z \setminus (S \cap S') = z_1 < z_2 < \ldots < z_k,
\]

where \( l = |S \Delta S'| \), and \( k = |Z \setminus (S \cap S')| = p + q - |S \cap S'| \).

The index set \( Z' = Z \setminus (S \cap S') \) may be presented as

\[
Z' = \bigcup_{i=0}^{l} \{s_i\} \cup ([s_i + 1, s_{i+1} - 1] \cap Z'),
\]

(B.3)

where \( s_0 = z_1 - 1 \), \( s_{l+1} = z_k + 1 \), and the symbol \([s, s']\) stands for the interval in the set \( N = \{1, 2, \ldots, n\} \). It is easy to show that \( l \equiv \kappa - \kappa' \pmod{2} \). Cases of even and odd \( l \) require separate analysis, since the representation of the set \( S \Delta S' \) as a union of intervals depends on the parity of \( l \) (see Eq.(A.5) from [3]):

\[
\Delta_{S \Delta S'} = \begin{cases} 
\bigcup_{i=1}^{l} [s_{2i-1} + 1, s_{2i}], & \text{if } l \text{ is even}, \\
[\bigcup_{i=0}^{\lfloor l/2 \rfloor} [s_{2i} + 1, s_{2i+1}], & \text{if } l \text{ is odd}.
\end{cases}
\]

(B.4)

Using decompositions (B.3)-(B.4), it is possible to express the sum on the right-hand side of Eq.(B.2) as a sum of binomials. We have

\[
[G_{p,q,\kappa,\kappa'}(Z)]_{SS'} = \begin{cases} 
\sum_{r_1, r_2, \ldots, r_{l+1} \geq 0} (-1)^{\sum_{i=1}^{l+1} r_i} \prod_{i=1}^{l+1} \binom{w_i}{r_i}, & \text{if } l \text{ is even}, \\
\sum_{r_1, r_2, \ldots, r_{l+1} \geq 0} (-1)^{\sum_{i=1}^{l+1} r_i} \prod_{i=1}^{l+1} \binom{w_i}{r_i}, & \text{if } l \text{ is odd},
\end{cases}
\]

(B.5)
where

\[ w_i = |[s_{i-1} + 1, s_i - 1] \cap (Z \setminus (S \cap S'))|. \]

By definition, \( w_i \geq 0 \) and \( \sum_{i=1}^{l+1} w_i = |Z \setminus (S \cup S')| \).

Performing summations on the right-hand side of Eq.(A.5) first over indices \( r \) with odd \( i \) and then over indices \( r \) with even \( i \) for the case of even \( l \), and in the backward succession for odd \( l \), we arrive to the following not very complicated expression

\[
[G_{p,q,x',x}(Z)]_{SS'} = (-1)^{pl} \sum_{r \geq 0} (-1)^r \left( \sum_{i=0}^{l-1} w_{2i+1} \right) \left( \sum_{i=1}^{l} w_{2i} \right). \tag{B.6}
\]

In Eqs.(B.5)-(B.6) the symbol \([x]\) stands for the function extracting integral part of \( x \).

If \( x = x' \) and \( S = S' \) then \( l = 0 \) and only \( w_1 = |[s_0 + 1, s_1 - 1] \cap (Z \setminus S)| = p + q - x \) differs from zero which means that \([G_{p,q,x,x}(Z)]_{SS'} = (p+q-x)\) in full accordance with Eq.(B.2). If \( x = q \) then for \( S \neq S' \) there is no room for \( p \)-electron subsets in the set \( Z \setminus (S \cup S') \) and in this case the only non-zero block is the diagonal one \((x' = q)\) coinciding with the \( q \)-electron identity matrix.

If \( Z = \{1, 2, \ldots, p+q\} \) then the sums of interval lengths involved in the right-hand side of Eq.(A.6) may be presented in a more transparent form. Indeed, in this case \( s_0 = 0, s_{i+1} = p + q + 1 \), and for even \( l \)

\[
\sum_{i=1}^{l} w_{2i} = \sum_{i=1}^{l} (-1)^i s_i - \frac{l}{2} - l_0,
\]

\[
\sum_{i=0}^{l} w_{2i+1} = p + q + \sum_{i=1}^{l} (-1)^{i+1} s_i - \frac{l}{2} - l_1,
\]

where \( l_0 \) and \( l_1 \) are the numbers of elements from \( S \cap S' \) belonging to 'even' intervals \([s_{2i-1} + 1, s_{2i} - 1]\) and 'odd' intervals \([s_{2i} + 1, s_{2i+1} - 1]\), respectively. For odd \( l \) we have

\[
\sum_{i=1}^{l+1} w_{2i} = p + q + 1 + \sum_{i=1}^{l} (-1)^i s_i - \frac{l + 1}{2} - l_0,
\]
\[ \sum_{i=0}^{l} \omega_{2i+1} = \sum_{i=1}^{l} (-1)^{i+1} s_i - \frac{l+1}{2} - l_1. \]

The final expression for the matrix elements under consideration may be written as

\[ [G_{p,q,\kappa,\kappa'}(Z)]_{SS'} = \begin{cases} 
\sum_{r \geq 0} (-1)^r (p+q+\sum_{i=1}^{r} (-1)^{i+1} s_i - \frac{l}{r} - l_0) (\sum_{i=1}^{r} (-1)^{i+1} s_i - \frac{l}{r} - l_0), & \text{if } l \text{ is even,} \\
\sum_{r \geq 0} (-1)^r (p+q+1+\sum_{i=1}^{r} (-1)^{i+1} s_i - \frac{l+1}{r} - l_0) (\sum_{i=1}^{r} (-1)^{i+1} s_i - \frac{l+1}{r} - l_0), & \text{if } l \text{ is odd.} 
\end{cases} \]

(B.7)

Directly from the definition (B.2) various recurrence relations involving matrix elements of metric matrices may be derived. Here we confine ourselves to the relations that are necessary for evaluation of relevant matrix elements. Let us suppose that subsets \( S, S' \subset Z \) are fixed and \( K(|K| = k) \) is some subset of the set \( Z \setminus (S \cup S') \). Then

\[ [G_{p,q,\kappa}(Z)]_{SS'} = \sum_{k_1=0}^{k} \sum_{K_1 \subset K} (-1)^{|K_1 \cap \Delta S \Delta S'|} [G_{p-k_1,q-k+2k_1,\kappa+k_1}(Z \setminus K_1) \cup K_1)]_{S \cup K_1 S' \cup K_1}. \]

(B.8)

In two most important particular cases \( K = \{i\} \) and \( K = \{i, j\} \) general relation (B.8) reduces to

\[ [G_{p,q,\kappa}(Z)]_{SS'} = [G_{p,q-1,\kappa}(Z \setminus \{i\})]_{SS'} + (-1)^{|\{i\} \cap \Delta S \Delta S'|} [G_{p-1,q+1,\kappa+1}(Z \setminus \{i, j\})]_{S \cup \{j\} S' \cup \{i\}}; \]

(B.9)

\[ [G_{p,q,\kappa}(Z)]_{SS'} = [G_{p,q-2,\kappa}(Z \setminus \{i, j\})]_{SS'} + (-1)^{|\{i\} \cap \Delta S \Delta S'|} [G_{p-1,q,\kappa+1}(Z \setminus \{j\})]_{S \cup \{j\} S' \cup \{i\}} + (-1)^{|\{j\} \cap \Delta S \Delta S'|} [G_{p-2,q+2,\kappa+2}(Z \setminus \{i, j\})]_{S \cup \{i, j\} S' \cup \{i, j\}}. \]

(B.10)
Appendix C

From Eq.(6) it follows that in expansion of q-germs phase prefactors of the type \((-1)^{|R\cap \Delta Z|}\) are involved. In Handy orbital representation \(R\) goes to \((R_\alpha, R_\beta)\) and \(Z\) goes to \((Z_\alpha, Z_\beta)\). Let us introduce the sets \(\bar{R}_\beta = m + R_\beta\) and \(\bar{Z}_\beta = m + Z_\beta\) with shifted by \(m = |M|\) elements. We have \(R = R_\alpha \Delta \bar{R}_\beta\) and \(Z = Z_\alpha \Delta \bar{Z}_\beta\). Using technique of manipulation with sign prefactors developed in [3], we obtain

\[ |R \cap \Delta Z| \equiv |R_\alpha \cap \Delta Z_\alpha| + |R_\beta \cap \Delta Z_\beta| + |\bar{R}_\alpha \cap \Delta Z_\alpha| + |\bar{R}_\beta \cap \Delta Z_\beta| \pmod{2}. \]

From Eq.(A.5) of [3] it follows that \(|\bar{R}_\beta \cap \Delta Z_\alpha| = 0\) and \(|R_\alpha \cap \Delta Z_\beta| \equiv |R_\alpha||Z_\beta| \pmod{2}\). As a result,

\[ |R \cap \Delta Z| \equiv |R_\alpha \cap \Delta Z_\alpha| + |R_\beta \cap \Delta Z_\beta| + |R_\alpha||Z_\beta| \pmod{2}. \quad (C.1) \]

Certain assymetry of this relation is connected with the use of Handy split determinant representation with \(\alpha\) indices always going first.

q-electron function

\[ \psi(Z_\alpha, Z_\beta) = \]

\[ (-1)^{p_\alpha |Z_\beta|} \sum_{R_\alpha \subset Z_\alpha} \sum_{R_\beta \subset Z_\beta} (-1)^{|R_\alpha \cap \Delta Z_\alpha| + |R_\beta \cap \Delta Z_\beta|} \bar{C}_{R_\alpha, R_\beta} |Z_\alpha \setminus R_\alpha, Z_\beta \setminus R_\beta \] \quad (C.2)

generates simple \((p, q)\)-sheaf with germs

\[ \psi(Z_\alpha, Z_\beta)(Z'_\alpha, Z'_\beta) = \]

\[ (-1)^{p_\alpha |Z'_\beta|} \sum_{R'_\alpha \subset Z'_\alpha \cap Z_\alpha} \sum_{R'_\beta \subset Z'_\beta \cap Z_\beta} (-1)^{|R'_\alpha \cap \Delta Z'_\alpha| + |R'_\beta \cap \Delta Z'_\beta|} \bar{C}'_{(R'_\alpha, R'_\beta)} |Z'_\alpha \setminus R'_\alpha, Z'_\beta \setminus R'_\beta \] \quad (C.3)

From Eq.(C.2) it follows that in the orbital representation with fixed \(M_S\) value only q-electron functions \(\psi(Z_\alpha, Z_\beta)\) from the vector space \(\mathcal{F}_{n,q}(Z_\alpha, Z_\beta)\) that are linear combinations of determinants \(|S_\alpha, S_\beta\) with \(|S_\alpha| = q_\alpha\) and \(|S_\beta| = q_\beta\) \((q_\alpha = |Z_\alpha| - p_\alpha, q_\beta = |Z_\beta| - p_\beta)\) are of actual interest.

In the orbital representation definitions (17) and (18) should be replaced by

\[ I_p(\psi(Z_\alpha, Z_\beta)) = \{(R_\alpha, R_\beta) \subset (Z_\alpha, Z_\beta) : \bar{C}_{(R_\alpha, R_\beta)} \neq 0\}; \quad (C.4) \]
\[ I^\alpha_p(\psi(Z_\alpha,Z_\beta)) = \{ R_\alpha \subset Z_\alpha : \bar{C}(R_\alpha,R_\beta) \neq 0 \text{ for some } R_\beta \subset Z_\beta \}; \quad (C.5) \]
\[ I^\beta_p(\psi(Z_\alpha,Z_\beta)) = \{ R_\beta \subset Z_\beta : \bar{C}(R_\alpha,R_\beta) \neq 0 \text{ for some } R_\alpha \subset Z_\alpha \}; \quad (C.6) \]
\[ L_\sigma(\psi(Z_\alpha,Z_\beta)) = \bigcup_{R_\sigma \in I^\sigma_p(\psi(Z_\alpha,Z_\beta))} R_\sigma \quad (\sigma = \alpha, \beta). \quad (C.7) \]

and each simple \((p,q)\)-sheaf \( \{ \psi(Z_\alpha,Z_\beta)(Z'_\alpha,Z'_\beta) \} \subset M \times M \) is generated by any of its
\[ \left( 2m - |L_\alpha(\psi(Z_\alpha,Z_\beta))| - |L_\beta(\psi(Z_\alpha,Z_\beta))| \right) \]
\[ + \left( p + q - |L_\alpha(\psi(Z_\alpha,Z_\beta))| - |L_\beta(\psi(Z_\alpha,Z_\beta))| \right) \quad (C.8) \]

ACKNOWLEDGMENTS

We gratefully acknowledge the Russian Foundation for Basic Research (Grant 00-03-32943a) and Ministry of Education of RF (Grant E00-5.0-62) for financial support of the present work.

References

[1] Panin, A.I. Int J Quantum Chem 2002,87,23.
[2] Panin, A. I. Int J Quantum Chem 1985,28,861.
[3] Panin, A.I. Int J Quantum Chem 2001,85,1.
[4] Coleman, A. J. Rev Mod Phys 1963, 35,668.
[5] Coleman, A. J. In Reduced Density Matrices With Applications to Physical and Chemical Systems; Coleman, A.J. and Erdahl,R.M.,Eds.;Queen’s Univ.: Kingston, Ontario, 1968;No 11,p.2.
[6] Coleman, A.J. J Math Phys 1972,13,214.
[7] Coleman, A. J. Reports on Math Phys 1973,4, 113.
[8] Knuth, D.E. The art of computer programming; Addison-Wesley Publishing Company: Reading, Massachusetts, Menlo Park, California, Don Mills, Ontario, 1968, Vol.1.
[9] Handy, N. C. Chem Phys Lett 1980, 74, 280.

[10] Schmidt, M. W.; Baldridge, K. K.; Boatz, J. A.; Elbert, S. T.; Gordon, M. S.; Jensen, J. H.; Koseki, S.; Matsunaga, N.; Nguyen, K. A.; Su, S. J.; Windus, T. L.; Dupuis, M.; Montgomery, J. A. J Comput Chem. 1993, 14, 1347.

[11] Davidson E. R., J. Comput. Phys. 17, 87 (1975).

[12] Stanley, P.S. Enumerative combinatorics; Wadsworth&Brooks/Cole, Advanced Books&Software: Monterey, California, 1986.
TABLE I
Results of ground state test calculations: Total energies.

| Species       | \( \kappa = 2 \) | \( \kappa = 3 \) | \( \kappa = 4 \) | \( \kappa = 5 \) | \( \kappa = 6 \) |
|---------------|------------------|------------------|------------------|------------------|------------------|
| \( Be(1S) \)  | -14.351880       | -14.366729       | -14.373701       | -14.403655       | -                |
| \( B(2P) \)   | -24.148989       | -24.152540       | -24.169145       | -24.161980       | -24.189265       |
| \( LiH(1\Sigma^+) \) | -7.862024       | -7.864463       | -7.868083       | -7.882402       | -                |
| \( NH_2(2B_2) \) | -54.834567      | -54.835048       | -54.839962       | -54.850959       | -54.882707       |
| \( NH_3(1A_1) \) | -55.447595      | -55.447969       | -55.449684       | -55.457770       | -55.468587       | -55.509590       |
| \( H_2O(1A_1) \) | -74.962992      | -74.965180       | -74.976319       | -75.012500       | -                |