THE HODGE OPERATOR IN FERMIONIC FOCK SPACE

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Received March 9, 2005
Accepted June 17, 2005

Dedicated to Professor Josef Paldus on the occasion of his 70th birthday.

The Hodge operator ("star" operator) plays an important role in the theory of differential forms, where it serves as a tool for the switching between the exterior derivative and co-derivative. In the theory of many-electron systems involving a finite-dimensional fermionic Fock space, one can define the Hodge operator as a unique (i.e., invariant with respect to linear transformations of the spin-orbital basis set) antilinear operator. The similarity transformation based on the Hodge operator results in the switching between the fermion creation and annihilation operators. The present paper gives a self-contained account on the algebraic structures which are necessary for the construction of the Hodge operator: the fermionic Fock space, the corresponding Grassmann algebra, and the generalized creation and annihilation operators. The Hodge operator is then defined, and its properties are reviewed. It is shown how the notion of the Hodge operator can be employed in a construction of the electronic time-reversal operator.

Keywords: Many-electron systems; Fermions; Fock space; Grassmann algebra; Hodge operator; Time-reversal operator; Spin-orbital bases; Quantum chemistry.

The Pauli exclusion principle[1] plays a crucial role in the quantum theory of many-electron systems – atoms, molecules, and solids. Electrons are spin-1/2 fermions, whose behavior is governed by the proper quantum statistics. In 1928, Jordan and Wigner[2] formulated the so-called second-quantization formalism for fermions, based on anticommuting fermion creation and annihilation operators, that automatically takes care of the Pauli principle. In 1932, Fock[3] introduced a vector space, then named after him, in which these operators act. Since then, the second-quantization approach (to fermion and to boson systems) has become a basic theoretical tool in quantum physics.

Parallel progress in quantum chemistry, on the other hand, has been for a long time associated exclusively with the "first-quantization" approach

based on the Schrödinger equation. For a many-electron system, the Pauli exclusion principle requires any N-electron wave function ($N \geq 2$) to be antisymmetric with respect to exchange of the spatial and spin coordinates of any pair of electrons. Thus, all the solutions of the Schrödinger equation which do not fulfill this condition, including the "mathematical ground state" (corresponding to the lowest eigenvalue), have to be discarded as nonphysical. The diffusion of the second-quantization techniques into the quantum-chemistry practice have been slow, one of the obstacles being the dominance of the time-dependent formalism, developed by physicists for studying relativistic particle-scattering problems. In 1975, Paldus and Čížek published an article entitled "Time-Independent Diagrammatic Approach to Perturbation Theory of Fermion Systems"[4], which set a standard for a second-quantization formalism tailored to the needs of quantum chemists (who are concerned mostly with the stationary states of nonrelativistic many-electron systems). The approach of ref.[4] employs the so-called algebraic approximation, in which the electronic creation and annihilation operators correspond to some finite basis of one-electron wave functions (spin orbitals). This results in the electronic Fock space of a finite dimension, and leads to a multitude of computational techniques that can be effectively translated into computer codes based on matrix algebra. One may safely state that almost all the contemporary post-Hartree–Fock methods of quantum chemistry have their roots in the '75 article of Paldus and Čížek. Many quantum chemists, including the present author, have made their first acquaintance with the second-quantization approach to many-electron systems by learning from that article, and also from the famous Paldus "orange book" of his '81 Nijmegen lectures[5].

In this paper, which I wish to dedicate to Prof. Paldus, the fermionic Fock space corresponding to the time-independent second-quantization approach of ref.[4] is analyzed. This is a *complex* vector space (i.e., the vector space over the field $\mathbb{C}$ of the complex numbers), of the dimension 2^M, where M is the number of spin orbitals used in its construction, endowed with a scalar product (as such, it is a *unitary* vector space). It turns out that the algebraic structure of such a vector space is quite rich, and has not yet been fully explored. In the present paper a formal algebraic construction of the Fock space, and the associated Grassmann algebra, is performed. Exploited are some analogies with the algebraic structures encountered in the theory of differential forms (which involves some *real*, *Euclidean* vector space E_1 of the dimension M), see, e.g., a book by Thirring[6], Chap. 1.2. The author would like also to acknowledge an invaluable inspiration due to the book of Komorowski[7]. In the theory of differential forms an important role

is played by the so-called Hodge operator[8], which converts the N-th-rank differential forms ω into the $(M - N)$-th-rank ones:

$$E_N \ni \omega \to * \omega \in E_{M-N} \qquad (1)$$

$N = 0, 1, 2, ..., M$. The star symbol $*$ denoting the Hodge operator was introduced by Weyl[9]. For real vector spaces E_N, the Hodge operator is a *linear* operator, invariant with respect to the linear transformations of the basis set spanning the vector space E_1. Thus, it is a nontrivial *unique* linear operator for the differential forms. Let us note that in a general Euclidean or unitary vector space there are only trivial unique linear operators: $\hat{0}$ (the *zero operator*) and $\hat{1}$ (the *unit operator*). On the other hand, the Hodge operator corresponding to the fermionic Fock space turns out to be a unique *antilinear* (and *antiunitary*) operator in that space.

According to the Wigner theorem[10] (see also ref.[11], Chap. 9-4), the symmetry operations of a quantum system may be represented by either linear (unitary) or antilinear (antiunitary) operators. An example of the antilinear symmetry operator is provided by the time-reversal operator[10] (see also ref.[11], Chaps 13-8 and 14-5). Let us note that if a nonsingular (i.e., reversible) antilinear operator $\hat{A}$ is defined in a complex vector space, an arbitrary antilinear operator $\hat{A}'$ acting in that space may be expressed as $\hat{A}' = \hat{L}\hat{A}$, where $\hat{L}$ is some linear operator. However, in a general complex vector space there is no antilinear operator $\hat{A}$ which is defined in a unique way. In a class of complex vector spaces generated by sets of complex-valued functions f (vector spaces of complex matrices, and $\mathbb{C}^M$ vector spaces belong also to that class), the operation of complex conjugation, $f \to f^*$, defines a unique antilinear operator. A nontrivial example of the unique antilinear operator may be found in the vector space of linear operators acting in a general unitary vector space: in this case $\hat{A}$ is a "superoperator" corresponding to calculating the Hermitian conjugate of a given linear operator, $\hat{L} \to \hat{L}^\dagger$. The Hodge operator defined in the fermionic Fock space provides another example of a nontrivial unique antilinear operator. When employed in a similarity transformation, this operator converts the fermion creation operators into the corresponding annihilation ones. The Hodge operator may thus be used to define the hole-particle conjugation operator corresponding to the so-called alternancy symmetry of alternant hydrocarbons, see the paper by Koutecký et al.[12] and references therein.

The plan of the present paper is as follows: In Section 1 we define some algebraic structures and objects which are necessary in the construction of the fermionic Fock space in Section 2. In Section 3, the Fock space is en-

dowed with a multiplicative algebraic structure, corresponding to the Grassmann algebra. With the help of the Grassmann *wedge product*, generalized definitions of the creation and annihilation operators are introduced in Section 4. The formal definition of the Hodge operator in the fermionic Fock space is given in Section 5, and some properties of this operator are discussed. Section 6 brings in an application of the Hodge operator: it is shown that the concept of the Hodge operator may be employed in constructing the electronic time-reversal operator. The paper ends with conclusions in Section 7.

1. ALGEBRAIC INGREDIENTS

The algebraic ingredients introduced in this section are devised for a transparent construction of a finite-dimensional fermionic Fock space and the corresponding Grassmann algebra. These ingredients include: (i) a biorthonormal approach, to cope with general (i.e., nonorthogonal) basis sets, (ii) a formalism explicitly covariant with respect to linear transformations of the basis sets, (iii) the Einstein summation convention (of implicitly summing over repeating upper and lower indices in algebraic expressions), (iv) an effective handling of antisymmetric objects, which are ubiquitous in the algebraic theory of many-fermion systems (some elements of the notation introduced by Stolarczyk and Monkhorst[13] are adapted for this purpose).

1.1. Biorthonormal Spin-Orbital Bases

The spin orbital corresponding to a fermion particle is a function of two variables, **r** and μ, where vector **r** represents the spatial coordinates of the particle, and μ is a discrete variable representing the spin and other internal degrees of freedom (e.g., the isospin). In the case of electrons, $\mu = -1/2, 1/2$ is the electron-spin coordinate. The spin orbitals are assumed to form a (complex) separable Hilbert space with a scalar product $\langle\psi_a|\psi_b\rangle$, which is antilinear in spin orbital ψ_a, and linear in spin orbital ψ_b. The algebraic properties of spin orbitals are discussed in more detail in subsection 6.1.

Within the algebraic approximation, one chooses a set of M linearly independent spin orbitals and defines an *ordered* basis set

$$(\phi_1, \phi_2, \ldots, \phi_M) . \qquad (2)$$

The above basis spans some complex vector space $\mathbb{V}^{(1)}$ which is a subspace, of the dimension M, of the full spin-orbital Hilbert space. With the scalar

product inherited from the parent Hilbert space, $\mathbb{V}^{(1)}$ has the algebraic structure of a *unitary* vector space. Remark (i): one may consider $\mathbb{V}^{(1)}$ to be a general unitary space, generated by basis (*2*). Thus, hereafter we shall refer to the elements of $\mathbb{V}^{(1)}$ as to vectors. Remark (ii): in applications to many-fermion systems, it is required that M is even; however, the condition $M = 2m_0$ (where m_0 is the dimension of the orbital space, see subsection 6.3) will be invoked only when necessary. Remark (iii): strictly speaking, there is no need to define any explicit order in the basis set (*2*): the set of integer indices {1, 2, ..., M} may be replaced by an *arbitrary* set of M distinguishable labels. For instance, in the case of the electronic spin orbitals one often uses labels of the form (p, σ), where $p = 1, 2, ..., m_0$ is an orbital index, and $\sigma = \alpha, \beta$ indicates the spin-function type. Thus, one may regard basis (*2*) as a mere *indexed* basis set. Only when one defines an *internal orientation* of the Fock space (see subsection 5.5), some ordering of basis (*2*) has to be assumed.

In general, the vectors of basis (*2*) are neither orthogonal nor normalized, and the corresponding overlap matrix **s** of elements

$$s_{k,l} = \langle \phi_k | \phi_l \rangle = (s_{l,k})^* \tag{3}$$

is a general Hermitian positive-definite $M \times M$ matrix (with determinant $\det \mathbf{s} > 0$). The elements of the inverse matrix, $\mathbf{s}^{-1}$, will be denoted by $s^{k,l}$ [$= (s^{l,k})^*$]. By definition, one has

$$s^{k,m} s_{m,l} = \delta^k{}_l \tag{4}$$

where $\delta^k{}_l$ ($= \delta_k{}^l = \delta_{k,l} = \delta^{k,l}$) is the Kronecker symbol. In Eq. (*4*), and throughout the paper, the Einstein summation convention is used. In a real (Euclidean) vector space, matrix **s**, often denoted by **g**, is a real symmetric matrix called the *metric matrix*.

One may now define another basis spanning the $\mathbb{V}^{(1)}$ space,

$$(\phi^1, \phi^2, \ldots, \phi^M) \tag{5}$$

which consists of vectors

$$\phi^k = \phi_m s^{m,k} \ . \tag{6}$$

One finds that the elements of the overlap matrix $\tilde{\mathbf{s}}$ corresponding to basis (*5*) read as

$$\langle \phi^k | \phi^l \rangle = s^{k,l} \tag{7}$$

and hence $\tilde{\mathbf{s}} = \mathbf{s}^{-1}$. Basis (*5*) may be transformed into basis (*2*) by applying the reverse transformation with respect to (*6*):

$$\phi_k = \phi^m s_{m,k} \ . \tag{8}$$

One finds that bases (*2*) and (*5*) fulfill the *biorthonormality* conditions:

$$\langle \phi^k | \phi_l \rangle = \delta^k{}_l \tag{9}$$

and thus will be referred to as the *biorthonormal bases*. The basis with lower indices is called a *covariant* basis, while that with upper indices – a *contravariant* one.

An arbitrary vector $\psi \in \mathbb{V}^{(1)}$ may be expressed as a linear combination of the vectors from either basis (*2*) or basis (*5*):

$$\psi = \phi_k c^k = \phi^k c_k \ . \tag{10}$$

The linear coefficients

$$c^k = \langle \phi^k | \psi \rangle, \quad c_k = \langle \phi_k | \psi \rangle \tag{11}$$

are related through formulas:

$$c^k = s^{k,m} c_m \ , \quad c_k = s_{k,m} c^m \tag{12}$$

and called the contravariant (c^k) and covariant (c_k) components of vector ψ. By using the vector representations given in Eq. (*10*), the scalar product of arbitrary vectors from $\mathbb{V}^{(1)}$ may be calculated as

$$\langle \psi_a | \psi_b \rangle = (c_a^k)^* s_{k,l} c_b^l = (c_{a,k})^* c_b^k = (c_{a,k})^* s^{k,l} c_{b,l} = (c_a^k)^* c_{b,k} \tag{13}$$

and no further reference to the scalar product in the full spin-orbital Hilbert space is necessary.

Linear operators acting in the $\mathbb{V}^{(1)}$ vector space may be conveniently represented by employing the Dirac ket-bra notation and the biorthonormal bases (*2*) and (*5*). The projection operator onto $\mathbb{V}^{(1)}$ may be written as

$$\hat{p} = \delta^k{}_l |\phi_k\rangle\langle\phi^l| = \delta_l{}^k |\phi^l\rangle\langle\phi_k| = \hat{p}^\dagger \ . \tag{14}$$

This operator plays a role of the unit operator in $\mathbb{V}^{(1)}$. For an arbitrary one-fermion operator $\hat{h}$ defined in the full spin-orbital space, one may build a projected operator,

$$\hat{h}_{(p)} = \hat{p}\hat{h}\hat{p} = h^{k}{}_{l}|\phi_k\rangle\langle\phi^l| = h_l{}^{k}|\phi^l\rangle\langle\phi_k| \tag{15}$$

which acts within $\mathbb{V}^{(1)}$. Quantities

$$h^{k}{}_{l} = \langle\phi^k|\hat{h}\phi_l\rangle, \quad h_l{}^{k} = \langle\phi_l|\hat{h}\phi^k\rangle \tag{16}$$

are related through formulas

$$h^{k}{}_{l} = s^{k,m}h_m{}^{n}s_{n,l}, \quad h_l{}^{k} = s_{l,n}h^{n}{}_{m}s^{m,k}. \tag{17}$$

For a Hermitian operator $\hat{h}$, one finds that

$$h^{k}{}_{l} = \langle\phi^k|\hat{h}\phi_l\rangle = \langle\hat{h}\phi^k|\phi_l\rangle = (h_l{}^{k})^*. \tag{18}$$

As seen in the above examples, the switching from a covariant basis to the corresponding contravariant one (and vice versa) may be accomplished by applying the "index-rising" ("index-lowering") procedure, involving the overlap-matrix elements $s^{k,l}$ ($s_{k,l}$). However, in comparison with analogous manipulations in a Euclidean vector space, more care has to be exercised in the case of a unitary vector space, because the overlap-matrix elements are now, in general, complex-valued. Quantities c^k and c_k may be treated as elements of (two different) single-column (or single-row) matrices. Similarly, quantities $h^k{}_l$, $h_k{}^l$, $h_{k,l}$ (= $h_k{}^m$, $s_{m,l}$), and $h^{k,l}$ (= $h^k{}_m$, $s^{m,l}$) may be treated as elements of (four different) $M \times M$ matrices (where indices k and l enumerate the rows and columns, respectively). Obviously, the symbols like h_l^k should be avoided, as they have no unique meaning.

When basis (*2*) is orthonormal, one has $s_{k,l} = s^{k,l} = \delta^k{}_l$, and the biorthonormal bases (*2*) and (*5*) coincide. In this case indices labeling various algebraic objects (vector components, matrix elements, etc.) may be raised or lowered at convenience, e.g., in order to suit the Einstein summation convention (ref.[13] provides an example of such a liberty in the use of lower and upper indices).

1.2. Linear Transformations of Spin-Orbital Bases

A linear transformation of the covariant basis (*2*),

$$\phi_k \rightarrow \underline{\phi}_k = \phi_m u^{m}{}_{k} \tag{19}$$

where the transformation matrix $\mathbf{u}$ is a nonsingular $M \times M$ matrix (det $\mathbf{u} \neq 0$), induces the following transformation of the contravariant basis (*5*):

$$\phi^k \rightarrow \underline{\phi}^k = (\tilde{u}^k{}_m)^* \phi^m \tag{20}$$

where $\tilde{\mathbf{u}} = \mathbf{u}^{-1}$, and hence

$$\tilde{u}^k{}_m u^m{}_l = \delta^k{}_l \ . \tag{21}$$

The biorthonormality of the new co- and contravariant bases is then preserved:

$$\langle \underline{\phi}^k | \underline{\phi}_l \rangle = \delta^k{}_l \ . \tag{22}$$

Matrices **u** corresponding to transformation (*19*) form the so-called general linear group $GL(M,\mathbb{C})$ of nonsingular complex $M \times M$ matrices.

The overlap matrix $\underline{\mathbf{s}}$ corresponding to the new covariant basis has elements

$$\underline{s}_{k,l} = \langle \underline{\phi}_k | \underline{\phi}_l \rangle = (u^m{}_k)^* s_{m,n} u^n{}_l \tag{23}$$

while the elements of matrix $\tilde{\underline{\mathbf{s}}}$ corresponding to the new contravariant basis read

$$\underline{s}^{k,l} = \langle \underline{\phi}^k | \underline{\phi}^l \rangle = \tilde{u}^k{}_m \, s^{m,n} (\tilde{u}^l{}_n)^* \ . \tag{24}$$

A new representation of vector ψ of Eq. (*10*) may now be written as

$$\psi = \underline{\phi}_k \underline{c}^k = \underline{\phi}^k \underline{c}_k \tag{25}$$

where the new linear coefficients

$$\underline{c}^k = \langle \underline{\phi}^k | \psi \rangle , \quad \underline{c}_k = \langle \underline{\phi}_k | \psi \rangle \tag{26}$$

may be obtained by transforming the old ones:

$$\underline{c}^k = \tilde{u}^k{}_m c^m \ , \quad \underline{c}_k = c_m (u^m{}_k)^* \ . \tag{27}$$

By comparing the transformation rules (*19*) and (*20*) for the basis vectors with those for the linear coefficients in Eqs (*27*), one finds some differences corresponding to the absence or appearance of the complex-conjugation symbol. Perhaps in a unitary space one should distinguish between the co- and contravariant objects of the first kind (represented by ϕ_k and c^k, respectively), and the co- and contravariant objects of the second kind (represented by c_k and ϕ^k, respectively).

The projection operator (*14*) does not change its form after being expressed in the transformed (underlined) bases. This operator is thus *invariant* with respect to the transformations of the $GL(M,\mathbb{C})$ group, and, as such, it is a unique operator in the $\mathbb{V}^{(1)}$ vector space. In the case of the projected operator (*15*), one arrives at the formula

$$\hat{h}_{(p)} = \hat{p}\hat{h}\hat{p} = \underline{h}^{k}{}_{l}|\underline{\phi}_{k}\rangle\langle\underline{\phi}^{l}| = \underline{h}_{l}{}^{k}|\underline{\phi}^{l}\rangle\langle\underline{\phi}_{k}| \tag{28}$$

where the matrix elements corresponding to the new bases,

$$\underline{h}^{k}{}_{l} = \langle\underline{\phi}^{k}|\hat{h}\underline{\phi}_{l}\rangle, \quad \underline{h}_{l}{}^{k} = \langle\underline{\phi}_{l}|\hat{h}\underline{\phi}^{k}\rangle \tag{29}$$

may be derived from those corresponding to the old bases by applying the following transformations:

$$\underline{h}^{k}{}_{l} = \tilde{u}^{k}{}_{m}h^{m}{}_{n}u^{n}{}_{l}, \quad \underline{h}_{l}{}^{k} = (\tilde{u}^{k}{}_{m})^{*}h_{n}{}^{m}(u^{n}{}_{l})^{*}. \tag{30}$$

It is seen that the representations of general vectors, given in Eqs (*10*) and (*25*), and that of general linear operators, given in Eqs (*15*) and (*28*), do not change under the concerted transformations (*19*) and (*20*) of the biorthonormal basis sets, providing that the corresponding linear parameters (c^{k}, $h^{k}{}_{l}$, etc.) are also properly transformed. It is customary to call that property, which is inherent to the biorthonormal formalism introduced in the previous subsection, the *covariance* with respect to the transformations of the $GL(M,\mathbb{C})$ group.

1.3. Index Strings and Antisymmetric Algebraic Objects

We shall consider finite ordered strings of indices, each index belonging to set {1, 2, ..., *M*}. Let us recall remark (iii) following the definition of the basis set (*2*): in general, the above set of integer indices may be replaced by an arbitrary set of *M* distinguishable labels. However, for simplicity, we shall hereafter use the integer indices. A string of *N* indices (i.e., arranged in a definite order) will be denoted by

$$X \equiv ij\cdots m \quad (n_{X} = N) \tag{31}$$

where n_X stands for the number of indices in the string *X* (the *length* of *X*, in short). The empty index string ($n_X = 0$) will be symbolized by $X = 0$.

For $n_X \geq 2$, if any two indices in the index string *X* are the same, *X* is called *degenerate*, otherwise *X* is called *nondegenerate*. Index strings corre-

sponding to $n_X = 0$ and $n_X = 1$ are considered nondegenerate. Two nondegenerate index strings X and Y of equal lengths are called *equivalent*, if one may be obtained by a *permutation* of the other. The parity of this permutation, $p(X,Y)$, calculated modulo 2, indicates two subcategories of equivalent index strings: X and Y may correspond either to $p(X,Y) = 0$ or to $p(X,Y) = 1$. The number of nondegenerate nonequivalent index strings of the length N is equal to $\binom{M}{N}$. The number of all the nondegenerate nonequivalent index strings (of the length $N = 0, 1, ..., M$) is equal to 2^M.

Any nondegenerate index string X of the length M is equivalent to the index string $12...M = \mathcal{M}$, which will be called the *maximal ordered index string*. In general (integer indices replaced by some distinguishable labels), the maximal ordered index string $\mathcal{M}$ may be chosen as some specified, but otherwise arbitrary, nondegenerate index string of the length M.

Let us consider a mapping

$$X \to c_X \tag{32}$$

where X are finite index strings (including the empty one), and c_X are elements of some (complex) vector space $\mathbb{V}$ (the case of $\mathbb{V} = \mathbb{C}$ is included). The zero vector is denoted by 0, and the vector reciprocal to c_X by $-c_X$. The following condition is assumed:

$$c_X = \begin{cases} 0, & X \text{ degenerate} \\ c_Y (-1)^{p(X,Y)}, & X, Y \text{ equivalent} \end{cases} . \tag{33}$$

Mapping (*32*) that fulfills the above condition is *antisymmetric*: any exchange of a pair of indices in string X, $X \to X'$, converts c_X into its reciprocal counterpart, $c_{X'} = -c_X$. The phrase "change of sign" should be avoided if c_X are not real numbers. In general, it will be said that mapping (*32*) defines an *antisymmetric algebraic object* of elements c_X.

As in subsection 1.1, it will be convenient to consider covariant antisymmetric objects of elements c_X, and contravariant antisymmetric objects of elements d^X. One may also extend the above construction to define antisymmetric objects with multiple index-string labels, e.g., $h^X{}_Y$; for such objects, the property of antisymmetry is associated with each index string separately. Among antisymmetric algebraic objects, a special role is played by the *antisymmetric Kronecker symbol*:

$$\delta^X{}_Y = \delta_X{}^Y = \delta_{X,Y} = \delta^{X,Y} = \begin{cases} 0, & X \text{ or } Y \text{ degenerate, or } n_X \neq n_Y \\ (-1)^{p(X,Y)}, & X, Y \text{ equivalent} \end{cases} \tag{34}$$

which will be frequently used in this paper.

Whenever it makes sense, one may define

$$S^{(N)} = c_X d^X \quad (n_X = N) \tag{35}$$

as the sum of products $c_X d^X$, extending over all nondegenerate nonequivalent strings X of the length N. Such a procedure may be called a *restricted summation* over index strings, since it includes only $\binom{M}{N}$ unique terms. The notation used in Eq. (*35*) will be referred to as the *generalized Einstein summation convention*. However, it is often advantageous to express $S^{(N)}$ by applying an *unrestricted summation* over individual indices, which gives

$$S^{(N)} = (N!)^{-1} c_{ij\cdots m} d^{ij\cdots m} \tag{36}$$

where the length of string $ij\cdots m$ is equal to N, and the usual Einstein summation convention is used. Such a summation formally includes M^N terms, the majority of which vanish (when string $ij\cdots m$ is degenerate); in addition, each nonzero term is repeated (N!) times (due to the repeating equivalent strings $ij\cdots m$, which necessitates a normalizing factor on the right-hand side of Eq. (*36*). A more general sum may be written as

$$\begin{aligned} S &= \sum_{N=0}^{M} S^{(N)} = c_X d^X = \\ &= c_0 d^0 + c_i d^i + \frac{1}{2} c_{ij} d^{ij} + \cdots + (N!)^{-1} c_{ij\cdots m} d^{ij\cdots m} + \cdots + c_{\mathcal{M}} d^{\mathcal{M}} \end{aligned} \tag{37}$$

where the restricted and unrestricted summations are employed. The former one reads simply $c_X d^X$, and involves 2^M unique terms. The last term, $c_{\mathcal{M}} d^{\mathcal{M}}$, corresponds to the maximal ordered index string $\mathcal{M}$, and may be written also as $c_{12\cdots M} d^{12\cdots M}$. The above notation may be applied to write down some useful identities involving the antisymmetrized Kronecker symbol defined in Eq. (*34*):

$$\delta^X{}_U \delta^Y{}_V \delta^{UV}{}_Z = \delta^{XY}{}_Z , \quad \delta^Z{}_{UV} \delta^U{}_X \delta^V{}_Y = \delta^Z{}_{XY} . \tag{38}$$

In each of the above formulas, the restricted summation over index strings U and V involves at most a single nonzero term.

For any nondegenerate index string $X = ij\cdots m$, one may find another nondegenerate index string $\overline{X} = kl\cdots n$, such that the composite string $X\overline{X} = ij\cdots mkl\cdots n$ is a nondegenerate index string of the length M. Strings X and $\overline{X}$ are called *complementary* to each other. However, string $\overline{X}$ is not defined uniquely, since any string equivalent to $\overline{X}$ is also complementary to

string X. In the case of an antisymmetric algebraic object corresponding to condition (*33*), one finds that

$$c_{X\bar{X}} = c_{\mathcal{M}} \delta^{\mathcal{M}}{}_{X\bar{X}} \ . \tag{39}$$

When the order of the complementary strings is reversed, the parity of the composite string may change:

$$(-1)^{p(X\bar{X},\bar{X}X)} = \delta^{X\bar{X}}{}_{\bar{X}X} = (-1)^{n_X (M-n_X)} \ . \tag{40}$$

No change of parity occurs when M is odd. However, we are concerned with the case of $M = 2m_0$, for which

$$(-1)^{p(X\bar{X},\bar{X}X)} = \delta^{X\bar{X}}{}_{\bar{X}X} = (-1)^{n_X} \ . \tag{41}$$

1.4. Antisymmetric Complexes of Matrices

Let us consider an $M \times M$ matrix $\mathbf{u}$ of (complex) elements $u^k{}_l$. For $2 \le N \le M$, we define quantities

$$u^{X}{}_{Y} \equiv u^{ij\cdots m}{}_{kl\cdots n} = u^{i}{}_{k'} u^{j}{}_{l'} \cdots u^{m}{}_{n'} \delta^{k'l'\cdots n'}{}_{kl\cdots n} = \delta^{ij\cdots m}{}_{i'j'\cdots m'} u^{i'}{}_{k} u^{j'}{}_{l} \cdots u^{m'}{}_{n} \tag{42}$$
$$(n_X = n_Y = N)$$

where unrestricted summations over individual indices are performed. Unlike in Eq. (*36*), no normalizing factor is required in this case. It can be shown that: (i) the two equalities in definition (*42*) are indeed equivalent, (ii) quantity $u^X{}_Y$ is antisymmetric with respect to permutations of the indices in string X or Y, (iii) for given two nondegenerate index strings X and Y, quantity $u^X{}_Y$ is equal to the *minor* of matrix $\mathbf{u}$, corresponding to the removal of all the columns and rows besides those corresponding to the index strings X and Y, respectively. For X and Y running (separately) through all the nondegenerate nonequivalent index strings of the length N, quantities $u^X{}_Y$ may be considered to be the elements of the *N-th antisymmetrized Kronecker power* of matrix $\mathbf{u}$. This matrix, denoted by $\mathbf{u}^{(N)}$, is thus a $\binom{M}{N} \times \binom{M}{N}$ matrix. The above definition may be extended to include $\mathbf{u}^{(1)} \equiv \mathbf{u}$, and a 1×1 matrix $\mathbf{u}^{(0)}$, of the element

$$u^0{}_0 = 1 \ . \tag{43}$$

For $N = M$, the construction defined in Eq. (*42*) gives

$$u^{X}{}_{Y} = \det \mathbf{u}\, \delta^{X}{}_{Y} \quad (n_X = n_Y = M)\,. \tag{44}$$

Thus, matrix $\mathbf{u}^{(M)}$ is a 1 × 1 matrix, equal to the matrix determinant det **u**.

By using definitions (*42*) and (*43*), and the identities given in Eq. (*38*), one may prove the following relations among the elements of matrices $\mathbf{u}^{(N)}$:

$$u^{X}{}_{U} u^{Y}{}_{V} \delta^{UV}{}_{Z} = u^{XY}{}_{Z}\,, \quad \delta^{Z}{}_{UV} u^{U}{}_{X} u^{V}{}_{Y} = u^{Z}{}_{XY} \tag{45}$$

where nonzero contributions may be obtained only when $n_U = n_X$ and $n_V = n_Y$. The above formulas may be employed in a recursive calculation of matrices $\mathbf{u}^{(N)}$. By combining Eqs (*44*) and (*45*), one may arrive at a generalized form of the Lagrange expansion of the matrix determinant.

For $\mathbf{u} = \mathbf{1}$ (the $M \times M$ unit matrix), definition (*42*) gives $u^{X}{}_{Y} = \delta^{X}{}_{Y}$. Thus, $\mathbf{1}^{(N)}$ is the $\binom{M}{N} \times \binom{M}{N}$ unit matrix. When matrix **u** is nonsingular, as in the case of the transformation matrix in subsection 1.2., one may calculate the inverse $\tilde{\mathbf{u}} = \mathbf{u}^{-1}$ and the corresponding antisymmetric Kronecker powers $\tilde{\mathbf{u}}^{(N)}$ for $N = 0, 1, 2, \ldots, M$. One finds that

$$\tilde{u}^{X}{}_{Z} u^{Z}{}_{Y} = \delta^{X}{}_{Y} \tag{46}$$

which is an analogue of Eq. (*21*).

For the overlap matrix **s** of the elements given in Eq. (*3*), one may use Eq. (*42*) to define the corresponding *N*-th antisymmetrized Kronecker power represented by matrix $\mathbf{s}^{(N)}$ of the elements $s_{X,Y}$. Similarly, for matrix $\tilde{\mathbf{s}} = \mathbf{s}^{-1}$, of the elements given in Eq. (*7*), one obtains matrix $\tilde{\mathbf{s}}^{(N)}$, of the elements $s^{X,Y}$. As before, we define $\mathbf{s}^{(1)} \equiv \mathbf{s}$, $\tilde{\mathbf{s}}^{(1)} \equiv \tilde{\mathbf{s}}$, and 1 × 1 matrices $\mathbf{s}^{(0)}$ and $\tilde{\mathbf{s}}^{(0)}$, of the elements

$$s_{0,0} = s^{0,0} = 1\,. \tag{47}$$

For $N = M$, an analogue of Eq. (*44*) reads

$$s_{X,Y} = \det \mathbf{s}\, \delta_{X,Y} \quad (n_X = n_Y = M)\,. \tag{48}$$

Matrices $\mathbf{s}^{(N)}$ and $\tilde{\mathbf{s}}^{(N)}$ are Hermitian. One finds also that $\tilde{\mathbf{s}}^{(N)} = (\mathbf{s}^{(N)})^{-1}$, which leads to an analogue of Eq. (*4*):

$$s^{X,Z} s_{Z,Y} = \delta^{X}{}_{Y}\,. \tag{49}$$

Let $\mathbf{u}^{(N)}$, $N = 0, 1, 2, \ldots, M$, be the antisymmetric Kronecker powers corresponding to a given matrix **u**. By requiring that $u^{X}{}_{Y} = 0$ for $n_X \neq n_Y$ and $n_X =$

$n_Y > M$, one makes quantity $u^X{}_Y$ defined for arbitrary index strings X and Y. This step completes the construction of $u^X{}_Y$ as an antisymmetric object (according to the definition given in the previous subsection). Such an object will be referred to as the *antisymmetric complex of matrix* **u**, and denoted by $\mathcal{A}(\mathbf{u})$. The antisymmetric complexes corresponding to the overlap matrices, $\mathcal{A}(\mathbf{s})$ and $\mathcal{A}(\tilde{\mathbf{s}})$, are defined exactly in the same way. By restricting X to the set of all the nondegenerate nonequivalent index strings of the length $\leq M$, and applying the same restriction to Y, one may regard $\mathcal{A}(\mathbf{u})$ as a $2^M \times 2^M$ matrix, which is block-diagonal, with diagonal blocks equal to the $\mathbf{u}^{(N)}$ matrices. The total number of elements corresponding to these diagonal blocks amounts to $\binom{2M}{M}$. Let us note that matrix $\mathcal{A}(\mathbf{u})$ inherits algebraic properties of its diagonal blocks, e.g., $\mathcal{A}(\mathbf{u}^{-1}) = \mathcal{A}^{-1}(\mathbf{u})$, etc. The antisymmetric complex $\mathcal{A}(\mathbf{1})$, of elements $\delta^X{}_Y$, may be treated as the $2^M \times 2^M$ unit matrix.

1.5. Antisymmetric Tensors

For $2 \leq N \leq M$, vectors of the basis set (*2*) may be used to define the following *N-th-rank antisymmetric tensors*:

$$\phi_X \equiv \phi_{ij\cdots m} = (N!)^{-1/2}\, \phi_k \otimes \phi_l \otimes \cdots \otimes \phi_n\, \delta^{kl\cdots n}{}_{ij\cdots m} \quad (n_X = N)\,. \tag{50}$$

Tensor ϕ_X behaves as an antisymmetric quantity with respect to permutations of the indices in string X. Tensors (*50*) are linearly independent for X belonging to the set of all nondegenerate nonequivalent index sets of the length N. The basis set $\{\phi_X\ (n_X = N)\}$ spans a complex vector space $\mathbb{V}^{(N)}$ of the dimension $\binom{M}{N}$, called the *N-th antisymmetric power* of the vector space $\mathbb{V}^{(1)}$. The N-th-rank antisymmetric tensors from $\mathbb{V}^{(N)}$ will be hereafter called the *N-vectors*. The scalar product in $\mathbb{V}^{(1)}$ induces the scalar product in $\mathbb{V}^{(N)}$, and it can be shown that

$$\langle \phi_X \,|\, \phi_Y \rangle = s_{X,Y} \tag{51}$$

where $s_{X,Y}$ is an element of matrix $\mathbf{s}^{(N)}$, the N-th antisymmetric Kronecker power of the overlap matrix **s**, see the previous subsection. In definition (*50*), constant $(N!)^{-1/2}$ is a prenormalizing factor: when basis (*2*) of the vector space $\mathbb{V}^{(1)}$ is orthonormal, the corresponding basis of the N-vectors defined in Eq. (*50*) becomes orthonormal as well. In general, basis $\{\phi_X\ (n_X = N)\}$ will be referred to as a covariant basis in $\mathbb{V}^{(N)}$; the definition of the N-vectors making the corresponding contravariant basis $\{\phi^X\ (n_X = N)\}$ is analogous to definition (*50*), with the vectors of basis (*5*) replacing those of

basis (*2*). Equivalently, one may obtain the contravariant basis by applying an "index-rising" procedure analogous to that of Eq. (*6*):

$$\phi^X = \phi_Z s^{Z,X} \quad (n_X = N) \tag{52}$$

where $s^{Z,X}$ are the elements of matrix $\tilde{\mathbf{s}}^{(N)}$, see Eq. (*49*). One finds that

$$\langle \phi^X | \phi_Y \rangle = \delta^X{}_Y \tag{53}$$

and thus bases $\{\phi_X \ (n_X = N)\}$ and $\{\phi^X \ (n_X = N)\}$ are biorthonormal.

Let us complete the family of $\mathbb{V}^{(N)}$ vector spaces ($2 \leq N \leq M$) by incorporating the $\mathbb{V}^{(1)}$ vector space, and adding a one-dimensional complex vector space corresponding to $N = 0$:

$$\mathbb{V}^{(0)} = \mathbb{C} \tag{54}$$

with the scalar product $\langle \psi_a^{(0)} | \psi_b^{(0)} \rangle = (\psi_a^{(0)})^* \psi_b^{(0)}$, where $\psi_a^{(0)}, \psi_b^{(0)} \in \mathbb{C}$. A natural choice for the 0-vector spanning the vector space $\mathbb{V}^{(0)}$ is

$$\phi_0 = \phi^0 = 1 \tag{55}$$

which is consistent with the definition of the overlap matrices $\mathbf{s}^{(0)}$ and $\tilde{\mathbf{s}}^{(0)}$ in Eq. (*47*). The 0-vectors corresponding to $\mathbb{V}^{(0)}$ are often referred to as *scalars*.

The algebraic considerations in subsection (1.1.), pertaining to the $\mathbb{V}^{(1)}$ vector space, may be extended to the whole family of the $\mathbb{V}^{(N)}$ vector spaces ($N = 0, 1, 2, \ldots, M$). Moreover, the $GL(M,\mathbb{C})$ transformations of the biorthonormal bases in the $\mathbb{V}^{(1)}$ space, see subsection (1.2.), induce analogous linear transformations of the corresponding biorthonormal bases in the $\mathbb{V}^{(N)}$ spaces, with the matrix elements $u^X{}_Y$ and $\tilde{u}^X{}_Y$, defined in subsection (1.4.), replacing the matrix elements $u^k{}_l$ and $\tilde{u}^k{}_l$:

$$\phi_X \rightarrow \underline{\phi}_X = \phi_Z u^Z{}_X \tag{56}$$

$$\phi^X \rightarrow \underline{\phi}^X = (\tilde{u}^X{}_Z)^* \phi^Z \ . \tag{57}$$

It can be shown that for $\mathbf{u} \in GL(M,\mathbb{C})$, the corresponding matrices $\mathbf{u}^{(N)}$ belong to certain irreducible representations of $GL(M,\mathbb{C})$, see the book by Hamermesh[14], Chap. 10.3. Thus, the $\mathbb{V}^{(N)}$ vector spaces are the carrier spaces for these irreducible representations.

Let us interpret vectors ϕ_k of basis (*2*) as electronic spin orbitals. Then one may treat the *N*-vectors defined in Eq. (*50*) as certain *N*-electron wave functions:

$$\phi_{ij\cdots m}(1, 2, \ldots, N) = (N!)^{-1/2}\, \phi_k(1)\, \phi_l(2) \cdots \phi_n(N)\, \delta^{kl\cdots n}{}_{ij\cdots m} \tag{58}$$

where $\phi_k(1) \equiv \phi_k(\mathbf{r}_1,\mu_1)$, etc., and pair $(\mathbf{r},\mu)$ represents the spatial and spin coordinates of electron. The wave function defined in Eq. (*58*) is antisymmetric with respect to permutations of the electronic coordinates (i.e., it fulfills the Pauli exclusion principle), and is identical with the Slater determinantal function for *N* electrons. One may thus refer to *N*-vectors (*50*) as to Slater determinants. In general, for $N = 0, 1, 2, \ldots, M$, one may built *N*-electron wave functions in the form of linear combinations,

$$\psi^{(N)} = \phi_X c^X = \phi^X c_X \quad (n_X = N) \tag{59}$$

in analogy to Eq. (*10*).

2. FERMIONIC FOCK SPACE

A system of *N* identical fermions, $0 \le N \le M$, obeying the Pauli exclusion principle and the laws of quantum mechanics, may be described within the algebraic approximation by employing the $\mathbb{V}^{(N)}$ vector spaces introduced in subsection 1.5. A better insight into the theory of many-fermion systems is provided by combining these vector spaces into their *direct sum*; the emerging algebraic structure is known as the (fermionic) Fock space:

$$\mathbb{F} = \mathbb{V}^{(0)} \oplus \mathbb{V}^{(1)} \oplus \mathbb{V}^{(2)} \oplus \cdots \oplus \mathbb{V}^{(M)}\,. \tag{60}$$

In fact, the fermionic Fock space is generated by the $\mathbb{V}^{(1)}$ vector space. When the the dimension of latter is *M*, the dimension of $\mathbb{F}$ is equal to 2^M. A general Fock-space vector may be written as an ordered set of $M + 1$ components

$$\Psi = (\psi^{(0)}, \psi^{(1)}, \psi^{(2)}, \ldots, \psi^{(M)}) \tag{61}$$

where $\psi^{(N)} \in \mathbb{V}^{(N)}$, for $N = 0, 1, 2, \ldots, M$. Each *N*-vector $\psi^{(N)}$ may be expressed as in Eq. (*59*). The scalar product in $\mathbb{F}$ is defined as

$$\langle \Psi_a | \Psi_b \rangle = \sum_{N=0}^{M} \langle \psi_a^{(N)} | \psi_b^{(N)} \rangle \tag{62}$$

where $\langle \psi_a^{(N)} | \psi_b^{(N)} \rangle$ is the scalar product in $\mathbb{V}^{(N)}$. We now define a covariant *Fock basis* which is related to the covariant basis sets introduced in the $\mathbb{V}^{(N)}$ vector spaces. The elements of the covariant Fock basis read

$$\begin{aligned}
\Phi_0 &= (\phi_0, 0, 0, \ldots, 0) \\
\Phi_k &= (0, \phi_k, 0, \ldots, 0) \quad (k = 1, 2, \ldots, M) \\
\Phi_{kl} &= (0, 0, \phi_{kl}, \ldots, 0) \quad (l > k = 1, 2, \ldots, M - 1) \\
\ldots &\qquad \ldots \\
\Phi_{\mathcal{M}} &= (0, 0, 0, \ldots, \phi_{\mathcal{M}})
\end{aligned} \tag{63}$$

where $\mathcal{M}$ = 12···M (in the case of integer indices). By applying definition (*62*), one finds that

$$\langle \Phi_X | \Phi_Y \rangle = s_{X,Y} \tag{64}$$

where $s_{X,Y}$ are the elements of the anisymmetric complex $\mathcal{A}(\mathbf{s})$ corresponding to the overlap matrix **s**. Thus, $\mathcal{A}(\mathbf{s})$ may be considered as the overlap matrix corresponding to the covariant Fock basis (*63*). The vectors of the corresponding contravariant Fock basis may be obtained as

$$\Phi^X = \Phi_Z s^{Z,X} \tag{65}$$

where $s^{X,Y}$ are the elements of the antisymmetric complex $\mathrm{A}(\tilde{\mathbf{s}})$ of the overlap matrix $\tilde{\mathbf{s}} = \mathbf{s}^{-1}$, see Eq. (*49*). Thus, one finds that

$$\langle \Phi^X | \Phi_Y \rangle = \delta^X{}_Y \tag{66}$$

which indicates that Fock bases $\{\Phi_X\}$ and $\{\Phi^X\}$ are biorthonormal. Because of definition (*55*), both Fock bases have at least one common element:

$$\Phi_0 = \Phi^0 = (1, 0, 0, \ldots, 0) . \tag{67}$$

When the Fock space $\mathbb{F}$ corresponds to an electronic system, Φ_0 is called the *electronic vacuum state*. A general vector in $\mathbb{F}$, see Eq. (*61*), may be written as

$$\Psi = \Phi_X C^X = \Phi^X C_X \tag{68}$$

where

$$C^X = \langle \Phi^X | \Psi \rangle , \quad C_X = \langle \Phi_X | \Psi \rangle . \tag{69}$$

The unit operator in the Fock space $\mathbb{F}$ may be written as

$$\hat{1} = \delta^{X}{}_{Y} |\Phi_X\rangle\langle\Phi^Y| . \tag{70}$$

The $GL(M,\mathbb{C})$ transformations corresponding to Eqs (*19*) and (*20*) induce transformations (*56*) and (*57*) of the corresponding bases in the $\mathbb{V}^{(N)}$ vector spaces, and lead to the following transformations of the co- and contravariant Fock bases,

$$\underline{\Phi}_X = \Phi_Z u^Z{}_X , \quad \underline{\Phi}^X = (\tilde{u}^X{}_Z)^* \Phi^Z \tag{71}$$

and the linear coefficients corresponding to Eq. (*68*),

$$\underline{C}^X = \tilde{u}^X{}_Z C^Z , \quad \underline{C}_X = C_Z (u^Z{}_X)^* . \tag{72}$$

In the above equations, $u^Z{}_X$ and $\tilde{u}^X{}_Z$ should be interpreted as the elements of the antisymmetric complexes $\mathcal{A}(\mathbf{u})$ and $\mathcal{A}(\tilde{\mathbf{u}})$ corresponding to matrices $\mathbf{u}$ and $\tilde{\mathbf{u}} = \mathbf{u}^{-1}$.

Let us introduce the following decomposition of a general Fock-space vector (*61*):

$$\Psi = \sum_{N=0}^{M} \Psi^{(N)} \tag{73}$$

where

$$\Psi^{(N)} = (0, \ldots, \psi^{(N)}, \ldots, 0) . \tag{74}$$

Vectors $\Psi^{(N)}$ span a certain subspace $\mathbb{F}^{(N)}$ of the Fock space $\mathbb{F}$. For $N = 0, 1, 2, \ldots, M$, there is a canonical isomorphism of vector spaces

$$\mathbb{V}^{(N)} \leftrightarrow \mathbb{F}^{(N)} \tag{75}$$

based on a one-to-one correspondence between the N-vectors $\psi^{(N)}$ and the Fock-space vectors $\Psi^{(N)}$. One may introduce the following resolution of the Fock space into a direct sum of its subspaces

$$\mathbb{F} = \mathbb{F}^{(\mathrm{even})} \oplus \mathbb{F}^{(\mathrm{odd})} \tag{76}$$

where (for $M = 2m_0$)

$$\begin{aligned} \mathbb{F}^{(\mathrm{even})} &= \mathbb{F}^{(0)} \oplus \mathbb{F}^{(2)} \oplus \mathbb{F}^{(4)} \oplus \cdots \oplus \mathbb{F}^{(M)} \\ \mathbb{F}^{(\mathrm{odd})} &= \mathbb{F}^{(1)} \oplus \mathbb{F}^{(3)} \oplus \mathbb{F}^{(5)} \oplus \cdots \oplus \mathbb{F}^{(M-1)} . \end{aligned} \tag{77}$$

Let us note a fundamental difference between Eq. (*60*), which corresponds to a *construction* of the Fock space from certain vectors spaces, and Eqs (*76*) and (*77*), which correspond to a *deconstruction* of the Fock space into its subspaces.

3. THE GRASSMANN ALGEBRA OF FOCK SPACE

In this section we define a multiplicative algebraic structure in the fermionic Fock space $\mathbb{F}$, associated with the so-called *wedge product*, which promotes this vector space to the rank of an algebra. The wedge product in $\mathbb{F}$ is assumed to be a binary product, distributive with respect to the addition of vectors, and commutative with respect to the multiplication of vectors by complex numbers. The wedge product will be introduced in two steps: In the first one, the so-called *exterior algebra* is defined, in which the wedge product acts within the family of the $\mathbb{V}^{(N)}$ vector spaces, $N = 0, 1, 2, ..., M$. In the second step the exterior-algebra structure becomes transferred into the $\mathbb{F}$ vector space, giving rise to the Grassmann algebra of the Fock space.

3.1. Exterior Algebra

Below we introduce a multiplicative structure within the family of the $\mathbb{V}^{(N)}$ vector spaces, $N = 0, 1, 2, ..., M$. In general, the wedge product of an N-vector and an N'-vector is a certain $(N + N')$-vector, which justifies the name of the exterior algebra for the emerging algebraic structure. In order to define the wedge product, it is sufficient to consider all pairs of N-vectors belonging to the bases spanning the $\mathbb{V}^{(N)}$ vector spaces (below we shall use the covariant bases). The definition of the wedge product employed in the present paper reads

$$\phi_X \wedge \phi_Y = \phi_{XY} \tag{78}$$

where $\phi_X \in \mathbb{V}^{(n_X)}$, $\phi_Y \in \mathbb{V}^{(n_Y)}$, and $\phi_{XY} \in \mathbb{V}^{(n_X + n_Y)}$; it is assumed that $\phi_{XY} = 0$ if any of X, Y, or XY is a degenerate index string. For general N-vectors, written as linear combinations of the basis vectors, see Eq. (*59*), one obtains by definition

$$\psi_a^{(N_a)} \wedge \psi_b^{(N_b)} = (\Phi_X \wedge \Phi_Y)\, C_a^X C_b^Y \quad (n_X = N_a, \quad n_Y = N_b)\,. \tag{79}$$

It should be noted that the definition of the wedge product in Eq. (*78*) takes into account the prenormalizing factor in Eq. (*50*): thus, ϕ_X, ϕ_Y, and ϕ_{XY} become normalized when the corresponding basis (*2*) in $\mathbb{V}^{(1)}$ is orthonormal.

The following properties of the wedge product may be derived from definition (*78*):

$$\phi_0 \wedge \phi_X = \phi_X \wedge \phi_0 = \phi_X \tag{80}$$

$$\phi_X \wedge \phi_Y = \phi_{XY} = (-1)^{n_X n_Y} \phi_Y \wedge \phi_X \tag{81}$$

$$\begin{aligned}(\phi_X \wedge \phi_Y) \wedge \phi_Z &= \phi_{XY} \wedge \phi_Z = \phi_{XYZ} = \\ &= \phi_X \wedge \phi_{YZ} = \phi_X \wedge (\phi_Y \wedge \phi_Z)\,.\end{aligned} \tag{82}$$

Equation (*80*) shows that ϕ_0 plays a role of the unit of the exterior algebra, which is consistent with definition (*55*). Equation (*81*) indicates that, in general, the wedge product is noncommutative; in particular,

$$\phi_k \wedge \phi_l = -\phi_l \wedge \phi_k\,. \tag{83}$$

As follows from Eq. (*82*), the wedge product is *associative*. The basis set (*2*) may be used to generate all the *N*-vectors ($N \geq 2$) since any antisymmetric tensor (*50*) may be written as:

$$\phi_{kl\cdots n} = \phi_k \wedge \phi_l \wedge \cdots \wedge \phi_n\,. \tag{84}$$

The definition of the wedge product given in Eq. (*78*) may be transformed into an analogous definition involving the contravariant basis set $\{\phi^X\}$. In either form, the definition of the wedge product is invariant with respect to the $GL(M,\mathbb{C})$ transformations (*56*) and (*57*) of the co- and contravariant bases in the $\mathbb{V}^{(N)}$ vector spaces. For example, for the transformed covariant basis one may prove that

$$\underline{\phi}_X \wedge \underline{\phi}_Y = \underline{\phi}_{XY}\,. \tag{85}$$

The proof makes use of Eqs (*56*), (*78*), and the second identity given in Eq. (*45*).

3.2. Grassmann Algebra

The algebraic structure of the exterior algebra may be, in a natural way, transferred into the Fock space $\mathbb{F}$. The counterpart of definition (*78*), involving the elements of the covariant Fock basis (*63*), now reads

$$\Phi_X \wedge \Phi_Y = \Phi_{XY} \ . \tag{86}$$

For general Fock-space vectors written as in Eq. (*68*), one may use an analogue of Eq. (*79*) and derive the following formula:

$$\Psi_a \wedge \Psi_b = \Psi_{ab} = \Phi_Z C_{ab}^Z \tag{87}$$

where

$$C_{ab}^Z = d^{Z}{}_{XY} C_a^X C_b^Y \ . \tag{88}$$

The wedge product endows the Fock space $\mathbb{F}$ with the structure called the Grassmann algebra.

The definition of the wedge product given above is invariant with respect to the $GL(M,\mathbb{C})$ transformations introduced in subsection 1.2. Analogs of Eqs (*80*), (*81*), (*82*) may be derived, showing that the Grassmann algebra of the Fock space is associative, noncommutative, and the vacuum vector $\Phi_0 = \Phi^0$ plays a role of the unit of this algebra. The vectors of the covariant Fock basis (*63*) may be written by using the wedge product,

$$\Phi_{kl\cdots n} = \Phi_k \wedge \Phi_l \wedge \cdots \wedge \Phi_n \tag{89}$$

cf. Eq. (*84*). The same holds, of course, for the vectors of the contravariant Fock basis $\{\Phi^X\}$.

In the literature, "exterior algebra" and "Grassmann algebra" are often considered as synonyms. However, the wedge product defined in the Fock space $\mathbb{F}$, although related to that corresponding to the family of the $\mathbb{V}^{(N)}$ vector spaces, has nothing "exterior" in its definition. Thus, we propose to make a distinction between the two algebras.

4. CREATION AND ANNIHILATION OPERATORS

The wedge product is helpful in defining two related families of linear operators acting in the Fock space $\mathbb{F}$: the (generalized) creation and annihilation operators. The creation operator corresponding to a Fock-space vector Φ is defined as:

$$\hat{c}[\Phi]\Psi = \Phi \wedge \Psi \,. \tag{90}$$

The annihilation operator corresponding to $\hat{c}[\Phi]$ is defined as the Hermitian conjugate:

$$\hat{a}[\Phi] = \hat{c}^{\dagger}[\Phi] \,. \tag{91}$$

The following properties may be derived from the above definitions:

$$\hat{c}[\Phi_a C_a + \Phi_b C_b] = C_a \hat{c}[\Phi_a] + C_b \hat{c}[\Phi_b] \tag{92}$$

(mapping $\Phi \rightarrow \hat{c}[\Phi]$ is thus linear);

$$\hat{a}[\Phi_a C_a + \Phi_b C_b] = C_a^* \hat{a}[\Phi_a] + C_b^* \hat{a}[\Phi_b] \tag{93}$$

(mapping $\Phi \rightarrow \hat{a}[\Phi]$ is thus antilinear);

$$\hat{c}[\Phi_a \wedge \Phi_b] = \hat{c}[\Phi_a]\, \hat{c}[\Phi_b] \tag{94}$$

$$\hat{a}[\Phi_a \wedge \Phi_b] = \hat{a}[\Phi_b]\, \hat{a}[\Phi_a] \,. \tag{95}$$

Below we shall discuss some properties of the creation operators corresponding to the covariant Fock basis, and the annihilation operators corresponding to the contravariant Fock basis. An abbreviated notation will be used:

$$\hat{c}[\Phi_X] \equiv \hat{c}_X \,, \quad \hat{a}[\Phi^X] \equiv \hat{a}^X = (\hat{c}^X)^{\dagger} \,. \tag{96}$$

In the case of the empty string $X = 0$, one finds that

$$\hat{c}_0 = \hat{a}^0 = \hat{1} \tag{97}$$

where $\hat{1}$ is the unit operator in $\mathbb{F}$, see Eq. (*70*). The action of the creation operators $\hat{c}_X$ on the vectors of the covariant Fock basis can be directly derived from definition (*90*):

$$\hat{c}_X \Phi_Y = \Phi_{XY} \,. \tag{98}$$

The case of the annihilation operators $\hat{a}^X$ requires some intermediate steps involving an insertion of the unit operator (*70*):

$$\begin{aligned}\hat{a}^X\Phi_Y &= \delta^Z{}_W\,|\Phi_Z\rangle\langle\Phi^W|\hat{a}^X\Phi_Y = \delta^Z{}_W\Phi_Z\langle\hat{c}^X\Phi^W|\Phi_Y\rangle = \\ &= \delta^Z{}_W\Phi_Z\langle\Phi^{XW}|\Phi_Y\rangle = \Phi_Z\delta^{XZ}{}_Y\ .\end{aligned} \tag{99}$$

The creation (annihilation) operators that correspond to elements of the $\mathbb{F}^{(1)}$ subspace of the Fock space (i.e., are related to spin orbitals belonging to $\mathbb{V}^{(1)}$) are called the *fermion creation operators* (*fermion annihilation operators*). In particular, the fermion operators

$$\hat{c}[\Phi_k] \equiv \hat{c}_k\ , \quad \hat{a}[\Phi^k] \equiv \hat{a}^k = (\hat{c}^k)^\dagger \tag{100}$$

may serve to generate the algebra of linear operators acting in the Fock space. The operators of Eq. (*96*), where $X \neq 0$, can be expressed in terms of products of the fermion operators:

$$\hat{c}_X = \hat{c}_{ij\cdots m} = \hat{c}_i\hat{c}_j\cdots\hat{c}_m\ , \quad \hat{a}^X = \hat{a}^{ij\cdots m} = \hat{a}^m\cdots\hat{a}^j\hat{a}^i \tag{101}$$

see Eqs (*89*), (*94*), and (*95*). The fermion operators (*100*) fulfill the following anticommutation relations:

$$\hat{c}_k\hat{c}_l + \hat{c}_l\hat{c}_k = \hat{0}\,, \quad \hat{a}^l\hat{a}^k + \hat{a}^k\hat{a}^l = \hat{0} \tag{102}$$

$$\hat{a}^k\hat{c}_l + \hat{c}_l\hat{a}^k = \delta^k{}_l\hat{1}\,. \tag{103}$$

Equations (*102*) are direct consequences of Eqs (*96*). A proof of Eq. (*103*) is given in the Appendix at the end of this paper. The above equations, together with the vacuum-annihilation condition

$$\hat{a}^k\Phi_0 = 0 \tag{104}$$

(which is a particular case of Eq. (*99*)), constitute a set of basic algebraic conditions characterizing the second-quantization formalism for fermions in a nonorthogonal spin-orbital basis. Moshinsky and Seligman[15] were the first to employ the biorthonormal spin-orbital bases to write the fermion-operator anticommutation relations in the form given in Eqs (*102*), (*103*). For a modern application of this formalism in many-electron theory, see the paper by Head-Gordon et al.[16]

A product of the fermion operators, in which all the annihilation operators precede the creation ones, is called the *normal product* (of fermion operators). By using operators (*101*) as building blocks, see also definitions (*96*) and (*97*), one writes the normal products as

$$\hat{c}_X \hat{a}^Y \ . \qquad (105)$$

For X and Y running (separately) through all the nondegenerate nonequivalent index strings of the length $N = 0, 1, ..., M$, one finds that there are exactly 2^{2M} different normal products of the form (*105*), which make a set of linearly independent operators. This set may be chosen as a basis set in the vector space of the linear operators acting in the Fock space $\mathbb{F}$; another basis set may be generated by the normal products of the form $\hat{c}^X \hat{a}_Y$. A general linear operator in $\mathbb{F}$ may be written as a linear combination of the normal products of fermion operators:

$$\hat{H} = h^X{}_Y \hat{c}_X \hat{a}^Y = h_Y{}^X \hat{c}^Y \hat{a}_X \ . \qquad (106)$$

Such a representation of a linear operator is called the second-quantized representation. In Eq. (*106*), the linear coefficients $h^X{}_Y$ and $h_Y{}^X$ are often referred to as the amplitudes of operator $\hat{H}$. When operator (*106*) is Hermitian, one has $h^X{}_Y = (h_Y{}^X)^*$, see Eq. (*18*).

An important linear operator in the Fock space is the particle-number operator:

$$\hat{N} = \delta^k{}_l \hat{c}_k \hat{a}^l \ . \qquad (107)$$

This operator is invariant with respect to the $GL(M,\mathbb{C})$ transformations of subsection 1.2.; thus, it is a nontrivial unique operator in $\mathbb{F}$. Each $\mathbb{F}^{(N)}$ subspace, see Eqs (*76*) and (*77*), is the invariant subspace of operator $\hat{N}$, corresponding to the eigenvalue N (equal to the number of the fermion particles). With the help of operator $\hat{N}$ one may also define the parity-number operator:

$$(-1)^{\hat{N}} = \exp(\mathrm{i}\pi\hat{N}) = \exp(-\mathrm{i}\pi\hat{N}) \qquad (108)$$

where i is the imaginary unit. The invariant subspaces of this operator are $\mathbb{F}^{(\mathrm{even})}$ and $\mathbb{F}^{(\mathrm{odd})}$, corresponding to the eigenvalues 1 and –1, respectively.

Let us note that for $\Phi^{(N)} \in \mathbb{F}^{(N)}$ and $\Psi^{(N')} \in \mathbb{F}^{(N')}$, one finds that $\hat{c}[\Phi^{(N)}]\Psi^{(N')} \in \mathbb{F}^{(N+N')}$ and $\hat{a}[\Phi^{(N)}]\Psi^{(N')} \in \mathbb{F}^{(N'-N)}$. Thus, by employing isomorphism (*75*), one may introduce the creation and annihilation operators that act among the $\mathbb{V}^{(N)}$ vector spaces:

$$\hat{c}[\phi^{(N)}]\psi^{(N')} \in \mathbb{V}^{(N+N')}, \quad \hat{a}[\phi^{(N)}]\psi^{(N')} \in \mathbb{V}^{(N'-N)} \qquad (109)$$

where $\phi^{(N)} \in \mathbb{V}^{(N)}$ and $\psi^{(N')} \in \mathbb{V}^{(N')}$. Alternatively, these creation and annihilation operators may be defined by using the analogy between the exterior algebra and the Grassmann algebra, see the previous section,

5. THE HODGE OPERATOR

5.1. The Orientation of Fock Space

In this subsection we focus on $\mathbb{F}^{(M)}$, which is a one-dimensional subspace of the Fock space $\mathbb{F}$. The projector on that subspace may be written in several equivalent forms:

$$\hat{P}^{(M)} = |\Phi_Z\rangle\langle\Phi^Z| = |\Phi^Z\rangle\langle\Phi_Z| = (\det \mathbf{s})^{-1}\ |\Phi_Z\rangle\langle\Phi_Z| = \det \mathbf{s}\ |\Phi^Z\rangle\langle\Phi^Z| \qquad (110)$$

where Z is an arbitrary nondegenerate index string of the length M. We introduce the following equivalence relation among the M-vectors in $\mathbb{F}^{(M)}$:

$$\Psi^{(M)} \sim \Psi'^{(M)} \quad \text{if} \quad \Psi^{(M)} = \lambda\, \Psi'^{(M)}, \quad \lambda \in \mathbb{R}, \quad \text{and} \quad \lambda > 0\,. \qquad (111)$$

Each equivalence class is called an *orientation* of the Fock space $\mathbb{F}$. A given nonzero orientation may be represented by a unique normalized vector

$$\Omega = (0, 0, 0, \ldots, 0, \omega) \qquad (112)$$

$$\langle\Omega|\,\Omega\rangle = \langle\omega|\omega\rangle = 1\,. \qquad (113)$$

Any two orientations Ω_a and Ω_b are related by a phase factor

$$\Omega_b = \Omega_a \exp(\mathrm{i}\varphi_{ab}) \qquad (114)$$

where $\varphi_{ab} \in [0,2\pi)$. If $\Omega_a = -\Omega_b$, the corresponding orientations will be called *opposite* with respect to each other. Let us note that in an Euclidean (real) Fock space there are only two different nonzero orientations, which are opposite with respect to each other.

5.2. The Definition of the Hodge Operator

Let Ω be some fixed nonzero orientation of the Fock space $\mathbb{F}$. The following operation

$$\mathbb{F} \ni \Psi \to *\Psi \in \mathbb{F} \qquad (115)$$

where

$$*\Psi = \hat{a}[\Psi]\Omega \tag{116}$$

will be called the Hodge operator in Fock space. The above definition makes some properties of the Hodge operator evident: operator $*$ is antilinear (see Eq. (*93*)), explicitly depends on Ω, and its definition does not involve any basis-set dependence. Thus, the Hodge operator is an unique antilinear operator in the Fock space, although its dependence on the orientation Ω introduces a freedom in the choice of the phase factor corresponding to Eq. (*114*):

$$*_b = \exp(i\varphi_{ab})*_a = *_a \exp(-i\varphi_{ab}) . \tag{117}$$

Let us note that in the case of an antilinear operator it makes a difference whether a complex factor is put before or after the symbol of the operator.

From definition (*116*) it follows that

$$*\Phi_0 = \Omega , \quad *\Omega = \Phi_0 . \tag{118}$$

In general, for the contravariant Fock basis corresponding to the covariant basis (*63*), the following formula may be derived:

$$*\Phi^X = \hat{a}[\Phi^X]\Omega = \hat{a}^X |\Phi_{X\bar{X}}\rangle\langle\Phi^{X\bar{X}}|\Omega\rangle = \eta^{X\bar{X}}\Phi_{\bar{X}} \tag{119}$$

where

$$\eta^Z = \langle\Phi^Z|\Omega\rangle \tag{120}$$

and the index string $\overline{X}$ is complementary with respect to the index string X, see the last paragraph of subsection 1.3. Thus, the (restricted) summation over $\overline{X}$ in Eq. (*119*) contributes only a single term, the ordering of indices in $\overline{X}$ being arbitrary. To derive Eq. (*119*), one uses a proper form of the projector of Eq. (*110*), and formula (*99*). An analogous derivation performed for the covariant Fock basis (*63*) gives

$$*\Phi_X = \hat{a}[\Phi_X]\Omega = \hat{a}_X |\Phi^{X\bar{X}}\rangle\langle\Phi_{X\bar{X}}|\Omega\rangle = \eta_{X\bar{X}}\Phi^{\bar{X}} \tag{121}$$

where

$$\eta_Z = \langle\Phi_Z|\Omega\rangle . \tag{122}$$

The η factors are subject to the following normalization condition:

$$(\eta_Z)^* \eta^Z = \langle\Omega|\Phi_Z\rangle\langle\Phi^Z|\Omega\rangle = \langle\Omega|\Omega\rangle = 1 \quad (n_Z = M) . \tag{123}$$

The Hodge transformation of a general Fock-space vector (*68*) may be written as

$$* \Psi = \Phi_X \overline{C}^X = \Phi^X \overline{C}_X \tag{124}$$

where

$$\overline{C}^X = (C_{\overline{X}})^* \eta^{\overline{X}X} , \quad \overline{C}_X = (C^{\overline{X}})^* \eta_{\overline{X}X} . \tag{125}$$

The square of the Hodge operator, $(*)^2$, is a linear operator. In an application to a many-fermion system ($M = 2m_0$), one finds that

$$(*)^2 \Phi_X = *(\eta_{X\overline{X}} \Phi^{\overline{X}}) = (\eta_{X\overline{X}})^* \eta^{\overline{X}X} \Phi_X = (-1)^{n_X} (\eta_{X\overline{X}})^* \eta^{X\overline{X}} \Phi_X = (-1)^{n_X} \Phi_X \tag{126}$$

which is a consequence of Eq. (*41*). Thus,

$$(*)^2 = (-1)^{\hat{N}} \tag{127}$$

and this result holds independently of the orientation Ω, i.e., it is independent of the phase factor in Eq. (*117*). The inverse of the Hodge operator reads as

$$(*)^{-1} = *(-1)^{\hat{N}} = (-1)^{\hat{N}} * . \tag{128}$$

One may define the *group of the Hodge operator*,

$$\left\{\hat{1}, *, (*)^2 = (-1)^{\hat{N}}, (*)^3 = (*)^{-1}\right\} \tag{129}$$

which is a cyclic group of the order 4.

By using Eqs (*124*), (*125*), and (*123*), the following identity may be proved:

$$\langle * \Psi_a | * \Psi_b \rangle = \langle \Psi_b | \Psi_a \rangle . \tag{130}$$

Thus, the Hodge operator is an antiunitary operator in the Fock space. From Eq. (*130*) one finds also that

$$\langle * \Psi_a | \Psi_b \rangle = \langle * \Psi_b | (*)^2 \Psi_a \rangle = \langle * \Psi_b | (-1)^{\hat{N}} \Psi_a \rangle . \tag{131}$$

Let us note that the left-hand side of Eq. (*131*) defines a *bilinear form* in the Fock space $\mathbb{F}$. This is a symmetric bilinear form for Ψ_a, $\Psi_b \in \mathbb{F}^{(\mathrm{even})}$, but it is an antisymmetric bilinear form for Ψ_a, $\Psi_b \in \mathbb{F}^{(\mathrm{odd})}$.

5.3. The Vector Product

One may introduce the Hodge operator as an operator acting among the $\mathbb{V}^{(N)}$ vector spaces:

$$\mathbb{V}^{(N)} \ni \psi^{(N)} \rightarrow *\psi^{(N)} \in \mathbb{V}^{(M-N)} \tag{132}$$

where

$$*\psi^{(N)} = \hat{a}[\psi^{(N)}]\omega \tag{133}$$

and $\omega \equiv \omega^{(M)}$ corresponds to Eq. (*112*). It may be said that vector ω defines the *orientation* of the $\mathbb{V}^{(M)}$ vector space. The above definition of the Hodge operator is now in line with that employed in the theory of differential forms, see Eq. (*1*).

With the help of the Hodge operator of Eq. (*133*), one may define the *vector product* in the vector space $\mathbb{V}^{(1)}$ of the dimension M. It is an $(M-1)$-argument operation: for arbitrary vectors $\psi_1, \psi_2, \ldots, \psi_{M-1} \in \mathbb{V}^{(1)}$, one calculates their vector product as

$$\psi_1 \times \psi_2 \times \cdots \times \psi_{M-1} = *(\psi_1 \wedge \psi_2 \wedge \cdots \wedge \psi_{M-1}) \in \mathbb{V}^{(1)} . \tag{134}$$

The following properties of the vector product can be deduced from the above definition: (i) it is antisymmetric with respect to the exchange of any pair of its arguments, (ii) it is antilinear for any of its arguments, (iii) it depends on the orientation ω.

For $M = 3$, the vector product is a binary operation in the respective vector space $\mathbb{V}^{(1)}$; in the case of the three-dimensional Euclidean space, definition (*134*) coincides with the usual definition of the vector product in $\mathbb{R}^{(3)} = \mathbb{V}^{(1)}$. For $M = 2$, definition (*134*) describes a single-argument antilinear operation, which corresponds to the time-reversal operation in the vector space of electronic spin functions, see subsection 6.1.

5.4. The Hodge Similarity Transformation

With the help of the Hodge operator one can define a similarity transformation of linear operators in the Fock space $\mathbb{F}$:

$$\hat{H} \to * \hat{H}(*)^{-1} \ . \tag{135}$$

The transformed operator $* \hat{H}(*)^{-1}$ is also a linear operator, but the transformation itself is antilinear:

$$*(C_a \hat{H}_a + C_b \hat{H}_b)(*)^{-1} = (C_a)^* * \hat{H}_a(*)^{-1} + (C_b)^* * \hat{H}_b(*)^{-1} \ . \tag{136}$$

It is easy to show that transformation (*135*) is independent of the choice of the orientation of the Fock space:

$$*_a \hat{H}(*_a)^{-1} = *_b \hat{H}(*_b)^{-1} \tag{137}$$

(see Eqs (*114*) and (*117*)). Thus, the Hodge similarity transformation is a truly unique antilinear transformation of linear operators in the Fock space. Another such unique antilinear transformation corresponds to calculating the Hermitian conjugate of a given linear operator. However, the two transformations behave in a different way for products of operators: one finds that

$$* \hat{H}_a \hat{H}_b (*)^{-1} = * \hat{H}_a (*)^{-1} * \hat{H}_b (*)^{-1} \tag{138}$$

while $(\hat{H}_a \hat{H}_b)^\dagger = \hat{H}_b^\dagger \hat{H}_a^\dagger$.

The following formulas can be derived for the Hodge-transformed operators of Eq. (*96*):

$$* \hat{c}_X (*)^{-1} = \hat{a}_X (-1)^{n_X \hat{N}} \ , \quad * \hat{a}^X (*)^{-1} = (-1)^{n_X \hat{N}} \hat{c}^X \ . \tag{139}$$

In particular, for the corresponding fermion operators one finds that

$$* \hat{c}_k (*)^{-1} = \hat{a}_k (-1)^{\hat{N}} \ , \quad * \hat{a}^k (*)^{-1} = (-1)^{\hat{N}} \hat{c}^k \ . \tag{140}$$

The Hodge similarity transformation of the normal products (*105*) gives

$$* \hat{c}_X \hat{a}^Y (*)^{-1} = \hat{a}_X (-1)^{(n_X - n_Y)\hat{N}} \hat{c}^Y \ . \tag{141}$$

In particular, one finds that

$$* \hat{c}_k \hat{a}^l (*)^{-1} = \hat{a}_k \hat{c}^l = \delta_k{}^l \hat{1} - \hat{c}^l \hat{a}_k \ . \tag{142}$$

For a Hermitian operator $\hat{H}^{(1)}$ being a special case of operator (*106*),

$$\hat{H}^{(1)} = h^k{}_l \hat{c}_k \hat{a}^l = h_l{}^k \hat{c}^l \hat{a}_k \tag{143}$$

where $h_l^k = (h^k{}_l)^*$, the Hodge similarity transformation gives

$$* \hat{H}^{(1)} (*)^{-1} = (\mathrm{tr}\, \mathbf{h})\, \hat{1} - \hat{H}^{(1)} \tag{144}$$

where

$$\mathrm{tr}\, \mathbf{h} = h_l^{\ k} \delta_k^{\ l} \tag{145}$$

is the trace of matrix $\mathbf{h} = (h_l^k)$ (this is not the trace of operator $\hat{H}^{(1)}$). In particular, the Hodge similarity transformation of the particle-number operator (*107*) reads

$$* \hat{N} (*)^{-1} = M\, \hat{1} - \hat{N} \,. \tag{146}$$

5.5. The Choice of the Orientation of Fock Space

Let us look closer at the action of the $GL(M,\mathbb{C})$ transformations (see subsection 1.2.) in the $\mathbb{V}^{(M)}$ vector space. A special case of Eqs (*71*) may be written as

$$\underline{\Phi}_Z = \Phi_Z \det \mathbf{u} \,, \quad \underline{\Phi}^Z = \Phi^Z (\det \mathbf{u})^{*(-1)} \tag{147}$$

where $n_Z = M$, and one makes use of Eqs (*44*) and (*46*). With the help of Eqs (*48*) and (*147*), the overlap integral for vector $\underline{\Phi}_Z$ can be expressed as

$$\langle \underline{\Phi}_Z | \underline{\Phi}_Z \rangle = \underline{s}_{Z,Z} = \det \underline{\mathbf{s}} = \det \mathbf{s}\, |\det \mathbf{u}|^2 \,. \tag{148}$$

For a given fixed orientation Ω, one calculates the transformed values of the η-factors of Eqs (*120*) and (*122*):

$$\underline{\eta}^Z = \langle \underline{\Phi}^Z | \Omega \rangle = (\det \mathbf{u})^{-1} \eta^Z \,, \quad \underline{\eta}_Z = \langle \underline{\Phi}_Z | \Omega \rangle = (\det \mathbf{u})^* \eta_Z \,. \tag{149}$$

The above formulas can be considered a special case of Eqs (*72*). Thus, under the action of the $GL(M,\mathbb{C})$ transformations, quantities η^Z and η_Z behave as ordinary contra- and covariant tensors, respectively. The same can be said about vectors $*\Phi^X$ of Eq. (*119*), and vectors $*\Phi_X$ of Eq. (*121*). This is the case of the orientation of the Fock space which is chosen independently of the choice of the basis set in the $\mathbb{V}^{(1)}$ vector space; such Ω will be called the *external orientation* of the Fock space.

However, it seems more practical to build Ω from the vectors of the covariant basis set (*2*), or the contravariant basis set (*5*):

$$\Omega = \Phi_{\mathcal{M}} (\det \mathbf{s})^{-1/2} = \Phi^{\mathcal{M}} (\det \mathbf{s})^{1/2} \tag{150}$$

where $\mathcal{M}$ is the maximal ordered index string. For the integer indices, it is natural to choose $\mathcal{M} = 12\cdots\mathrm{M}$; however, in fact $\mathcal{M}$ can be chosen arbitrarily. Orientation Ω defined in Eq. (*150*) will be called the *internal orientation* of the Fock space. The arbitrariness in the choice of $\mathcal{M}$ has a limited effect since for two different nondegenerate strings $\mathcal{M}$ and $\mathcal{M}'$ the corresponding internal orientations Ω and Ω' may be either identical or opposite. In the present paper, this is the first instance of a definition that truly depend on the choice of $\mathcal{M}$. Let us now define analogs of the η-factors of Eqs (*120*) and (*122*), calculated for Ω defined in Eq. (*150*):

$$\varepsilon^{Z} = \langle \Phi^{Z} | \Omega \rangle = \delta^{Z}{}_{\mathcal{M}} (\det \mathbf{s})^{-1/2} \tag{151}$$

$$\varepsilon_{Z} = \langle \Phi_{Z} | \Omega \rangle = \delta_{Z}{}^{\mathcal{M}} (\det \mathbf{s})^{1/2} \tag{152}$$

where the new symbols are introduced to make a distinction between the external and internal orientation. The Hodge operator may be defined by assuming the internal orientation of the Fock space, in this case we rewrite Eqs (*119*) and (*121*) with the help of the ε-factors:

$$*\Phi^{X} = \varepsilon^{X\bar{X}} \Phi_{\bar{X}} \tag{153}$$

$$*\Phi_{X} = \varepsilon_{X\bar{X}} \Phi^{\bar{X}} \,. \tag{154}$$

Let us note that while the η-factors of Eqs (*120*) and (*122*) may assume complex values, the corresponding ε-factors of Eqs (*151*) and (*152*) are always real.

Under the action of the $GL(M,\mathbb{C})$ transformations (*147*), the internal orientation (*150*) transforms according to the following formula:

$$\Omega \to \underline{\Omega} = \underline{\Phi}_{\mathcal{M}} (\det \underline{\mathbf{s}})^{-1/2} = \Omega \det \mathbf{u} |\det \mathbf{u}|^{-1} \,. \tag{155}$$

It is seen that the initial and final internal orientations may differ by a phase factor; cf. Eq. (*114*). The transformed ε-factors read as

$$\underline{\varepsilon}^{Z} = \delta^{Z}{}_{\mathcal{M}} (\det \underline{\mathbf{s}})^{-1/2} = |\det \mathbf{u}|^{-1} \varepsilon^{Z} \tag{156}$$

$$\underline{\varepsilon}_{Z} = \delta_{Z}{}^{\mathcal{M}} (\det \underline{\mathbf{s}})^{1/2} = |\det \mathbf{u}| \varepsilon_{Z} \,. \tag{157}$$

One finds that there is a subtle difference in the transformation rule for the ε-factors, in comparison with that of the η-factors, see Eqs (*149*). It is thus customary to refer to the ε-factors as to *pseudotensors*. As long as the Hodge operator of Eq. (*116*) is defined by assuming the internal orientation Ω of Eq. (*150*), the Hodge-transformed vectors defined in Eqs (*153*) and (*154*) also behave as pseudotensors. The difference between tensors and pseudotensors disappears for those $GL(M,\mathbb{C})$ transformations $\mathbf{u}'$, for which det $\mathbf{u}'$ is real and positive. Such transformations make a subgroup of $GL(M,\mathbb{C})$, which we denote by $GL^{(+)}(M,\mathbb{C})$. A general $GL(M,\mathbb{C})$ transformation $\mathbf{u}$ may be written as

$$\mathbf{u} = \exp(\mathrm{i}\varphi)\,\mathbf{u}' \qquad (158)$$

where $\exp(\mathrm{i}\varphi)$ is a phase factor, and $\mathbf{u}' \in GL^{\wedge(+)}(M,\mathbb{C})$. This phase factor causes the appearance of the phase factor $\det \mathbf{u}|\det \mathbf{u}|^{-1} = \exp(\mathrm{i}M\varphi)$ in Eq. (*155*). Thus, as long as $\varphi \neq 2\pi m/M$, $m = 0, 1, \ldots, M-1$, the corresponding $GL(M,\mathbb{C})$ transformation causes a change of the internal orientation Ω.

6. TIME-REVERSAL OPERATOR

In Chapters 13-8 and 14-5 of his book[11], Jauch invokes physical and mathematical arguments that help to define the time-reversal operator for a spin-1/2 particle. For such a particle (e.g., electron), spin functions span a two-dimensional unitary vector space. Below we show how to express this operator by means of the Hodge operator corresponding to that space.

6.1. Time-Reversal Operator for Electronic Spin Functions

The spin function of electron is a complex function of a discrete variable $\mu = -1/2, 1/2$ (in principle, one may assume *any* two distinct values for μ, e.g., $\mu = 1, 2$). Such functions may be treated as vectors in the $\mathbb{C}^2$ vector space, endowed with a natural scalar product. In $\mathbb{C}^2$ one may define a simple antiunitary operator corresponding to the complex conjugation of the vector components. However, for our purposes it will be sufficient to treat the space of one-electron spin functions as an abstract two-dimensional unitary vector space, without any additional algebraic structure. Within this subsection, we shall assume that this is simply the $\mathbb{V}^{(1)}$ vector space introduced at the beginning of the dimension $M = 2$. Let

$$(\sigma_1, \sigma_2) \qquad (159)$$

be a covariant basis in that space, with the corresponding overlap matrix 2×2 positive-definite Hermitian matrix. The $\mathbb{V}^{(2)}$ vector space is now a one-dimensional space spanned by a (covariant) basis vector $\sigma_{12} = \sigma_1 \wedge \sigma_2$; cf. Eq. (*84*).

We consider the Hodge operator defined in Eqs (*132*) and (*133*). The internal orientation ω of the $\mathbb{V}^{(2)}$ vector space, corresponding to the covariant basis (*159*), may be defined by using an analogue of Eq. (*150*):

$$\omega = \sigma_{12} (\det \mathbf{s})^{-1/2} = \sigma^{12} (\det \mathbf{s})^{1/2} \tag{160}$$

where $\sigma^{12} = \sigma^1 \wedge \sigma^2$, and $\{\sigma^1,\sigma^2\}$ is the contravariant basis set corresponding to basis (*159*). For $M = 2$, the vector product (*134*) is a single-argument operation in $\mathbb{V}^{(1)}$, equal to the Hodge operator itself. For a general spin function $\sigma \in \mathbb{V}^{(1)}$, the following formula may be derived:

$$\begin{aligned} *\sigma &= *(\sigma_1 c^1 + \sigma_2 c^2) = \varepsilon_{12} (c^1)^* \sigma^2 + \varepsilon_{21} (c^2)^* \sigma^1 = \\ &= (\det \mathbf{s})^{1/2} [(c^1)^* \sigma^2 - (c^2)^* \sigma^1] \end{aligned} \tag{161}$$

and we make use of (an analogue of) Eq. (*154*), with

$$\varepsilon_{kl} = \delta_{kl}^{\ 12} (\det \mathbf{s})^{1/2} \tag{162}$$

see Eq. (*152*). Operator $*$ is an antiunitary operator in the two-dimensional unitary vector space $\mathbb{V}^{(1)}$, and it can be shown that

$$(*)^2 = -\hat{1} \tag{163}$$

where $\hat{1}$ is the unit operator in $\mathbb{V}^{(1)}$. The operation defined in Eq. (*161*) represents the action of the time-reversal operator in the vector space of one-electron spin functions. The above definition is covariant with respect to the $GL^{(+)}(2,\mathbb{C})$ transformations, see the previous section. However, general $GL(2,\mathbb{C})$ transformations, of the form given in Eq. (*158*), may change the phase of the internal orientation ω defined in Eq. (*160*). It seems that there is no physical argument that would help in removing that phase-factor arbitrariness from the definition of the time-reversal operator.

6.2. Time-Reversal Operator for Electronic Spin Orbitals

The vector space of electronic spin orbitals is a tensor product of the orbital vector space and the vector space of one-electron spin functions. Orbitals are square-integrable complex-valued functions of variable $\mathbf{r}$ representing

the spatial coordinates of electron. By employing the covariant basis set (*159*), one may write a general spin orbital as

$$\psi = f^1 \otimes \sigma_1 + f^2 \otimes \sigma_2 \tag{164}$$

where f^1 and f^2 are certain orbitals (not necessarily linearly independent). The value of function (*164*) is calculated as

$$\psi(\mathbf{r}, \mu) = f^1(\mathbf{r})\,\sigma_1(\mu) + f^2(\mathbf{r})\,\sigma_2(\mu)\,. \tag{165}$$

By making use of definition (*161*), we now define the time-reversal operator $\hat{\tau}$ for the spin orbitals:

$$\begin{aligned} \hat{\tau}\psi &= (f^1)^* \otimes (*\sigma_1) + (f^2)^* \otimes (*\sigma_2) = \\ &= (\det \mathbf{s})^{1/2}[(f^1)^* \otimes \sigma^2 - (f^2)^* \otimes \sigma^1]\,. \end{aligned} \tag{166}$$

The above definition invokes the complex-conjugation operation, $f \rightarrow f^*$, in the vector space of orbitals. Because of Eq. (*163*),

$$\hat{\tau}^2 = -\hat{1} \tag{167}$$

where $\hat{1}$ is the unit operator in the spin-orbital vector space. Operator $\hat{\tau}$ is a unique antilinear operator in that space, but it is subject to the phase-factor arbitrariness discussed at the end of the previous subsection.

The scalar product of simple spin orbitals $\psi_a = f_a \otimes \sigma_a$ and $\psi_b = f_b \otimes \sigma_b$ reads as a product of the scalar products corresponding to the orbital and spin parts:

$$\langle \psi_a | \psi_b \rangle = \langle f_a | f_b \rangle \langle \sigma_a | \sigma_b \rangle\,. \tag{168}$$

It is easy to show that operator $\hat{\tau}$ is antiunitary,

$$\langle \hat{\tau}\psi_a | \hat{\tau}\psi_b \rangle = \langle \psi_b | \psi_a \rangle\,. \tag{169}$$

Moreover, due to Eq. (*167*), the following formula is true:

$$\langle \hat{\tau}\psi_a | \psi_b \rangle = -\langle \hat{\tau}\psi_b | \psi_a \rangle \tag{170}$$

which defines an antisymmetric bilinear form in the spin-orbital vector space. It follows from the above formula that for an arbitrary spin orbital ψ one has

$$\langle \hat{\tau}\psi | \psi \rangle = 0 \tag{171}$$

which means that vectors ψ and $\hat{\tau}\psi$ are always orthogonal to each other. Thus, operator $\hat{\tau}$ has no eigenvectors. Operator $\hat{\tau}$ defines some unique *pairing* in the spin-orbital space: the whole space is a union of different two-element sets $\{\psi,\hat{\tau}\psi\}$, and a single-element set $\{\psi = 0\}$.

6.3. Time-Reversal Operator in Fock Space

When choosing the (covariant) basis set (*2*), one has to make sure that the $\mathbb{V}^{(1)}$ vector space of spin orbitals, spanned by this basis, is invariant with respect to the $GL(2,\mathbb{C})$ transformations of the one-electron spin functions. This condition requires that $\mathbb{V}^{(1)}$ is a tensor product of an orbital vector space, spanned by a certain orbital basis,

$$(f_1, f_2, \ldots, f_{m_0}) \tag{172}$$

and the vector space of the one-electron spin functions, spanned by basis (*159*). Thus, basis (*2*) should consist of tensor products of the members of bases (*172*) and (*159*), which fixes the dimension of the resulting $\mathbb{V}^{(1)}$ vector space at $M = 2m_0$. In order to make $\mathbb{V}^{(1)}$ invariant also with respect to the time-reversal operator $\hat{\tau}$, the corresponding orbital vector space of the dimension m_0 should be closed with respect to the complex-conjugation operation. This in turn requires basis (*172*) to be equivalent, by means of some linear transformation, to a basis set of real functions. That condition is not fulfilled by some orbital basis sets, e.g. by the so-called GIAO basis set used in the gauge-independent calculations of molecular magnetic properties (see ref.[17] and references therein).

Let us assume that our $\mathbb{V}^{(1)}$ vector space of spin orbitals is invariant with respect to the time-reversal operator $\hat{\tau}$ defined in Eq. (*166*). The corresponding time-reversal operator $\hat{\tau}^{(N)}$ acting in the $\mathbb{V}^{(N)}$ vector space ($2 \le N \le M$) can now be defined by means of the following formulas:

$$\hat{\tau}^{(N)}\phi_{kl\cdots n} = \hat{\tau}^{(N)}(\phi_k \wedge \phi_l \wedge \cdots \wedge \phi_n) = (\hat{\tau}\phi_k) \wedge (\hat{\tau}\phi_l) \wedge \cdots \wedge (\hat{\tau}\phi_n) \tag{173}$$

$$\hat{\tau}^{(N)}\psi^{(N)} = (c^X)^* \hat{\tau}^{(N)}\phi_X \quad (n_X = N) \tag{174}$$

where we make use of representation (*84*) for the (covariant) antisymmetric tensors (*50*), and formula (*59*) for a general *N*-vector of $\mathbb{V}^{(N)}$. In addition, we put $\hat{\tau}^{(1)} \equiv \hat{\tau}$, and define $\hat{\tau}^{(0)}$ as the complex-conjugation operation in $\mathbb{V}^{(0)} \equiv \mathbb{C}$.

Let us consider a general vector (*61*) in the Fock space $\mathbb{F}$. One can define the time-reversal operator $\hat{\mathcal{T}}$ in this vector space by means of the following formula:

$$\hat{\mathcal{T}}\,\Psi = (\hat{\tau}^{(0)}\psi^{(0)}, \hat{\tau}^{(1)}\psi^{(1)}, \hat{\tau}^{(2)}\psi^{(2)}, \ldots, \hat{\tau}^{(M)}\psi^{(M)})\,. \qquad (175)$$

Operator $\hat{\mathcal{T}}$ is an antiunitary operator in the Fock space, and it can be shown that

$$\hat{\mathcal{T}}^2 = (-1)^{\hat{N}} \qquad (176)$$

cf. Eq. (*127*). Operator $*\hat{\mathcal{T}}$ is a linear operator in the Fock space $\mathbb{F}$. It can be proved that the Hodge operator and the time-reversal operator commute

$$*\,\hat{\mathcal{T}} = \hat{\mathcal{T}}* \qquad (177)$$

if the internal orientation Ω of Eq. (*150*) is chosen in the Fock space, and the internal orientation ω of Eq. (*160*) is chosen for the spin functions.

7. CONCLUSIONS

Due to a special algebraic structure which corresponds to definition (*60*), the fermionic Fock space $\mathbb{F}$ has a family of nontrivial unique linear and antilinear operators. This family is generated by the particle-number operator $\hat{N}$, and the Hodge operator $*$. In addition, another unique antilinear operator, the time-reversal operator $\hat{\mathcal{T}}$, emerges due to a special algebraic structure of the spin-orbital space. Operator $\hat{\mathcal{T}}$ is related to the Hodge operator in the two-dimensional unitary space of the electronic spin functions. A peculiar feature of the Hodge operator acting in a given vector space is its dependence on the so-called orientation of that space, see the discussion in subsection 5.5.

Two antilinear operators, $*$ and $\hat{\mathcal{T}}$, play complementary roles in the Fock space: the former is a “global” one, since it exchanges states corresponding to different numbers of particles, while the latter is a “local” one, since it acts via a transformation of the single-particle states.

8. APPENDIX

A proof of Eq. (*103*) requires several steps of derivation, analogous to those in Eq. (*99*):

$$\hat{a}^k \hat{c}_l = \delta^V{}_{V'} |\Phi_V\rangle\langle\Phi^{V'}| \hat{a}^k \hat{c}_l \Phi_W\rangle\langle\Phi^{W'}| \delta^W{}_{W'} = \\ = |\Phi_V\rangle\langle\Phi^{kV}|\Phi_{lW}\rangle\langle\Phi^W| = \delta^{kV}{}_{lW} |\Phi_V\rangle\langle\Phi^W| \tag{178}$$

$$\hat{c}_l \hat{a}^k = \delta^V{}_{V'} |\Phi_V\rangle\langle\Phi^{V'}| \hat{c}_l \Phi_Z\rangle \delta^Z{}_{Z'} \langle\Phi^{Z'}| \hat{a}^k \Phi_W\rangle\langle\Phi^{W'}| \delta^W{}_{W'} = \\ = |\Phi_V\rangle\langle\Phi^V|\Phi_{lZ}\rangle\langle\Phi^{kZ}|\Phi_W\rangle\langle\Phi^W| = \delta^V{}_{lZ}\, \delta^{kZ}{}_W |\Phi_V\rangle\langle\Phi^W| . \tag{179}$$

Thus,

$$\hat{a}^k \hat{c}_l + \hat{c}_l \hat{a}^k = (\delta^{kV}{}_{lW} + \delta^V{}_{lZ}\, \delta^{kZ}{}_W) |\Phi_V\rangle\langle\Phi^W| . \tag{180}$$

By examining four possible cases: ($k = l$, $V = W$), ($k = l$, $V \neq W$), ($k \neq l$, $V = W$), and ($k \neq l$, $V \neq W$), one finds that

$$\delta^{kV}{}_{lW} + \delta^V{}_{lZ}\, \delta^{kZ}{}_W = \delta^k{}_l\, \delta^V{}_W \tag{181}$$

which leads to Eq. (*103*).

Let us now consider general fermion creation and annihilation operators, of the form $\hat{c}[\Psi^{(1)}]$ and $\hat{a}[\Psi^{(1)}]$, where $\Psi^{(1)} \in \mathbb{F}^{(1)}$ corresponds, through isomorphism (*75*), to $\psi^{(1)} \equiv \psi \in \mathbb{V}^{(1)}$. By employing Eqs (*10*) and (*13*), as well as Eqs (*92*) and (*93*), one may write down the anticommutation relations (*102*) and (*103*) for such general fermion operators. In particular, the general form of Eq. (*103*) reads

$$\hat{a}[\Psi_a^{(1)}]\, \hat{c}[\Psi_b^{(1)}] + \hat{c}[\Psi_b^{(1)}]\, \hat{a}[\Psi_a^{(1)}] = \langle\Psi_a^{(1)}|\Psi_b^{(1)}\rangle \hat{1} = \langle\psi_a|\psi_b\rangle \hat{1} . \tag{182}$$

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