Orthogonalization of fermion k-body operators and representability

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The reduced k-particle density matrix of a density matrix on finite-dimensional, fermion Fock space can be defined as the image under the orthogonal projection in the Hilbert-Schmidt geometry onto the space of k-body observables. A proper understanding of this projection is therefore intimately related to the *representability problem*, a long-standing open problem in computational quantum chemistry. Given an orthonormal basis in the finite-dimensional one-particle Hilbert space, we explicitly construct an orthonormal basis of the space of Fock space operators which restricts to an orthonormal basis of the space of k-body operators for all k.

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I. INTRODUCTION

A. Motivation: Representability problems

In quantum chemistry, molecules are usually modeled as nonrelativistic many-fermion systems (Born-Oppenheimer approximation). More specifically, the Hilbert space of these systems is given by the fermion Fock space $\mathcal{F} = \mathcal{F}_f(\mathfrak{h})$, where $\mathfrak{h}$ is the (complex) Hilbert space of a single electron [e.g., $\mathfrak{h} = L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$], and the Hamiltonian $\mathbb{H}$ is usually a two-body operator or, more generally, a k-body operator on $\mathcal{F}$. A key physical quantity whose computation is an important task is the ground-state energy

$$E_0(\mathbb{H}) \doteq \inf_{\varphi \in \mathcal{S}} \varphi(\mathbb{H}) \tag{1}$$

of the system, where $\mathcal{S} \subseteq \mathcal{B}(\mathcal{F})'$ is a suitable set of states on $\mathcal{B}(\mathcal{F})$, where $\mathcal{B}(\mathcal{F})$ is the Banach space of bounded operators on $\mathcal{F}$ and $\mathcal{B}(\mathcal{F})'$ its dual. A direct evaluation of (1) is, however, practically impossible due to the vast size of the state space $\mathcal{S}$.

1. Abstract representability problem

As has been widely observed, this problem can be reduced drastically by replacing the states $\tau \in \mathcal{S}$ by a quantity r_τ, the *k-body reduction* of τ, that only encodes the expectation values of k-body operators in the state τ. More precisely, denote by $\mathcal{O}_k(\mathcal{F}) \subseteq \mathcal{B}(\mathcal{F})$ the subspace of k-body operators on $\mathcal{F}$ and let $\tau \in \mathcal{B}(\mathcal{F})'$, then r_τ can be defined as the restriction $\tau|_{\mathcal{O}_k(\mathcal{F})} \in \mathcal{O}_k(\mathcal{F})'$. In other words, if $i_k : \mathcal{O}_k(\mathcal{F}) \to \mathcal{B}(\mathcal{F})$ denotes the inclusion map then the mapping $\tau \mapsto r_\tau$ is given by the dual map $i_k' : \mathcal{B}(\mathcal{F})' \to \mathcal{O}_k(\mathcal{F})'$, which we call the *k-body reduction map*. Now, if $\mathbb{H} \in \mathcal{O}_k(\mathcal{F})$ then $\tau(\mathbb{H}) = (i_k'\tau)(\mathbb{H})$ for all $\tau \in \mathcal{B}(\mathcal{F})'$ and (1) can be rewritten as

$$E_0(\mathbb{H}) = \inf_{\tau \in \mathcal{S}} \tau(\mathbb{H}) = \inf_{\tau \in \mathcal{S}} r_\tau(\mathbb{H}) = \inf_{r \in i_k'(\mathcal{S})} r(\mathbb{H}), \tag{2}$$

thus the evaluation of (1) is, in principle, simplified, because the infimum has to be taken over the much smaller set $i_k'(\mathcal{S})$. To explicitly compute the right hand side of (2), however, one has to find an efficient parametrization of the set $i_k'(\mathcal{S})$. The *representability problem for* $\mathcal{S}$ (and $k \in \mathbb{N}_0$) amounts to characterize the image $i_k'(\mathcal{S})$ of *representable* functionals on $\mathcal{O}_k(\mathcal{F})$ in a computationally efficient way.

2. Traditional representability problems

The general framework of representability problems as discussed here is usually invisible in the pertinent literature because in concrete applications $\mathcal{S}$ is almost always chosen to be (a subset of) the set of density matrices on $\mathcal{F}$ and $\mathcal{O}_k(\mathcal{F})'$ is identified with a suitable subspace of $\mathcal{B}(\mathcal{F})$. Moreover, in applications of physics or chemistry the by far most important case is $k = 2$, as the Hamiltonian usually is a two-body operator. In this case the two-body reduction $i_k'(\rho)$ of an N-particle density matrix can be identified with the (customary) 2-RDM, which is a bounded operator on $\bigwedge^2 \mathfrak{h}$.

3. Erdahl's representability framework

In this paper, only the case $\dim \mathfrak{h} < \infty$ is considered, which is sufficient for many important applications. For example, in quantum chemistry one commonly starts by choosing a finite subset of $L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$ of *spin orbitals* and then considers their span $\mathfrak{h}$. In the finite-dimensional case, the reduced k-body reduction of a density matrix ρ can be introduced as the image $\pi_k(\rho)$ under the orthogonal projection onto $\mathcal{O}_k(\mathcal{F})$ (see [1]),

$$\pi_k : \mathcal{L}^2(\mathcal{F}) \to \mathcal{O}_k(\mathcal{F}) \subseteq \mathcal{L}^2(\mathcal{F}). \tag{3}$$

As it turns out, in the finite-dimensional case π_k is an equivalent description of the map i_k' introduced above. The reason for this is that in the finite-dimensional case $\mathcal{B}(\mathcal{F}) = \mathcal{L}^2(\mathcal{F})$, where $\mathcal{L}^2(\mathcal{F})$ denotes the Hilbert space of Hilbert-Schmidt operators on $\mathcal{F}$, and we may identify $\mathcal{B}(\mathcal{F})' \cong \mathcal{L}^2(\mathcal{F})$ and $\mathcal{O}_k(\mathcal{F})' \cong \mathcal{O}_k(\mathcal{F})$ via the Riesz isomorphisms. Under these identifications, the k-body reduction map i_k' is given by the adjoint i_k^* of i_k and $\pi_k = i_k i_k^*$. This geometric interpretation of the representability problem is visualized in Fig. 1. Note that Erdahl's representability framework breaks down in the

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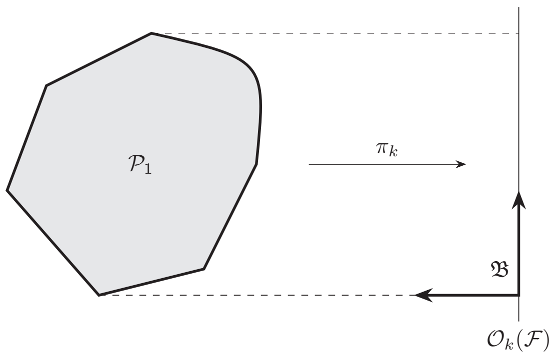

FIG. 1. Geometric interpretation of the representability problem for density matrices in finite dimensions: The mapping of density matrices $\rho \in \mathcal{P}_1$ to its k-body reduction as orthogonal projection π_k onto the subspace $\mathcal{O}_k(\mathcal{F}) \subseteq \mathcal{L}^2(\mathcal{F})$ of k-body operators. The representability problem amounts to find an efficient characterization of the image $\pi_k(\mathcal{P}_1)$ within $\mathcal{O}_k(\mathcal{F})$. The orthonormal basis $\mathfrak{B}$ given in Theorem I.1 is adapted to this situation as it restricts to an orthonormal basis $\mathfrak{B} \cap \mathcal{O}_k(\mathcal{F})$ of $\mathcal{O}_k(\mathcal{F})$ for every $k \in \mathbb{N}_0$.

infinite-dimensional case because then k-body operators are generally not Hilbert-Schmidt anymore.

B. Related work

The idea of replacing density matrices by their reduced density matrices to simplify the evaluation of (1) can be traced back to Husimi [2]. First extensive analyses were carried out in the 1950's and 1960's and lead, e.g., to the solution of the representability problem for one-body reduced density matrices of N-particle density matrices [3–5] and the development of (still very inaccurate) lower bound methods based on representability conditions. In 1978, Erdahl introduced a new class of representability conditions [1], which were found to significantly increase the accuracy of lower bound methods [6]. In 2005 the representability problem for the one-body reduced density matrices of *pure* states was solved by Klyachko [7] based on results from quantum information theory. In 2012 Mazziotti established a hierarchy of representability conditions providing a formal solution of the representability problem for the two-body RDMs of N-particle density matrices [8]. However, the general representability problem has been found to be computationally intractible [8], even on a quantum computer [9]. Computational advances [10] enabled a range of recent applications [11–13]. Representability methods have also proved useful in Hartree-Fock theory [14]. For a more detailed overview on the history of representability problems, we refer to [15,16].

C. Goal and main results

The goal of the present work is to shed more light on the projection π_k in the finite-dimensional case. As a result, we explicitly diagonalize the orthogonal projections π_k simultaneously for all $k \in \mathbb{N}_0$. More specifically, we prove the following.[1]

Theorem I.1 (Main Theorem). Let $\dim_{\mathbb{C}} \mathfrak{h} = n < \infty$ and $\varphi_1, \ldots, \varphi_n$ be an orthonormal basis of $\mathfrak{h}$. For $I = \{i_1 < \ldots < i_j\} \subseteq \{1, \ldots, n\}$ define $\mathbf{c}_I \doteq c(\varphi_{i_j}) \cdots c(\varphi_{i_1})$ and $n_I \doteq \mathbf{c}_I^* \mathbf{c}_I$, where $c(\varphi)$ denotes the usual fermion annihilation operator. Then the following is found.

(1) An orthonormal basis $\mathfrak{B}$ of $\mathcal{L}^2(\mathcal{F})$ is given by the elements

$$\frac{1}{\sqrt{2^{n-|I \dot\cup J|}}} \sum_{A \subseteq L} (-2)^{|A|} \mathbf{n}_A \mathbf{c}_I^* \mathbf{c}_J, \tag{4}$$

where I, J, L run over all mutually disjoint subsets of $\{1, \ldots, n\}$.

(2) For any $k \in \mathbb{N}_0$, $\mathfrak{B} \cap \mathcal{O}_k(\mathcal{F})$ is an orthonormal basis of $\mathcal{O}_k(\mathcal{F})$.

Orthogonal decompositions of $\mathcal{L}^2(\mathcal{F})$ as implied by Theorem I.1 have already been introduced, e.g., in [1], Sec. 8, where an orthogonal decomposition $\mathcal{B}(\mathcal{F}) = \bigoplus_{n,m} \Lambda(n, m)$ is used to derive new classes of representability conditions. The spaces $\Lambda(n, m)$ are generated by elements of the form (66), see Sec. V. The orthonormal basis elements given in Theorem I.1, however, have the additional property of being *normal ordered*, which can be used to express $\pi_k(\rho)$ in terms of the customary reduced density matrices, as in the following example.

Corollary I.2. Let ρ be a particle number-preserving density matrix, $\gamma \in \mathcal{B}(\mathfrak{h})$ its 1-RDM and $d\Gamma(\gamma) = \sum_{i,j} \gamma_{ji} c_i^* c_j$ the (differential) second quantization of γ. Then

$$2^n \pi_1(\rho) = (n+1) - 2\,\mathrm{tr}\{\gamma\} - 2\hat{\mathbb{N}} + 4 d\Gamma(\gamma), \tag{5}$$

where $\hat{\mathbb{N}} = \sum_i c_i^* c_i$ denotes the particle number operator.

A similar formula for $\pi_2(\rho)$ exists, but is much more complicated.

D. Overview of the paper

In Sec. II, we introduce the necessary terminology and notation of fermion many-particle systems and general density matrix theory, as well as, some features specific to the finite-dimensional setting. In Sec. III, we compute the Hilbert-Schmidt scalar product of specific monomials in creation and annihilation operators (Proposition III.8). In Sec. IV we prove Theorem I.1 in two steps, as follows.

(1) The orthonormal basis $\mathfrak{B}$ of $\mathcal{L}^2(\mathcal{F})$ is constructed in Theorem IV.2.

(2) In Theorem IV.4 we show that $\mathfrak{B} \cap \mathcal{O}_k(\mathcal{F})$ is a basis of $\mathcal{O}_k(\mathcal{F})$ for all $k \in \mathbb{N}_0$.

In many cases one also considers the space $\mathcal{O}_k^{\mathbb{R}}(\mathcal{F})$ of *self-adjoint* k-body operators. We generalize the above results in Theorem IV.7, where we apply a suitable unitary transformation U on $\mathcal{L}^2(\mathcal{F})$ and show that the orthonormal basis $U(\mathfrak{B})$ of $\mathcal{L}^2(\mathcal{F})$ restricts to an orthonormal basis of $\mathcal{O}_k^{\mathbb{R}}(\mathcal{F})$ for all $k \in \mathbb{N}_0$. Finally, in Sec. V we present an alternative approach for constructing an orthonormal basis of $\mathcal{L}^2(\mathcal{F})$ with properties as in Theorem I.1, which was first communicated to us by Gosset[2] and turned out to be already present in [1].

[1]See Fig. 1 for a geometric interpretation of this result and its relation to the representability problem.

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E. Motivating application

We illustrate the virtue of having orthonormal bases of the space of operators explicitly available on the following example: Consider a fermionic many-particle system with finite-dimensional one-particle Hilbert space $\mathfrak{h}$, a two-body Hamiltonian of the form

$$\mathbb{H} = \sum_{i,j} t_{ij} c_i^* c_j + \frac{1}{2} \sum_{i,j,k,l} V_{ij;kl} c_i^* c_j^* c_l c_k, \tag{6}$$

where $V_{ij;kl} \doteq \langle \varphi_i \otimes \varphi_j \mid V(\varphi_k \otimes \varphi_l) \rangle$ is a matrix element of a repulsive two-body potential $V \geqslant 0$. Let $\mathcal{B}$ be an orthonormal basis of $\mathcal{L}^2(\mathcal{F})$. Then for any $\mathcal{A} \subseteq \mathcal{B}$ we have $P_\mathcal{A} \doteq \sum_{\theta \in \mathcal{A}} |\theta\rangle\langle\theta| \leqslant \sum_{\theta \in \mathcal{B}} |\theta\rangle\langle\theta| = \mathbb{1}_{\mathcal{L}^2(\mathcal{F})}$ and, under suitable positivity requirements on the potential V, we obtain

$$\mathbb{H} \geqslant \sum_{i,j} t_{ij} c_i^* c_j + \frac{1}{2} \sum_{i,j,k,l} V_{ij;kl} c_i^* c_j^* P_\mathcal{A} c_l c_k \doteq \mathbb{H}_\mathcal{A}. \tag{7}$$

Thus $E_0(\mathbb{H}_\mathcal{A})$ is a lower bound, which are usually more difficult to derive than upper bounds, for the ground-state energy $E_0(\mathbb{H})$ of the original quantum system. In many situations, after a suitable choice of an orbital basis $\varphi_1, \ldots, \varphi_n$ of $\mathfrak{h}$, the orthonormal basis $\mathfrak{B}$ given by Theorem I.1 and a suitable choice of $\mathcal{A} \subset \mathcal{B}$ leads to a nontrivial lower bound $E_0(\mathbb{H}_\mathcal{A})$ of $E_0(\mathbb{H})$.

II. FOUNDATIONS

Throughout this work, $\mathfrak{h}$ denotes the one-particle Hilbert space, i.e., a separable complex Hilbert space. We consider only the *finite-dimensional case* here and assume $n \doteq \dim_\mathbb{C} \mathfrak{h} < \infty$ throughout the paper.

A. General notions

In this subsection, we will recall some relevant notions from general density matrix theory of fermion many-particle systems that are also valid when $\dim \mathfrak{h} = \infty$.

1. Hilbert spaces

If not stated otherwise, all Hilbert spaces are assumed to be complex. For a Hilbert space $\mathcal{H}$, the inner product between elements $\varphi, \psi \in \mathcal{H}$ is denoted by $\langle \varphi \mid \psi \rangle_\mathcal{H}$ and is assumed to be *antilinear* in the first and *linear* in the second component. When there is no risk of confusion, we will freely omit the subscript $\mathcal{H}$ of the inner product. By $\mathcal{B}(\mathcal{H})$ we denote the C*-algebra of linear bounded operators on $\mathcal{H}$.

2. Hilbert-Schmidt operators

The space of Hilbert-Schmidt operators on a Hilbert space $\mathcal{H}$ is denoted by $\mathcal{L}^2(\mathcal{H})$ and is a Hilbert space with respect to the inner product $\langle a \mid b \rangle_{\mathcal{L}^2(\mathcal{H})} \doteq \mathrm{tr}\{a^* b\}$. Furthermore, $\mathcal{L}^2(\mathcal{F})$ is endowed with a natural real structure (i.e., a complex conjugate involution) given by the Hermitian adjoint.

3. Fermion Fock space

For a Hilbert space $\mathfrak{h}$, the associated *fermion Fock space* $\mathcal{F} \doteq \mathcal{F}(\mathfrak{h})$ is the completion of the Grassmann algebra $\bigwedge \mathfrak{h} = \bigoplus_{k \geqslant 0} \bigwedge^k \mathfrak{h}$ with respect to the inner product defined by

$$\langle \varphi_1 \wedge \cdots \wedge \varphi_k \mid \psi_1 \wedge \cdots \wedge \psi_l \rangle \doteq \begin{cases} \det(\langle \varphi_i \mid \psi_j \rangle)_{i,j=1}^k & \text{if } k = l, \\ 0 & \text{otherwise.} \end{cases} \tag{8}$$

The neutral element $1 \in \mathbb{C} \doteq \bigwedge^0 \mathfrak{h} \subset \mathcal{F}$ of the wedge product on $\mathcal{F}$ is also called the *(Fock) vacuum* and denoted by $\Omega_\mathcal{F}$.

4. CAR

Associated with $\mathcal{F}$, there are natural linear, respectively antilinear, maps $c^*, c : \mathfrak{h} \to \mathcal{B}(\mathcal{F})$ called the *creation-* and *annihilation operators* which are defined for $f \in \mathfrak{h}$ and $\omega \in \mathcal{F}$ by $c(\varphi) \doteq [c^*(\varphi)]^*$ and $c^*(f)\omega \doteq f \wedge \omega$, respectively. They satisfy the *canonical anticommutation relations* (CAR)

$$\{c^*(\varphi), c^*(\psi)\} = \{c(\varphi), c(\psi)\} = 0\{c^*(\varphi), c(\psi)\} = \langle \varphi \mid \psi \rangle, \quad \forall \varphi, \psi \in \mathfrak{h}, \tag{9}$$

and $c(\varphi)\Omega_\mathcal{F} = 0$ for all $\varphi \in \mathfrak{h}$. The mappings $c^*, c : \mathfrak{h} \to \mathcal{B}(\mathcal{F})$ induce a representation of the (abstract) CAR algebra generated by $\mathfrak{h}$ (see [17], Sec. 5.2.2), called the *Fock representation*.

5. Density matrices

We denote by $\mathcal{P} \doteq \mathcal{L}_+^1(\mathcal{F}) \subseteq \mathcal{L}^2(\mathcal{F})$ the cone of positive, trace-class operators on $\mathcal{F}$. Elements ρ from the convex subset $\mathcal{P}_1 \subseteq \mathcal{P}$ which are *normalized* in the sense that $\mathrm{tr}\{\rho\} = 1$ are called *density matrices on* $\mathcal{F}$. Elements of $\mathcal{P}_1$ uniquely represent the *normal states* on the C*-algebra $\mathcal{B}(\mathcal{F})$ (see [18], Theorem 2.7).

B. Finite-dimensional features

We conclude this section by summarizing some more specific notions, which (partly) depend on the finite-dimensionality of $\mathfrak{h}$.

1. Generalized creation and annihilation operators

By the CAR, we may extend c, c^* to linear, respectively, antilinear, maps $\mathbf{c}^*, \mathbf{c} : \mathcal{F} \to \mathcal{B}(\mathcal{F})$ via

$$\mathbf{c}^*(\omega)\eta \doteq \omega \wedge \eta, \quad \mathbf{c}(\omega) \doteq [\mathbf{c}^*(\omega)]^*. \tag{10}$$

Note that the definition of $\mathbf{c}$ is such that $\mathbf{c}(\varphi_1 \wedge \cdots \wedge \varphi_k) = c(\varphi_k) \cdots c(\varphi_1)$, for all $\varphi_1, \ldots \varphi_k \in \mathfrak{h}$. We call $\mathbf{c}^*, \mathbf{c}$ the *generalized* creation and annihilation operators[3]. Note that the CAR (9) do *not* hold for $\mathbf{c}^*$ and $\mathbf{c}$, when $\varphi, \psi \in \mathfrak{h}$ are replaced by general $\omega, \eta \in \mathcal{F}$.

2. Polynomials in creation and annihilation operators

We are particularly interested in operators on $\mathcal{F}$, which are "polynomials in creation and annihilation" operators, i.e., elements in the complex $*$-subalgebra $\mathcal{A} \subseteq \mathcal{B}(\mathcal{F})$ generated by $\{c^*(\varphi) \mid \varphi \in \mathfrak{h}\}$. In the finite-dimensional case, $\mathcal{A} = \mathcal{B}(\mathcal{F})$ (see [17], Theorem 5.2.5) and we have a natural linear map

$$\Theta : \mathcal{F} \otimes \bar{\mathcal{F}} \ni \omega \otimes \bar{\eta} \mapsto \mathbf{c}^*(\omega)\mathbf{c}(\eta) \in \mathcal{A}, \tag{11}$$

[3]This terminology is also used, e.g., in [19].

where $\bar{\mathcal{F}}$ denotes the *conjugate* Hilbert space of $\mathcal{F}$ (see [20], Sec. 1.2). In fact, by the Wick Theorem, Θ is surjective and therefore an isomorphism, as the vector spaces involved are all finite-dimensional.

3. k-body operators

Let $k \in \mathbb{N}_0$. We call a sum of operators of the form $\mathbf{c}^*(\omega)\mathbf{c}(\eta)$ with $\omega \in \mathcal{F}_r$, $\eta \in \mathcal{F}_s$ and $r + s = 2k$ a *k-particle operator*. More generally, a sum of l-particle operators with $l \leqslant k$ is called a *k-body operator*, and we denote the space of k-body operators by $\mathcal{O}_k(\mathcal{F})$. We also consider the $\mathbb{R}$-subspace $\mathcal{O}_k^{\mathbb{R}}(\mathcal{F}) \subseteq \mathcal{O}_k(\mathcal{F})$ of self-adjoint (or *real*) elements of $\mathcal{O}_k(\mathcal{F})$, which are called *k-body observables*.

Remark II.1 (On the Terminology of k-Body Operators). There are different conventions regarding the notion of a *k-body operator*. Especially in the physics literature this terminology usually refers to what we call a k-particle operator. For example, a typical Hamiltonian in second quantization is given by (6). In the physical literature, this operator would then often be considered as a sum of a one- and two-body operator, whereas in our convention (6) is a sum of a one- and two-*particle* operator and therefore a two-body operator.

4. Hilbert-Schmidt geometry

Since in the finite-dimensional case we have $\mathcal{L}^2(\mathcal{F}) = \mathcal{B}(\mathcal{F})$, the mappings Θ, $\mathbf{c}^*$ and $\mathbf{c}$ introduced above are in fact mappings between (finite-dimensional) complex Hilbert spaces. In particular, using the natural isomorphism $\mathcal{F} \otimes \bar{\mathcal{F}} \cong \mathcal{L}^2(\mathcal{F})$ the map Θ defined in (11) gives rise to a linear automorphism

$$\alpha : \mathcal{L}^2(\mathcal{F}) \ni |\omega\rangle\langle\eta| \mapsto \mathbf{c}^*(\omega)\mathbf{c}(\eta) \in \mathcal{L}^2(\mathcal{F}). \tag{12}$$

III. TRACE FORMULAS

The goal of this section is to prove Proposition III.8, which provides a formula for the Hilbert-Schmidt inner product $\langle a \mid b\rangle_{\mathcal{L}^2(\mathcal{F})}$ between certain monomials a, b in creation and annhiliation operators. Our approach is to evaluate

$$\langle a \mid b\rangle_{\mathcal{L}^2(\mathcal{F})} = \mathrm{tr}\{a^* b\} = \sum_I \langle \varphi_I \mid a^* b \varphi_I\rangle_{\mathcal{F}} \tag{13}$$

for a suitable basis $(\varphi_I)_I$ of $\mathcal{F}$ (Proposition III.4). The main work then is to characterize the set $\mathfrak{M}$ of those I with nonvanishing contributions in (13) (Proposition III.5).

A. Basic notation

1. Set-theory

For a set X, we denote by $|X| \in \mathbb{N} \cup \{0, \infty\}$ the number of elements in X and by $\mathfrak{P}(X)$ the system of all subsets of X. Given sets $A_1, \ldots, A_\Lambda \in \mathfrak{P}(X)$, we write $A_1 \dot\cup \cdots \dot\cup A_\Lambda$ for their union $A_1 \cup \cdots \cup A_\Lambda$ when we want to indicate or require the $A_1, \ldots, A_\Lambda$ to be *mutually disjoint*, i.e., $A_\alpha \cap A_\beta = \emptyset$ for all $1 \leqslant \alpha < \beta \leqslant \Lambda$. Given a proposition p (e.g., a set-theoretic relation like $x \in A \cap B$) we write

$$\mathbb{1}(p) \doteq \begin{cases} 1 & \text{if } p \text{ is true,} \\ 0 & \text{otherwise.} \end{cases} \tag{14}$$

In the case where p is of the form $a = b$, we also write $\delta_{a,b}$ for $\mathbb{1}(p)$ (the *Kronecker Delta*).

2. Orbital bases and induced Fock bases

For the remainder of this paper, let $\mathfrak{h}$ be finite-dimensional, $\dim \mathfrak{h} \doteq n < \infty$, and assume that $\{\varphi_1, \ldots, \varphi_n\}$ is a fixed orthonormal basis. Let $\mathbb{N}_n \doteq \{1, \ldots, n\}$ and $\mathfrak{P}(\mathbb{N}_n)$ be the family of subsets of $\mathbb{N}_n$. For $A = \{a_1, \cdots, a_k\} \subseteq \mathbb{N}_n$ with $a_1 < \cdots < a_k$ we define

$$\varphi_A \doteq \begin{cases} \varphi_{a_1} \wedge \cdots \wedge \varphi_{a_k} & A \neq \emptyset, \\ \Omega_{\mathcal{F}} & \text{for } A = \emptyset. \end{cases} \tag{15}$$

Then, by definition (8) of the inner product on $\mathcal{F}$, $(\varphi_A)_{A\subseteq\mathbb{N}_n}$ is an *orthonormal* basis of $\mathcal{F}$ and, using Diracs Bra-ket notation, $(|\varphi_A\rangle\langle\varphi_B|)_{A,B\subseteq\mathbb{N}_n}$ is an orthonormal basis of $\mathcal{L}^2(\mathcal{F})$. Applying the generalized creation and annihilation operators, we further define for $A, B \subseteq \mathbb{N}_n$ the monomials

$$\mathbf{c}_A^* \doteq \mathbf{c}^*(\varphi_A), \quad \mathbf{c}_A \doteq \mathbf{c}(\varphi_A), \quad \mathbf{c}_{A,B} \doteq \mathbf{c}_A^*\mathbf{c}_B, \quad \mathbf{n}_A \doteq \mathbf{c}_{A,A}. \tag{16}$$

B. Monomials acting on the induced Fock bases

To efficiently deal with the signs occurring in computations with the monomials of the form (16), we introduce for $A_1, \ldots, A_k, B_1, \ldots, B_l \subseteq \mathbb{N}_n$ the *multisign*

$$\begin{bmatrix} A_1 \ldots A_k \\ B_1 \ldots B_l \end{bmatrix} \doteq \langle \varphi_{A_1} \wedge \cdots \wedge \varphi_{A_k} \mid \varphi_{B_1} \wedge \cdots \wedge \varphi_{B_l}\rangle. \tag{17}$$

The main use of these multisigns is to account for the signs occurring when reordering products of elements of the form (15), which is made precise by the following.

Lemma III.1. The multi-sign (17) vanishes, unless $A_1 \dot\cup \cdots \dot\cup A_k = B_1 \dot\cup \cdots \dot\cup B_l$. However, if $A_1 \dot\cup \cdots \dot\cup A_k = B_1 \dot\cup \cdots \dot\cup B_l$, then

$$\begin{bmatrix} A_1 \cdots A_k \\ B_1 \cdots B_l \end{bmatrix} (\varphi_{A_1} \wedge \cdots \wedge \varphi_{A_k}) = \varphi_{B_1} \wedge \cdots \wedge \varphi_{B_l}. \tag{18}$$

Proof. Since the φ_i anticommute as elements in $\mathcal{F}$, its clear that $\varphi_{A_1} \wedge \cdots \wedge \varphi_{A_k} = 0$ whenever the A_i are not mutually disjoint (and similarly for the B_i). Therefore the right-hand side of (17) trivially vanishes unless the A_i and B_i are mutually disjoint, respectively. Now consider the case where the A_i and B_i are mutually disjoint, but their unions A respectively B are not equal, say there is $a \in A \setminus B$ for some $a \in \mathbb{N}_n$. Then $\langle \varphi_a \mid \varphi_b\rangle = 0$ for all $b \in B$, thus $\langle \varphi_A \mid \varphi_B\rangle = 0$ by definition (8) and

$$\begin{bmatrix} A_1 \cdots A_k \\ B_1 \cdots B_l \end{bmatrix} = \pm\langle \varphi_A \mid \varphi_B\rangle = 0, \tag{19}$$

which proves the first part. For the second part, assume that $A_1 \dot\cup \cdots \dot\cup A_k = B_1 \dot\cup \cdots \dot\cup B_l$. Then, by anticommuting the φ_i, there is $\lambda \in \{-1, +1\}$ such that

$$\varphi \doteq \varphi_{A_1} \wedge \cdots \wedge \varphi_{A_k} = \lambda \cdot \varphi_{B_1} \wedge \cdots \wedge \varphi_{B_l} \doteq \lambda \cdot \tilde{\varphi}. \tag{20}$$

Using the same argument, we find that $\tilde{\varphi} = \pm\varphi_A$, thus $\|\tilde{\varphi}\|^2 = 1$. Consequently,

$$\begin{bmatrix} A_1 \cdots A_k \\ B_1 \cdots B_l \end{bmatrix} \varphi_{A_1} \wedge \cdots \wedge \varphi_{A_k} = \langle \varphi \mid \tilde{\varphi} \rangle \varphi = \lambda^2 \|\tilde{\varphi}\|^2 \tilde{\varphi} = \tilde{\varphi} = \varphi_{B_1} \wedge \cdots \wedge \varphi_{B_l}. \tag{21}$$

Lemma III.2. For $A, B, I \subseteq \mathbb{N}_n$ we have

$$\mathbf{c}_A^* \varphi_I = \mathbb{1}(A \cap I = \emptyset) \begin{bmatrix} A & I \\ A \cup I \end{bmatrix} \varphi_{A \cup I}, \tag{22}$$

$$\mathbf{c}_A \varphi_I = \mathbb{1}(A \subseteq I) \begin{bmatrix} A & I \setminus A \\ I \end{bmatrix} \varphi_{I \setminus A}. \tag{23}$$

Proof. If $A \cap I \neq \emptyset$ then $\mathbf{c}_A^* \varphi_I = 0$ and also the right hand side of (22) vanishes due to Lemma III.1. Otherwise, if $A \cap I = \emptyset$ then Lemma III.1 implies

$$\mathbf{c}_A^* \varphi_I = \varphi_A \wedge \varphi_I = \begin{bmatrix} A & B \\ A \cup B \end{bmatrix} \varphi_{A \cup B}, \tag{24}$$

which completes the proof of (22).

To prove (23) note that since $(\varphi_J)_{J \subseteq \mathbb{N}_n}$ is an orthonormal basis of $\mathcal{F}$, we have

$$\mathbf{c}_A \varphi_I = \sum_{J \subseteq \mathbb{N}_n} \langle \mathbf{c}_A \varphi_I \mid \varphi_J \rangle \varphi_J. \tag{25}$$

Unwinding the definitions and using Lemma III.1, we compute

$$\langle \mathbf{c}_A \varphi_I \mid \varphi_J \rangle \varphi_J = \langle \varphi_I \mid \varphi_A \wedge \varphi_J \rangle = \begin{bmatrix} & I \\ A & J \end{bmatrix} = \mathbb{1}(A \subseteq I) \mathbb{1}(J = A \setminus I) \begin{bmatrix} & I \\ A & I \setminus A \end{bmatrix}, \tag{26}$$

thus (23) follows by combining (25) and (26). ■

Remark III.3. Definition (15) of the Fock space basis elements φ_A naturally generalizes to the case where A is a *string* over the alphabet $\mathbb{N}_n$. Within this generalized framework, the multisign (17) can be interpreted as the antisymmetric Kronecker Delta (see, e.g., the "algebraic framework" in [21]).

C. Derivation of the trace formula

Proposition III.4. Let $A, B, C, D \subseteq \mathbb{N}_n$, then

$$\langle \mathbf{c}_{A,B} \mid \mathbf{c}_{C,D} \rangle_{\mathcal{L}^2(\mathcal{F})} = \sum_{I \in \mathfrak{M}} \begin{bmatrix} A & I \setminus B \\ C & I \setminus D \end{bmatrix} \begin{bmatrix} & I \\ B & I \setminus B \end{bmatrix} \begin{bmatrix} & I \\ D & I \setminus D \end{bmatrix}, \tag{27}$$

where $\mathfrak{M} \doteq \mathfrak{M}(A, B, C, D)$ is the family of all $I \subseteq \mathbb{N}_n$ such that

(1) $B \cup D \subseteq I$ and

(2) $A \,\dot{\cup}\, (I \setminus B) = C \,\dot{\cup}\, (I \setminus D)$.

Proof. Since $(\varphi_I)_{I \subseteq \mathbb{N}_n}$ is an orthonormal basis of $\mathcal{F}$, we have

$$\langle \mathbf{c}_{A,B} \mid \mathbf{c}_{C,D} \rangle = \mathrm{tr}\{\mathbf{c}_B^* \mathbf{c}_A \mathbf{c}_C^* \mathbf{c}_D\} = \sum_{I \subseteq \mathbb{N}_n} \langle \mathbf{c}_A^* \mathbf{c}_B \varphi_I \mid \mathbf{c}_C^* \mathbf{c}_D \varphi_I \rangle. \tag{28}$$

Using Lemma III.2, we compute for arbitrary $I \subseteq \mathbb{N}_n$

$$\mathbf{c}_{A,B} \varphi_I = \mathbf{c}_A^* (\mathbf{c}_B \varphi_I) = \mathbb{1}(B \subseteq I) \begin{bmatrix} & I \\ B & I \setminus B \end{bmatrix} \mathbf{c}_A^* \varphi_{I \setminus B} = \mathbb{1}(B \subseteq I) \mathbb{1}(A \cap (I \setminus B) = \emptyset) \begin{bmatrix} & I \\ B & I \setminus B \end{bmatrix} \varphi_A \wedge \varphi_{I \setminus B}, \tag{29}$$

and similarly for $\mathbf{c}_{C,D} \varphi_I$, which yields

$$\langle \mathbf{c}_{A,B} \varphi_I \mid \mathbf{c}_{C,D} \varphi_I \rangle = \mathbb{1}(I \in \mathfrak{M}) \begin{bmatrix} A & I \setminus B \\ C & I \setminus D \end{bmatrix} \begin{bmatrix} & I \\ B & I \setminus B \end{bmatrix} \begin{bmatrix} & I \\ D & I \setminus D \end{bmatrix}. \tag{30}$$

Combining (30) with (28), the assertion follows. ■

As stated in Proposition III.4, the contributing sets $I \subseteq \mathbb{N}_n$ in (27) must satisfy certain set-theoretic compatibility relations with the given sets A, B, C and D. Moreover, Proposition III.4 is of limited use because of the complicated signs occuring in (27). The main part of this paper therefore is to overcome these difficulties by a careful analysis of the set $\mathfrak{M}$ of contributing subsets $I \subseteq \mathbb{N}_n$.

Proposition III.5. Let $\mathfrak{M} = \mathfrak{M}(A, B, C, D)$ as in Proposition III.4. Then the following conditions are equivalent:

(1) $\mathfrak{M} \neq \emptyset$,

(2) $A \,\dot{\cup}\, (D \setminus B) = C \,\dot{\cup}\, (B \setminus D)$,

(3) $B \cup D \in \mathfrak{M}$,

(4) $A \setminus B = C \setminus D$ and $B \setminus A = D \setminus C$.

In any of these cases,

$$\mathfrak{M} = \{(B \cup D) \,\dot{\cup}\, N \mid N \cap (A \cup C) = \emptyset\}. \tag{31}$$

Proof. We will first show the equivalence of the conditions 1 to 3. The equivalence of 2 and 4 follows from a purely set-theoretic argument, see Lemma III.6 below.

1⇒2: Choose $M \in \mathfrak{M}$. By definition of $\mathfrak{M}$, $B \cup D \subseteq M$, we may write $M = (B \cup D) \,\dot{\cup}\, N$ so that $M \setminus B = (D \setminus B) \,\dot{\cup}\, N$. Since $A \cap (M \setminus B) = \emptyset$ by definition of $\mathfrak{M}$, also $A \cap (D \setminus B) \subseteq A \cap (M \setminus B) = \emptyset$, and similarly $C \cap (B \setminus D) = \emptyset$. Moreover, we have $A \cap N \subseteq A \cap [(D \setminus B) \cup N] = A \cap (M \setminus B) = \emptyset$ and similarly $C \cap N = \emptyset$. In summary, we have $[A \cup (D \setminus B)] \,\dot{\cup}\, N = A \cup (M \setminus B) = C \cup (M \setminus D) = [C \cup (B \setminus D)] \,\dot{\cup}\, N$ and therefore $A \cup (D \setminus B) = C \cup (B \setminus D)$.

2 ⇒ 3: By definition of $\mathfrak{M}$, $M \doteq B \cup D \in \mathfrak{M}$ if and only if $A \,\dot{\cup}\, (M \setminus B) = C \,\dot{\cup}\, (M \setminus D)$, but by construction $M \setminus B = D \setminus B$ and $M \setminus D = B \setminus D$.

3 ⇒ 1: this follows trivially.

Now it remains to prove (31), given the conditions 1-4 hold. Denote the right-hand side of (31) by $\tilde{\mathfrak{M}}$.

$\mathfrak{M} \subseteq \tilde{\mathfrak{M}}$: Choose some $M \in \mathfrak{M}$. Since $B \cup D \subseteq M$, we can write $M = (B \cup D) \,\dot{\cup}\, N$ for some $N \subseteq I \setminus (B \cup D)$ and now need to show that $N \cap (A \cup C) = \emptyset$. Since $A \cap (M \setminus B) = \emptyset$ by definition of $\mathfrak{M}$, also $A \cap (D \setminus B) \subseteq A \cap (M \setminus B) = \emptyset$, and similarly $C \cap (B \setminus D) = \emptyset$. Moreover, we have $A \cap N \subseteq A \cap [(D \setminus B) \cup N] = A \cap (M \setminus B) = \emptyset$ and similarly $C \cap N = \emptyset$, thus $N \cap (A \cup C) = \emptyset$.

$\tilde{\mathfrak{M}} \subseteq \mathfrak{M}$: Let $M \doteq (B \cup D) \,\dot{\cup}\, N \in \tilde{\mathfrak{M}}$, i.e., $N \cap (A \cup C) = \emptyset$. Clearly, $B \cup D \subseteq M$. Moreover, by assumption we have

$A \,\dot\cup\, (D \setminus B) = C \,\dot\cup\, (B \setminus D)$, thus

$$A \cap (M \setminus B) = A \cap [(D \setminus B) \cup N] = [A \cap (D \setminus B)] \cup (A \cap N) = \emptyset. \quad (32)$$

Similarly, $C \cap (M \setminus D) = \emptyset$. Finally,

$$A \cup (M \setminus B) = A \cup [(D \setminus B) \cup N] = [A \cup (D \setminus B)] \cup N = [C \cup (B \setminus D)] \cup N = C \cup (M \setminus D), \quad (33)$$

thus $M \in \mathfrak{M}$, which completes the proof. ■

Lemma III.6. Let X be a set and $A, B, C, D \subseteq X$. Then the following conditions are equivalent

(1) $A \,\dot\cup\, (D \setminus B) = C \,\dot\cup\, (B \setminus D)$,

(2) $A \setminus B = C \setminus D$ and $B \setminus A = D \setminus C$.

Proof. $1 \Rightarrow 2$: Let $x \in A \setminus B$. Then $x \in A \subseteq A \,\dot\cup\, (D \setminus B) = C \,\dot\cup\, (B \setminus D)$, thus $x \in C$. Moreover, since $(A \setminus B) \cap D = A \cap (D \setminus B) = \emptyset$, we have $x \notin D$, hence $x \in C \setminus D$. This shows that $A \setminus B \subseteq C \setminus D$. Exchanging the roles of A, C and B, D, respectively, also $C \setminus D \subseteq A \setminus B$.

Moreover, let $x \in B \setminus A$. If $x \notin D$ then $x \in B \setminus D \subseteq C \,\dot\cup\, (B \setminus D) = A \,\dot\cup\, (D \setminus B)$, i.e., $x \in A$, contradicting our assumption $x \in B \setminus A$. Hence, $x \in D$. Also, if $x \in C$ then $x \in C \,\dot\cup\, (B \setminus D) = A \,\dot\cup\, (D \setminus B)$, so $x \in D \setminus B$, which contradicts $x \in B$, hence $x \notin C$. This shows $B \setminus A \subseteq D \setminus C$. Again, by renaming A, B, C and D, we also see $D \setminus C \subseteq B \setminus A$.

$2 \Rightarrow 1$: We compute

$$A \cap (D \setminus B) = A \cap D \cap B^c = (A \setminus B) \cap D = (C \setminus D) \cap D = \emptyset. \quad (34)$$

Exchanging the roles of A, C and B, D, we also get $C \cap (B \setminus D) = \emptyset$. To show that $A \cup (D \setminus B) = C \cup (B \setminus D)$, first note that

$$A \cap D^c = (A \cap D^c \cap B) \cup (A \cap D^c \cap B^c) \subseteq (B \setminus D) \cup (A \setminus B) = (B \setminus D) \cup (C \setminus D) \subseteq C \cup (B \setminus D) \quad (35)$$

and

$$A \cap B = A \cap (A \cap B) \subseteq A \cap (B \setminus A)^c = A \cap (D \setminus C)^c = A \cap (C \cup D^c) = (A \cap C) \cup (A \cap D^c) \subseteq C \cup B \setminus D, \quad (36)$$

where we used (35) in the last step. Consequently, we conclude

$$A \overset{(34)}{\subseteq} A \cap (D \setminus B)^c = A \cap (D^c \cup B) = (A \cap D^c) \cup (A \cap B) \subseteq C \cup (B \setminus D), \quad (37)$$

where we used (35) and (36) in the last step. Moreover, we have

$$D \setminus B \overset{(34)}{\subseteq} (D \setminus B) \cap A^c = [(D \setminus B) \cap A^c \cap C] \cup [(D \setminus B) \cap A^c \cap C^c] \subseteq C \cup (D \cap C^c \cap A^c) = C \cup (B \cap A^c) \subseteq C \cup B, \quad (38)$$

and intersecting both sides of this inclusion with B^c, we obtain $D \setminus B \subseteq C \setminus B \subseteq C$. Combined with (37), this shows $A \cup (D \setminus B) \subseteq C \cup (B \setminus D)$ and, by exchanging the roles of A, C and B, D, the converse inclusion follows as well. ■

Remark III.7. Lemma III.6 can be further generalized by noting that the given conditions are also equivalent to the following (equivalent) conditions:

(1) $B \setminus D = A \setminus C$ and $D \setminus B = C \setminus A$,

(2) $B \,\dot\cup\, (A \setminus C) = D \,\dot\cup\, (C \setminus A)$.

Proposition III.8 (Trace Formula). Let $K, A, B \subseteq \mathbb{N}_n$ and $L, C, D \subseteq \mathbb{N}_n$ be mutually disjoint, respectively. Then

$$\langle \mathbf{n}_K \mathbf{c}_{A,B} \mid \mathbf{n}_L \mathbf{c}_{C,D} \rangle_{\mathcal{L}^2(\mathcal{F})} = \delta_{A,C}\delta_{B,D} \cdot 2^{n-|A\cup B\cup K\cup L|}. \quad (39)$$

Proof. Using Lemma III.1 and Lemma III.2, we find for any $I \subseteq \mathbb{N}_n$

$$\mathbf{n}_K \varphi_I = \mathbf{c}_K^*(\mathbf{c}_K \varphi_I) = \mathbb{1}(K \subseteq I) \begin{bmatrix} & I \\ K & I \setminus K \end{bmatrix} \mathbf{c}_K^* \varphi_{I\setminus K} = \mathbb{1}(K \subseteq I) \begin{bmatrix} & I \\ K & I \setminus K \end{bmatrix} \varphi_K \wedge \varphi_{I\setminus K} = \mathbb{1}(K \subseteq I)\varphi_I. \quad (40)$$

Combined with Lemma III.2, we therefore get for any $I \subseteq \mathbb{N}_n$

$$\mathbf{n}_K \mathbf{c}_{A,B} \varphi_I = \mathbb{1}(K \subseteq A \cup (I \setminus B))\mathbb{1}(B \subseteq I)\mathbb{1}(A \cap I \setminus B = \emptyset) \cdot \begin{bmatrix} & I \\ B & I \setminus B \end{bmatrix} \varphi_A \wedge \varphi_{I\setminus B}. \quad (41)$$

Consequently, we have with $\mathfrak{M} = \mathfrak{M}(A, B, C, D)$ as in Proposition III.5

$$\langle \mathbf{n}_K \mathbf{c}_{A,B} \varphi_I \mid \mathbf{n}_L \mathbf{c}_{C,D} \varphi_I \rangle = \mathbb{1}(I \in \mathfrak{M})\mathbb{1}[K \subseteq A \cup (I \setminus B)]\mathbb{1}[L \subseteq C \cup (I \setminus D)] \cdot \begin{bmatrix} A & I \setminus B \\ C & I \setminus D \end{bmatrix} \begin{bmatrix} & I \\ B & I \setminus B \end{bmatrix} \begin{bmatrix} & I \\ D & I \setminus D \end{bmatrix}. \quad (42)$$

Since $A \cap B = C \cap D = \emptyset$ by assumption, Proposition III.5 implies that $\mathbb{1}(I \in \mathfrak{M}) = \delta_{A,C}\delta_{B,D}\mathbb{1}(B \subseteq I)\mathbb{1}(I \cap A = \emptyset)$. Thus (42) equals

$$\delta_{A,C}\delta_{B,D}\mathbb{1}(B \subseteq I)\mathbb{1}(I \cap A = \emptyset)\mathbb{1}[K \cup L \subseteq A \cup (I \setminus B)]. \quad (43)$$

Now observe that for $A = C$ we have $L \cap A = L \cap C = \emptyset$, i.e., $K \cup L \subseteq A \cup (I \setminus B)$ is equivalent to $K \cup L \subseteq I \setminus B$, which is further equivalent to $K \cup L \subseteq I$. Hence (42) equals

$$\delta_{A,C}\delta_{B,D}\mathbb{1}(I \cap A = \emptyset)\mathbb{1}(B \cup K \cup L \subseteq I) \quad (44)$$

and, by summing (44) over all $I \subseteq \mathbb{N}_n$, we find

$$\langle \mathbf{n}_K \mathbf{c}_{A,B} \mid \mathbf{n}_L \mathbf{c}_{C,D} \rangle = \delta_{A,C}\delta_{B,D}|\mathfrak{P}[\mathbb{N}_n \setminus (A \cup B \cup K \cup L)]|. \quad (45)$$

■

Example III.9 (Trace of the Particle Number Operator). Let $\dim \mathfrak{h} = n < \infty$. By Lemma III.2, the *particle number operator* $\hat{\mathbb{N}} \doteq \sum_{i=1}^n n_i$ can be written as $\hat{\mathbb{N}} = \bigoplus_{k=0}^n k \cdot \mathrm{id}_{\wedge^k \mathfrak{h}}$. Consequently, its trace is given by $\sum_{k=0}^n k \cdot \binom{n}{k}$. On the other hand, Proposition III.8 implies $\mathrm{tr}\{\hat{\mathbb{N}}\} = \sum_{i=1}^n \langle \mathbb{1} \mid n_i \rangle = n \cdot 2^{n-1}$. Thus we proved the well-known identity

$$\sum_{k=0}^n k \binom{n}{k} = \mathrm{tr}\{\hat{\mathbb{N}}\} = n \cdot 2^{n-1}, \quad (46)$$

which also follows from differentiating $(1 + x)^n$ with respect to x and evaluating at $x = 1$.

IV. ORTHONORMALIZATION

In this section, given an orthonormal basis in $\mathfrak{h}$, we will construct explicit orthogonal bases of $\mathcal{L}^2(\mathcal{F})$ which restrict to the spaces of k-body operators and k-body observables, respectively.

A. Orthonormal basis of $\mathcal{L}^2(\mathcal{F})$

As implied by Proposition III.8, the monomials $(\mathbf{n}_K)_{K\subseteq\mathbb{N}_n}$ are *not* pairwise orthogonal. Inspired by computer algebraic experiments using Gram-Schmidt orthogonalization in low-dimensional cases, we introduce for $K\subseteq\mathbb{N}_n$ the element

$$b_K \doteq \sum_{I\subseteq K}(-2)^{|I|}\mathbf{n}_I \in \mathcal{L}^2(\mathcal{F}). \tag{47}$$

As we will see in Theorem IV.2, the b_K are pairwise orthogonal and can be used to construct an orthogonal basis of $\mathcal{L}^2(\mathcal{F})$. The key ingredient is the following lemma, which is essentially a consequence of the binomial formula.

Lemma IV.1. Let K, L be finite sets. Then

$$\sum_{I\subseteq K}\sum_{J\subseteq L}(-2)^{|I|+|J|}2^{-|I\cup J|} = \delta_{KL}. \tag{48}$$

Proof. Let $M \doteq K\cap L$. We compute

$$S \doteq \sum_{\substack{I\subseteq K\\ J\subseteq L}}(-2)^{|I|+|J|}2^{-|I\cup J|} = \sum_{\substack{I\subseteq K\\ J\subseteq L}}\frac{(-1)^{|I|+|J|}}{2^{-|I\cap J|}}, \tag{49}$$

where we used that $|I\cup J| = |I|+|J|-|I\cap J|$. Since every $I\subseteq K$ can be written uniquely as $I = I_1\,\dot{\cup}\, I_2$ with $I_1 \doteq (I\cap M)\subseteq M$ and $I_2 \doteq I\setminus I_1 \subseteq K\setminus M$ and (similarly for $J\subseteq L$), we find

$$S = \sum_{I_1,J_1\subseteq M}\frac{(-1)^{|I_1|+|J_1|}}{2^{-|I_1\cap J_1|}}\sum_{I_2\subseteq K\setminus M}(-1)^{|I_2|}\sum_{J_2\subseteq K\setminus M}(-1)^{|J_2|}. \tag{50}$$

By the binomial formula, for any finite set X and $a\in\mathbb{C}$ we have

$$\sum_{Y\subseteq X}a^{|Y|} = (1+a)^{|X|}. \tag{51}$$

In particular, for $a=-1$ we have $\sum_{Y\subseteq X}(-1)^{|Y|} = \mathbb{1}(X=\emptyset)$. Hence

$$\begin{aligned}\sum_{I_2\subseteq K\setminus M}(-1)^{|I_2|}\sum_{J_2\subseteq L\setminus M}(-1)^{|J_2|} &= \mathbb{1}(K\setminus M=\emptyset)\mathbb{1}(L\setminus M=\emptyset)\\ &= \mathbb{1}(K\subseteq L)\mathbb{1}(L\subseteq K) = \delta_{KL}.\end{aligned} \tag{52}$$

Inserting (52) in (50), we find

$$S = \delta_{KL}\sum_{I,J\subseteq M}\frac{(-1)^{|I|+|J|}}{2^{-|I\cap J|}}. \tag{53}$$

To evaluate the sum in (53), instead of summing over all $I,J\subseteq M$, we sum over all $X\doteq I\cap J\subseteq M$, $I_3\doteq I\setminus X\subseteq M\setminus X$ and $J_3\doteq J\setminus(X\,\dot{\cup}\, I_3)\subseteq M\setminus(X\,\dot{\cup}\, I_3)$ and apply (51) once again:

$$\begin{aligned}\sum_{\substack{I\subseteq M\\ J\subseteq M}}\frac{(-1)^{|I|+|J|}}{2^{-|I\cap J|}} &= \sum_{X\subseteq M}2^{|X|}\sum_{I_3\subseteq M\setminus X}(-1)^{|I_3|}\sum_{J_3\subseteq M\setminus(X\dot{\cup} I_3)}(-1)^{|J_3|}\\ &= \sum_{X\subseteq M}2^{|X|}\sum_{I_3\subseteq M\setminus X}(-1)^{|I_3|}\mathbb{1}(I_3 = M\setminus X)\\ &= \sum_{X\subseteq M}2^{|X|}(-1)^{|M\setminus X|} = (-1)^{|M|}\sum_{X\subseteq M}(-2)^{|X|}\\ &= (-1)^{|M|}(-1)^{|M|} = 1.\end{aligned} \tag{54}$$

Combining (53) and (54), the assertion follows. ■

Theorem IV.2. Let b_K be defined as in (47), then an orthonormal basis of $\mathcal{L}^2(\mathcal{F})$ is explicitly given by

$$\mathfrak{B} = \left\{\frac{b_K\mathbf{c}_{I,J}}{\sqrt{2^{n-|I\dot{\cup}J|}}}\in\mathcal{L}^2(\mathcal{F})\,\middle|\, K,I,J\subset\mathbb{N}_n \text{ pairwise disjoint}\right\}. \tag{55}$$

Proof. Let $K,A,B\subseteq\mathbb{N}_n$ and $L,C,D\subseteq\mathbb{N}_n$ be mutually disjoint, respectively. By definition of b_K and using Proposition III.8, we obtain

$$\begin{aligned}\langle b_K\mathbf{c}_{A,B}\mid b_L\mathbf{c}_{C,D}\rangle &= \sum_{I\subseteq K}\sum_{J\subseteq L}(-2)^{|I|+|J|}\langle\mathbf{n}_I\mathbf{c}_{A,B}\mid\mathbf{n}_J\mathbf{c}_{C,D}\rangle\\ &= \sum_{I\subseteq K}\sum_{J\subseteq L}(-2)^{|I|+|J|}\delta_{AC}\delta_{BD}2^{n-|(A\dot{\cup}B)\cup(I\cup J)|}\\ &= \delta_{AC}\delta_{BD}2^{n-|A\dot{\cup}B|}\left(\sum_{I\subseteq K}\sum_{J\subseteq L}(-2)^{|I|+|J|}2^{-|I\cup J|}\right)\\ &= \delta_{AC}\delta_{BD}2^{n-|A\dot{\cup}B|}\delta_{KL},\end{aligned} \tag{56}$$

where we used that for $A=C$, $B=D$, $I\subseteq K$ and $J\subseteq L$ we have $|A\cup B\cup I\cup J| = |A\cup B|+|I\cup J|$ in the third step and Lemma IV.1 (see below) in the last step. This shows that (55) is an orthonormal basis of its span S. Noting that

$$\dim S = |\mathfrak{B}| = |\{f:\mathbb{N}_n\to\{1,2,3,4\}\}| = 4^n = \dim\mathcal{L}^2(\mathcal{F}), \tag{57}$$

we conclude that $S=\mathcal{L}^2(\mathcal{F})$. ■

B. Orthonormal basis of k-body operators

Having established $\mathfrak{B}$ as an orthonormal basis of $\mathcal{L}^2(\mathcal{F})$, we now proceed and show that $\mathfrak{B}$ restricts to a basis of $\mathcal{O}_k(\mathcal{F})$ for all $k\in\mathbb{N}_0$ (Theorem IV.4).

Lemma IV.3. A basis of $\mathcal{O}_k(\mathcal{F})$ is explicitly given by

$$\mathfrak{B}_0 \doteq \{\mathbf{c}_{I,J}\,|\,I,J\subseteq\mathbb{N}_n,\ |I|+|J| = 2l \text{ with } 0\leqslant l\leqslant k\}, \tag{58}$$

in particular, we have $\dim_{\mathbb{C}}\mathcal{O}_k(\mathcal{F}) = \sum_{l=0}^{k}\binom{2n}{2l}$.

Proof. Since the mapping α defined in (12) is a linear automorphism of $\mathcal{L}^2(\mathcal{F})$, the $\mathbf{c}_{I,J} = \alpha(|\varphi_I\rangle\langle\varphi_J|)$ with $I,J\subseteq$

$\mathbb{N}_n$ form a basis of $\mathcal{L}^2(\mathcal{F})$. An element $A \in \mathcal{L}^2(\mathcal{F})$ of the form

$$A = \sum_{I,J\subseteq\mathbb{N}_n} A_{I,J}\mathbf{c}_{I,J} \tag{59}$$

is a k-body operator if and only if $A_{I,J} = 0$ whenever $|I| + |J|$ is odd or $|I| + |J| > 2k$. In other words, (58) a basis of $\mathcal{O}_k(\mathcal{F})$ and

$$\dim_{\mathbb{C}} \mathcal{O}_k(\mathcal{F}) = |\mathfrak{B}_0| = \sum_{l=0}^{k}\sum_{i=0}^{2l}\binom{n}{i}\binom{n}{2l-i} = \sum_{l=0}^{k}\binom{2n}{2l}, \tag{60}$$

where we used Vandermonde's identity. ■

Theorem IV.4. The orthonormal $\mathbb{C}$-basis $\mathfrak{B}$ of $\mathcal{L}^2(\mathcal{F})$ given in Theorem IV.2 restricts to an orthonormal basis $\mathfrak{B}_k$ of the space $\mathcal{O}_k(\mathcal{F})$ of k-body operators. More specifically, we have

$$\mathfrak{B}_k \doteq \mathfrak{B} \cap \mathcal{O}_k(\mathcal{F}) = \left\{ \frac{b_K\mathbf{c}_{I,J}}{\sqrt{2^{n-|I\cup J|}}} \,\middle|\, \begin{matrix} K, I, J \subset \mathbb{N}_n \text{ pairwise disjoint,} \\ |I| + |J| + 2|K| = 2l \text{ with } 0 \leqslant l \leqslant k \end{matrix} \right\}. \tag{61}$$

Proof. Let $b \in \mathfrak{B}$, i.e.,

$$b = b_K\mathbf{c}_{I,J} = \sum_{L\subseteq K} \frac{(-2)^{|L|}}{\sqrt{2^{n-|I\cup J|}}} n_L\mathbf{c}_{I,J} \tag{62}$$

for $K, I, J \subseteq \mathbb{N}_n$ pairwise disjoint. Since $n_L\mathbf{c}_{I,J} = \pm\mathbf{c}_{I\dot\cup L,J\dot\cup L}$ for every $L \subseteq K$, Lemma IV.3 implies that $b \in \mathcal{O}_k(\mathcal{F})$ if and only if $|I| + |J| + 2|K| = 2l$ for some $0 \leqslant l \leqslant k$, which proves (61). Finally, noting that we have a bijection $\mathfrak{B} \ni b_K\mathbf{c}_{I,J} \to \mathbf{c}_{I\dot\cup K,J\dot\cup K} \in \mathfrak{B}_0$ with inverse $\mathbf{c}_{I,J} \mapsto b_{I\cap J}\mathbf{c}_{I\setminus J,J\setminus I}$, we conclude that $|\mathfrak{B}_k| = |\mathfrak{B}_0| = \dim \mathcal{O}_k(\mathcal{F})$ and therefore $\mathfrak{B}_k$ is a basis of $\mathcal{O}_k(\mathcal{F})$. ■

C. Orthonormal basis of k-body observables

The orthonormal $\mathbb{C}$-basis $\mathfrak{B}$ of $\mathcal{L}^2(\mathcal{F})$ as given in Theorem IV.2 does not immediately restrict to bases of k-body *observables*, since $\mathfrak{B}_{\mathbb{C}}$ contains elements which are not self-adjoint. For example, if $I \subset \mathbb{N}_n$ is nonempty, then

$$(b_\emptyset\mathbf{c}_{I,\emptyset})^* = \mathbf{c}_I \neq \mathbf{c}_I^* = b_\emptyset\mathbf{c}_{I,\emptyset}.$$

However, $\mathfrak{B}_{\mathbb{C}}$ has the special property that $\mathfrak{B}_{\mathbb{C}} = \{b^* \mid b \in \mathfrak{B}_{\mathbb{C}}\}$, which allows us to obtain an orthonormal basis of self-adjoint elements by a suitable unitary transformation of $\mathcal{L}^2(\mathcal{F})$. The general principle of this idea is given by the following.

Lemma IV.5. Let $\mathcal{H}$ be a finite-dimensional, complex Hilbert space with real structure J and $\mathfrak{B}$ an orthonormal $\mathbb{C}$-basis with $J(\mathfrak{B}) \subseteq \mathfrak{B}$. Then

(1) $\mathfrak{B}$ is of the form

$$\mathfrak{B} = (a_1, \dots, a_k, b_1, b_1^*, \dots, b_l, b_l^*) \text{ with } a_i = a_i^* \quad \forall 1 \leqslant i \leqslant k. \tag{63}$$

(2) An orthonormal $\mathbb{R}$-basis of $V_{\mathbb{R}} \doteq \{v \in V \mid J(v) = v\}$ is given by

$$\mathfrak{B}_{\mathbb{R}} \doteq (a_1, \dots, a_k, \sqrt{2}\mathrm{Re}(b_1), \sqrt{2}\mathrm{Im}(b_1), \dots, \sqrt{2}\mathrm{Re}(b_l), \sqrt{2}\mathrm{Im}(b_l)). \tag{64}$$

[Here, $\mathrm{Re}(a) \doteq \frac{1}{2}(a + a^*)$ and $\mathrm{Im}(a) \doteq \frac{1}{2i}(a - a^*)$ denote the real- and imaginary part of a, respectively]

Proof. 1 Since $J(\mathfrak{B}) \subseteq \mathfrak{B}$ and $J^2 = 1$, J defines an action of $\mathbb{Z}/2\mathbb{Z}$ on $\mathfrak{B}$. The set $\mathfrak{B}$ is decomposed into the orbits of this action, which are either of length 1 or length 2 by the orbit-stabilizer Theorem. By construction, the orbits of length 1 are of the form $\{a = a^*\}$ and the orbits of length 2 are of the form $\{b, b^*\}$, hence the desired form (63) is obtained by selecting an element in each orbit of $\mathfrak{B}$.

2 Let $f : V \to V$ be the $\mathbb{C}$-linear map mapping $\mathfrak{B}$ to $\mathfrak{B}_{\mathbb{R}}$. Then f is represented with respect to $\mathfrak{B}$ by the unitary matrix

$$\mathbb{1}_k \oplus \underbrace{U \oplus \cdots \oplus U}_{l \text{ times}} \quad \text{with} \quad U \doteq \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} \in U(2). \tag{65}$$

In particular, with $\mathfrak{B}$ also $\mathfrak{B}_{\mathbb{R}}$ is an orthonormal $\mathbb{C}$-basis of V and $|\mathfrak{B}_{\mathbb{R}}| = |\mathfrak{B}|$. By construction we have $\mathfrak{B}_{\mathbb{R}} \subseteq V_{\mathbb{R}}$, thus $\mathfrak{B}_{\mathbb{R}}$ is an orthonormal $\mathbb{R}$-basis of its $\mathbb{R}$-span U. Since U is an $\mathbb{R}$-subspace of $V_{\mathbb{R}}$ of dimension $|\mathfrak{B}_{\mathbb{R}}| = |\mathfrak{B}| = \dim_{\mathbb{C}} V = \dim_{\mathbb{R}} V_{\mathbb{R}}$, we have $U = V_{\mathbb{R}}$, i.e., $\mathfrak{B}_{\mathbb{R}}$ is an orthonormal $\mathbb{R}$-basis of $V_{\mathbb{R}}$. ■

Remark IV.6. The ordering (63) of the basis $\mathfrak{B}$ in Lemma IV.7 is not uniquely determined. However, if $\mathfrak{B}$ is endowed with a prescribed ordering, then $\mathfrak{B}$ can can be uniquely reordered in the form (63) by requiring $a_1 < \cdots < a_k$ and $b_i < b_i^*$ for all $1 \leqslant i \leqslant l$.

Theorem IV.7. An orthonormal $\mathbb{C}$-basis of $\mathcal{L}^2(\mathcal{F})$ is explicitly given by

$$\mathfrak{B}^{\mathbb{R}} = \{2^{-n/2}b_K \mid K \subseteq \mathbb{N}_n\} \,\dot\cup\, \left\{ \frac{b_K(\mathbf{c}_{I,J} \pm \mathbf{c}_{J,I})}{2^{(n+1-|I\cup J|)/2}} \,\middle|\, \begin{matrix} K, I, J \subset \mathbb{N}_n \text{ mutually} \\ \text{disjoint and } I < J \end{matrix} \right\}.$$

$\mathfrak{B}^{\mathbb{R}}$ restricts to an orthonormal basis of the space $\mathcal{O}_k^{\mathbb{R}}(\mathcal{F})$ of k-body observables for every $k \in \mathbb{N}_0$. More specifically, an orthonormal $\mathbb{R}$-basis of $\mathcal{O}_k^{\mathbb{R}}(\mathcal{F})$ is given by

$$\mathfrak{B}_k^{\mathbb{R}} \doteq \mathfrak{B}^{\mathbb{R}} \cap \mathcal{O}_k^{\mathbb{R}}(\mathcal{F}) = \{b_K \mid K \subseteq \mathbb{N}_n \text{ and } |K| \leqslant k\} \,\dot\cup\, \left\{ \frac{b_K(\mathbf{c}_{I,J} \pm \mathbf{c}_{J,I})}{2^{(n+1-|I\cup J|)/2}} \,\middle|\, \begin{matrix} K, I, J \subset \mathbb{N}_n \text{ pairwise disjoint, } I < J \\ \text{and } |I| + |J| + 2|K| = 2l \text{ with } 0 \leqslant l \leqslant k \end{matrix} \right\},$$

where $I < J$ is to be understood with respect to the lexicographic ordering.

Proof. The first statement follows immediately from Lemma IV.7 applied to the orthonormal $\mathbb{C}$-basis $\mathfrak{B}$ as given in Theorem IV.2, which has been ordered according to Remark IV.6 by defining $b_K\mathbf{c}_{A,B} < b_L\mathbf{c}_{C,D} \Leftrightarrow (K, A, B) < (L, C, D)$ (lexicographic order). ■

V. ALTERNATIVE CONSTRUCTION OF AN ORTHONORMAL BASIS

In this section, we provide an alternative construction of an orthonormal basis of $\mathcal{L}^2(\mathcal{F})$ which restricts to an orthonormal basis of $\mathcal{O}_k(\mathcal{F})$ in the sense of Theorem IV.4. This construction was already presented in Sec. 8 of [1], but the corresponding proofs were deferred to a somewhat obscure reference.

Fix an orthonormal basis $\varphi_1, \dots, \varphi_n$ of the one-particle Hilbert space $\mathfrak{h}$ and consider for $j = 1, \dots, 2n$ the operator

$$a_j \doteq \begin{cases} c_k^* + c_k & \text{if } j = 2k \text{ is even,} \\ \mathrm{i}(c_k^* - c_k) & \text{if } j = 2k+1 \text{ is odd.} \end{cases} \tag{66}$$

By definition, the a_j are self-adjoint and, by the CAR (9), satisfy

$$\{a_j, a_k\} = 2\delta_{jk},\, a_j^2 = \mathbb{1}. \tag{67}$$

Moreover, for a subset $J = \{j_1 < \cdots < j_l\} \subseteq \mathbb{N}_{2n}$ we define $a_J \doteq a_{j_1} \cdots a_{j_l}$ where $a_\emptyset \doteq \mathbb{1}$ by convention. The following result has been suggested to us by Gosset. We present a proof which only relies on the algebraic properties (67) of the elements a_j.

Theorem V.1. An orthonormal $\mathbb{C}$-basis of $\mathcal{L}^2(\mathcal{F})$ is given by

$$\widetilde{\mathfrak{B}} \doteq \{2^{-n/2} a_J \mid K \subseteq \mathbb{N}_{2n}\}. \tag{68}$$

Moreover, $\widetilde{\mathfrak{B}}$ restricts to an orthonormal basis $\widetilde{\mathfrak{B}}_k$ of $\mathcal{O}_k(\mathcal{F})$ for every $k \in \mathbb{N}_0$, where

$$\widetilde{\mathfrak{B}}_k \doteq \widetilde{\mathfrak{B}} \cap \mathcal{O}_k(\mathcal{F}) = \left\{ a_J \,\middle|\, \begin{matrix} J \subseteq \mathbb{N}_{2n} \text{ and} \\ |J| = 2l \text{ with } 0 \leqslant l \leqslant \mathrm{k} \end{matrix} \right\}. \tag{69}$$

Proof. We will first show that $\langle a_J \mid a_K\rangle = 2^n \delta_{JK}$ for all $J, K \subseteq \mathbb{N}_{2n}$. If $J = K = \{j_1 < \cdots < j_l\}$ then, by self-adjointness of the a_j and $a_j^2 = \mathbb{1}_\mathcal{F}$ we have

$$\begin{aligned} \langle a_J \mid a_K\rangle &= \mathrm{tr}\{a_J^* a_J\} = \mathrm{tr}\{a_{j_l} \cdots a_{j_1} a_{j_1} \cdots a_{j_l}\} \\ &= \mathrm{tr}\{\mathbb{1}_\mathcal{F}\} = 2^n. \end{aligned} \tag{70}$$

Now consider the case $J \neq K$. Without loss of generality, we may assume $J \cap K = \emptyset$ because if $i \in J \cap K$ then, by (67),

$$\langle a_J \mid a_K\rangle_{\mathcal{L}^2(\mathcal{F})} = \mathrm{tr}\{a_J^* a_K\} = \pm\, \mathrm{tr}\{a^*_{J\setminus\{i\}} a_{K\setminus\{i\}}\}. \tag{71}$$

Moreover, by setting $I \doteq J \dot\cup K$ and noting that $\langle a_J \mid a_K\rangle = \pm\,\mathrm{tr}\{a_I\}$, it suffices to show that $\mathrm{tr}\{a_I\} = 0$ for all nonempty $I \subseteq \mathbb{N}_{2n}$. First, consider the case where $|I| = l > 0$ is even. Then, writing $I = \{i_1 < \cdots < i_l$ we obtain, using (67) and cyclicity of trace,

$$\begin{aligned} \mathrm{tr}\{a_I\} &= \mathrm{tr}\{a_{i_1} \cdots a_{i_l}\} = (-1)^{l-1}\,\mathrm{tr}\{a_{i_l} a_{i_1} \cdots a_{i_{l-1}}\} \\ &= (-1)^{l-1}\,\mathrm{tr}\{a_{i_1} \cdots a_{i_l}\} = -\,\mathrm{tr}\{a_I\}, \end{aligned} \tag{72}$$

thus $\mathrm{tr}\{a_I\} = 0$. On the other hand, if $|I|$ is odd, then consider the natural $\mathbb{Z}_2$-grading $\mathcal{F} = \mathcal{F}_+ \oplus \mathcal{F}_-$ on $\mathcal{F}$ induced by $\chi \doteq (-1)^{\hat{\mathbb{N}}}$, i.e., $\mathcal{F}_\pm \doteq \ker\{\chi \mp \mathbb{1}\}$. By definition, a_i is *odd* with respect to this grading for any $i \in \mathbb{N}_{2n}$, hence also a_I is odd when $|I|$ is odd and therefore $\mathrm{tr}\{a_I\} = 0$. We have thus proved that

$$\langle a_J \mid a_K\rangle = 2^n \delta_{JK}, \quad J, K \subseteq \mathbb{N}_{2n}. \tag{73}$$

In particular, since $|\widetilde{\mathfrak{B}}_k| = 2^{2n} = \dim \mathcal{L}^2(\mathcal{F})$, $\widetilde{\mathfrak{B}}_k$ is an ONB of $\mathcal{L}^2(\mathcal{F})$.

To prove (69) note that, by definition, an element a_J is an j-particle operator with $j \doteq |J|$ for any $J \subseteq \mathbb{N}_{2n}$, hence a_J is a k-body operator if and only if $|J| = 2l$ for some $0 \leqslant l \leqslant k$. By (69) and Lemma IV.3,

$$|\widetilde{\mathfrak{B}}_k| = \sum_{l=0}^{k} \binom{2n}{2l} = \dim \mathcal{O}_k(\mathcal{F}), \tag{74}$$

thus $\widetilde{\mathfrak{B}}_k$ is an orthonormal basis of $\mathcal{O}_k(\mathcal{F})$. ■

Remark V.2 (Relation between $\mathfrak{B}$ and $\widetilde{\mathfrak{B}}$). If $n > 0$, the orthonormal bases $\widetilde{\mathfrak{B}}$ and $\mathfrak{B}$ are different. In fact, $\mathfrak{B} \cap \widetilde{\mathfrak{B}} = \{2^{-n/2}\mathbb{1}_\mathcal{F}\}$ since the elements of $\mathfrak{B}$ are homogeneous with respect to the natural grading $\mathcal{F} = \bigoplus_{k\geqslant 0} \bigwedge^k \mathfrak{h}$, whereas the elements $a_J \in \widetilde{\mathfrak{B}}$ are inhomogeneous whenever $J \neq \emptyset$.

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