Orthogonalization of fermion $k$-Body operators
and representability

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Abstract

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 $k$.

1 Introduction

1.1 Motivation: Representability problems

In quantum chemistry, molecules are usually modeled as non-relativistic many-fermion systems (Born-Oppenheimer approximation). More specifically, the Hilbert space of these systems is given by the fermion Fock space $\mathcal{F} = \mathcal{F}_\Lambda(\mathcal{h})$, where $\mathcal{h}$ is the (complex) Hilbert space of a single electron (e.g. $\mathcal{h} = L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$), and the Hamiltonian $\hat{H}$ 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

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

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

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 $r_\tau$, the $k$-body reduction of $\tau$, that only encodes the expectation values of
The representability problem for way. As it turns out, in the finite-dimensional case tor. In this case the two-body reduction i of) the set of density matrices on k most important case is B subspace of k because in concrete applications S sentability problems as discussed here is usually invisible in the pertinent litera- T raditional representability problems The general framework of repre- nsability framework breaks down in the infinite-dimension case, because

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

**Traditional representability problems** The general framework of representability problems as discussed here is usually invisible in the pertinent literature, because in concrete applications \( S \) is almost always chosen to be (a subset of) the set of density matrices on \( F \) and \( O_k(F)' \) is identified with a suitable subspace of \( B(F) \). 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 \( \wedge^2 \mathfrak{h} \).

**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 \( \rho \) can be introduced as the image \( \pi_k(\rho) \) under the orthogonal projection onto \( O_k(F) \) [see §8],

\[
\pi_k : \mathcal{L}^2(F) \to O_k(F) \subseteq \mathcal{L}^2(F).
\]

As it turns out, in the finite-dimensional case \( \pi_k \) is an equivalent description of the map \( i'_k \) introduced above. The reason for this is that in the finite-dimensional case \( B(F) = \mathcal{L}^2(F) \), where \( \mathcal{L}^2(F) \) denotes the Hilbert space of Hilbert-Schmidt operators on \( F \), and we may identify \( B(F)' = \mathcal{L}^2(F) \) and \( O_k(F)' \cong O_k(F) \) 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 infinite-dimensional case, because then \( k \)-body operators are generally not Hilbert-Schmidt anymore.
1.2 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 [10]. 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 \[5, 9, 21\] and the development of (still very inaccurate) lower bound methods based on representability conditions. In 1978 Erdahl introduced a new class of representability conditions \[8\], which were found to significantly increase the accuracy of lower bound methods \[4\]. In 2005 the representability problem for the one-body reduced density matrices of pure states was solved by Klyachko \[11\] 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 \[15\]. However, the general representability problem has been found to be computationally intractible \[15\], even on a quantum computer \[12\]. Computational advances \[13\] enabled a range of recent applications \[17, 18, 16\]. Representability methods have also proved useful in Hartree-Fock theory \[2\]. For a more detailed overview on the history of representability problems, we refer to \[14\] and \[6\].

1.3 Goal and main results

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

**Theorem 1 (Main Theorem)** Let \( \dim \mathfrak{h} = n < \infty \) 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 \( c_I \doteq c(\varphi_{i_1}) \cdots c(\varphi_{i_j}) \) and \( n_I \doteq c_I^* c_I \), where \( c(\varphi) \) denotes the usual fermion annihilation operator. Then the following is found

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

\[
\frac{1}{\sqrt{2^{n-|I\cup J|}}} \sum_{A \subseteq L} (-2)^{|A|} n_A c_I^* c_J,
\]

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

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

Orthogonal decompositions of \( \mathcal{L}^2(\mathcal{F}) \) as implied by **Theorem 1** have already been introduced, e. g., in \[8\] 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 \( (69) \), see Sec. 5. The

\[1\] See Fig. 1 for a geometric interpretation of this result and its relation to the representability problem.
Figure 1: Geometric interpretation of the representability problem for density matrices in finite dimensions: the mapping of density matrices $\rho \in P_1$ to its $k$-body reduction as orthogonal projection $\pi_k$ onto the subspace $O_k(F) \subseteq L^2(F)$ of $k$-body operators. The representability problem amounts to finding an efficient characterization of the image $\pi_k(P_1)$ within $O_k(F)$. The orthonormal basis $\mathfrak{B}$ given in Theorem 1 is adapted to this situation as it restricts to an orthonormal basis $\mathfrak{B} \cap O_k(F)$ of $O_k(F)$ for every $k \in \mathbb{N}_0$.

Orthonormal basis elements given in Theorem 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 2** Let $\rho$ 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 $\gamma$. Then

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

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

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

**1.4 Overview of the paper**

In Sec. 2 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. 3 we compute the Hilbert-Schmidt scalar product of specific monomials in creation and annihilation operators (Proposition 11). In Sec. 4 we prove Theorem 1 in two steps, as follows.

1. The orthonormal basis $\mathfrak{B}$ of $L^2(F)$ is constructed in Theorem 14.

2. In Theorem 16 we show that $\mathfrak{B} \cap O_k(F)$ is a basis of $O_k(F)$ for all $k \in \mathbb{N}_0$.

In many cases one also considers the space $O_k^R(F)$ of selfadjoint $k$-body operators. We generalize the above results in Theorem 19 where we apply a suitable
unitary transformation $U$ on $\mathcal{L}^2(\mathcal{F})$ and show that the orthonormal basis $U(\mathcal{B})$ of $\mathcal{L}^2(\mathcal{F})$ restricts to an orthonormal basis of $\mathcal{O}_k^2(\mathcal{F})$ for all $k \in \mathbb{N}_0$. Finally, in Sec. 5 we present an alternative approach for constructing an orthonormal basis of $\mathcal{L}^2(\mathcal{F})$ with properties as in Theorem 1, which was first communicated to us by Gosset \footnote{dgosset@uwaterloo.ca} and turned out to be already present in \cite{8}.

1.5 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

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

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

$$
H \geq \sum_{i,j} t_{ij} c_i^* c_j + \frac{1}{2} \sum_{i,j,k,l} V_{ij;kl} c_i^* c_j^* P_{\mathcal{A}c_l c_k} \equiv H_{\mathcal{A}}.
$$

Thus $E_0(H_{\mathcal{A}})$ is a lower bound, which are usually more difficult to derive than upper bounds, for the ground-state energy $E_0(H)$ 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 $\mathcal{B}$ given by Theorem 1 and a suitable choice of $\mathcal{A} \subset \mathcal{B}$ leads to a nontrivial lower bound $E_0(H_{\mathcal{A}})$ of $E_0(H)$.

2 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 $n \equiv \text{dim}_\mathbb{C} \mathfrak{h} < \infty$ throughout the paper.

2.1 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 $\text{dim} \mathfrak{h} = \infty$. \footnote{dgosset@uwaterloo.ca}
**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 $\langle \varphi | \psi \rangle_{\mathcal{H}}$ and is assumed to be anti-linear 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 $\mathcal{H}$.

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

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

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

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

**CAR** Associated with $\mathcal{F}$, there are natural linear, respectively anti-linear, 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 $c(\varphi) = [c^*(\varphi)]^*$ and $c^*(f)\omega = f \wedge \omega$, respectively. They satisfy the canonical anti-commutation relations (CAR)

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

and $c(\phi)\Omega_\mathcal{F} = 0$ for all $\phi \in \mathfrak{h}$. The mappings $c^*, c : \mathfrak{h} \to \mathcal{B}(\mathcal{F})$ induce a representation of the (abstract) CAR algebra generated by $\mathfrak{h}$ [see [3, Sec. 5.2.2]], called the Fock representation.

**Density matrices** We denote by $\mathcal{P} \doteq L^1_+(\mathcal{F}) \subseteq L^2(\mathcal{F})$ the cone of positive, trace-class operators on $\mathcal{F}$. Elements $\rho$ from the convex subset $\mathcal{P}_1 \subseteq \mathcal{P}$ which are normalized in the sense that $\text{tr}\{\rho\} = 1$ 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 [1, Theorem 2.7]].

### 2.2 Finite-dimensional features

We conclude this section by summarizing some more specific notions, which (partly) depend on the finite-dimensionality of $\mathfrak{h}$.
Generalized creation- and annihilation operators  By the CAR, we may extend $c, c^*$ to linear, respectively anti-linear, maps $c^*, c : \mathcal{F} \to \mathcal{B}(\mathcal{F})$ via
\[
c^*(\omega)\eta = \omega \wedge \eta, \quad c(\omega) = [c^*(\omega)]^*.
\] (10)
Note that the definition of $c$ is such that $c(\phi_1 \wedge \cdots \wedge \phi_k) = c(\phi_k) \cdots c(\phi_1)$, for all $\phi_1, \ldots, \phi_k \in \mathfrak{h}$. We call $c^*, c$ the generalized creation- and annihilation operators.\(^3\) Note that the CAR (9) do not hold for $c^*$ and $c$, when $\phi, \psi \in \mathfrak{h}$ are replaced by general $\omega, \eta \in \mathcal{F}$.

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 $\{c^*(\phi) \mid \phi \in \mathfrak{h}\}$. In the finite-dimensional case, $\mathcal{A} = \mathcal{B}(\mathcal{F})$ [see \cite{3}, Theorem 5.2.5] and we have a natural linear map
\[
\Theta : \mathcal{F} \otimes \bar{\mathcal{F}} \ni \omega \otimes \bar{\eta} \mapsto c^*(\omega)c(\eta) \in \mathcal{A},
\] (11)
where $\bar{\mathcal{F}}$ denotes the conjugate Hilbert space of $\mathcal{F}$ [see \cite{7}, Sec. 1.2]. In fact, by the Wick Theorem, $\Theta$ is surjective and therefore an isomorphism, as the vector spaces involved are all finite-dimensional.

$k$-Body Operators  Let $k \in \mathbb{N}_0$. We call a sum of operators of the form $c^*(\omega)c(\eta)$ 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 $l \leq k$ 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 $\mathcal{O}_k^R(\mathcal{F}) \subseteq \mathcal{O}_k(\mathcal{F})$ of selfadjoint (or real) elements of $\mathcal{O}_k(\mathcal{F})$, which are called $k$-body observables.

Remark 3 (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. □

The Hilbert-Schmidt geometry  Since in the finite-dimensional case we have $\mathcal{L}^2(\mathcal{F}) = \mathcal{B}(\mathcal{F})$, the mappings $\Theta, c^*, c$ 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 $\Theta$ defined in (11) gives rise to a linear automorphism
\[
\alpha : \mathcal{L}^2(\mathcal{F}) \ni |\omega\rangle\langle \eta| \mapsto c^*(\omega)c(\eta) \in \mathcal{L}^2(\mathcal{F}).
\] (12)
\(^3\)This terminology is also used, e.g, in \cite{13}.
3 Trace Formulas

The goal of this section is to prove Proposition 11 which provides a formula for the Hilbert-Schmidt inner product \( \langle a \mid b \rangle_{L^2(F)} \) between certain monomials \( a, b \) in creation and annihilation operators. Our approach is to evaluate

\[
\langle a \mid b \rangle_{L^2(F)} = \text{tr}\{a^* b\} = \sum_{I} \langle \varphi_I \mid a^* b \varphi_I \rangle_F \tag{13}
\]

for a suitable basis \((\varphi_I)_I\) of \( F \) (Proposition 7). The main work then is to characterize the set \( M \) of those \( I \) with non-vanishing contributions in (13) (Proposition 8).

3.1 Basic notation

Set-theory For a set \( X \), we denote by \(|X| \in \mathbb{N} \cup \{0, \infty\}\) the number of elements in \( X \) and by \( \mathcal{P}(X) \) the system of all subsets of \( X \). Given sets \( A_1, \ldots, A_\Lambda \in \mathcal{P}(X) \), we write \( \bigcupdot_{\ell=1}^{\Lambda} A_\ell \) for their union 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 \( 1 \leq \alpha < \beta \leq \Lambda \). Given a proposition \( p \) (e.g., a set-theoretic relation like \( x \in A \cap B \)) we write \( 1(p) = \begin{cases} 1 & \text{if } p \text{ is true}, \\ 0 & \text{otherwise}. \end{cases} \tag{14} \)

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

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

\[
\varphi_A \doteq \begin{cases} 
\varphi_{a_1} \wedge \cdots \wedge \varphi_{a_k} & A \neq \emptyset, \\
\Omega_F & A = \emptyset.
\end{cases} \tag{15}
\]

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

\[
c_A^* \doteq c^*(\varphi_A), \quad c_A \doteq c(\varphi_A), \quad c_{A,B} \doteq c_A^* c_B, \quad n_A \doteq c_{A,A}. \tag{16}
\]

3.2 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 \( A_1, \ldots, A_k, B_1, \ldots, B_l \subseteq \mathcal{N}_n \) the multi-sign

\[
\begin{bmatrix} A_1 & \cdots & A_k \\ B_1 & \cdots & B_l \end{bmatrix} \doteq (\varphi_{A_1} \wedge \cdots \wedge \varphi_{A_k} \mid \varphi_{B_1} \wedge \cdots \wedge \varphi_{B_l}). \tag{17}
\]
The main use of these multi-signs is to account for the signs occurring when reordering products of elements of the form \((15)\), which is made precise by the following.

**Lemma 4** The multi-sign \((17)\) vanishes, unless \(A_1 \cup \cdots \cup A_k = B_1 \cup \cdots \cup B_l\). However, if \(A_1 \cup \cdots \cup A_k = B_1 \cup \cdots \cup B_l\), then

\[
\begin{bmatrix}
A_1 & \cdots & A_k \\
B_1 & \cdots & B_l
\end{bmatrix}
(\varphi_{A_1} \land \cdots \land \varphi_{A_k}) = \varphi_{B_1} \land \cdots \land \varphi_{B_l}.
\] (18)

**Proof** Since the \(\varphi_i\) anti-commute as elements in \(\mathcal{F}\), it’s clear that \(\varphi_{A_1} \land \cdots \land \varphi_{A_k} = 0\) 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 \(\langle \varphi_a | \varphi_b \rangle = 0\) for all \(b \in B\), thus \(\langle \varphi_A | \varphi_B \rangle = 0\) by definition \((8)\) and

\[
\begin{bmatrix}
A_1 & \cdots & A_k \\
B_1 & \cdots & B_l
\end{bmatrix}
\varphi_{A_1} \land \cdots \land \varphi_{A_k} = \pm \langle \varphi_A | \varphi_B \rangle = 0,
\] (19)

which proves the first part. For the second part, assume that \(A_1 \cup \cdots \cup A_k = B_1 \cup \cdots \cup B_l\). Then, by anti-commuting the \(\varphi_i\), there is \(\lambda \in \{-1, +1\}\) such that

\[
\varphi \equiv \varphi_{A_1} \land \cdots \land \varphi_{A_k} = \lambda \cdot \varphi_{B_1} \land \cdots \land \varphi_{B_l} \equiv \lambda \cdot \tilde{\varphi}
\] (20)

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

\[
\begin{bmatrix}
A_1 & \cdots & A_k \\
B_1 & \cdots & B_l
\end{bmatrix}
\varphi_{A_1} \land \cdots \land \varphi_{A_k} = \langle \varphi | \tilde{\varphi} \rangle \varphi = \lambda^2 \|\tilde{\varphi}\|^2 \varphi = \tilde{\varphi}
\] (22)

\[= \varphi_{B_1} \land \cdots \land \varphi_{B_l}.
\]

**Lemma 5** For \(A, B, I \subseteq \mathbb{N}_n\) we have

\[
c_A^* \varphi_I = 1(A \cap I = \emptyset) \begin{bmatrix} A & I \end{bmatrix} \varphi_{A \cup I} \] (23)

\[
c_A^* \varphi_I = 1(A \subseteq I) \begin{bmatrix} A & I \setminus A \end{bmatrix} \varphi_{I \setminus A}.
\] (24)

**Proof** If \(A \cap I \neq \emptyset\) then \(c_A^* \varphi_I = 0\) and also the right hand side of \((23)\) vanishes due to [Lemma 4]. Otherwise, if \(A \cap I = \emptyset\) then [Lemma 4] implies

\[
c_A^* \varphi_I = \varphi_A \land \varphi_I = \begin{bmatrix} A & B \end{bmatrix} \varphi_{A \cup B},
\] (25)
which completes the proof of (23).

To prove (24) note that, since \((\varphi_J)_{J \subseteq \mathbb{N}_n}\) is an orthonormal basis of \(\mathcal{F}\), we have
\[
c_A \varphi_I = \sum_{J \subseteq \mathbb{N}_n} \langle c_A \varphi_I | \varphi_J \rangle \varphi_J.
\] (26)

Unwinding the definitions and using Lemma 4, we compute
\[
\langle c_A \varphi_I | \varphi_J \rangle \varphi_J = \langle \varphi_I | \varphi_A \wedge \varphi_J \rangle = [I \ A \ J] [A \ I \ A \ I \ A].
\] (28)

thus (24) follows by combining (26) and (28).

\[\square\]

Remark 6 Definition (15) of the Fock space basis elements \(\varphi_A\) naturally generalizes to the case where \(A\) is a string over the alphabet \(\mathbb{N}_n\). Within this generalized framework, the multi-sign (17) can be interpreted as the anti-symmetric Kronecker Delta (see, e.g., the “algebraic framework” in [20]).

3.3 Derivation of the trace formula

Proposition 7 Let \(A, B, C, D \subseteq \mathbb{N}_n\), then
\[
\langle c_{A,B} | c_{C,D} \rangle_{L^2(\mathcal{F})} = \sum_{I \in \mathfrak{M}} [A \ I \ B][C \ I \ D][B \ I \ B][D \ I \ D].
\] (29)

where \(\mathfrak{M} = \mathfrak{M}(A, B, C, D)\) is the family of all \(I \subseteq \mathbb{N}_n\) such that
1. \(B \cup D \subseteq I\) and
2. \(A \cup (I \ \setminus B) = C \cup (I \ \setminus D)\).

Proof Since \((\varphi_I)_{I \subseteq \mathbb{N}_n}\) is an orthonormal basis of \(\mathcal{F}\), we have
\[
\langle c_{A,B} | c_{C,D} \rangle = \text{tr}\{c_B^* c_A c_C^* c_D\} = \sum_{I \subseteq \mathbb{N}_n} \langle c_A^* c_B \varphi_I | c_C^* c_D \varphi_I \rangle.
\] (30)

Using Lemma 5 we compute for arbitrary \(I \subseteq \mathbb{N}_n\)
\[
c_{A,B} \varphi_I = c_A^* (c_B \varphi_I) = \mathbb{1}(B \subseteq I) [B \ I \ B] c_A^* \varphi_I \setminus B
\]
\[
= \mathbb{1}(B \subseteq I) \mathbb{1}(A \cap (I \ \setminus B) = \emptyset) [B \ I \ B] \varphi_A \wedge \varphi_I \setminus B,
\] (31)

and similarly for \(c_{C,D} \varphi_I\), which yields
\[
\langle c_{A,B} \varphi_I | c_{C,D} \varphi_I \rangle = \mathbb{1}(I \in \mathfrak{M}) [A \ I \ B][C \ I \ D][B \ I \ B][D \ I \ D].
\] (32)

Combining (32) with (30), the assertion follows.

\[\square\]
As stated in Proposition 7, the contributing sets $I \subseteq \mathbb{N}_n$ in (29) must satisfy certain set-theoretic compatibility relations with the given sets $A, B, C$ and $D$. Moreover, Proposition 7 is of limited use because of the complicated signs occurring in (29). The main part of this paper therefore is to overcome these difficulties by a careful analysis of the set $\mathcal{M}$ of contributing subsets $I \subseteq \mathbb{N}_n$.

**Proposition 8** Let $\mathcal{M} = \mathcal{M}(A, B, C, D)$ as in Proposition 7. Then the following conditions are equivalent:

1. $\mathcal{M} \neq \emptyset$,
2. $A \cup (D \setminus B) = C \cup (B \setminus D)$,
3. $B \cup D \in \mathcal{M}$,
4. $A \setminus B = C \setminus D$ and $B \setminus A = D \setminus C$.

In any of these cases,

$$\mathcal{M} = \{(B \cup D) \cup N \mid N \cap (A \cup C) = \emptyset\}. \quad (33)$$

**Proof** We will first show the equivalence of the conditions. The equivalence of $2$ and $1$ follows from a purely set-theoretic argument, see Lemma 9 below.

$\mathcal{M} \subseteq \mathcal{M}$: Choose $M \in \mathcal{M}$. By definition of $\mathcal{M}$, $B \cup D \subseteq M$, we may write $M = (B \cup D) \cup N$ so that $M \setminus B = (D \setminus B) \cup N$. Since $A \cap (M \setminus B) = \emptyset$ by definition of $\mathcal{M}$, 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 $(A \cup (D \setminus B)) \cup N = A \cup (M \setminus B) = C \cup (M \setminus D) = (C \cup (B \setminus D)) \cup N$ and therefore $A \cup (D \setminus B) = C \cup (B \setminus D)$.

$\mathcal{M} \subseteq \mathcal{M}$: By definition of $\mathcal{M}$, $M \vdash B \cup D \in \mathcal{M}$ if and only if $A \cup (M \setminus B) = C \cup (M \setminus D)$, but by construction $M \setminus B = D \setminus B$ and $M \setminus D = B \setminus D$.

This follows trivially.

Now it remains to prove (33), given the conditions hold. Denote the right-hand side of (33) by $\mathcal{M}$.

$\mathcal{M} \subseteq \mathcal{M}$: Choose some $M \in \mathcal{M}$. Since $B \cup D \subseteq M$, we can write $M = (B \cup D) \cup N$ 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 $\mathcal{M}$, 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 $N \cap (A \cup C) = \emptyset$.

$\mathcal{M} \subseteq \mathcal{M}$: Let $M \vdash (B \cup D) \cup N \in \mathcal{M}$, i.e., $N \cap (A \cup C) = \emptyset$. Clearly, $B \cup D \subseteq M$. Moreover, by assumption we have $A \cup (D \setminus B) = C \cup (B \setminus D)$, thus

$$A \cap (M \setminus B) = A \cap (D \setminus B \cup N) = (A \cap (D \setminus B)) \cup (A \cap N) = \emptyset. \quad (34)$$

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

$$A \cup (M \setminus B) = A \cup (D \setminus B \cup N) = (A \cup (D \setminus B)) \cup N = (C \cup (B \setminus D)) \cup N = C \cup (M \setminus D), \quad (35)$$
thus \( M \in \mathfrak{M} \), which completes the proof. \hfill \blacksquare

**Lemma 9** Let \( X \) be a set and \( A, B, C, D \subseteq X \). Then the following conditions are equivalent

1. \( A \cup (D \setminus B) = C \cup (B \setminus D) \),
2. \( A \setminus B = C \setminus D \) and \( B \setminus A = D \setminus C \).

**Proof** \( \text{[1]} \Rightarrow \text{[2]} \). Let \( x \in A \setminus B \). Then \( x \in A \subseteq A \cup (D \setminus B) = C \cup (B \setminus D) \), 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 \( x \in D \setminus C \). Let \( x \notin D \), thus \( x \notin A \). Moreover, since \( (D \setminus C) \setminus A = A \cup (D \setminus B) \), i.e., \( x \notin B \setminus A \). Hence, \( x \in D \). Also, if \( x \in C \) then \( x \in C \setminus (B \setminus D) = A \cup (D \setminus B) \), so \( x \in D \setminus B \), which contradicts \( x \notin D \). This shows \( D \setminus C \subseteq B \setminus A \). Again, by renaming \( A, B, C \) and \( D \), we also see \( D \setminus C \subseteq B \setminus A \).

\( \text{[2]} \Rightarrow \text{[1]} \). We compute

\[
A \cap (D \setminus B) = A \cap D \cap B^c = (A \setminus B) \cap D = (C \setminus D) \cap D = \emptyset. \tag{37}
\]

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

\[
A \cap D^c = (A \cap D^c \cap B) \cup (A \cap D^c \cap B^c) \subseteq (B \setminus D) \cup (A \setminus B) = (B \setminus D) \cup (C \setminus D) \subseteq C \cup (B \setminus D) \tag{38}
\]

and

\[
A \cap B = A \cap (A \cap B) \subseteq A \cap (B \setminus A)^c = A \cap (D \setminus C)^c = A \cap (C \cup D^c) = (A \cap C) \cup (A \cap D^c) \subseteq C \cup (B \setminus D), \tag{39}
\]

where we used \( \text{[38]} \) in the last step. Consequently, we conclude

\[
A \subseteq A \cap (D \setminus B)^c = A \cap (D^c \cup B) = (A \cap D^c) \cup (A \cap B) \subseteq C \cup (B \setminus D), \tag{40}
\]

where we used \( \text{[38]} \) and \( \text{[39]} \) in the last step. Moreover, we have

\[
D \setminus B \subseteq (D \setminus B) \cap A^c = [(D \setminus B) \cap A^c \cap C] \cup [(D \setminus B) \cap A^c \cap C^c] \subseteq C \cup (D \cap C^c \cap A^c) = C \cup (B \cap A^c) \subseteq C \cup B, \tag{41}
\]

and intersecting both sides of this inclusion with \( B^c \), we obtain \( D \setminus B \subseteq C \setminus B \subseteq C \). Combined with \( \text{[1]} \), 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. \hfill \blacksquare
Remark 10 Lemma 9 can be further generalized by noting that the given conditions are also equivalent to the following (equivalent) conditions:

1. \( B \triangleleft D = A \triangleleft C \) and \( D \triangleleft B = C \triangleleft A \),

2. \( B \cup (A \cap C) = D \cup (C \cap A) \).

Proposition 11 (Trace Formula) Let \( K, A, B \subseteq \mathbb{N}_n \) and \( L, C, D \subseteq \mathbb{N}_n \) be mutually disjoint, respectively. Then

\[
\langle n_K c_{A,B} | n_L c_{C,D} \rangle_{\mathcal{L}^2(F)} = \delta_{A,C} \delta_{B,D} \cdot 2^{n-|A \cup B \cup K \cup L|}.
\] (42)

Proof Using Lemma 4 and Lemma 5, we find for any \( I \subseteq \mathbb{N}_n \)

\[
n_K \varphi_I = c_K^* (c_K \varphi_I) = \mathbb{1}(K \subseteq I) \begin{bmatrix} I \\ K \end{bmatrix} c_K^* \varphi_{I \setminus K} = \mathbb{1}(K \subseteq I) \begin{bmatrix} I \\ K \end{bmatrix} \varphi_{K \cap \varphi_{I \setminus K}} = \mathbb{1}(K \subseteq I) \varphi_I.
\] (43)

Combined with Lemma 6 we therefore get for any \( I \subseteq \mathbb{N}_n \)

\[
n_K c_{A,B} \varphi_I = \mathbb{1}(K \subseteq A \cup (I \setminus B)) \mathbb{1}(B \subseteq I) \mathbb{1}(A \cap I \setminus B = \emptyset) \cdot \begin{bmatrix} I \\ B \end{bmatrix} \varphi_{A \cap \varphi_{I \setminus B}}.
\] (44)

Consequently, we have with \( \mathcal{M} = \mathcal{M}(A, B, C, D) \) as in Proposition 8

\[
\langle n_K c_{A,B} \varphi_I | n_L c_{C,D} \varphi_I \rangle = \mathbb{1}(I \in \mathcal{M}) \mathbb{1}[K \subseteq A \cup (I \setminus B)] \mathbb{1}[L \subseteq C \cup (I \setminus D)] \cdot \begin{bmatrix} A \\ C \end{bmatrix} \begin{bmatrix} I \\ B \end{bmatrix} \mathbb{1}[I \subseteq D \cap I \setminus D] \] (45)

Since \( A \cap B = C \cap D = \emptyset \) by assumption, Proposition 8 implies that \( I \in \mathcal{M} \) = \( \delta_{A,C} \delta_{B,D} \mathbb{1}(B \subseteq I) \mathbb{1}(A \cap I = \emptyset) \). Thus (15) equals

\[
\delta_{A,C} \delta_{B,D} \mathbb{1}(B \subseteq I) \mathbb{1}(A \cap I = \emptyset) \mathbb{1}[K \cup L \subseteq A \cup (I \setminus B)].
\] (46)

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 (15) equals

\[
\delta_{A,C} \delta_{B,D} \mathbb{1}(I \cap A = \emptyset) \mathbb{1}(B \cup K \cup L \subseteq I)
\] (47)

and, by summing (47) over all \( I \subseteq \mathbb{N}_n \), we find

\[
\langle n_K c_{A,B} | n_L c_{C,D} \rangle = \delta_{A,C} \delta_{B,D} \mathcal{M}[\mathbb{N}_n \setminus (A \cup B \cup K \cup L)].
\] (48) ■
Example 12 (Trace of the Particle Number Operator) Let \( \text{dim } \mathfrak{h} = n < \infty \). By Lemma 5, the particle number operator \( \hat{N} = \sum_{k=0}^{n} k \cdot \text{id}_{A^k \mathfrak{h}} \). Consequently, its trace is given by \( \sum_{k=0}^{n} k \cdot \binom{n}{k} \). On the other hand, Proposition 11 implies \( \text{tr}\{\hat{N}\} = \sum_{i=1}^{n} \langle 1 | n_i \rangle = n \cdot 2^{n-1} \). Thus we proved the well-known identity

\[
\sum_{k=0}^{n} k \binom{n}{k} = \text{tr}\{\hat{N}\} = n \cdot 2^{n-1}, \tag{49}
\]

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

\[\Box\]

4 Orthonormalization

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

4.1 Orthonormal basis of \( L^2(\mathcal{F}) \)

As implied by Proposition 11 the monomials \( (n_K)_{K \subseteq \mathbb{N}_n} \) 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

\[
b_K = \sum_{I \subseteq K} (-2)^{|I|} n_I \in L^2(\mathcal{F}). \tag{50}
\]

As we will see in Theorem 14 the \( b_K \) are pairwise orthogonal and can be used to construct an orthogonal basis of \( L^2(\mathcal{F}) \). The key ingredient is the following lemma, which is essentially a consequence of the binomial formula.

Lemma 13 Let \( K, L \) be finite sets. Then

\[
\sum_{I \subseteq K} \sum_{J \subseteq L} (-2)^{|I|+|J|} 2^{-|I \cup J|} = \delta_{KL}. \tag{51}
\]

Proof Let \( M = K \cap L \). We compute

\[
S = \sum_{I \subseteq K \cap L} (-2)^{|I|+|J|} 2^{-|I \cup J|} = \sum_{I \subseteq K \cap L} \frac{(-1)^{|I|+|J|}}{2^{-|I \cap J|}}, \tag{52}
\]

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

\[
S = \sum_{I_1, J_1 \subseteq M} \frac{(-1)^{|I_1|+|J_1|}}{2^{-|I_1 \cap J_1|}} \sum_{I_2 \subseteq K \setminus M} (-1)^{|I_2|} \sum_{J_2 \subseteq K \setminus M} (-1)^{|J_2|}. \tag{53}
\]
By the binomial formula, for any finite set $X$ and $a \in \mathbb{C}$ we have
\[ \sum_{Y \subseteq X} a^{|Y|} = (1 + a)^{|X|}. \quad (54) \]
In particular, for $a = -1$ we have $\sum_{Y \subseteq X} (-1)^{|Y|} = 1(X = \emptyset)$. Hence
\[ \sum_{I_2 \subseteq K \setminus M} \sum_{J_2 \subseteq L \setminus M} (-1)^{|I_2|} (-1)^{|J_2|} = 1(K \setminus M = \emptyset) 1(L \setminus M = \emptyset) \]
\[ = 1(K \subseteq L) 1(L \subseteq K) = \delta_{KL}. \quad (55) \]
Inserting (55) in (53), we find
\[ S = \delta_{KL} \sum_{I,J \subseteq M} \frac{(-1)^{|I|+|J|}}{2^{-|I|+|J|}}. \quad (56) \]
To evaluate the sum in (56), instead of summing over all $I,J \subseteq M$, we sum over all $X = I \cap J \subseteq M$, $I_3 = I \setminus X \subseteq M \setminus X$ and $J_3 = J \setminus (X \cup I_3) \subseteq M \setminus (X \cup I_3)$ and apply (54) once again:
\[ \sum_{I,J \subseteq M} \frac{(-1)^{|I|+|J|}}{2^{-|I|+|J|}} = \sum_{X \subseteq M} 2^{|X|} \sum_{I_3 \subseteq M \setminus X} (-1)^{|I_3|} \sum_{J_3 \subseteq M \setminus (X \cup I_3)} (-1)^{|J_3|} \]
\[ = \sum_{X \subseteq M} 2^{|X|} \sum_{I_3 \subseteq M \setminus X} (-1)^{|I_3|} \mathbb{1}(I_3 = M \setminus X) \]
\[ = \sum_{X \subseteq M} 2^{|X|} (-1)^{|M\setminus X|} = (-1)^{|M|} \sum_{X \subseteq M} (-2)^{|X|} \]
\[ = (-1)^{|M|} (-1)^{|M|} = 1. \quad (57) \]
Combining (56) and (57), the assertion follows.

**Theorem 14** Let $b_K$ be defined as in (50), then an orthonormal basis of $L^2(F)$ is explicitly given by
\[ \mathcal{B} = \left\{ \frac{b_K e_{I,J}}{\sqrt{2^n-|I|+|J|}} \in L^2(F) \right| K, I, J \subseteq \mathbb{N}_n \text{ pairwise disjoint} \right\}. \quad (58) \]

**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 11 we obtain
\[ \langle b_K e_{A,B} | b_L e_{C,D} \rangle = \sum_{I \subseteq K} \sum_{J \subseteq L} (-2)^{|I|+|J|} \langle n_I e_{A,B} | n_J e_{C,D} \rangle \]
\[ = \sum_{I \subseteq K} \sum_{J \subseteq L} (-2)^{|I|+|J|} \delta_{AC} \delta_{BD} 2^{n- |A \cup B|} 2^{- |I|+|J|} \]
\[ = \delta_{AC} \delta_{BD} 2^{n- |A \cup B|} \left( \sum_{I \subseteq K} \sum_{J \subseteq L} (-2)^{|I|+|J|} 2^{- |I|+|J|} \right) \]
\[ = \delta_{AC} \delta_{BD} 2^{n- |A \cup B|} \delta_{KL}, \quad (59) \]
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 13 (see below) in the last step. This shows that (58) is an orthonormal basis of its span $S$. Noting that

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

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

\[\blacksquare\]

### 4.2 Orthonormal basis of $k$-body operators

Having established $\mathcal{B}$ as an orthonormal basis of $L^2(\mathcal{F})$, we now proceed and show that $\mathcal{B}$ restricts to a basis of $\mathcal{O}_k(\mathcal{F})$ for all $k \in \mathbb{N}_0$ (Theorem 16).

**Lemma 15** A basis of $\mathcal{O}_k(\mathcal{F})$ is explicitly given by

$$\mathcal{B}_0 = \{ c_{I, J} | I, J \subseteq \mathbb{N}_n, |I| + |J| = 2l \text{ with } 0 \leq l \leq k \},$$

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

**Proof** Since the mapping $\alpha$ defined in (12) is a linear automorphism of $L^2(\mathcal{F})$, the $c_{I, J} = \alpha (|\psi_I\rangle\langle \psi_J|)$ with $I, J \subseteq \mathbb{N}_n$ form a basis of $L^2(\mathcal{F})$. An element $A \in L^2(\mathcal{F})$ of the form

$$A = \sum_{I, J \subseteq \mathbb{N}_n} A_{I, J} c_{I, J}$$

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, (61) a basis of $\mathcal{O}_k(\mathcal{F})$ and

$$\dim \mathcal{O}_k(\mathcal{F}) = |\mathcal{B}_0| = \sum_{l=0}^{k} \sum_{i=0}^{2l} \binom{n}{i} \binom{n}{2l-i} = \sum_{l=0}^{k} \binom{2n}{2l},$$

where we used Vandermonde’s identity.

\[\blacksquare\]

**Theorem 16** The orthonormal C-space $\mathcal{B}$ of $L^2(\mathcal{F})$ given in Theorem 14 restricts to an orthonormal basis $\mathcal{B}_k$ of the space $\mathcal{O}_k(\mathcal{F})$ of $k$-body operators. More specifically, we have

$$\mathcal{B}_k \equiv \mathcal{B} \cap \mathcal{O}_k(\mathcal{F}) = \left\{ \frac{b_K c_{I, J}}{\sqrt{2^{n-|I\cup J|}}} \bigg| K, I, J \subseteq \mathbb{N}_n \text{ pairwise disjoint, } |I| + |J| + 2|K| = 2l \text{ with } 0 \leq l \leq k \right\}.$$  

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

$$b = b_K c_{I, J} = \sum_{L \subseteq K} \frac{(-1)^{|L|}}{\sqrt{2^{n-|I\cup J|}}} n_L c_{I, J}$$

for $K, I, J \subseteq \mathbb{N}_n$ pairwise disjoint. Since $n_L c_{I, J} = \pm c_{I \cup L, J \cup L}$ for every $L \subseteq K$, Lemma 15 implies that $b \in \mathcal{O}_k(\mathcal{F})$ if and only if $|I| + |J| + 2|K| = 2l$ for some $0 \leq l \leq k$, which proves (64). Finally, noting that we have a bijection $\mathcal{B} \ni b_K c_{I, J} \mapsto c_{I \cup K, J \cup K} \in \mathcal{B}_0$ with inverse $c_{I, J} \mapsto b_{I \cup J} c_{I, J}$, we conclude that $|\mathcal{B}_k| = |\mathcal{B}_0| = \dim \mathcal{O}_k(\mathcal{F})$ and therefore $\mathcal{B}_k$ is a basis of $\mathcal{O}_k(\mathcal{F})$.

\[\blacksquare\]
4.3 Orthonormal basis of $k$-body observables

The orthonormal $C$-basis $\mathcal{B}$ of $L^2(\mathcal{F})$ as given in [Theorem 14] does not immediately restrict to bases of $k$-body observables, since $\mathcal{B}_C$ contains elements which are not self-adjoint. For example, if $I \subset \mathbb{N}_n$ is non-empty, then

$$(b_0 \epsilon I, 0)^* = c_I \neq c_I^* = b_0 \epsilon I, 0.$$

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

**Lemma 17** Let $\mathcal{H}$ be a finite-dimensional, complex Hilbert space with real structure $J$ and $\mathcal{B}$ an orthonormal $C$-basis with $J(\mathcal{B}) \subseteq \mathcal{B}$. Then

1. $\mathcal{B}$ is of the form

$$\mathcal{B} = (a_1, \ldots, a_k, b_1, b_1^*, \ldots, b_l, b_l^*) \text{ with } a_i = a_i^* \quad \forall 1 \leq i \leq k. \quad (66)$$

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

$$\mathcal{B}_R \doteq \left( a_1, \ldots, a_k, \sqrt{2} \Re(b_1), \sqrt{2} \Im(b_1), \ldots, \sqrt{2} \Re(b_l), \sqrt{2} \Im(b_l) \right) \quad (67)$$

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

**Proof** Since $J(\mathcal{B}) \subseteq \mathcal{B}$ and $J^2 = 1$, $J$ defines an action of $\mathbb{Z}/2\mathbb{Z}$ on $\mathcal{B}$. The set $\mathcal{B}$ 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 (66) is obtained by selecting an element in each orbit of $\mathcal{B}$.

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

$$1_k \oplus \underbrace{U \oplus \cdots \oplus U}_{l \text{ times}} \text{ with } U \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} \in U(2). \quad (68)$$

In particular, with $\mathcal{B}$ also $\mathcal{B}_R$ is an orthonormal $C$-basis of $\mathcal{V}$ and $|\mathcal{B}_R| = |\mathcal{B}|$. By construction we have $\mathcal{B}_R \subseteq \mathcal{V}_R$, thus $\mathcal{B}_R$ is an orthonormal $\mathbb{R}$-basis of its $\mathbb{R}$-span $U$. Since $U$ is an $\mathbb{R}$-subspace of $\mathcal{V}_R$ of dimension $|\mathcal{B}_R| = |\mathcal{B}| = \dim_C \mathcal{V} = \dim_R \mathcal{V}_R$, we have $U = \mathcal{V}_R$, i.e., $\mathcal{B}_R$ is an orthonormal $\mathbb{R}$-basis of $\mathcal{V}_R$. $\blacksquare$

**Remark 18** The ordering (66) of the basis $\mathcal{B}$ in Theorem 14 is not uniquely determined. However, if $\mathcal{B}$ is endowed with a prescribed ordering, then $\mathcal{B}$ can be uniquely reordered in the form (66) by requiring $a_1 < \cdots < a_k$ and $b_i < b_i^*$ for all $1 \leq i \leq l. \quad \square$
Theorem 19 An orthonormal \( \mathbb{C} \)-basis of \( L^2(\mathcal{F}) \) is explicitly given by

\[
\mathcal{B}^R = \left\{ 2^{-n/2} b_K \mid K \subseteq \mathbb{N}_n \right\} \cup \left\{ \frac{b_K (c_{I,J} \pm c_{J,I})}{2(n+1-|I\cup J|)/2} \mid K, I, J \subseteq \mathbb{N}_n \text{ mutually disjoint and } I < J \right\}.
\]

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

\[
\mathcal{B}^k = \mathcal{B}^R \cap \mathcal{O}_k^R(\mathcal{F}) = \left\{ b_K \mid K \subseteq \mathbb{N}_n \text{ and } |K| \leq k \right\} \cup \left\{ \frac{b_K (c_{I,J} \pm c_{J,I})}{2(n+1-|I\cup J|)/2} \mid K, I, J \subseteq \mathbb{N}_n \text{ pairwise disjoint, } I < J \text{ and } |I| + |J| + 2|K| = 2l \text{ with } 0 \leq l \leq k \right\},
\]

where \( I < J \) is to be understood with respect to the lexicographic ordering.

Proof The first statement follows immediately from Theorem 19 applied to the orthonormal \( \mathbb{C} \)-basis \( \mathcal{B} \) as given in Theorem 14, which has been ordered according to Remark 13 by defining \( b_K c_{A,B} < b_L c_{C,D} \Leftrightarrow (K, A, B) < (L, C, D) \) (lexicographic order).

5 Alternative construction of an orthonormal basis

In this section, we provide an alternative construction of an orthonormal basis of \( L^2(\mathcal{F}) \) which restricts to an orthonormal basis of \( \mathcal{O}_k(\mathcal{F}) \) in the sense of Theorem 16. This construction was already presented in [8, Sec. 8], but the corresponding proofs were deferred to a somewhat obscure reference.

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

\[
a_j = \begin{cases} 
  c_k^* + c_k & \text{if } j = 2k \text{ is even,} \\
  i(c_k^* - c_k) & \text{if } j = 2k + 1 \text{ is odd.}
\end{cases} \tag{69}
\]

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

\[
\{a_j, a_k\} = 2\delta_{jk}, \quad a_j^2 = \mathbb{1}. \tag{70}
\]

Moreover, for a subset \( J = \{j_1 < \cdots < j_l\} \subseteq \mathbb{N}_{2n} \) we define \( a_J = a_{j_1} \cdots a_{j_l} \), where \( a_{\emptyset} \equiv \mathbb{1} \) by convention. The following result has been suggested to us by Gosset. We present a proof which only relies on the algebraic properties \( \text{(70)} \) of the elements \( a_j \).

Theorem 20 An orthonormal \( \mathbb{C} \)-basis of \( L^2(\mathcal{F}) \) is given by

\[
\widetilde{\mathcal{B}} = \left\{ 2^{-n/2} a_J \mid K \subseteq \mathbb{N}_{2n} \right\}. \tag{71}
\]
Moreover, \( \mathfrak{B} \) restricts to an orthonormal basis \( \mathfrak{B}_k \) of \( \mathcal{O}_k(\mathcal{F}) \) for every \( k \in \mathbb{N}_0 \), where

\[
\mathfrak{B}_k = \mathfrak{B} \cap \mathcal{O}_k(\mathcal{F}) = \left\{ a_J \middle| J \subseteq \mathbb{N}_{2n} \text{ and } |J| = 2l \text{ with } 0 \leq l \leq k \right\}, \tag{72}
\]

**Proof** We will first show that \( \langle a_J | a_K \rangle = 2^n \delta_{JK} \) 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 \( a_j^2 = 1_F \) we have

\[
\langle a_J | a_K \rangle = \text{tr} \{ a_J^* a_J \} = \text{tr} \{ a_{j_1} \cdots a_{j_l} a_{j_l} \cdots a_{j_1} \} = \text{tr} \{ 1_F \} = 2^n.
\tag{73}
\]

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 (70),

\[
\langle a_J | a_K \rangle_{\mathcal{L}^2(\mathcal{F})} = \text{tr} \{ a_J^* a_K \} = \pm \text{tr} \{ a_{J \setminus \{ i \}} a_{K \setminus \{ i \}} \}. \tag{74}
\]

Moreover, by setting \( I = J \cup K \) and noting that \( \langle a_J | a_K \rangle = \pm \text{tr} \{ a_I \} \), it suffices to show that \( \text{tr} \{ a_I \} = 0 \) for all non-empty \( I \subseteq \mathbb{N}_{2n} \). First, consider the case where \( |I| = l > 0 \) is even. Then, writing \( I = \{ i_1 < \cdots < i_l \} \) we obtain, using (70) and cyclicity of trace,

\[
\text{tr} \{ a_I \} = \text{tr} \{ a_{i_1} \cdots a_{i_l} \} = (-1)^{l-1} \text{tr} \{ a_{i_l} a_{i_1} \cdots a_{i_{l-1}} \} = (-1)^{l-1} \text{tr} \{ a_{i_1} \cdots a_{i_l} \} = -\text{tr} \{ a_I \}, \tag{75}
\]

thus \( \text{tr} \{ a_I \} = 0 \). 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 \( \chi \doteq (-1)^{\mathbb{N}} \), i.e. \( \mathcal{F}_\pm \doteq \ker \{ \chi \doteq 1 \} \). 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 \( \text{tr} \{ a_I \} = 0 \). We have thus proved that

\[
\langle a_J | a_K \rangle = 2^n \delta_{JK} \quad J, K \subseteq \mathbb{N}_{2n}. \tag{76}
\]

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

To prove (72) 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 \( 0 \leq l \leq k \). By (72) and Lemma 15

\[
|\mathfrak{B}_k| = \sum_{l=0}^{k} \binom{2n}{2l} = \dim \mathcal{O}_k(\mathcal{F}), \tag{77}
\]

thus \( \mathfrak{B}_k \) is an orthonormal basis of \( \mathcal{O}_k(\mathcal{F}) \). \[ \blacksquare \]

**Remark 21 (Relation between \( \mathfrak{B} \) and \( \mathfrak{B} \))** If \( n > 0 \), the orthonormal bases \( \mathfrak{B} \) and \( \mathfrak{B} \) are different. In fact, \( \mathfrak{B} \cap \mathfrak{B} = \{ 2^{-n/2} 1_F \} \), since the elements of \( \mathfrak{B} \) are homogeneous with respect to the natural grading \( \mathcal{F} = \bigoplus_{k \geq 0} \mathfrak{h}^k \), whereas the elements \( a_J \in \mathfrak{B} \) are inhomogeneous whenever \( J \neq \emptyset \). \[ \square \]
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