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.

Motivation: The Representability Problem in Quantum Chemistry

In quantum chemistry, atoms or molecules are usually considered as many-fermion quantum systems:

- **Hilbert space:** fermion Fock space

$$\mathcal{F} = \bigoplus_{N\geq 0} \bigwedge^N \mathfrak{h} \qquad \text{with } \mathfrak{h} = \text{1-particle Hilbert space, e.g. } \mathfrak{h} = L^2(\mathbb{R}^3)\otimes\mathbb{C}^2$$

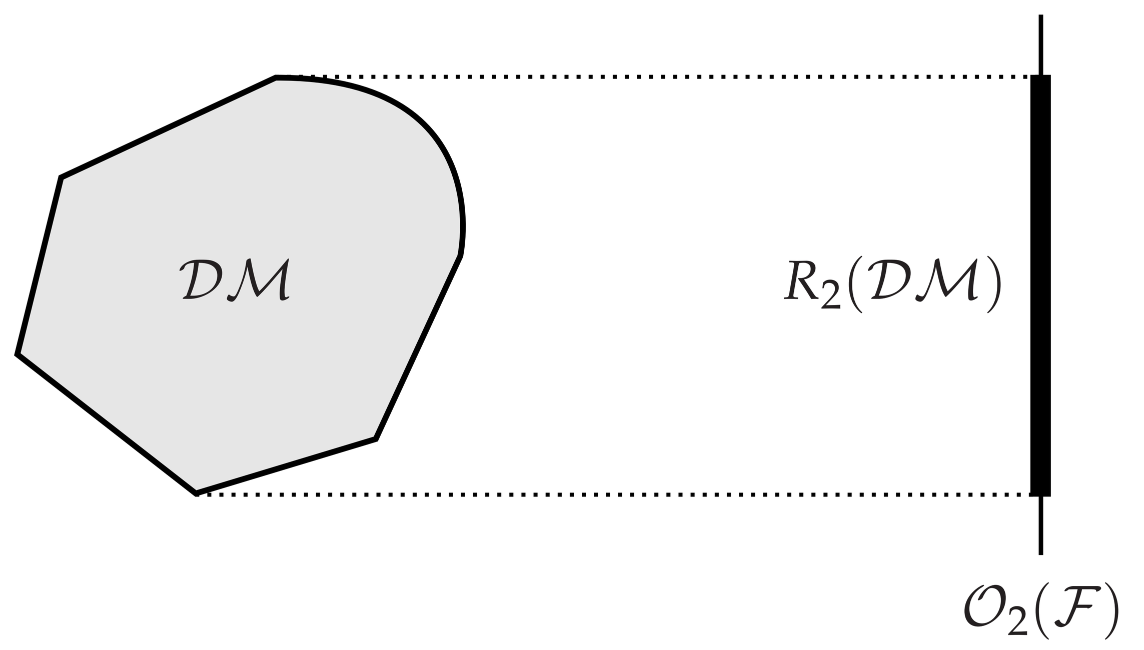
- **Hamiltonian:** a 2*-body operator* $\mathbb{H} = \mathbb{H}^* = \bigoplus_{N\geq 0} \mathbb{H}_N$, e.g.

$$\mathbb{H}_N = \sum_{i=1}^{N}\left(-\Delta_i - \sum_{j=1}^{K}\frac{Z_j}{|x_i - R_j|}\right) + \sum_{1\leq i<j\leq N}\frac{1}{|x_i - x_j|}.$$

States of these systems are usually modeled as elements ρ of the set $\mathcal{DM}$ of density matrices on $\mathcal{F}$. However, practically all physically relevant information can be obtained by expectation values of 2*-body operators*. Therefore, one would like to replace density density matrices ρ with its 2*-body reductions* $R_2(\rho)$, which encode precisely the 2-body expectation values of ρ. For example, the ground state energy is given by

$$E_0 \doteq \inf_{\rho\in\mathcal{DM}}\langle\rho,\mathbb{H}\rangle = \inf_{r\in R_2(\mathcal{DM})}\langle r,\mathbb{H}\rangle.$$

In order to exploit this observation, one has to find a computationallly efficient characterization of $R_2(\mathcal{DM})$, which is called the *representability problem*. When $\dim\mathfrak{h} < \infty$, then $R_2(\rho)$ can be identified with the orthogonal projection of ρ onto the space of 2-body operators $\mathcal{O}_2(\mathcal{F})$ within the Hilbert-Schmidt geometry:



Goal & Results

In order to gain a deeper understanding of the representability problem and related questions, one would like to have a more concrete formula of the orthogonal projection

$$R_k : \mathcal{L}^2(\mathcal{F}) \to \mathcal{O}_k(\mathcal{F}) \subseteq \mathcal{L}^2(\mathcal{F}),$$

e.g. by means of an orthogonal basis of $\mathcal{O}_k(\mathcal{F})$.

Theorem 1 *Let $\dim\mathfrak{h} \doteq n < \infty$ and $\varphi_1,\dots,\varphi_n$ an orthonormal basis of $\mathfrak{h}$. Then an orthogonal basis of $\mathcal{L}^2(\mathcal{F})$ is given by*

$$\mathfrak{B} \doteq \left\{ \sum_{L\subseteq K}(-2)^{|L|}\mathbf{c}_L^*\mathbf{c}_L\mathbf{c}_I^*\mathbf{c}_J \;\middle|\; \begin{array}{c} I,J,K\subseteq\{1,\dots,n\} \\ \text{mutually disjoint}\end{array}\right\}.$$

Here, $c^*, c : \mathfrak{h} \to \mathcal{B}(\mathcal{F})$ denote the creation- and annihilation operators and for $I = \{i_1 < \cdots < i_l\} \subseteq \{1,\dots,n\}$ we define $\mathbf{c}_I^* \doteq c^*(\varphi_{i_1})\cdots c^*(\varphi_{i_l})$ and $\mathbf{c}_I \doteq c(\varphi_{i_l})\cdots c(\varphi_{i_1})$.

Corollary 1 *Let $k\in\mathbb{N}_0$. Then an orthogonal basis of $\mathcal{O}_k(\mathcal{F})$ is given by $\mathfrak{B}\cap\mathcal{O}_k(\mathcal{F})$.*

Current Research

The above results are an important first step for our current research. More specifically, we are currently working on

1. finding a characterization of of $\pi_k(\mathcal{DM})$ in terms of the orthogonal basis $\mathfrak{B}$,
2. identifying classical representability conditions as boundary conditions,
3. obtaining new representability conditions, which are important for lower bound methods, and
4. studying the action of Bogoliubov transformations on the space of representability conditions.

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