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Orthogonalization of Fermion k-Body Operators and Representabilty

The reduced k-particle density matrix (k-RDM) of a density matrix ρ on fermion Fock space $\mathcal{F}$ can be defined as the image under the orthogonal projection

$$\pi_k : \mathcal{L}^2(\mathcal{F}) \to \mathcal{O}_k \subset \mathcal{L}^2(\mathcal{F})$$

onto the space $\mathcal{O}_k$ of k-body observables on $\mathcal{F}$ within the space of Hilbert-Schmidt operators $\mathcal{L}^2(\mathcal{F})$. A proper understanding of π_k is intimately related to the *representability problem*, a long-standing open problem in computational quantum chemistry, which amounts to give a computationally efficient characterization of the cone $\pi_k(\mathcal{P})$ of *representable* k-RDMs, where $\mathcal{P}$ denotes the cone of positive trace-class operators on $\mathcal{F}$.

The goal of this joint work with V. Bach is the derivation of new representability conditions and the characterization of π_k in the finite-dimensional case. We have recently completed the first step towards this goal by explicitly constructing a distinguished orthonormal basis of $\mathcal{L}^2(\mathcal{F})$ which restricts to a basis adapted to the flag $0 \subsetneq \mathcal{O}_1 \subsetneq \mathcal{O}_2 \subsetneq \cdots$ of k-body observables. This orthonormal basis serves as a tool for the study of the cone $\pi_k(\mathcal{P})$ of representable density-matrices.