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Orthogonalization of Fermion k-Body Operators and Representabilty

The reduced k-particle density matrix (k-RDM) of a density matrix  $\rho$  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  $\pi_k$  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  $\pi_k$  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  $0 \subseteq \mathcal{O}_1 \subseteq \mathcal{O}_2 \subseteq \cdots$  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.