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Workshop on Quantum Marginals and Numerical Ranges 2015

Monday, August 17, 14:50 – 15:15

Title: N-representability conditions on the three-particle density matrix constrained to wave functions of the DOCI class.

Abstract: The DOCI (in full: doubly occupied configuration interaction) class of N-fermion wave functions is a subspace of the N-fermion Fock space consisting of all linear combinations of Slater determinants in which each spatial orbital is doubly occupied. The DOCI class entails great simplifications in the structure of its two- and three-particle density matrices. These simplifications allow a computationally feasible variational determination of the three-particle density matrix subject to all the semidefinite positivity constraints that are familiar when treating the two-particle density matrix. This feature can elucidate, for the first time, the convergence when considering variational higher-order density matrices in N-fermion systems.