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Quantum Information Theoretical Approach to Functional Theories

Julia Liebert[1], Christian Schilling[2]

[1]*Princeton University, USA*
[2]*Ludwigs-Maximilians Universität München, Germany*

Density functional approximations often struggle with strong static correlation, whereas systematically improvable wave function methods become increasingly costly as system size and multireference character grow. One-particle reduced density matrix functional theory (RDMFT) offers a complementary route by using the one-particle reduced density matrix (1RDM) as its basic variable. This richer description, however, raises the one-body N-representability problem: which 1RDMs arise from valid N-fermion states? Characterizing this domain is central both to the foundations of RDMFT and to the construction of reliable approximations. In this talk, we develop a unified geometric framework for functional theories in which the scope, which is specified by the basic observables and the fixed part of the Hamiltonian, determines the reduced variable, universal functional, and representability domain. For spin-1/2 fermions at fixed total spin, we use this framework to identify the orbital 1RDM with the moment map for the action of the corresponding unitary group on the many-fermion state space. The admissible ordered spectra form a moment polytope, yielding symmetry-adapted constraints for pure and ensemble one-body N-representability. We then extend this construction to ensembles of low-lying excited states. For a chosen weighting of the low-lying energies, one obtains a restricted domain of admissible orbital 1RDMs, whose ordered spectra form a convex polytope. Its facets provide weight-dependent, mixed-state generalizations of Pauli's exclusion principle. We discuss their structure and implications for excited state RDMFT. Finally, we introduce an ensemble Hartree-Fock theory for excited states as a tractable mean-field counterpart and derive the associated functional approximation. Together, these results establish symmetry, convex geometry, and N-representability as a common foundation for functional theories of ground and excited states.