Ensemble reduced density matrix functional theory for excited states and hierarchical generalization of Pauli's exclusion principle

We propose and work out a reduced density matrix functional theory (RDMFT) for calculating energies of eigenstates of interacting many-particle systems beyond the ground state. Various obstacles which historically have doomed such an approach to be unfeasible are overcome. First, we resort to a generalization of the Ritz variational principle to ensemble states with fixed weights. This in combination with the constrained search formalism allows us to establish a universal functional of the one-particle reduced density matrix. Second, we employ tools from convex analysis to circumvent the too involved N-representability constraints. Remarkably, this identifies Valone's pioneering work on RDMFT as a special case of convex relaxation and reveals that crucial information about the excitation structure is contained in the functional's domain. Third, to determine the crucial latter object, a methodology is developed which eventually leads to a generalized exclusion principle. The corresponding linear constraints are calculated for systems of arbitrary size.