

## Generalized Pauli constraints: do they have an effect on Reduced Density Matrix Functional Theory minimization?

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Functionals of the one-body reduced density matrix (1-RDM) are routinely minimized under Coleman's ensemble N-representability conditions. Recently, the topic of pure-state N-representability conditions, also known as generalized Pauli constraints, received increased attention following the discovery of a systematic way to derive them for any number of electrons and any finite dimensionality of the Hilbert space. In this presentation we assess the potential impact of the enforcement of the pure-state conditions on the results of reduced density-matrix functional theory calculations. In particular, we examine whether the standard minimization of typical 1-RDM functionals under the ensemble N-representability conditions violates the pure-state conditions for prototype 3-electron systems. We also enforce the pure-state conditions, in addition to the ensemble ones, for the same systems and functionals and compare the correlation energies and optimal occupation numbers with those obtained by the enforcement of the ensemble conditions alone[1].

[1] I. Theophilou, N. N. Lathiotakis, M. A. L. Marques and N. Helbig, *J. Chem. Phys.* 142, 154108 (2015)