Playing with the reduced density-matrix: representability, functionals and embedding

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Résumé

Going beyond Density-Functional Theory appear today as an important challenge for theoretical chemists and physicists, in particular to improve the accuratie for strongly correlated systems and to access to beyond ground-states properties. In that context, theories based on the reduced density-matrix are appealing but necessitates developments to become practical. In this presentation we present our recent work on the resolution of the density matrix functional theory variational equations and our strategy to construct a density-matrix-based embedding theory. Proofs of concept are presented in the framework of the periodic Hubbard model.

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