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Implementing Reduced Density Matrix Functional Theory within a Kohn–Sham like Framework

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Density functional theory (DFT) has been one of the central pillars of electronic structure theory for decades. Its remarkable balance between accuracy and computational efficiency has made it the method of choice across chemistry, materials science, and condensed matter physics. Despite its tremendous success, however, DFT faces well-known limitations, particularly in the description of strongly correlated systems, where static and dynamic correlation cannot be treated on equal footing.
Reduced density matrix functional theory (RDMFT) offers a promising alternative by replacing the electronic density with the one-body reduced density matrix as the fundamental variable. While this richer descriptor naturally incorporates key aspects of electronic correlation, the theoretical framework of RDMFT has historically lacked some of the foundational structures that have made Kohn–Sham DFT so successful.
I will present a reformulation of RDMFT built from first principles, introducing a fictitious partially interacting reference system analogous to the Kohn–Sham construction. The resulting effective Hamiltonian provides a rigorous foundation for developing the theory and, crucially, enables the construction of an adiabatic connection within the RDMFT framework. We explore the properties of this adiabatic connection and demonstrate how it can be used to analyze correlation effects and guide functional development.
By establishing an adiabatic connection for RDMFT, we recover one of the most powerful conceptual tools of modern electronic structure theory in a density-matrix setting. This creates a systematic pathway for constructing and benchmarking new functionals and brings RDMFT significantly closer to becoming a practical and broadly applicable successor to conventional density functional theory.