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Wavefunctions, Adiabatic Connections, and Universal Functionals for 1-Matrix Functional Theory

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In Kohn-Sham density functional theory, a reference system of noninteracting electrons with the same density as the physical system is used as a zeroth-order approximation to the system. Using an adiabatic connection to the target system, one can then correct the Kohn-Sham approximation. In this talk, I will establish an analogous approach for the 1-electron reduced density matrix (DM1). The reference system now contains *interacting* electrons, which we choose to describe with the Richardson Hamiltonian. The Richardson Hamiltonian includes the noninteracting-electrons limit (Kohn-Sham) and strictly-correlated-electrons limit (antisymmetrized geminal power). Any singlet-state DM1 can be reproduced by a Richardson Hamiltonian, and an adiabatic connection from the Richardson Hamiltonian to the target physical system provides a rigorous definition for the correlation functional in 1-density matrix functional theory (DM1FT). Preliminary numerical results are favorable. Because DM1FT treats both the strongly correlated and weakly correlated limits exactly, it seems to be a very promising avenue for research.