Time-dependent renormalized natural orbital theory for laser-driven correlated few-body quantum dynamics

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Reduced density matrix functional theory (RDMFT) can be formulated in terms of the eigenfunctions of the 1-RDM, the "natural orbitals" (NO), leading to natural orbital theory (NOT). In many-body strong-field physics we are mainly interested in time-dependent, correlated phenomena far beyond linear response. Hence, a full time-dependent version of NOT, i.e., TDNOT, or TDRDMFT, is needed, especially in cases where simpler TDDFT fails [1,2].

In our presentation, we test the TDNOT approach with the help of numerically exactly solvable model systems and well-known, "worst-case" resonant or correlated strong-field phenomena [3-5]. In cases where the exact wave function is available, (TD)NOT is useful to analyze the role of correlation in the system. The effective two-particle case is of particular importance because the 2-RDM functional is known there. We also explain how the highly nonlinear equations of motion for the time-dependent NO are actually solved for these systems.