

Abstract Submitted
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Time-Resolved Dynamics in Exact TDDFT: Studies of Two-Electron Systems ERNESTO SANDOVAL, JOHANNA FUKS, KAI LUO, NEEPA MAITRA, Hunter College and CUNY Graduate Center, PETER ELLIOTT, Max-Planck Institute for Microstructure Physics — An exact decomposition of the exchange-correlation potential in time-dependent density functional theory (TDDFT) into kinetic and hole contributions is derived, with the goal of a better understanding of features of the TDDFT functionals, leading eventually to improved approximations. We study the kinetic and hole contributions for a range of dynamical situations in two-electron systems in one-dimension, from models of Rabi oscillations to local excitations, charge-transfer excitations, and resonance energy transfer, and compare them to their adiabatically-exact approximation. We find that dynamical step structures are present in both terms, that require a non-adiabatic functional approximation. In many cases, the kinetic contribution dominates the step structure, but not in all. The adiabatically-exact approximation is generally worse for the kinetic contribution than for the hole contribution.

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