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Transition densities in time-dependent density functional theory
YONGHUI LI, CARSTEN ULLRICH, Department of Physics and Astronomy, University of Missouri, Columbia, MO 65211 — Real-space density-matrix analysis is a useful computational tool to visualize and interpret the induced charges and electron-hole coherences of electronic excitations in molecules. We extend this technique into the nonlinear, real-time domain and define the time-dependent transition densities in the context of time-dependent density-functional theory. This provides a real-time visualization tool for optical excitation processes in molecules, which will be illustrated for simple one-dimensional lattice model systems. Comparisons with numerically exact many-body benchmark solutions will be carried out by constructing the corresponding exact time-dependent Kohn-Sham transition density matrix. This work is supported by NSF Grant DMR-0553485

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