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Time-Resolved Dynamics in Time-Dependent Density Functional Theory: Significance of Non-locality in Space and Time¹

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The usual approximations in Time-Dependent Density Functional Theory (TDDFT) have achieved an unprecedented balance between accuracy and efficiency for calculating excitation spectra and response. We show however that these approximations are less successful for time-resolved dynamics beyond the linear response regime. Step and peak structures develop in the exact exchange-correlation potential that have a density-dependence that is non-local both in time and in space, missed by all approximations in use today. The lack of these structures leads to their incorrect predictions of dynamics, such as faster time-scales, and incomplete charge-transfer. [P. Elliott, J.I. Fuks, A. Rubio, N.T. Maitra arXiv:1211.2012; J. I. Fuks, P. Elliott, A. Rubio, N. T. Maitra, arXiv:1211.2849]

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