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Studies of spuriously time-dependent resonances in TDDFT

NEEPA MAITRA, Hunter College and the Graduate Center of the City University of New York, JOHANNA FUKS, Hunter College of the City University of New York — Recently the failure of some exchange-correlation functionals to accurately capture non-perturbative dynamics in time-dependent density functional theory (TDDFT) was shown to be correlated with their violation of an exact condition [1]: that the resonance positions of the system remain fixed during the evolution. Closely related is the inconsistent prediction of excitation frequencies in linear response when the reference state is an excited state of the system. We discuss this and the effect on dynamics in a range of molecular systems, exploring system-size dependence of the violation. [1] Time-resolved spectroscopy in time-dependent density functional theory: An exact condition, J. I. Fuks, K. Luo, E. D. Sandoval, N. T. Maitra, Phys. Rev. Lett. **114**, 183002 (2015).

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