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Non-adiabatic approximations and exact conditions in TDDFT[1]
JOHANNA I. FUKS, Hunter College of City University of New York, SOEREN E. B. NIELSEN, Max Planck Institute for the Structure and Dynamics of Matter , NEEPA T. MAITRA, Hunter College of City University of New York — Almost all calculations today in time-dependent Density Functional Theory (TDDFT) utilize an adiabatic approximation for the exchange-correlation potential, however it is known that non-adiabatic features of the exact potential can have a large impact on the dynamics, especially when a system is driven far from its ground state. In this work, we explore the development of non-adiabatic functional approximations based on the decomposition of the exact exchange-correlation potential in terms of an interaction component and a kinetic component [J. Chem. Phys. 140, 18A515 (2014)]. In particular, we investigate different approximations to these two components in the light of the fulfilment of the following exact conditions: zero force theorem, harmonic potential theorem, memory condition and constant resonances condition. We study several cases of non-equilibrium dynamics and correlate poor performance with the violation of one or more of these exact conditions.

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