

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Kinetic and Hole Contributions to the Exact TDDFT Correlation Potential¹ KAI LUO, CUNY-Graduate Ctr, JOHANNA FUKS, CUNY-Graduate Ctr and Hunter College, ERNESTO SANDOVAL, CUNY-Hunter College, PETER ELLIOTT, Max-Planck Institute for Microstructure Physics, NEEPA MAITRA, CUNY-Graduate Ctr and Hunter College — The recent report[1-2] that dynamical steps generically develop in the exact correlation potential of time-dependent density functional theory (TDDFT) triggers the present work on the investigation on correlation potential and its adiabatic approximation. We hope this understanding will be of use in the construction of new non-adiabatic functionals capable of modeling non-linear electron dynamics using time-resolved TDDFT. We decompose the exact correlation potential into kinetic and hole contributions, analogously to what was done in the ground-state some years ago (e.g.[3]). In the ground-state, it was found that the dominant contribution was typically from the correlation hole potential, except in cases of strong correlation, when the system is far from single Slater determinant. However, this is not true in the time-dependent case: the dynamical step feature is independent of the deviation from a single-Slater determinant. Instead, the steps appear to be correlated with local oscillations of time-dependent natural orbital occupation numbers and further understanding of this connection is part of on-going investigations. [1] Elliott, Phys. Rev. Lett. 109,266404(2012) [2] Fuks, J. Phys. Chem. Lett. 4, 735(2013) [3] Gritsenko, J. Chem. Phys. 104, 8535-8545(1996)

¹Supported by National Science Foundation CHE-1152784 and Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences

Kai Luo
CUNY-Graduate Ctr

Date submitted: 14 Nov 2013

Electronic form version 1.4