

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Dynamical Steps in the Time-Dependent Exchange-Correlation Potential¹ KAI LUO, NEENA MAITRA, Hunter College and CUNY Graduate Center, PETER ELLIOTT, Max-Planck Institute for Microstructure Physics, JOHANNA FUKS, ANGEL RUBIO, Dpto. Física de Materiales, Universidad del País Vasco — It was recently demonstrated that the exact correlation potential of time-dependent density functional theory (TDDFT) generically develops step and peak features that have a density-dependence that is non-local in space and time [arXiv:589981]. Usual adiabatic functional approximations fail to capture these steps, yet these same functionals work quite well for excitation spectra. We investigate the role of the steps in the linear response regime.

¹NSF CHE-1152784 & DOE DE-SC0008623.

Kai Luo
Hunter College and CUNY Graduate Center

Date submitted: 17 Nov 2012

Electronic form version 1.4