Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Exploiting initial-state dependence to improve the performance of adiabatic TDDFT JOHANNA I. FUKS, Hunter college City University of New York, SOEREN E.B. NIELSEN, MICHAEL RUGGENTHALER, Max-Planck-Institut fr Struktur und Dynamik der Materie, Hamburg, NEEPA T. MAITRA, Hunter college City University of New York, HUNTER COLLEGE CITY UNIVERSITY OF NEW YORK COLLABORATION, MAX-PLANCK-INSTITUT FR STRUKTUR UND DYNAMIK DER MATERIE, HAMBURG COLLABORATION — Although time-dependent density functional theory (TDDFT) descriptions of dynamics in non-equilibrium situations have seen exciting successes recently, there have also been studies that throw into doubt the reliability of the approximate exchange-correlation functionals to accurately describe the dynamics. Here we study exact exchange-correlation potentials for few electron systems, found using the global fixed-point iteration method [NRL]. We find that the size of dynamical correlation features that are missing in the currently-used adiabatic approximations depend strongly on the choice of the initial Kohn-Sham wavefunction. With a judicious choice, the dynamical effects can be small over a finite time duration, but sometimes they can get large at longer times. We also examine different starting points, in particular an orbital-dependent potential directly obtained from the Kohn-Sham hole [LFSEM14], for approximate xc functionals: instead of building on an adiabatic approximation.

Johanna I. Fuks
Hunter college City University of New York

Date submitted: 24 Nov 2015 Electronic form version 1.4