Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Curing pathologies of TDDFT with semiclassical electron correlation PETER ELLIOTT, NEEPA MAITRA, Hunter College, City University of New York — Time-dependent density functional theory (TDDFT) has been identified as a prime candidate for describing the dynamics of atoms and molecules in strong laser fields. It would be especially useful in predicting the highly non-intuitive fields needed in the optimal control problem for photonic reagents. However TDDFT encounters a number of problems when simulating these systems, both in the functional approximation of the exchange and correlation potentials, but also for observables of interest, such as momentum distributions or ionization probabilities. Recently a method to overcome some of these problems was proposed[1], whereby an auxiliary semiclassical dynamics calculation produces a correlation potential, which is then used to drive a density-matrix propagation. This method incorporates memory, initial-state dependence, changing occupation numbers, all of which are known issues for TDDFT. In this talk we build on previous work[2] and examine this scheme for a number of model 1D systems including calculations for strong field dynamics, optimal control, non-sequential ionization, and double excitations [1] A.K. Rajam, I. Raczkowska,and N.T. Maitra, Phys. Rev. Lett. 105, 113002 (2010). [2] P. Elliott and N.T. Maitra, J. Chem. Phys. 135, 104110 (2011).

Peter Elliott
Hunter College, City University of New York

Date submitted: 11 Nov 2011 Electronic form version 1.4