Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Phase-Space Density Functional Theory: A Quasiclassical Approach[1] IZABELA RACZKOWSKA, Hunter College, City University of New York, ARUN RAJAM, City University of New York , NEEPA MAITRA, City University of New York and Hunter College — In time-dependent density functional theory, one obtains all observables pertaining to an interacting electronic system from one that is non-interacting, in principle exactly. In practice approximations are needed for the exchange-correlation potential and also observable-functionals. Although presently used functionals have been successful for many applications, they perform poorly for several phenomena of interest eg. momentum distributions, electronic quantum control problems, and where there is strong memory-dependence. We propose and explore a possible solution to these problems by extending TDDFT to phase-space densities, and discuss dynamical quasiclassical and semiclassical approximations for the correlation functional in phase-space.

[1]Funded by the National Science Foundation and a Cottrell Scholar Award from the Research Foundation

Neepa Maitra
City University of New York and Hunter College

Date submitted: 19 Nov 2009 Electronic form version 1.4