

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

TDDFT in Phase-Space¹ ARUN RAJAM, Graduate Center of the City University of New York, CHRISTIAN GAUN, NEEPA MAITRA, Hunter College of the City University of New York — We explore the possibility of a density-functional theory in phase-space, where the basic variable is a phase-space density rather than the usual coordinate-space density. In this way information about the momentum distribution is directly captured, rather than being hidden in the form of the exchange-correlation functionals, which often complicates the functional, making it hard to approximate. We give examples to motivate this approach, and discuss initial stages in the development of the functionals.

¹Supported by the National Science Foundation and the Research Corporation Cottrell Scholar Program

Neepa Maitra
Hunter College of the City University of New York

Date submitted: 27 Nov 2007

Electronic form version 1.4