Phase-Space Explorations in Time-Dependent Density Functional Theory

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Time-Dependent Density Functional Theory is increasingly popular for calculating excitation and response properties of atoms, molecules, clusters and solids. It has achieved an unprecedented balance between accuracy and efficiency for a wide range of systems, but not all. Although not limited to the linear response regime, there are particular challenges for applications to strongfield processes: for example obtaining momentum distributions, certain electronic quantum control problems, and including memory-dependence necessary in the functional dependence. In this talk we will discuss some of these, and introduce a new extension of the theory where the basic variable is the phase-space density \( W(r,p,t) \) (that contains information on both the co-ordinate- and momentum distributions of the electrons), instead of the usual co-ordinate space density \( n(r,t) \), to deal with these challenges.

\(^1\)Funded by NSF and Research Corporation