

Abstract Submitted
for the DAMOP17 Meeting of
The American Physical Society

Correlated two-electron quantum dynamics in intense laser fields

DIETER BAUER, MARTINS BRICS, JULIUS RAPP, ADRIAN HANUSCH, University of Rostock — Two electrons interacting with each other, a binding potential, and a laser field turn out to be a real buzzkill for time-dependent many-body approaches. In particular, TDDFT with known and practicable exchange-correlation potentials fails in reproducing typical strong-field laser-atom phenomena of current interest such as photoelectron or transient absorption spectra. Even high-harmonics spectra, commonly believed to be an “easy” observable for TDDFT, can be qualitatively wrong. Failures of that kind will be illustrated in the talk. The challenge is to overcome these troubles with TDDFT. Working methods like MCTDHF or TDCI are quite expensive. As TDDFT is based on the single-particle density and MCTDHF/TDCI on the wavefunction, the obvious idea is to go just one “small” step beyond TDDFT and consider the one-body reduced density matrix (1-RDM) as the basic variable. Deriving equations of motion for the eigenfunctions and eigenvalues of the 1-RDM leads to time-dependent natural orbital theory (TDNOT). It will be shown in the talk that TDNOT indeed overcomes all the problems TDDFT has with two electrons in intense laser fields.

Dieter Bauer
University of Rostock

Date submitted: 06 Apr 2017

Electronic form version 1.4