

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

A Density Functional Approach to High Harmonic Generation¹

MICHAEL MACK, DANIEL WHITENACK, Purdue University, ADAM WASSERMAN, Purdue University, THE SUSPENDERS TEAM — The role of the asymptotic behavior of the ground state exchange-correlation (xc) potential is examined for the case of high harmonic generation (HHG) in N₂ via Time-dependent Density Functional Theory (TDDFT) within the adiabatic approximation. High harmonic generation (HHG) is a high-energy phenomenon that has been theoretically investigated using the strong-field approximation (SFA) within the single active electron approximation (SAEA) for small molecules. In the case of N₂, experimental results for characteristic features of the harmonic emission suggest a breakdown of those approximations. TDDFT bypasses the need for such approximations as it accounts for all the electrons in the system; however, it requires approximations to the xc-potential. We investigate how asymptotic corrections to the Local Density Approximation (LDA) xc-potential influence the HHG spectrum.

¹Purdue Research Foundation

Michael Mack
Purdue University

Date submitted: 09 Nov 2011

Electronic form version 1.4