Recent Advances in Computational Methods for the Solution of the Time-Dependent Schrödinger Equation for the Interaction of Short, Intense Radiation with One and Two Electron Systems: Application to He and H_2^+

Barry I. Schneider, Johannes Feist, Stefan Nagele, Renate Pazourek, Suxing Hu, Lee A. Collins, and Joachim Burgdörfer

Abstract In the past few years new and efficient algorithms have been developed to solve the time-dependent Schrödinger equation (TDSE) for few-electron systems. When coupled with the advances in and availability of high performance computing platforms, it is now possible to numerically calculate nearly exact solutions to the interactions of short, intense laser pulses with simple one and two-electron systems. In addition, somewhat less accurate treatments of the heavier rare gases and simple two-electron molecules are also becoming available. The proceedings from this workshop have provided a unique opportunity to describe the substantial numerical

Barry I. Schneider
Office of Cyberinfrastructure and Physics Division, National Science Foundation, 4201 Wilson Blvd., Arlington, VA 22230, USA, e-mail: bschneid@nsf.gov

Johannes Feist
ITAMP, Harvard–Smithsonian Center for Astrophysics, Cambridge, MA 02138, USA, e-mail: jfeist@cfa.harvard.edu

Stefan Nagele
Institut für Theoretische Physik, Technische Universität Wien, Wiedner Hauptstraße 8, 1040 Wien, Austria, e-mail: stefan.nagele@tuwien.ac.at

Renate Pazourek
Institut für Theoretische Physik, Technische Universität Wien, Wiedner Hauptstraße 8, 1040 Wien, Austria, e-mail: renate.pazourek@tuwien.ac.at

Suxing Hu
Laboratory for Laser Energetics, University of Rochester, 250 E. River Road, PO Box 278871, Rochester, NY 14623-1212 USA, e-mail: shu@lle.rochester.edu

Lee A. Collins
Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, e-mail: lac@lanl.gov

Joachim Burgdörfer
Institut für Theoretische Physik, Technische Universität Wien, Wiedner Hauptstraße 8, 1040 Wien, Austria, e-mail: burg@dollywood.itp.tuwien.ac.at

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and algorithmic progress that has been achieved over the past few years to solve the TDSE and to illustrate them on the He atom and H_2^+ molecule.

1 Introduction

In recent years, revolutionary new technologies have made coherent, ultrashort, and intense pulses in the vacuum and extreme ultraviolet (VUV-XUV) region available. These pulses are currently generated from two quite different types of sources.

One are free electron lasers (FEL) [1–7]. Currently, there are two FELs in the VUV-XUV and X-ray regime (XFELs) in operation: FLASH at DESY in Hamburg, Germany [8, 9], and LCLS in Stanford, USA [10, 11]. FLASH has reached focused intensities of up to $10^{16}\,\mathrm{W/cm^2}$, and photon energies as high as 190 eV, while LCLS reaches even higher energies up to 8 keV and intensities of up to $10^{18}\,\mathrm{W/cm^2}$. The duration and temporal structure of the individual FEL pulses is not well known, but is of the order of 10–50 femtoseconds for FLASH. In addition, there have been a number of proposals aimed to decrease the duration of these pulses to a few hundred attoseconds [12–18].

The other approach to produce intense ultrashort pulses at XUV wavelengths is to use high harmonic generation (HHG) from a driving infrared (IR) laser [19–28]. This technique has been successfully used to create the shortest pulses available today, with durations down to 80 as [27]. With current technology, attosecond pulses are much less intense than FEL pulses. The focused intensities are not well known but typically do not exceed $\approx 10^{12}\,\mathrm{W/cm^2}$, although various ways to increase the maximally available intensity have been proposed [29–36].

The continuing development of these novel light sources has led to an increased interest in multiphoton processes at high photon energies. Simultaneously, the ultrashort duration of the pulses in the femtosecond ($1\,\mathrm{fs} = 10^{-15}\,\mathrm{s}$) or even attosecond ($1\,\mathrm{as} = 10^{-18}\,\mathrm{s}$) domain enables the study of *time-resolved* electron dynamics, starting the field of *attosecond science* [37–41].

In this contribution, we report on some of our recent theoretical and numerical investigations, motivated by the availability of these pulses. We study relatively simple systems (He and H_2^+), for which the Schrödinger equation including all relevant degrees of freedom can be fully solved. This necessitates the use of numerical approaches that take advantage of modern high-performance computing facilities. The work that is reviewed in this manuscript has been previously published in the diploma theses of Stefan Nagele [42] and Renate Pazourek [43] and the PhD thesis of Johannes Feist [44], as well as some journal publications [45–50].

We start by giving an overview of the numerical methods we are using to discretize the spatial (Sect. 2) and temporal (Sect. 3) degrees of freedom. We then comment on some numerical details of our implementation (Sect. 4).

For the case of helium (Sect. 5), we focus on two-photon double ionization. Double ionization of helium has long been of great interest in atomic physics since it provides fundamental insights into the role of electronic correlation in the full three-