Outline of selected topics for current and future research

The investigation of the interaction of atoms and molecules with intense laser fields is one of the most interesting areas of the current research in atomic and molecular physics. The general motivation for studying molecules in laser fields lies in the possibility of gaining fundamental understanding of the dynamics and the intermediate processes involved in various physical, chemical and biological reactions.

Research Interests:

My main research interests lie in

(i) numerically modeling dissociation dynamics of heavier diatomic molecular ions (such as H_2^+, O_2^+, N_2^+, Ar_2^+ …) in intense IR and XUV laser fields by calculating their fragment kinetic energy release (KER) spectra as a function of pump-probe delay τ (the calculated results are compared with pump-probe experimental data), [1-12] and

(ii) Theoretical investigation of photoionization of atoms, and fullerenes, endohedral fullerenes in laser fields mainly focusing on time delay from different subshells of atoms, or atoms confined in C_{60} or C_{240} fullerenes [13-16].

In the first project we numerically solve time dependent Schrodinger equation (TDSE) using Crank-Nicolson method, that is a finite difference method which is used to solve differential equations [2,4,10]. By solving the TDSE, the time evolution of the nuclear wave packet can be calculated theoretically (Fig.1a). We calculate the time evolution of an initial nuclear vibrational wave packet in molecular ion (H_2^+, O_2^+ ,...) generated by rapid ionization of neutral molecule (H_2,O_2,...) in an ultrashort (femtosecond) pump-laser pulse based on quantum-mechanical model. The quantum beat frequency and internuclear distance-dependent power spectra (Fig.1b) are obtained by Fourier transformation of the nuclear probability density with respect to the time delay between pump and delayed probe pulses. One can convert R-dependent spectra in kinetic energy release (KER) spectra that is measured experimentally for comparison to study dissociation dynamics of the molecules [3-11].

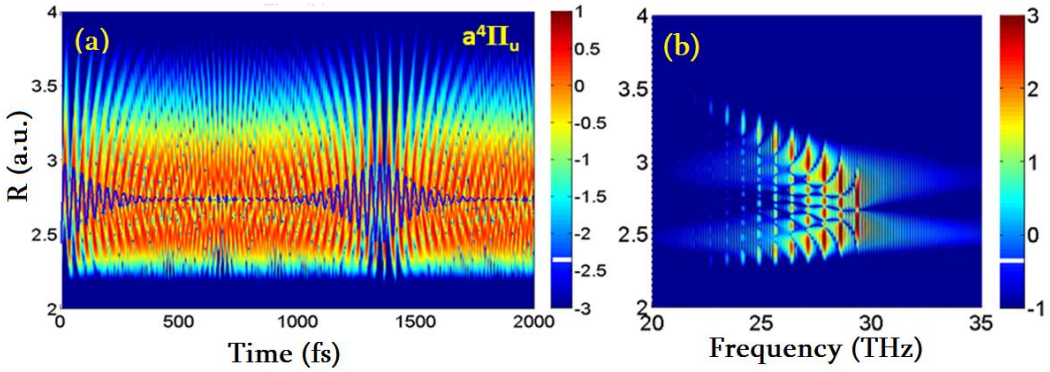

Figure1. (a) Evolution of the nuclear wave packet on $a^4\Pi_u$ curve of O_2^+ (b) corresponding power spectra.

Second project involves calculations with so called jellium model (since large number of electrons are involved). For the ground state calculations we use local density approximation (LDA). In LDA the core ions are smeared into classical jellium, the valence electrons are delocalized and Kohn-Sham equations are solved for 240 valence electrons for C_{60} and 960 valence electrons for C_{240} [13-16]. In our Photoionization calculations we use time dependent local density approximation (TDLDA) with Leewen and Baerends exchange correlation functional, that produces accurate asymptotic behavior of ground and continuum electrons [13-16]. With TDLDA we obtain dynamical response of the system to the external electromagnetic field. We investigate photoemission quantum phases and associated Wigner-Smith time delays Figure 2 shows example of the phases and the delays for HOMO-1 electrons of a C_{60} molecule. These calculations are unique to grasp insights of the time scales of electron photoionization. It has large importance in nanotechnology as it promises a convergence of science, medicine, and engineering that may allow the development of a new generation of scientific approaches, experimental and simulation research tools, and clinical devices.

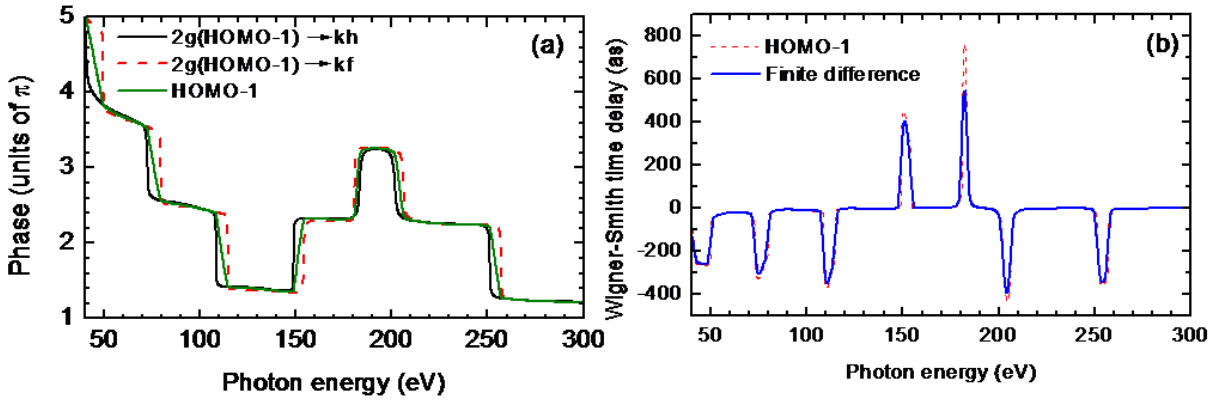

Figure 2. (a) Quantum TDLDA phases and (b) Wigner-Smith delays for HOMO-1 electrons of C_{60}.

Future Plans:

A. In the future I plan to improve the quantum model used for KER calculations. The current model does not include more than two electronic states, nor molecular rotations. A next step would be to implement three and more electronic states in the calculations. Including molecular rotation in the current code without doing full *ab*-initio calculations [12] will be more challenging. I want to extend my research and try heavier molecules with more than one active degree of freedom that require potential surface calculations. It would be interesting to figure out how current models can be extended to investigate the dissociation dynamics of large molecules.

B. On the fullerene side of the research, plan to investigate:

1. Time-dependent local density approximation (TDLDA) studies of quantum phases and time delays in bound-continuum transitions of noble gas atoms.
2. Confinement and cavity effects in time-domain photoionization of Kr@C_{60} and Xe@C_{60}.

3. Quantum phase shifts and Wigner-Smith time delays in the photoionization versus radiative recombination of Ar, Kr and Xe (and @C_{60}) valence electrons.

Applications of this research are being developed in such fields as energy production, medicine, photography, optoelectronics, and information storage, there are many directions to pursue. The time delay studies in combination with emerging nanotechnology, could serve as a bridge to developing a new science discipline that combines nanoscience and attoscience.

Student involved in either of these projects will learn not only the physics behind the laser-matter interactions but how to program in FORTRAN as well.

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