Theoretical Studies on the Dynamics of Atoms and Molecules in Strong Laser Fields

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1. Project Purpose
   a) Collaborate with the experiment group at Griffith University to search an efficient way to produce metastable states of Ar atoms in strong fields.
   b) Collaborate with the experiment group in RIKEN to understand the structure and dynamics of muonic Ar atomic ions.
   c) Collaborate with the experiment group in the University of Electro-Communication to investigate the interference effects between radiative and di-electronic recombinations.
   d) Simulate high-order harmonic generation in multiscale grids.

2. Results
   a) We studied the atomic excitation in a strong field. The goal of this work is to find an efficient way to produce the metastable state of Ar atoms with the experimental conditions in Griffith University. Since the parameters space is too large, we could not find a reasonable excitation probability after many simulations. Recent, we used Genetic Algorithm to search over the large parameter space and the preliminary results are very encourage. We will work on this direction.

   b) Based on our developed relativistic density functional theory with self-interaction correction, we simulated the energy structures of muonic Ar atomic ions over a board energy region. The results are used to analyze the recent experiment performed by an experiment group in RIKEN. The project is almost finished, and we are working on writing the paper.

   c) We performed a systematical study for the polarization of x rays emitted when a free electron is captured by Be-like highly charged ions theoretically. We focus on the dielectronic recombination of $J = 1/2 \rightarrow J = 1/2$ transition because its polarization is zero due to the axial symmetry. Including the interference between the dielectronic and radiative recombinations, the polarization changes dramatically when the electron energy crosses the resonant energy. We extended our previous results to a broad iso-electron sequence and found that for low-Z

ions, the configuration interaction of the DR states affects the polarization greatly while for high-Z ions, the configuration interaction of the ground state of Be-like ions plays an important role. This work has been published in Physical Review A [10.1103/PhysRevA.107.052801]

d) We theoretically studied the high-order harmonic generation (HHG) from a gas target in an intense laser pulse. We obtain the microscopic HHG by solving the time-dependent Schrodinger equation with a single-active-electron approximation and the macroscopic HHG by summing over all the microscopic HHG with phase matching and self-absorption in two scales. One is in the laser wavelength scale, within which the laser peak intensity does not change while the propagation phase changes. Another is in the laser beam waist scale, within which the laser intensity and Gouy phase shift change. Taking Ar atom as an example, we calculate the macroscopic HHG energy distribution and divergence. We also discuss the dependency of the macroscopic HHG on the gas pressure and gas jet position. This work has been published in Physical Review A [10.1103/PhysRevA.108.023118]

３．Roles of the MCRP and its significance

Most of the theoretical works involved large scale simulations using supercomputers. Results b) were performed on Wisteria since the kinds of muonic atomic ion is close to one million. The results a) and d) were performed on Cygnas and Pegasus. Given the total CPU time used in the simulation, the works could not be done with a high-performance workstation. So, without the support of the MCRP, we couldn't do the research.

４．Future plan

a) Search an effective way to produce more metastable Ar atoms using genetic algorithm (GA). This research is a joint research project funded by Australia Research Council. GA is evolution method, which needs many simulations with different parameters.

b) Recently, we started to collaborate with an experiment group in Max Planck Institute for Nuclear Physics on the optical transition of He in two-color laser fields. The energy resolution covers six orders, so we must do a high precision simulation to compare with the experiment.

5. Publications and conference presentations

(1) Journal papers

a) XM Tong, "Multiscale simulation of high-order harmonic generation: From microscopic to macroscopic", Phys. Rev. A **108**, 023118:1-9 (2023).

b) XM Tong, X Gao, D Kato, and N Nakamura, "Interference between dielectronic and radiative recombination of Be-like highly charged ions", Phys. Rev. A 107, 052801:1-5 (2023).

(2) Presentations

a) D. Chetty, *et. al.,* "Carrier-Envelope-Phase Effects for Multiphoton and Tunnel Excitation of Argon", ICPEAC 2023 (XXXIII International conference on photonic, electronic, and atomic collisions), July 25-Aug. 1, 2023, Ottawa, Canada

b) XM Tong, D. Kato, T. Okumura, S. Okada, T. Azuma, "Electronic K x rays emitted from muonic atoms: an application of density functional theory", ICPEAC 2023 (XXXIII International conference on photonic, electronic, and atomic collisions), July 25-Aug. 1, 2023, Ottawa, Canada

c) T. Okumura*, et. al.*, "High-resolution spectroscopy of electronic K x rays from muonic atoms using transition-edge sensor microcalorimeters ", ICPEAC 2023 (XXXIII International conference on photonic, electronic and atomic collisions), July 25-Aug. 1, 2023, Ottawa, Canada (invited talk)

(3) Others

Supercomputer	Use	Allocated resources*	
		Initial resources	Additional resources
Cygnus	Yes	4,800	--
Wisteria/BDEC-01	Yes	12,800	6,400
*in units of node-hour product			