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

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1. Project Purpose

a) Collaborate with the experimental group at Griffith University to fully uncover the atomic excitation in intense laser fields.

b) Investigate the X-ray polarization emitted by dielectronic recombination of highly charged Bi ions. The goal of the work is to understand the unexpected polarization observed in Tokyo EBITs.

c) Study atoms in arbitrary fields by the previously developed method with single active electron approximation or density functional theory.

d) Investigate the energy structure of hyper-satellite K_α^h muonic Ar atomic ions and uncover the mechanisms observed in the muon experiment performed by the RIKEN experiment group.

2. Results

a) We have studied atomic excitation in a strong field. Through numerical simulations, we show that the resulting bound-state population is sensitive to both the intensity and the CEP. The experimental data agree with the theoretical prediction, and the results encourage the use of precisely tailored laser fields to coherently control the strong-field excitation process. We find a markedly different behavior for the CEP-dependent bound-state population at low and high intensities with a clear boundary, which we attribute to the transition from the multiphoton to the tunneling regime. This work has been published in Physical Review Letters [10.1103/PhysRevLett.128.173201].

b) We perform 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 and its polarization is zero due to axial symmetry. Including the interference between the dielectronic and radiative recombinations, the polarization changes dramatically when the electron energy crosses the resonant energy. By comparing the simulations with or without certain interactions, we 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 Letters [10.1103/PhysRevLett.130.113001].

c) We develop a method of the relativistic density functional theory with self-interaction correction, which is simple and fast yet with reasonable accuracy. Comparison with measured K_α lines and their hyper-satellites of several atoms, from low-Z to high-Z, reveals that the relativistic local density approximation is suitable for K_α lines. In contrast, the relativistic local spin density approximation with self-interaction correction is better for K_α^h hyper-satellites. Compared with the non-relativistic density functional theory, we found that the relativistic effect is significant (about 100 eV) even for middle Z atoms, like Cu. The screening effects, from inner-shell to outer-shell, and conduction band, are also discussed. The present work provides all the transition lines of muonic atoms, which can be used to narrow down the possible transitions by comparing them with the measurements. This work is published on Phys. Rev. A [10.1103/PhysRevA.107.012804].

3. Roles of the MCRP and its significance

Most of the simulations in Result a) were performed on GPU in Cygnus. Without the large-scale simulation, it is difficult to understand how the strong field excitation depends on the laser parameter and what is the excitation mechanism for different laser intensities. Most in the simulations of Result c) were performed on wisteria since the simulation code was written for conventional CPU. Each simulation does not take much time but there are about 1 million transition lines. The work could not be done with a high-performance workstation.

4. Future plan

a) Investigate how the laser pulse shape affects the atomic excitation and how to optimize the excitation probability. This is joint work with an experimental group at Griffith University.

b) Simulate the hypersatellite structures of muonic atoms in the gas phase to understand the measurement by a group in RIKEN.

c) Investigate the multipole contribution in dielectronic recombination to collaborate with the ongoing experiment at the University of Electron-Communications.

5. Publications and conference presentations

(1) Journal papers

1) XM Tong, D Kato, T Okumura, S Okada, and T Azuma, *"Electronic K x rays emitted*

from muonic atoms: an application of relativistic density functional theory", Phys. Rev. A **107**, 012804 (2023).

2) N Nakamura, N Numadate, S Oishi, XM Tong, X Gao, D Kato, H Odaka, T Takahashi,Y Tsuzuki, Y Uchida, H. Watanabe, S Watanabe, and Hiroki Yoneda, "Strong Polarization of a J=1/2 to 1/2 Transition Arising from Unexpectedly Large Quantum Interference", Phys. Rev. Lett. **130**, 113001:1-6 (2023).
3) D Chetty, RD Glover, XM Tong, BA deHarak, H Xu, N Haram, K Bartschat, AJ Palmer, AN Luiten, PS Light, IV Litvinyuk, and RT Sang, *"Carrier-Envelope-Phase Dependent Strong-Field Excitation"*, Phys. Rev. Lett. **128**, 173201:1-6 (2022).

(2) Presentations

1) T. Okumura, *et. al.* "Formation dynamics of highly charged muonic Ar ions", The Physical Society of Japan, Annal meeting, March 22-25, 2023 (online).
2) Okumura, *et. al.* "Formation of H, He, Li-like muonic Ar ions", The Physical Society of Japan, Annal meeting, September 10, 2022 (online)
3) Okumura, *et. al.* "High-resolution spectroscopy of electronic K x rays from muonic atoms", 20th International Conference on the Physics of Highly Charged Ions, Aug. 29 – Sep. 2, 2022, Matsue, Japan

(3) Others

Supercomputer	Use	Allocated resources*	
		Initial resources	Additional resources
Cygnus	Yes	3,600	0
Wisteria/BDEC-01	Yes	36,000	0
*in units of node-hour product			