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

Xiao-Min Tong
Center for Computational Sciences, University of Tsukuba

1. Project Purpose

a) To study the non-dipole contribution in intense laser atom interaction and to investigate how the retardation affects the photoelectron momentum distribution along the laser propagation direction. Such a work needs a high precision simulation since the retardation is a high order effect.

b) To investigate the exotic atomic structure of muon captured in materials by developing a relativistic local spin density functional method. The purpose of the work is to understand the ongoing experiments in RIKEN

2. Results

a) We have studied the momentum distribution along the laser propagation direction which is induced by the non-dipole interaction of the ionized electron with the laser field. By changing the model potential, we find that the momentum shifts along the laser propagation direction have structure which depends on the detailed motion of the electron or model potential used in the simulation. The theoretical prediction with the model potential generated by our previous work is in good agreement with the experiment. The dip structure observed in the experiment is attributed to the back scattering of the electron by the nucleus. This is a joint wok with other groups around the world and the work is published in Physical Review Letter [**128**, 023301:1-6 (2022)], a prestige journal in physical society. The work was selected as editor's suggestion.

b) We have simulated the energy structures of exotic atoms of negative muon captured by Fe and Cu at various ionic states. Due to the mass difference between the muon and electron, the muon moves closer to the nucleus than the electron. The emitted K_α and K_β X-rays encode the information of the muon position. Our structure simulations are used to simulate the dynamic process of muon de-excitation, which reflects the time-dependent screening effect of nuclear charge by the negative muon and the L-shell electrons. Although Fe and Cu are low$-Z$ atoms, the relativistic effect is unexpected important due to the muon moves very closer to the nucleus. This is a joint wok with an experiment

group in RIKEN and other theoretical group in Europe. The work is also published in Physical Review Letter [127, 053001:1-6 (2021)], a prestige journal in physical society. The work is also selected as editor's suggestion.

3. Roles of the MCRP and its significance

Both above works involved large scale numerical simulations. Project a) was a full 3-dimension time-dependent problem and it took one month for a test run on a workstation. So, the work could not be done without running on Cygnus. Project b) was also time-consuming work due to the two different space grids of electron and muon, plus there are about several ten thousand configures. The simulation was executed on OFP. With the MCRP support, we could speed-up the simulation time and made the impossible work on a workstation possible.

4. Future plan

We will continue our present theoretical work on the laser material interaction, mainly focus on the strong field excitation process, which is a hot topic in the strong field society. The work is also stimulated by the recent experiments performed in Griffith University. Meanwhile, we will restart our previous work on di-electron recombination of highly charged Bi ions. The goal of this work is to understand the unexpected polarization observed in Tokyo EBITs by the experiment group in the University of Electro-Communications.

5. Publications and conference presentations

(1) Journal papers

1) K Lin, S Brennecke, HC Ni, X Chen, A Hartung, D Trabert, K Fehre, J Rist, XM Tong, J Burgdorfer, LPH Schmidt, MS Schoffler, T Jahnke, M Kunitski, F He, M Lein, S Eckart, and R Dorner, "Magnetic-field effect in high-order above-threshold ionization", Phys. Rev. Lett. **128**, 023301:1-6 (2022).

2) T Okumura,T Azuma, DA Bennett, P Caradonna, I. Chiu, WB Doriese, MS Durkin, JW Fowler, JD Gard, T Hashimoto, R Hayakawa, GC Hilton, Y Ichinohe, P Indelicato, T Isobe, S Kanda, D. Kato, M Katsuragawa, N Kawamura, Y Kino, MK Kubo, K Mine, Y Miyake, KM Morgan, K Ninomiya, H Noda, GC O'Neil, S. Okada, K Okutsu, T Osawa, N Paul, CD Reintsema, DR Schmidt, K Shimomura, P Strasser, H Suda, DS Swetz, T Takahashi, S Takeda, S Takeshita, M. Tampo, H. Tatsuno, XM Tong, Y Ueno, JN Ullom, S Watanabe, and S Yamada, "De-excitation dynamics of muonic atoms revealed

by high precision spectroscopy of electronic K x rays using superconducting transition-edge sensor microcalorimeters", Phys. Rev. Lett. **127**, 053001:1-7 (2021).

(2) Presentations

1) H Ni, S Brennecke, X Gao, PL He, S Sonsa, I Brezinova, F He, J Wu, M Lein, XM Tong and J Burgdorfer, "Noadiabatic Subcycle Linear Momentum Transfer in Tunneling Ionization", 32nd International Conference on photonic, electronic and atomic collision, July 20-23, 2021(online).
2) T Okumura, T Azuma, DA Bennet, P Caradonna, I Chiu, WB Doriese, MS Durkin, JW Fowler, JD Gard, T Hashimoto, R Hayakawa, GC Hilton, Y Ichinohe, P Indelicato, T Isobe, S Kanda, D Kato, M Katsuragawa, N Kawamura, Y Kino, KM Kubo, K Mine, Y Miyake, KM Morgan, K Ninomiya, H Noda, GC O'Neil, S Okada, K Okutsu, T Osawa, N Paul, CD Reintsema, D R Schmidt, K Shimomura, P Strasser, H Suda, DS Swetz, T Takahashi, S Takeda, S Takeshita, M Tampo, H Tatsuno, XM Tong, Y Ueno, JN Ullom, S Watanabe, and S. Yamada, "High resolution measurement of electronic K x rays from muonic atoms in metal", 32nd International Conference on photonic, electronic and atomic collision, July 20-23, 2021(online).
3) XM Tong, "Exchange-correlation functional with self-interaction corrections for many-atom systems", 32nd International Conference on photonic, electronic and atomic collision, July 20-23, 2021(online).

(3) Others

Supercomputer	Use	Allocated resources*	
		Initial resources	Additional resources
Cygnus	Yes	2,592	0
Oakforest-PACS	Yes	36,720	0
*in units of node-hour product			