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) Collaborate with the experiment group at Griffith University to study atomic excitation in a strong laser field, mainly focusing on how to search for the best experimental condition to get the largest atomic excitation probability.

b) Collaborate with the experiment group in RIKEN to study the K x-ray emission from muonic atoms in the gas phase, especially in the 3 keV region, in which the neutral Ar K_α, μAr electronic hyper-satellite, K_α^h and muon X-ray transitions are mixed.

c) Continue our collaboration with Tokyo EBITs to investigate how the interference between radiative and dielectronic recombination affects other isoelectronic systems of highly charged ions. This year, we will focus on the Li-like ions to investigate the QED effects.

2. Results

a) We studied the atomic excitation of Ar atoms in a two-color laser field using a Genetic Algorithm (GA). With the help of the GA method, we found that a strong 400 nm and a weak 800 nm laser can produce more excited states than a weak 400 nm and a strong 800 nm. This conclusion contradicts our original plan, so the experiment is reset to confirm the findings.

b) After a long time of discussion with our experimental colleagues, we finally found that the discrepancies between the experimental measurement and the theoretical results originated from the initial muon capture states. We found that the muon orbital collapse plays an important role. This finding results in two papers (one theory and one experiment) accepted by Physical Review Letters.

c) Following our previous works, we found that the interference between dielectronic and radiative recombination improves the agreement between the experiment and theoretical simulations for the Li-like ions. We still cannot conclude if the full Breit interaction is better than the Breit interaction with zero frequency approximation. We consider the multipole transitions, and the agreement does not improve.

d) We started a new collaboration with an experiment group at Max-Planck Institute of Nuclear Physics to study the single-photon double excitation of He atoms in a combined XUV and IR pulse. With the help of the IR laser, the experiment can observe a weak

transition. Based on our full two-electron quantum simulation, we found that the observable of the weak transition is due to the indirect two-photon IR transition. This finding is accepted for publication in Nature Communications.

3. Roles of the MCRP and its significance

Most of the simulation codes are ready to run on a GPU machine. Most of the simulations were carried out on Cygnus. Especially for results a), it had to run the GA method, which solved the time-dependent Schrodinger equations several million times. The code for result d) only works on a CPU machine, and the simulation was performed on Wisteria. Without the support of the MCRP, we couldn't perform the present research.

4. Plan

a) Continue our collaboration with the experiment group at Griffith University to study atomic excitation in a strong laser field, mainly focusing on how to search for the best experimental condition to get the largest atomic excitation probability. This is a long-term collaboration project supported by the Austrian Research Council under the Discovery Project Grand ID: DP230101253. This year, we will focus on how the chirped pulse affects the excitation probability.

b) Continue our collaboration with the experiment group at RIKEN to investigate the muon-heavy atom collision. We would like to confirm if the orbital collapse also works for the heavy atoms, as our theory suggests.

c) Continue our collaboration with the experiment group at the University of Electro-Communications to solve the discrepancies between the observations and our simulations.

d) Start a new research project to collaborate with the research group at EPFL in Lausanne, Switzerland, to study the two-photon excitation of Hydrogen atoms in a strong-short laser field. This project is for plasma diagnosis using LIF.

e) Start a new research project to collaborate with a research group at Kyoto University to provide atomic data for the explanation of observations in astrophysics.

5. Publications and conference presentations

(1) Journal papers

- X. M. Tong, K. Tokesi, D. Kato, T. Okumura, S. Okata and T. Azuma, *"Orbital Collapse in Exotic Atoms and Its Effect on Dynamics"*, Phys. Rev. Lett. accepted.

- Yu He, Xiao-Min Tong, Shuyuan Hu, Gergana D. Borisova, Hao Liang, Maximilian Hartmann, Veit Stooss, Chunhai Lyu, Zoltan Harman, Christoph H. Keitel, Kenneth J. Schafer, Mette B. Gaarde, Christian Ott, and Thomas Pfeifer, *"Bring Weak Transitions*

to Light", Nature Communications (accepted).

- T. Okumura, T. Azuma, D. A. Bennett, W. B. Doriese, M. S. Durkin, J. W. Fowler, J. D. Gard, T. Hashimoto, R. Hayakawa, Y. Ichinohe, P. Indelicato, T. Isobe, S. Kanda, D. Kato, M. Katsuragawa, N. Kawamura, Y. Kino, N. Kominato, Y. Miyake, K. M. Morgan, H. Noda, G. C. O'Neil, S. Okada, K. Okutsu, N. Paul, C. D. Reintsema, T. Sato, D. R. Schmidt, K. Shimomura, P. Strasser, D. S. Swetz, T. Takahashi, S. Takeda, S. Takeshita, M. Tampo, H. Tatsuno, K. Tokei, X. M. Tong, Y. Toyama, J. N. Ullom, S. Watanabe, S. Yamada, and T. Yamashita, *"Few-electron highly charged muonic Ar atoms verified by electronic K x rays"*, Phys. Rev. Lett. (accepted).

(2) Presentations

- X. M. Tong, *"Theory on Dynamics of Atoms in Strong Laser Field",* 32nd Summer School and International Symposium on the Physics of Ionized Gases, Belgrade, Serbia, Aug 26-30, 2024 (**Plenary Talk**).
- X. M. Tong, D. Kato, T. Okumura, X, Gao, S. Okada, N. Nakamura, T. Azuma, "Theories on the Polarization of Dielectronic Recombination and Structures of Muonic Highly Charged Ions", 21st Highly Charged Ions Conference, Egmond aan Zee, Netherlands, Sept 1-6, 2024 **(invited talk**).
- T. Okumura, T. Azuma, D. A. Bennett, W. B. Doriese, M. S. Durkin, J. W. Fowler, J. D. Gard, T. Hashimoto, R. Hayakawa, Y. Ichinohe, P. Indelicato, T. Isobe, S. Kanda, D. Kato, M. Katsuragawa, N. Kawamura, Y. Kino, N. Kominato, Y. Miyake, K. M. Morgan, H. Noda, G. C. O'Neil, S. Okada, K. Okutsu, N. Paul, C. D. Reintsema, T. Sato, D. R. Schmidt, K. Shimomura, P. Strasser, D. S. Swetz, T. Takahashi, S. Takeda, S. Takeshita, M. Tampo, H. Tatsuno, X. M. Tong, Y. Toyama, J. N. Ullom, S. Watanabe, S. Yamada, and T. Yamashita, *"X-ray spectroscopy of highly charged muonic atoms with transition-edge sensor microcalorimeters"*, 21st Highly Charged Ions Conference, Egmond aan Zee, Netherlands, Sept 1-6, 2024 (**invited talk**).
- X. M. Tong, D. Kato, T. Okumura, X. Gao, S. Okada, N. Nakamura, T. Azuma, "Polarization induced by the interference of dielectronic and radiative recombinations for highly charged ions", 2024 年 9 月 16～19 日、第７９回日本物理学会　北海道大学　札幌キャンパス(**invited talk**).
- 奥村拓馬, 東俊行, D.A. Bennett, W.B. Doriese, M.S. Durkin, J.W. Fowler, J.D. Gard,橋本直, 早川亮大,一戸悠人, P. Indelicato, 磯部忠昭, 神田聡太郎, 加藤太治, 桂川美穂, 河村成肇, 木野康志, 小湊菜央, 三宅康博, K.M. Morgan, 野田博文, G.C. O'Neil, 岡田信二, 奥津賢一, N. Paul, C.D. Reintsema, 佐藤寿紀,

D.R. Schmidt,下村浩一郎, P. StrasserC, D.S. SwetzB, 高橋忠幸 F, 武田伸一郎, 竹下聡史, 反保元伸, 竜野秀行, X.M. Tong, 外山裕一, J.N. UllomB, 渡辺伸, 山田真也, 山下琢磨, “TES 型 X 線マイクロカロリメータによるミュオニック多価イオン形成メカニズムの解明”, 2024 年 9 月 16〜19 日、第７９回日本物理学会　北海道大学　札幌キャンパス(**invited talk**).

- X. M. Tong, K. Tokesi, 加藤太治, 奥村拓馬, 岡田信二, 東俊行, “エキゾチック原子における Orbital Collapse とそのダイナミクスへの影響”, 3 月１８～２１日、日本物理学会 2025 年春季大会。

(3) Others

Supercomputer	Use	Allocated resources*		
		Initial resources	Transferred resources**	Additional resources
Cygnus	Yes	2560	0	0
Pegasus	No	-	-	-
Wisteria/BDEC-01	Yes	15360	0	0
	*in units of node-hour product ** If the budget transfer was performed, fill in here, such as “+2000” and “−1000”.			