

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) Collaborate with an experimental group in the Max-Planck-Institute for Nuclear Physics to study the enhancement of a weak transition assisted by a strong, short IR laser pulse.

2. Results

- a) We studied the atomic excitation of Ar atoms in a two-color laser field using a Genetic Algorithm (GA). Using the GA method, we found that a strong 400 nm laser and a weak 800 nm laser produce more excited states than a weak 400 nm laser and a strong 800 nm laser. Generally speaking, the shorter the pulse duration, the larger the excitation probability is. But it reaches a limit when the pulse is shorter than 5 fs. So far, the experiment has been 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) published in Physical Review Letters.
- c) Using the large-scale simulation, we confirmed that the weak transition can be enhanced by 2-3 orders by adding a second IR pulse. Further investigation in the simulation by turning off certain autoionization states, we illustrate the mechanics of the enhancement: the observable of the weak transition is due to the indirect two-photon IR transition. This finding is published 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 and Miyabi-G. Especially for result 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 Miyabi-C.

Without the support of the MCRP, we couldn't perform the present research.

4. Future plan

- 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.
- We will investigate how to describe the multi-photon excitation process in a short laser field when Fermi's golden rule fails. By productive simulation, we hope to find a general rule for multi-photon excitation in a short weak laser field. Such research is very important for plasma diagnosis.

5. Publications and conference presentations

(1) Journal papers

- Yu He, Xiao-Min Tong, Shuyuan Hu, Gergana D. Borisova, Hao Liang, Maximilian Hartmann, Veit Stooss, Chunhai Lyu, Zoltán Harman, Christoph H. Keitel, Kenneth J. Schafer, Mette B. Gaarde, Christian Ott & Thomas Pfeifer, "Bring weak transitions to light", *Nature Communications*, **16**, 5322 (2025).
- 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, (43), "Few-electron highly charged muonic Ar atoms verified by electronic K x rays", *Phys. Rev. Lett.* **134**, 243001:1-7 (2025).
- 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.* **134**, 193001:1-6 (2025).

(2) Presentations

- 奥村拓馬, 東俊行, 橋本直, 早川亮大, 加藤太治, 金子真太郎, 岡田信二, 齋藤岳志, 高橋嶺, X.M. Tong, 外山裕一, 山田真也, for HEATES collaboration, "超伝導転移端検出器を用いたミュオンキセノン原子の高分解能硬X線分光", 日本物理学会第80回年次大会 (2025年) 9月16~19日、広島大学、東広島キャンパス。
- Y He, XM Tong, S Hu, G D Borisova, H Liang, Y Zhang, M Rebolz, M Hartmann, V Stooss, Z Liu, C Lyu, Z Harman, C H Keitel, K J Schafer, M B Gaarde, C Ott, and T

Pfeifer, “Bring weak transitions to light”, 34th International Conference on Photonic, Electronic and Atomic Collisions, July 29-Aug. 5, 2025, in Sapporo, Japan.

- CW Hogle, L Martin, WK Peters, XM Tong, T Miteva, K Ueda, LS Cederbaum, and P Ranitovic, “Laser-Enabled Control of Interatomic-Coulomb-Decay Dynamics”, 34th International Conference on Photonic, Electronic and Atomic Collisions, July 29-Aug. 5, 2025, in Sapporo, Japan.
- YN Yang, AJ David, XM Tong, IV Litvinyuk, RT Sang, “Excitation of Argon using strong-field light”, 34th International Conference on Photonic, Electronic and Atomic Collisions, July 29-Aug. 5, 2025, in Sapporo, Japan.
- XM Tong and N Toshima, “Efficient way to create H 3d excited state in strong laser fields”, 34th International Conference on Photonic, Electronic and Atomic Collisions, July 29-Aug. 5, 2025, in Sapporo, Japan.
- XM Tong, T. Károly, D. Kato, T. Okumura, S. Okada, T. Azuma, “Orbital collapse in exotic atoms”, 34th International Conference on Photonic, Electronic and Atomic Collisions, July 29-Aug. 5, 2025, in Sapporo, Japan (**invited talk**).
- Y He, XM Tong, S Hu, G D Borisova, H Liang, Y Zhang, M Rebholz, M Hartmann, V Stooss, Z Liu, C Lyu, Z Harman, C H Keitel, K J Schafer, M B Gaarde, C Ott, and T Pfeifer, “Attosecond transient absorption spectroscopy of laser-dressed dense helium: spectral lineshape modification and weak transitions brought to light”, 10th International Conference on Attosecond Science and Technology (ATTO X), July 6th to 11th, 2025 in Lund, Sweden.

(3) Others

Supercomputer	Use	Allocated resources*		
		Initial resources	Transferred resources**	Purchased resources
Pegasus	Yes/No	2816		0
Miyabi-G	Yes/No	6336	0	0
Miyabi-C	Yes/No	1584	0	0
*in units of node-hour product				
** If the budget transfer was performed, fill in here, such as “+2000” and “-1000”.				