Canadian Association of Physicists

Association canadienne des physiciens et physiciennes

Contribution ID: **145** Type: **Oral Competition (Graduate Student) / Compétition orale (Étudiant(e) du 2e ou 3e cycle)**

(G*) Accurate numerical method for the calculation of the doubly excited states in atoms

Wednesday 9 June 2021 15:59 (4 minutes)

We investigate in the present work the doubly excited states (DES) in the Helium-like O6+ and F7+ ions. The interaction of these systems with X-ray laser pulses can cause the DES to appear in their energy spectra due to the strong correlation between the electrons. The formation of the DES can be followed by a decay by electron emission (autoionization) causing the parent ion to lose its electrons.
The recent advent of free electron lasers (FELs) sources capable to generate laser pulses of durations comparable to the ultrashort lifetimes of the autoionizing DES in atoms will open the opportunity to investigate the autoionization mechanisms and to understand the importance of the role the DES play in the ionization process. Accurate theoretical knowledge of where these states can be located in the energy spectrum of the targeted system and their precise lifetime decay will be a support to the future experiments on the laser-atom processes involving the DES.
To date, theoretical data of the energy position E and the lifetime decay τ for the DES in the O6+ and F7+ ions and other heavier systems are still lacking. In order to locate and investigate the DES in the energy spectrum of an Helium-like ion, we have developed an efficient method based on the numerical resolution of the Schrödinger equation with a B-splines discretization technique [1,2] combined with the complex rotation method [3]. Our method has the numerical advantage to generate the parameters (E, τ) in a single calculation. It also allows the identification of the DES that share similar angular correlation pattern, which helps in their classification into distinct series.
We present our recently published results on the detection of DES in the O6+ion [4] and other recent results of our investigation of the DES in the F7+ ion. The theoretical results generated in this work will be of great interest to the future experiments on the O6+ and F7+ with X-ray FELs laser pulses.

[1] S. Barmaki, M.-A. Albert, S. Laulan, Chem.Phys. 517, 24 (2019)
[2] S. Barmaki, M.-A. Albert, S. Laulan, J. Phys. B: At. Mol. Opt. Phys. 51, 105002 (2018)
[3] M.- A. Albert, S. Laulan, S. Barmaki, Radiat. Phys. Chem. 166, 108453 (2020)
[4] S. Barmaki, M.- A. Albert, S. Laulan, Phys. Scr. 95, 055403 (2020)

Author: ALBERT, Marc-André

Co-authors: Dr LAULAN, Stéphane; Dr BARMAKI, Samira

Presenter: ALBERT, Marc-André

Session Classification: W3-1 Quantum Information: Theory (DAMOPC) / Information quantique: théorie (DPAMPC)

Track Classification: Atomic, Molecular and Optical Physics, Canada / Physique atomique, moléculaire et photonique, Canada (DAMOPC-DPAMPC)