Beitrag ID: **33** Typ: **Poster**

A Pedestrian Approach to Modeling Atomic Processes and Behavior

Montag, 15. September 2025 16:30 (1 h 30m)

Synopsis While the interaction of atoms with particles and light has been extensively studied over the past decades, making precise and reliable predictions about the behavior and dynamics of atoms and ions remains a challenge. Serious difficulty arise not only from the complexity of most atomic processes but also from the intricate nature of inter-electronic interactions. In this work, we introduce, emonstrate, and advance computational tools designed for providing consistent and reliable atomic data.

Atomic data and information are essential in fields such as astrophysics, plasma physics or fusion research, where an accurate modeling of atomic interactions, radiation processes, and energy transfer is more or less urgently required, but also at many places elsewhere. Whereas, at least in principle, this information could be obtained through (spectrocopic) measurements, computational methods need to be developed in order to solve the quantum many-electron problem with sufficient accuracy. Despite recent progress, however, detailed predictions in atomic and plasma physics are challenging due to the complex interplay of many-body interactions, relativistic effects as well as quantum correlations, which altogether often require sophisticated models and extensive computational resources.To overcome these difficulties, powerful opensource codes are required to incorporate manybody interactions and relativistic contributions into the modeling of atoms, and especially into their coupling to the electron continuum. With JAC, the Jena Atomic calculator [1,2], we now supports atomic (structure) calculations of different kinds and complexities. Indeed, this toolbox can be readily applied also to model a good number of atomic excitation and decay processes within the same computational ramework. With the design and implementation of JAC, we aimed also to develop a “descriptive language”that is (i) user-friendly, (ii) emphasizes the underlying atomic physics, and (iii) avoids most technical jargon, as is common for other established codes.

All these goals are relevant in order to ensure a good (self-)consistency of the data generated for different atomic roperties, processes and cascade [3].

Figure 1. Features of the JAC toolbox [1,2].

In this talk, I shall explain how JAC can be utilized to model many, if not most, of the known processes. Explicit examples will include collective Auger processes [4], the decay dynamics of double core-hole states [5], or various types of hyperfine-induced transitions. In particular, I shall demonstrate that such a collaborative approach is not only desirable but also feasible and highly beneficial for the atomic physics community.

References

[1] Fritzsche S 2019 Comp. Phys. Commun. 240 1

[2] JAC: https://github.com/OpenJAC/JAC.jl

[3] Fritzsche S et al 2024 Eur. J. Phys. D78 75

[4] Hikosaka Y and Fritzsche S 2025 Phys. Rev. Lett.134 in print

[5] Mazza et al 2024 J. Phys. B 57 225001

Autor: FRITZSCHE, Stephan

Vortragende(r): FRITZSCHE, Stephan

Sitzung Einordnung: Poster Session