Project Title:

Atomic database for X-ray astrophysics

Name:
〇Liyi Gu (1)
Laboratory at RIKEN:
(1) **Tamagawa high energy astrophysics laboratory**

1. Background and purpose of the project, relationship of the project with other projects

The research aims to elevate the precision of atomic data utilized in X-ray astronomy, ensuring the requisite accuracy for the accurate interpretation of high-resolution spectroscopic data anticipated from upcoming missions. As XRISM was just launched, the SPEX team is intensifying efforts to incorporate updates on atomic data. This includes refining calculations on L-shell collisional excitation, photoionization cross sections, and innershell ionization cross sections for cosmic abundant elements. While the atomic data have undergone testing in single temperature calculations before integration into SPEX, a more comprehensive verification is necessary to establish their alignment with observations under varied conditions. Obtaining errors on theoretical rates can be achieved through comparisons with observational data.

2. Specific usage status of the system and calculation method

We carried out a systematic calculation of photoionization cross sections and innershell ionization cross sections for a number of cosmic abundant elements. The flexible atomic code (FAC) has been used. It allows relativistic configuration interaction which is needed to solve the innershell atomic structure.

3. Result

The photoionization cross section in SPEX has been improved mainly in two aspects:

1. The ground-based measurements of the absorption edge energies has been incorporated in the new dataset.
2. The new data include resonance contributions in the photoionization rates. These resonances are calculated by evaluating the photoexcitation-autoionization routes.

The free-bound emission and the photoionization heating has been improved in the similar way.

The innershell ionization rates are calculated for Fe. Systematic crosscheck will be needed to validate the new calculation.

4. Conclusion

The new atomic data calculated based on RIKEN's super computer has been implemented into the popular X-ray code supporting the science of XRISM mission. The photoionization model but also other plasma models have been improved.

5. Schedule and prospect for the future

The innershell ionization calculation towards the neutral species requires high-order approaches such as many-body pertubative theory. This approach will be utilized in the coming year.

6. If no job was executed, specify the reason.

Usage Report for Fiscal Year 2023

Fiscal Year 2023 List of Publications Resulting from the Use of the supercomputer

[Paper accepted by a journal]

Gu, Liyi, Kaastra, Jelle, Rogantini, Daniele, Mehdipour, Missagh, Juráňová, Anna, Costantini, Elisa, Li, Chen, 2023, Time-dependent photoionization spectroscopy of the Seyfert galaxy NGC 3783, Astronomy & Astrophysics, 679, 43, 12

[Conference Proceedings]

[Oral presentation]

[Poster presentation]

[Others (Book, Press release, etc.)]