Usage Report for Fiscal Year 2019

Project Title: Atomic database for X-ray astrophysics

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

Precise interpretation of X-ray spectra from the cosmic sources rests crucially on the accurate modeling of atomic processes. Increasing reach of X-ray astrophysics, to be allowed by the high-resolution X-ray spectrometer on-board XRISM (2022, JAXA/ISAS), is making the demand for robust modeling of the atomic spectrum more stringent than ever. The **goal** of the research is to bridge the gap between requirement and current quality of the plasma modeling, through systematic improvement, extension, and validation of the atomic data and software of the SPEX code. These new developments will result in a fundamental improvement of our capability to perform frontline science with the new challenging data obtained with XRISM.

This project and its successors are a part of the RIKEN pioneering project "evolution of matters in the universe".

2. Specific usage status of the system and calculation method

We calculate atomic data of the basic atomic structure (level energies, transition probability) and collision cross sections (electron-impact collision excitation, dielectronic recombination, radiative recombination, Auger auto-ionization, innershell ionization/excitation) using the flexible atomic code (FAC, a free open source code).

The current run uses 15363.0 core-hours in the past FY year. The calculation time is on the same order as the proposed amount in the application.

3. Result

A bulk of atomic data has been produced with the calculation. The current calculation focuses on the collisional excitation (including pure electron-impact and resonant excitations) and dielectronic recombination for Fe XVI to Fe XXIV, all visible in the X-ray spectrum at the Fe-L complex. The new calculation is substantially more complete than the current database in the SPEX atomic code.

The new calculations are compared to the existing results with the R-matrix method, as well as to the controlled laboratory measurements obtained with the EBIT experiments, and the stellar corona grating spectrum of Capella. The comparison reveals difference of 10-20% for the main emission lines. The discrepancies are much larger for the weaker lines. This proves that the uncertainties in the atomic database now contribute a main component for the systematics in the science outcome of future X-ray missions.

4. Conclusion

We performed the theoretical calculation of X-ray spectrum of the Fe-L complex. We calibrated the theoretical cross sections through the EBIT measurement and Chandra grating observation of Capella. We conclude that the present Fe-L atomic calculation is almost ready to be delivered to the community, except for a few issues on wavelengths and rates, which are to be addressed with the follow-up calculations and dedicated lab measurements.

5. Schedule and prospect for the future

A follow-up project is proposed in FY2020 to continue the theoretical calculation of the atomic structure. We plan to spend the computing time in the first half year on the other Fe ions and the late half year on the K-shell (and L-shell when applicable) of O, Ne, Mg, Si, S, Ar, and Ca.

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

Fiscal Year 2019 List of Publications Resulting from the Use of the supercomputer

[Paper accepted by a journal]

Gu, L., Raassen, A. J. J., Mao, J., de Plaa, J., Shah, C., Pinto, C., Werner, N., Simionescu, A., Mernier, F., and Kaastra, J. S. X-ray spectra of the Fe-L complex, Astronomy & Astrophysics, 627, A51:24, July 2019.

[Conference Proceedings]

[Oral presentation]

Gu, L. "Plasma and atomic astrophysics", XCalibur 2019, Winchester, 2019/07/15

[Poster presentation]

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