Usage Report for Fiscal Year 2022

Project Title:

Atomic database for X-ray astrophysics

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

The objective of the research is to enhance the quality of atomic data utilized in X-ray astronomy, thereby achieving the necessary level of accuracy for correctly interpreting the high-resolution spectroscopic data obtained from the forthcoming missions. As the launch of XRISM is approaching (expected May 2023), the SPEX team is accelerating our activities implementing the updates on atomic data, including the calculation carried out on the L-shell collisional excitation for cosmic abundant elements. The atomic data have been tested in single temperature calculations before imported to SPEX, however, a more extensive verification is required to ensure the data match well with the observations in all conditions. The errors on the theoretical rates can also be obtained by comparing with the observations.

2. Specific usage status of the system and calculation method

We suggest that the atomic data uncertainties can be inferred by a statistical sampling of discrepancies between the models and well-calibrated, well-understood spectra, which can be treated as the absolute true values within their quoted uncertainties. This approach is valid when (1) the sampling size of spectral feature measurements is statistical significant, and (2) the observed discrepancies are not driven by other types of uncertainties, such as statistical uncertainty and systematic uncertainties from astrophysics and instrumental calibration.

We perform comparison on the following data: for the collision excitation forming Fe-L, we choose the Chandra high energy transmission grating (HETG) data of Capella and HR 1099; the Chandra low energy transmission grating (LETG) data of Capella are used to calibrate the L-shell data of Mg, Si, S, and Ca, as well as lowly-ionized Fe. Both targets are well-studied X-ray bright stellar corona mostly in quiescent.

We run a large set of calculations of atomic constants (collisional rates and level energies) and compare the spectra with the observed Capella data.

3. Result

For strong transitions, the fractional uncertainties are found to be around 10%, while for the weak lines, the uncertainties increase to unity or larger. To describe the observed uncertainty-emissivity relation, we divide the emissivity range into a number of bins, and assume for each bin that the distribution of uncertainties follows a Gaussian function with zero mean value. The derived variances of the systematic uncertainties, as plotted in Figure 1, can be approximated by a simple power-law function,

$$\sigma = a \times \left(\frac{I}{10^{41}}\right)^{b}$$

Where σ is the variance, I is the line emissivity in unit of photons per second, a and b are the free parameters. This relation holds for both Capella and HR 1099.

4. Conclusion

The collision excitation calculation by L. Gu on L-shell lines should be considered valid in general as the discrepancies between model and data are ~10% for strong lines. The line diagnostics using weak lines, on the other hands, would be caveated as the uncertainties increase, which is not surprising given the complexity in atomic physics concerning the weak transitions. The routine for error calculation has been implemented in SPEX. This will improve the interpretation of the data from upcoming XRISM and Athena missions.

5. Schedule and prospect for the future

Our proposed follow-up project for FY2023 aims to further theoretical calculations of atomic constants. Specifically, we plan to devote computing time to innershell ionization and the transition from meta-stable levels. As time allows, we will also calculate E- and B-dependent transition rates.

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

Fiscal Year 2022 List of Publications Resulting from the Use of the supercomputer

[Paper accepted by a journal]

Gu, L., Shah, C., Mao, J., et al. 2022, X-ray spectra of the Fe-L complex. III. Systematic uncertainties in atomic data, Astronomy and Astrophysics, 664, A62.

[Conference Proceedings]

[Oral presentation]

[Poster presentation]

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

Gu, L. & Shah, C. 2023, Charge exchange in X-ray astrophysics, chapter to the Springer book “High-Resolution X-ray Spectroscopy” (edited by Cosimo Bambi and Jiachen Jiang)