Uncertainty Calculations for Theoretical Atomic Data toward the Applications of Astrophysical Spectroscopy

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Most of our knowledge about our universe comes from observing the photons (light) emitted by the atoms in astrophysical objects. Using theoretical models, such observations can return a wealth of information on temperatures, densities, velocities, and plasma composition. However, there is usually not an estimate of the uncertainty in the theoretical calculations. Consequently, we often lack a meaningful range of values for the diagnosed parameters. In this work, we develop methods to assign uncertainties on atomic data and carry such uncertainties through to diagnosed plasma parameters. The difficulty in assigning uncertainties to theoretical atomic data lies in the complexity of the Schrödinger equation. This second order partial differential equation,

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\boldsymbol{r},t)+V_0(\boldsymbol{r},t)\Psi(\boldsymbol{r},t)=i\hbar\frac{\partial}{\partial t}\Psi(\boldsymbol{r},t),$$

where $-\frac{\hbar^2}{2m}\nabla^2$ is the kinetic energy operator and $V_0(\boldsymbol{r},t)$ is the potential energy, is challenging to solve and does not propagate uncertainties linearly on the wavefunctions. The solution may be very sensitive to the initial conditions. In this project, helium-like oxygen (O^{6+}) was considered. This two-electron system is an important temperature diagnostic in X-ray emitting plasmas. The atomic data for O^{6+} were calculated (excitation, ionization, and recombination), and uncertainties were assigned to the data. A Monte-Carlo method, with randomized input values within our uncertainty range, was used to compute the diagnostic line ratios. One million Monte-Carlo iterations were sufficient to cover the parameter space, and standard statistical methods were employed to analyze the data. A spectral line ratio as a function of plasma electron temperature was generated along with an uncertainty estimate on the line ratio. This will allow astrophysicists to assign a meaningful temperature range to their plasmas.

In exploring a new direction for this work we investigated the effects of correlation on the atomic data. Small changes were made to the orbital wavefunctions that were used in the atomic structure code [1], and the effects were carried through to spontaneous emission and electron-impact excitation rate coefficients. A case study on a controversial line ratio of Fe16+ was also investigated, and it was found that a counter-correlation (Figure 1) may help to explain much of the discrepancies in the literature [2].

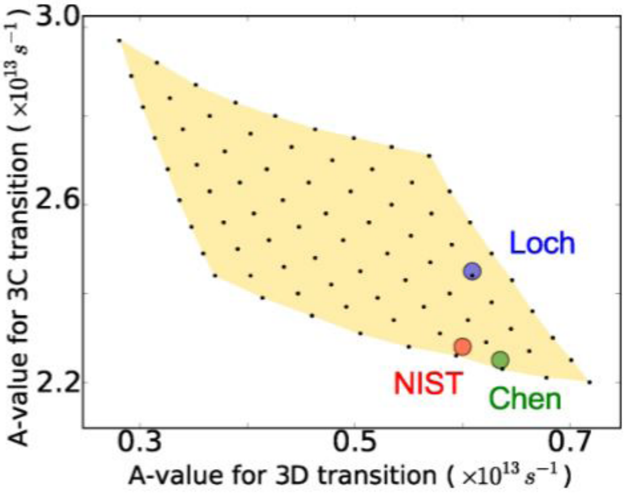

Figure 1. A-values for the 3C and 3D transitions for Fe^{16+}. The negative slope shows the counter-correlation in the values.

Statement of Research Advisor:

I guided the overall project direction and taught Mr. Yang how to run the large computer codes, with the exception for the ionization balance codes, which Mr. Yang wrote by himself
—*Hans-Werner van Wyk, Mathematics and Statistics and Stuart Loch, Physics*

References:

[1] Badnell et al., Astronomy and Astrophysics, 406, 1151 (2003)
[2] S. Bernitt et al., Nature, 492, 7428 (2012)