A Synergistic Approach to Modeling X-Ray Spectra


This paper was prepared for submittal to the Proceeding of the Laboratory Space Science Workshop Cambridge, MA April 1-3, 1998

July 1, 1998
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A Synergistic Approach to Modeling X-Ray Spectra

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Plasma emission models used in X-ray astronomy need to simulate X-ray spectra from at least thirteen elements. Development of comprehensive models requires large-scale calculations; for example, Fe M-shell spectra, Kα fluorescence from near-neutral ions, and dielectronic recombination satellite spectra from L-shell ions. Current and recent missions (EUVE, ASCA, DXS, etc.) have already demonstrated the need for major, rapid improvements in spectral models. The high-resolution spectra to be acquired with the next generation of X-ray observatories (AXAF, XMM, Astro-E) promise to push spectral models to their limits. Essential to ensuring the quality of calculations used in spectral codes is corroboration in the laboratory, where controlled and precisely measured plasma conditions can be attained. To this end, we are capitalizing on a three-way synergistic relationship that links astrophysical observations, atomic modeling, and experiments using the LLNL Electron Beam Ion Trap (EBIT). After providing a brief orientation concerning the role of plasma emission models in X-ray astronomy, we discuss one example of this interplay.

1. X-Ray Astrophysics and Atomic Modeling

Successful extractions of astrophysical information from X-ray spectra hinge upon the existence of a reliable atomic “database.” Highly-ionized species of the cosmically abundant metals C, N, O, Ne, Na, Mg, Al, Si, S, Ar, Ca, Fe, and Ni radiate in the X-ray band. Lower charge states also produce X rays through fluorescence following inner-shell ionization. Given that over a hundred charge states need to be accommodated, and that the range of physical conditions under which observable X-ray line emission can be produced in cosmic X-ray sources — ~10^6-10^8 K, ~10^{-3}-10^{18} cm^{-3} — is so large, it is clear that the assemblage of an accurate, versatile database poses considerable challenges.

Access to and manipulation of the vast retinue of atomic data currently used in spectroscopic analysis are provided by plasma emission codes. Along with a host of important astrophysical results, the ASCA, EUVE, and DXS missions have demonstrated our reliance on plasma emission codes, and the frustration that can result when satisfactory fits cannot be found. In fact, confrontations with spectra acquired during these missions have led us to conclude that the atomic data used in plasma codes are in need of a thorough overhaul. Atomic modeling problems derive from limitations in our abilities to achieve adequate levels of accuracy and completeness simultaneously. By accuracy, we refer to the degree to which quantities such as wavelengths or collision strengths are correct. Completeness can refer to
the degree to which the entirety of observational data is accommodated by the plasma code (e.g., wavelength or temperature coverage), or to the degree to which the code accounts for the total radiative power in a given spectral bin. In this context, it is worth emphasizing the distinction between atomic modeling and theoretical atomic physics. To first order, atomic modeling strives for completeness while maintaining an acceptable level of accuracy, while theoretical work strives for “first-principles” accuracy, with less attention paid to completeness. In developing a robust atomic model, all processes that contribute substantially to a given line emissivity must be included in a reasonably accurate way. Therefore, in harnessing what accurate atomic data exists to synthesize model spectra that are diagnostically reliable, a great deal of “engineering” is necessary. An example of engineering might be referred to as “hybridization,” where detailed calculations are augmented by interpolated or extrapolated approximations. Obviously, it is desirable that such a hybridized model be subjected to rigorous testing in the laboratory — before astrophysical conclusions are drawn.

2. Testing Modeling Schemes with the LLNL EBIT

We have identified non-negligible contributors to the line power that have simply been left out of plasma emission models (thus bearing on the issue of completeness), and which may underlie recent problems encountered in attempting to fit ASCA data (Liedahl & Brickhouse 1998). We find that the neglect of $nd \rightarrow 2p$ transitions from levels of high principal quantum number (high-$n$ or Rydberg levels), which are populated by electron impact excitation from low-lying levels, contribute to observable emission. For a given ion, the missing lines lie between the line of highest energy that is currently included in the spectral code and the ionization limit. Therefore, the line power in a set of narrow spectral bands is underpredicted by plasma models. This new component, when added to the current models, “fills in” regions of missing flux. In attempting to fit data with the MEKAL code (Mewe, Kaastra, & Liedahl 1995), evidence for these spectral regions of missing flux have been identified in at least three objects: Capella (Brickhouse et al. 1998), the cluster of galaxies A3581 (Johnstone, Fabian, and Taylor 1998), and the elliptical galaxy M87 (Hwang et al. 1997), where, for all three sources, the discrepancies lie in the 1.1–1.5 keV spectral region.

Using the HULLAC atomic physics package, we have re-calculated iron spectra for the eight L-shell ions Fe XVII–XXIV over temperature ranges appropriate to collisional ionization equilibrium (Liedahl, Osterheld, & Goldstein 1995). Typically, these models consist of all energy levels up to and including the fifth atomic shell, amounting to several hundred levels for most of the L-shell ions. Since we do not have the freedom to calculate accurate distorted wave collisional cross-sections for arbitrarily large models, emissivities for higher $nd \rightarrow 2p$ series members are obtained by extrapolating from the detailed calculations. Line positions are assigned according to a hydrogenic approximation. Our preliminary results suggest that the regions of missing flux in the 1.1–1.5 keV band can be attributed to the omission of $nd \rightarrow 2p$ lines in Fe XVII–XIX.

The LLNL EBIT facility was used to measure the radiative properties of Ne-like Fe XVII (Brown et al. 1998). The controllable, well-characterized conditions available on EBIT
allow us to isolate specific line-formation processes in specific ions. In this case, we studied Fe XVII spectra as produced almost entirely through collisional excitation from the 1s²2s²2p⁶ ground level. The brightest lines are those resulting from transitions of the type 1s²2s²2p⁵3l \rightarrow \text{ground}. Comparing the experimental intensity ratios to HULLAC calculations, good agreement was found for \( nd \rightarrow 2p \) transitions up to and including \( n = 6 \). For higher \( n \), however, the calculations overestimated the intensities. In fact, we find, for \( n \geq 8 \), an overestimate of \( \sim 40 \% \) for the summed \( nd \rightarrow 2p \) line flux. The reasons for the discrepancies are still under examination, but are thought to reflect an inadequate treatment of configuration interaction. As \( n \) increases, configurations in different shells begin to overlap in energy. Since energy levels in shells not included in the models can interact with levels in shells that are in the models, the calculations neglect a potentially important effect.

3. Synergy in Action

The example discussed in the previous section exemplifies the synergistic approach that has evolved. To summarize, motivated by difficulties encountered in astrophysical data, especially the ASCA spectrum of Capella, a series of calculations were performed, which apparently resolved the problem. Precision measurements obtained with EBIT, however, showed that the methods employed in obtaining the proposed solution were too simplistic. The atomic modeling results can be modified so as to be in accord with the EBIT measurements, where the modifications are currently assumed to mimic the effects of configuration interaction between high-lying energy levels. The new atomic models are being incorporated into plasma emission models, which, coming full circle, will then be brought to bear on the Capella spectrum (Brickhouse et al. 1998), the first astrophysical testbed for the improved plasma codes.

The synergy extends further, however. Problems such as that discussed in this paper, have contributed to a “community awareness” of the likelihood that plasma codes are missing a substantial fraction of the actual radiative power. In response to this awareness, the AXAF Science Center will conduct a series of observations comprising the “X-Ray Emission Line Project” (XELP). This program consists of several long-duration grating exposures of Procyon, Capella, and HR1099, three bright stars chosen to span a wide range in stellar coronal temperatures. The aim of the XELP is to assess the spectral content of an astrophysical plasma over a broad bandpass (1–140 Å). By “assess the spectral content” we mean the systematic evaluation — bin-by-bin — of emission-line flux in a plasma under coronal conditions. The evaluation addresses the problems of, first, discerning observable contributions to X-ray spectra, and, second, identifying the source of the emission. (It is worth emphasizing that failures to account fully for the spectral content of astrophysical plasmas, such as the \( n \rightarrow 2 \) lines discussed above, are among the chief impediments to obtaining satisfactory interpretations of several current datasets.) Based upon our experience with ASCA, EUVE, and DXS, we expect to uncover further shortcomings in the atomic database. The XELP will largely supersede the aggregate solar coronal database, owing primarily to the fact that spectra are to be obtained from well-calibrated grating instruments, the High Energy Transmission Grating (HETG) and the Low Energy Transmission Grating (LETG),
and will cover a large bandpass. We anticipate that results from the XELP will provide impetus for further spectroscopic investigations, on both the modeling and experimental fronts.

4. Concluding Remarks

The overlap of astrophysical data, laboratory data, and the results of atomic modeling works to maximize the utility of plasma emission models used for interpreting high-resolution spectra from complex (uncontrolled) environments found in high-energy astrophysics. The difficulties encountered with recent spectroscopic datasets, and the imminent launches of AXAF (1998), XMM (1999), and Astro-E (2000), have instigated worldwide efforts to develop new spectroscopic models, and to improve upon old ones. The accelerated pace of X-ray spectral code development should be accompanied by an equally accelerated worldwide program of laboratory testing and benchmarking.

References:

Acknowledgments:
We wish to thank Nancy Brickhouse for useful discussions. Work at LLNL was performed under the auspices of the U.S. Department of Energy Contract No. W-7405-ENG-48, and was supported by the NASA High Energy Astrophysics X-Ray Astronomy Research and Analysis grant NAG5-5123 (Columbia University) and work order W-19127 (LLNL).