Improved Simulations of Astrophysical Plasmas: Computation of New Dielectronic Recombination Data

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Abstract

Here we recap the works of two posters presented at the 2002 NASA Laboratory Astrophysics Workshop. The first was *Shortcomings of the R-Matrix Method for Treating Dielectronic Recombination*. The second was *Computation of Dielectronic Recombination Data for the Oxygen-Like Isoelectronic Sequence*.

1. Introduction

Most hard astrophysical numbers come from the quantitative analysis and interpretation of spectra, frequently of emitting plasmas that are at extremely low density by laboratory standards, and as a result the gas is in a profoundly non-equilibrium state. The physical conditions and the resulting spectrum cannot be predicted by analytical theory, and large-scale numerical simulations must be done instead. The results can be directly compared with a broad range of X-ray, UV, and IR observations, but rely on a vast sea of basic atomic and molecular cross sections and rates.

We have initiated a program to carry out detailed theoretical calculations for dielectronic recombination (DR) of specific 2nd, 3rd, and 4th row ions. These are investigated using a radiation-damped R-matrix approach as well as the perturbative AUTOSTRUCTURE package. These independently-determined DR rates are benchmarked against each other and, where possible, against experimental results. Here we detail two projects along these lines. First, a comparison between R-matrix, perturbative, and experimental results is made for DR of Fe XVIII, where certain shortcomings of these and other R-matrix methods are discovered. Second, we have used the perturbative program AUTOSTRUCTURE to compute DR and radiative recombination (RR) data along the entire O-like sequence, giving a single table of fitting coefficients.

2. Shortcomings of the R-Matrix Method for Treating Dielectronic Recombination

By performing new radiation-damped R-matrix scattering calculations for the photorecombination of Fe XVIII forming Fe XVII, we have demonstrated the difficulties and fundamental inaccuracies associated with the R-matrix method for treating dielectronic recombination (DR). Our new R-matrix results (Gorczyca *et al.* 2002) have significantly improved upon earlier R-matrix results (Pradhan *et al.* 2001; Zhang *et al.* 2001) for this ion. However, we have shown theoretically that all R-matrix methods are unable to account accurately for the phenomenon of radiative decay followed by autoionization. For Fe XVIII, we have demonstrated numerically that this results in an overestimate of the DR cross section at the series limit, which tends to our analytically predicted amount of 40%. We have further found the need for fine resonance resolution and the inclusion of radiation damping effects. Overall, slightly better agreement with experiment (Savin *et al.* 1999) is still found with the results of perturbative calculations, which are computationally more efficient than R-matrix calculations by more than two orders of magnitude.

3. Computation of Dielectronic Recombination Data for the Oxygen-Like Isoelectronic Sequence

We have systematically calculated rate coefficients for dielectronic recombination (DR) along the oxygenlike sequence. A recent benchmarking of DR resonance strength and energies between our theoretical techniques and the experimental results from the Test Storage Ring in Heidelberg has already shown fairly good agreement for the most highly-ionized oxygen-like system we consider here, DR of Fe XIX forming Fe XVIII (Savin *et al.* 2002). At the low-charge end of this isoelectronic sequence, we benchmark our results using F II DR data which are determined from measured neutral fluorine photoionization measurements and the principle of detailed balance. To assess the reliability of our calculations for intermediate oxygenlike ionization stages, we compare between theoretical R-matrix and perturbative results. All calculations have been performed in intermediate-coupling, so that fine structure effects are incorporated. Furthermore, both $\Delta n = 0$ and $\Delta n > 0$ core transitions are included in order to span a higher temperature range. Final-state-resolved rate coefficients and total rate coefficients have been tabulated, and these data are available in either format from our web site (`http://homepages.wmich.edu/~gorczyca/drdata`).

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