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Improved Collisional Line Broadening for Low-Temperature Ions and Neutrals in the spectral modeling code ATOMIC

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The Los Alamos National Laboratory (LANL) spectral modeling code ATOMIC, a part of the LANL suite of atomic physics codes, produces emissivity and opacity calculations for plasmas based on *ab-initio* atomic data from CATS and ionization cross-sections from GIPPER. It uses this atomic data to solve collisional-radiative atomic kinetics rate equations in either LTE or NLTE for single or multi-element plasmas. The ability to model complex systems with many thousands of lines in a reasonable computational time has required compromises in the treatment of Stark line broadening. The approximate model currently used[1] is based on the assumption that the complete set of all available transitions will contribute to the broadening, yielding a line width based on matrix elements proportional to the effective n, l quantum numbers of the levels of the transition in question and the electron temperature and density of the system. While this has been a reasonable estimate for high temperature systems, for low temperature (~ 1eV) plasmas, this approximation appears to overestimate the amount of broadening. This is because the threshold characterized by the ratio between the transition energy and the temperature of the system is much larger, so that the amount of Stark broadening a given state imparts is strongly correlated to its distance in energy from the transition in question. However, with improvements in computational resources it becomes possible to improve ATOMIC's treatment of line broadening for low temperature plasmas comprised of neutral atoms and low-charged ions (+1 and +2). For this purpose, we have implemented two collisional line-broadening models based on the impact parameter approximation. For neutral radiators, we utilize a variation of Griem's semi-empirical model[2]. For ion radiators, we utilize a semi-classical approach incorporating the hyperbolic curvature of the incoming electron's path[3]. We will compare widths extracted from each model to published experimental line widths for Ca I and Ca II lines[4]. As a real world test, we will model Ca spectra from a low temperature CaF_2 plasma produced in laser-induced breakdown spectroscopy (LIBS) experiments. We will compare the results of ATOMIC with and without the new collisional broadening routines against an independent line shape model[5].

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