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Completeness of the Configuration Interaction / Close Coupling expansion versus the relativistic formalism in R-matrix calculations

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Synopsis R-matrix calculations have different sources of inaccuracy. We analyze the differences in the final results caused by differences in three aspects of the calculation: the atomic structure of the target, the completeness of the close coupling expansion, and the method used to include relativistic effects in the Hamiltonian. We present the electron-impact excitation of the ion Be-like Al^{9+} as a case study. We conclude that the completeness of the CI/CC expansion plays the most important role for the reliability of the results, mainly for the most highly-excited levels.

Reliable and accurate electron-impact excitation data are key to the successful spectroscopic diagnostic modeling of non-LTE plasmas.

We have compared and contrasted differences in such data for the benchmark Be-like Al^{9+} ion which we have calculated using the R-matrix method [1]. Such differences arise through: 1) differing degrees of approximation of relativistic effects, 2) uncertainties in atomic structure / configuration interaction (CI) expansion and 3) errors due to the lack of convergence of the close-coupling (CC) expansion. Error 3) is quantifiable and can be reduced systematically and reliably — to illustrate this we compare a new 98-level and previous 238-level CC Intermediate Coupling Frame Transformation (ICFT) R-matrix calculations [2]. We find that effective collision strengths to $n = 4$ levels are significantly enhanced over a wide range of temperatures by coupling to $n > 4$ levels. Uncertainty 2) is quantifiable but is more difficult to reduce and constrain as an error. To illustrate this, we compared 98-level and 238-level CI expansion calculations of line strengths and infinite energy plane-wave Born collision strengths. Again, transitions to $n = 4$ levels are most susceptible to lack of convergence but of the CI expansion this time. Differences 1) between different R-matrix treatments of relativistic effects are small, and negligible relative to 2) and 3). We illustrate this by a comparison of new 98-level CI/CC ICFT and Breit–Pauli (BP) R-matrix effective collision strengths which use the exact same atomic structure. This is to be expected for an element which lies below Zn.

Thus, we find to be false a recent conjecture that the ICFT approach may not be completely robust [3]. The conjecture was based upon a comparison of 98-level CI/CC Dirac Atomic R-matrix Code (DARC) effective collision strengths for Al^{9+} [4] with those from the 238-level CI/CC ICFT R-matrix calculations of [2]. The disagreement found recently is due to a lack of convergence of the CC expansion in the 98-level CI/CC DARC work, mainly for the $n = 4$ levels.

Similar considerations need to be made for other Be-like ions, and for other sequences.

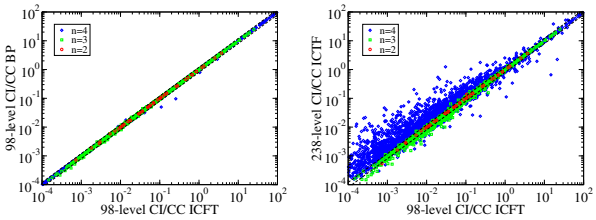

Figure 1. Comparison for the electron impact-excitation effective collision strengths for all transitions between the lowest 98 IC levels of the ion Al^{9+} at temperature $T = 10^6$ K. Left panel: BP vs ICFT, both for 98-level CI/CC expansion; right panel: 98- vs 238-level CI/CC expansion, both ICFT.

References

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