Accurate Transition Probabilities from Large-scale Multiconfiguration Calculations

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Abstract. The quality and resolution of solar, stellar, and other types of plasma observations, has so improved that the accuracy of atomic data is frequently a limiting factor in the interpretation of these new observations. An obvious need is for accurate transition probabilities. Laboratory measurements, e.g. using ion/traps, beam-foil or laser techniques, have been performed for isolated transitions and atoms, but no systematic laboratory study exists or is in progress. Instead the bulk of these atomic data must be calculated. Multiconfiguration methods, either non-relativistic with Breit-Pauli corrections (MCHF+BP) or fully relativistic (MCDHF), are useful to this end. The main advantage of multiconfiguration methods is that they are readily applicable to excited and open-shell systems, including open f-shells, across the whole periodic table, thus allowing for mass production of atomic data. The accuracy of these calculations depends on the complexity of the shell structure and on the underlying model for describing electron correlation. By systematically increasing the number of basis functions in large-scale calculations, as well as exploring different models for electron correlation, it is often possible to provide both transition energies and transition probabilities with some error estimate.

The success of the calculations also depends on available computer software. In this talk we will describe a collaborative effort to continue the important and acclaimed work of Prof. Charlotte Froese Fischer and to develop state-of-the-art multiconfiguration codes. In the latest versions of the non-relativistic (ATSP2K) and relativistic (GRASP2K) multiconfiguration codes angular integration is performed using second quantization in the coupled tensorial form, angular momentum theory in three spaces (orbital, spin and quasispin), and a generalized graphical technique that allows open f-shells. In addition it is possible to transform results given in the relativistic jj-coupling to the more useful *LSJ*-coupling. Biorthogonal transformation techniques are implemented and initial and final states in a transition can be separately optimized. The main parts of the codes are also adapted for parallel execution using MPI. Results from recent large-scale calculations using these codes will be presented for systems of different complexity. Of special interest are spectrum calculations, where all states up to a certain level are computed at the same time. Finally, we look at new computational developments that allow basis functions in multiconfiguration methods to be built on several independent and non-orthogonal sets of one-electron orbitals. Initial calculations indicate that the increased flexibility of the orbital sets allows transition energies, as well as other atomic properties, to be predicted to a much higher accuracy than before.

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