Massive Calculations of Atomic Properties with High Accuracy for Boron-like Iron and other Ions of Astrophysical Interest

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Synopsis Recent progress in relativistic multiconfiguration methods makes it possible to compute transition energies with very high accuracy. We apply these methods to compute spectroscopic data for the 291 lowest states in the astrophysically important Fe XXII as well as in other ions. Results are compared with other works.

Information about physical processes in astrophysical and fusion plasmas can be inferred from high resolution spectra. The X-ray spectra from iron L-shell ions are particularly important for astrophysics as they are in the wave length range covered by telescopes on board the space observatories Chandra and XMM-Newton. The analysis of high-resolution X-ray spectra requires knowledge of a large number of accurate transition data and transition probabilities, either from theory or experiment, to identify spectral lines, produce synthetic spectra, and carry out plasma diagnostics.

During the last years a number of calculations have been carried out to provide more complete sets of energies and transition data for highly charged iron [1, 2, 3, 4, 5]. Although theoretical data are available it is still very difficult to analyze spectra, unambiguously identify transitions, and deduce energy levels with the proper labels. Looking at the NIST Atomic Spectra Database [6] there remain large gaps that need to be filled. Also there are misidentifications.

This work reports from a long term theoretical effort to attain "spectroscopic accuracy", i.e. calculated transition energies that are accurate enough to confirm or revise experimental identifications. The basis for the work are large scale relativistic multiconfiguration methods [7] with hundreds of thousands of configuration states functions. By accurately balancing electron correlation effects it now is possible to compute transition energies with an inaccuracy of fractions of a per mille [8]. As an application, calculations were performed for the 291 lowest states in boron-like ions, including Fe XXII, belonging to the configurations $1s^22s^22p$, $1s^22s2p^2$, $1s^22p^3$, $1s^22s^23l$, $1s^22s2p3l$, $1s^22p^23l$, $1s^22s^24l'$, $1s^22s2p4l'$, $1s^22p^24l'$ ($l = 0,1,2$ and $l' = 0,1,2,3$). Results are presented and discussed in relation to other works.

References

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