Photoionization of neutral iron from ground and metastable states

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Synopsis The B-spline R-matrix method is used to investigate the photoionization of neutral iron from the ground and metastable states in the energy region from the ionization thresholds to 2 Ry. The sensitivity of the results is checked by comparing the predictions obtained in different approximations. Inclusion of all terms from the $3d^6 4p$ and $3d^5 4s4p$ configurations considerably changes the low-energy resonance structure.

Neutral Fe and its ions play important roles in many aspects of astrophysics. Within fundamental atomic physics, the large number of possible terms resulting from the approximately half-open 3d shell, in combination with the near degeneracy of the $3d^x$, $3d^{x-1}4s$, $3d^{x-2}4s^2$, and other configurations for the neutral elements and the lowly-charged ions, result in very complex spectra that are strongly influenced by configuration interaction. Therefore, the calculations become extremely cumbersome and the spectra very rich in structure and difficult to analyze.

Accurate photoionization cross sections are required for the analysis and interpretation of spectroscopic observations. Thus far, the only data available for the photoionization of Fe I are limited to transitions between *LS* states. The most extensive calculations, presented by Bautista [1], involved 52 *LS* terms of the Fe II target. This is only a small part of the Fe II spectrum, which raises the question of the convergence of results.

The purpose of the present work was to perform elaborate and extensive calculations for the photoionization of neutral iron by using highly accurate target wave functions and by including fine-structure effects in the close-coupling expansions directly. The calculations were performed with the advanced BSR code [2], which employs the R-matrix method in a B-spline basis. To represent the target states, we used term-dependent non-orthogonal orbital sets. This allowed us to generate a more accurate description of the Fe I target states than those previously employed.

The target expansion included all states of the $3d^6 4s$, $3d^7$, $3d^6 4p$, $3d^5 4s^2$, and $3d^5 4s4p$ configurations. This adds up to 261 *LS* terms or 716 fine-structure levels. The convergence of the results was checked by comparing data obtained in different approximations. As an example, Fig. 1 compares the predicted photoionization cross section of the ground state of Fe I in two *LS* approximations. BSR-39 includes all relevant terms of the $3d^6 4s$, $3d^7$, and $3d^5 4s^2$ configurations, as well as the low-lying states of the $3d^6 4p$ and $3d^5 4s4p$ configurations as in [1], whereas BSR-112 also includes all terms of the $3d^6 4p$ and $3d^5 4s4p$ configurations. Note that both the resonance structure and the background cross sections change considerably, with the BSR-39 results being only in qualitative agreement with the cross sections obtained in [1]. This is due to the different target representations.

Ultimately, the present work aims to provide systematic data for photoionization of the fine-structure levels. Further details of the calculation and some preliminary results for ground-state and metastable photoionization in the Breit-Pauli approximation will be presented at the conference.

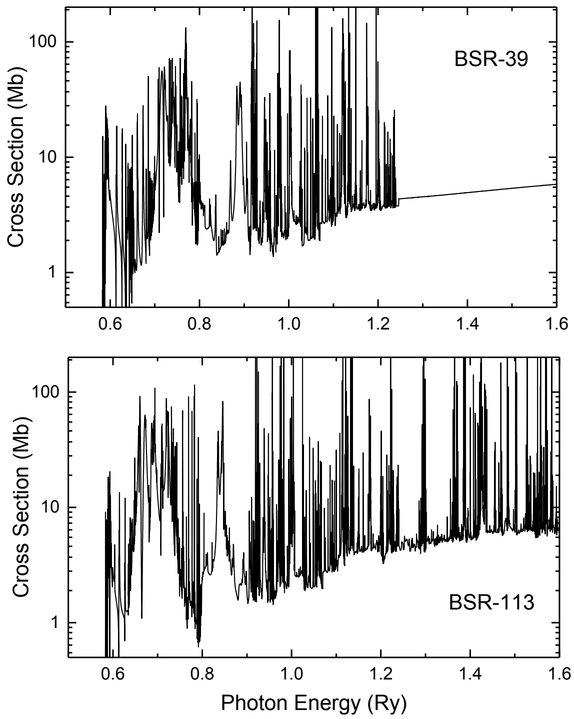

Figure 1. Comparison of the photoionization cross section of the ground state $(3d^6 4s^2)^5D$ of Fe I between two scattering models, BSR-39 and BSR-112.

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References

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