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LETTER

Letter to the Editor

K-shell photoejection cross section for neutral iron

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Abstract. This *Letter* presents the first *ab initio* calculation, using the R-matrix method, of the cross section for photoejection of a K-shell electron from neutral iron. A 9-state target state approximation is employed, and the results are compared with recent theoretical values, namely the Hartree-Dirac-Slater method data of Verner and co-workers (1993, 1995). At the highest photon energy considered (640 Ryd), agreement is excellent. However, with decreasing photon energy the two calculations diverge, and the behaviour of the present cross section near threshold shows a rapid rise from threshold in contrast to earlier work for which the behaviour of the cross section as a function of photon energy is approximately linear.

Key words: atomic data – atomic processes

1. Introduction

The Kα emission lines of Fe I at 1.936 and 1.940 Å are produced when a K-shell electron is removed by a photon having an energy larger than the iron K-shell binding energy (7.12 keV), and the vacancy is filled by an electron previously in the L-shell (see, for example, Phillips et al. 1994). These lines are observed during solar flares (Parmar et al. 1984), as well as in a variety of astronomical sources such as active galactic nuclei (Mushotzky et al. 1993). The reliable modeling of the Kα emission clearly requires accurate atomic data for the K-shell photoionization cross sections (Bai 1979).

The calculation of photoionization cross sections involving the removal of inner-shell electrons presents significant problems for theorists. However, the difficulty in obtaining experimental data obliges the theorists to investigate such processes. In this *Letter* we investigate the photoejection of the K-shell electrons of neutral iron. To the best of our knowledge, only central-field theoretical approximation work exists for this process, the most recent calculation being that of Verner et al. (1993) and Verner & Yakovlev (1995). They used the relativistic Hartree-Dirac-Slater method to calculate partial cross-sections for photoionization from each individual subshell of several ions of elements between helium and zinc, and thus included $1s$-photoejection of neutral iron. Assessment of the accuracy of this approximation is exceedingly difficult, but it has been shown that the background cross section (the approximation does not support resonance phenomena) for $1s$-photoejection from highly ionized ions of iron, namely Fe XXIII and Fe XXIV (Black et al. 1997), is accurate to approximately 5%. In contrast, the R-matrix method results of Bautista & Pradhan (1995) for photoionization of the outer shells of neutral iron differed by up to several orders of magnitude from the central field approximation values. It is therefore essential that further calculations be carried out for photoejection of the K-shell electrons of neutral iron. In this *Letter* we restrict consideration to the following process:

$$h\nu \; + \; \mathrm{Fe\ I}\ (1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 4s^2\ ^5D) \rightarrow \\ e^- + \mathrm{Fe\ II}\ (1s 2s^2 2p^6 3s^2 3p^6 3d^6 4s^{2\ 2S+1}L) \qquad (1)$$

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2. Method

The calculation was performed within the framework of the R-matrix method, using the computer codes described by Berrington et al. (1987), with the associated theory being given by Seaton (1987). LS coupling was adopted, while spin-orbit coupling and other relativistic effects were neglected. The total wavefunctions describing both the initial bound state and the final state of the system are expanded in the R–matrix internal region ($r < a$) in terms of the following basis (Burke & Robb 1975; Berrington et al. 1978, 1987):

$$\Psi_k \; = \; A \sum_{ij} C_{ijk} \overline{\Phi_i}(x_1, x_2 ..., x_N, r_{N+1}\sigma_{N+1}) u_{ij}(r_{N+1}) \\ + \sum_j d_{jk} \phi_j(x_1, x_2 ..., x_{N+1}) \qquad (2)$$

A is the antisymmetrisation operator which ensures the total wavefunction satisfies the Pauli exclusion principle. The $\overline{\Phi_i}$ are channel functions formed by coupling the target states to the angular and spin function of the scattered electron. The u_{ij} are the continuum basis orbitals representing the scattered electron and the ϕ_j are (N+1)–electron bound configurations formed from the atomic orbital basis, and are included to ensure completeness of the total wavefunction and to allow for short range correlation.

The continuum orbitals u_{ij} are solutions of the radial differential equation:

$$\left[\frac{d^2}{dr^2} - \frac{l_i(l_i+1)}{r^2} + V(r) + k_i^2\right] u_{ij}(r) = \sum_k \lambda_{ijk} P_k(r) \quad (3)$$

which satisfies the boundary conditions:

$$u_{ij}(0) = 0 \quad (4)$$

$$\frac{a}{u_{ij}} \frac{du_{ij}}{dr}\bigg|_{r=a} = b. \quad (5)$$

In Eq. (3), l_i is the angular momentum of the scattered electron and $V(r)$ is the static potential of the target in its ground state. The λ_{ijk} are Lagrange multipliers, which are obtained by imposing the orthogonality of the continuum orbitals to the bound radial orbitals with the same value of l_i. The coefficients C_{ijk} and d_{jk} in Eq. (2) are found by diagonalizing the (N+1)–electron non-relativistic Hamiltonian within the inner region. The R–matrix is then calculated on the boundary between the inner and outer regions.

The major problem connected with the present work lies in the choice of singly ionized iron target state wavefunctions to be included in the expansion of Eq. (2). Customarily, one would include the ground state of Fe II, and the bound state of Fe I is then relatively easy to obtain within the framework of the R-matrix method. However, if this state were included in the present calculation, then (because of the large ionization threshold for $1s$ electron removal) it becomes completely impossible to take account of the excessively large number of continuum basis orbitals required to span the R-matrix box, and achieve a convergent description of the final (e^-+Fe II) state of the system. Numerically, the determination of the set of continuum basis orbitals becomes unstable. The alternative approach adopted in the present work is to retain *only* 'hole' target states. This somewhat simplified the problem associated with the continuum basis orbitals, although considerable care was needed to ensure that an adequate number were included to obtain convergent results. A potential difficulty now arises in the bound state determination, since we are seeking a bound state approximately 7 keV relative to the lowest 'hole' Fe II state. However, it was found that the bound state was largely determined by the (N+1)-electron bound configuration corresponding to the Fe I ground state.

We included the nine target states given in Table 1 in the R-matrix expansion. Each of the states was represented by a single configuration constructed from one-electron orbitals. The radial part of these one-electron functions is given by a linear combination of Slater-type orbitals

$$P_{nl}(r) = \sum_{j=1}^{k} c_{jnl} \left[\frac{(2\zeta_{jnl})^{2I_{jnl}+1}}{(2I_{jnl})!}\right]^{\frac{1}{2}} r^{I_{jnl}} e^{-\zeta_{jnl} r} \quad (6)$$

The parameters c_{jnl}, I_{jnl}, ζ_{jnl} were taken to be the Hartree-Fock values obtained by Bunge et al. (1993). Table 1 gives the energies corresponding to the target states.

Table 1. Target state energies (in Ryd) relative to the '$1s$-hole' ^6D state of Fe II.

Number	Target state	Energy
1	$1s2s^22p^63s^23p^63d^6(a^5D)4s^2\ ^6D$	0.00000
2	$1s2s^22p^63s^23p^63d^6(a^5D)4s^2\ ^4D$	0.00345
3	$1s2s^22p^63s^23p^63d^6(a^3H)4s^2\ ^4H$	0.20045
4	$1s2s^22p^63s^23p^63d^6(a^3P)4s^2\ ^4P$	0.22339
5	$1s2s^22p^63s^23p^63d^6(a^3F)4s^2\ ^4F$	0.23036
6	$1s2s^22p^63s^23p^63d^6(a^3G)4s^2\ ^4G$	0.25361
7	$1s2s^22p^63s^23p^63d^6(a^3D)4s^2\ ^4D$	0.32833
8	$1s2s^22p^63s^23p^63d^6(b^3F)4s^2\ ^4F$	0.54414
9	$1s2s^22p^63s^23p^63d^6(b^3P)4s^2\ ^4P$	0.55112

In constructing the total wavefunction in the R-matrix internal region, 64 continuum orbitals were then used for each incident electron orbital angular momentum, and convergence of the cross section was found to be achievable over the photon energy range from threshold to 640 Ryd. The R-matrix boundary was found to be 26.0 Ryd, and the $1s$ ionization energy of the ground state of neutral iron was calculated to be 7112 eV, in good agreement with the experimental result of 7124 eV (Sevier 1979) and the theoretical result of 7083 eV obtained by Verner et al (1993, 1995).

3. Results and discussion

We feel confident that we have successfully overcome all of the difficulties discussed above in applying the R-matrix codes to this inner-shell photoejection problem. Using a photon energy resolution of 0.001 Ryd, the photoionization cross section for photoejection of the $1s$ electron from the ground state of neutral iron was calculated from threshold to 640 Ryd. Fig. 1 compares the present results with the earlier Hartree-Dirac-Slater (HDS) method data of Verner et al. (1993) and Verner & Yakovlev (1995). This comparison is interesting in that the central-field approximation values are almost linear as a function of energy, whereas the present results increase more rapidly as one approaches the region of the $1s$ ionization threshold and a sharp peak is observed close to threshold. An explanation for this near-threshold behaviour may be obtained from Fig. 2, where the cross section in this energy region is presented together with the positions of the thresholds as calculated by the R-matrix method and tabulated in Table 1. This figure illustrates that at the first $1s$ ionization threshold the cross section has a magnitude (0.0287 Mb) which is approximately 16% lower than that found by Verner et al. However, once the threshold (only 0.00345 Ryd above the first $1s$ ionization threshold) allowing the ion to be left in the excited $1s2s^22p^63s^23p^63d^6(a^5D)4s^2\ ^4D$ state is reached, the cross section demonstrates a dramatic and extremely sharp increase (to approx. 0.04932 Mb) (see inset to Fig. 2). It is the coupling to this excited state which explains the difference between the present work and the earlier central field approximation results. We note also that the resolution

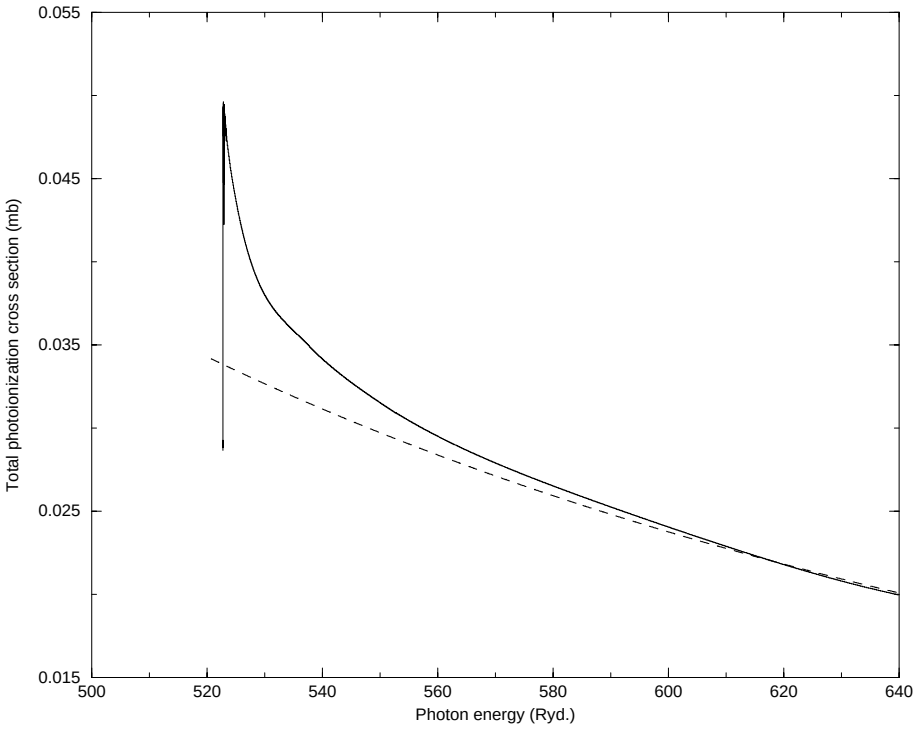

Fig. 1. Photoionization cross section for photoejection of the $1s$ electron from the ground state of neutral iron. Solid line: present calculation; dashed line: Verner et al. (1993) and Verner & Yakovlev (1995)

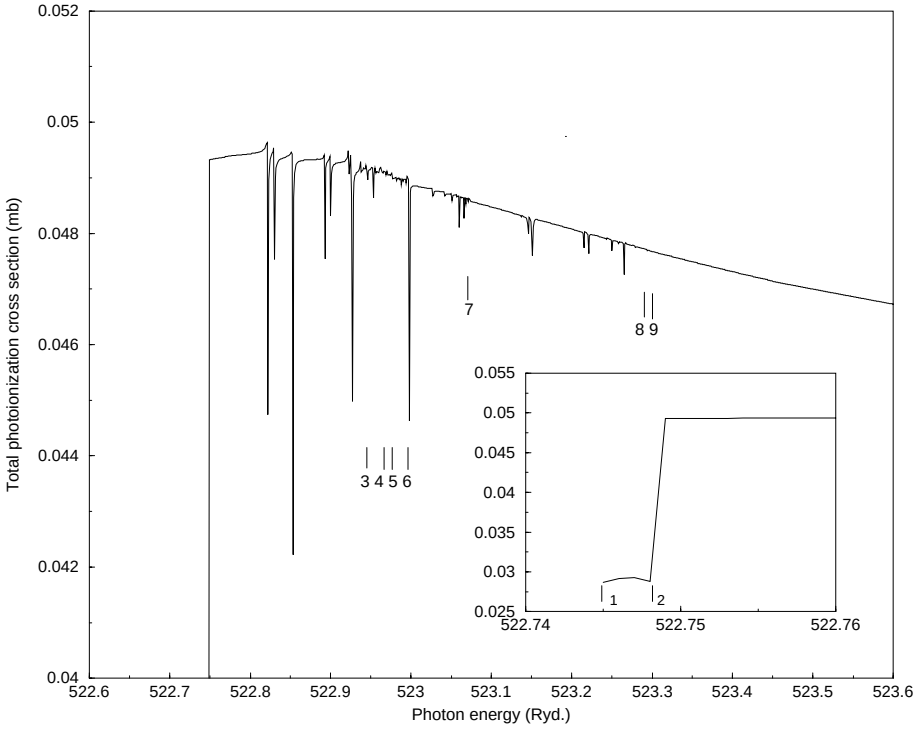

Fig. 2. Photoionization cross section for photoejection of the $1s$ electron from the ground state of neutral iron in the region of the $1s$ ionization thresholds

used in the present calculation is sufficient to resolve any resonance structure associated with the included thresholds. Such structure is observed in Fig. 2 and has not been obtained in any previous investigation.

From the point of view of modellers using the data, it is interesting to note that the two theoretical approximations rapidly reach agreement as the photon energy increases and above about 550 Ryd the difference is less than 10%. Verner & Yakovlev (1995) have pointed out that the data frequently employed by modellers in astrophysical codes are those of Daltabuit & Cox (1972), which give cross sections differing from experiment by large factors at high photon energies. The present calculation, therefore, confirms the correctness of the work of Verner and co-workers at photon energies away from threshold, but does emphasise caution when values close to thresholds are used. It is difficult to assess the accuracy of the present work near

threshold and unfortunately experiment is not directly available to assist in any assessment. To our knowledge the only experimental work in the energy region near the K-shell threshold are experiments on iron X-ray attenuation coefficients (Wang Dachun et al. 1992). These coefficients allow the calculation of the *total* X-ray cross section and, at threshold, the data point (Fig. 5 of Wang Dachun et al.), $\mu = 420$ cm^2/g, corresponds to a cross section value of 0.039 Mb in excellent agreement with the *total* cross section of 0.0384 Mb obtained by Verner and Yakovlev (1995). If we were to adopt the ratio of 0.89 found by Verner and Yakovlev (1995) for the ratio of the K-shell photoejection cross section to the total cross section and apply it to the experimental point, then the resulting value of 0.035 Mb would be approximately 22% above the present K-shell photoejection cross section. It is not possible to comment further. In particular, the experimental resolution is not sufficiently fine enough that the rapid rise in the current work near threshold can be verified.

4. Summary

In summary, we have performed the first *ab initio* close-coupling calculation for photoejection of the $1s$ inner-shell electron from the ground state of neutral iron. The present results are seen to deviate from previous investigations near threshold and resonance structure is resolved for the first time.

The solution of problems associated with application of the method now encourages us to improve the calculation. However, such improvement presents a formidable challenge and will require substantial effort, both in the improvement of the target state wavefunctions and in the number of target states included in the R-matrix wavefunction expansion.

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