Theoretical studies on photoionization of Na-like iron ion

J J Wan, C Z Dong, C C Sang, X B Ding, L Y Xie and J Jiang

College of Physics and Electronic Engineering, Northwest Normal University, Lanzhou 730070, China
E-mail: dongcz@nwnu.edu.cn

Abstract. The ionization energies and the corresponding photoionization cross sections from the 1s, 2s, 2p and 3s subshells of Fe\(^{15+}\) are calculated systematically using a newly developed program RERR06 for the first time, which is based on the widely used GRASP92 and RATIP packages. In the calculation, the effects of configuration interaction and orbital relaxation have been considered. As a result, the shake-up processes accompanied by the main photoionization processes have been treated as unified. It is found that the present calculations for ionization energies are in good agreement with existing data and the photoionization (PI) cross sections for the 2p electron are also in good accordance with recent computations. The contribution from the shake-up processes are found to be not important for the photoionization of Fe\(^{15+}\), but an enhancement feature is noticed for the 2p to 3p shake-up process accompanied by the PI of the 3s electron.

1. Introduction
Photoionization (PI) can be regarded as the inverse process of radiative recombination (RR), in which a continuum electron is captured into a discrete state of the ion and the excess energy is radiated as a photon simultaneously. The PI cross section not only provides much information of electron correlation in multielectron atoms, but also plays an important role in modeling dynamic equilibrium in laboratory and astrophysical plasmas, especially in the astrophysical plasmas called 'photoionized plasmas' [1]. For example, the iron group elements are known to occur frequently in the universe [2], and Fe\(^{16+}\) is a dominant ionized state over a broad temperature range in coronal equilibrium [1]. This ion can be produced via a PI process of Fe\(^{15+}\), and its x-ray spectra have been observed in a wide range of astrophysical sources [3]. If an inner electron of Fe\(^{15+}\) is ionized, a great deal of hollow states of Fe\(^{16+}\) are produced, which can decay by emitting x-ray photons to a lower state of Fe\(^{16+}\) or an Auger electron to Fe\(^{17+}\). In the PI process, due to the removal of the inner electron, rearrangement of the residual electrons will occur (i.e. orbital relaxation). As a result, some higher order processes, such as shake-down, shake-up, or even shake-off, will accompany the main PI process.

In the past, there were many investigations on the properties of various iron ions due to its high abundance in the solar corona and fusion plasmas, especially for the Na-like Fe\(^{15+}\) with a relatively simple structure. Recently, because of the need for atomic data in astrophysical and laboratory plasmas modeling, people have paid more attention to the inner-shell photoionization of highly charged ions. For example, Inal et al. [4] have studied the linear polarization of the 2p\(^5\)3s − 2p\(^6\) lines following the photoionization of 2p electron of Fe\(^{15+}\) ion. They found that
the inner-shell photoionization can induce a relatively low linear polarization of the emitted photons. In the present work, all the ionization thresholds and corresponding photoionization cross sections from the 1s, 2s, 2p and 3s subshells are calculated systematically, using a newly developed program RERR06 [5] based on the widely used GRASP92 [6] and RATIP packages [7]. In the calculations, the effects of main configuration interaction and orbital relaxation have been considered. As a result, some important shake-up processes have also been studied.

2. Theoretical method
In calculations of the wavefunctions and energies of the present ions of interest, the multi-conﬁguration Dirac-Fock (MCDF) method and the corresponding computational package GRASP92 [6] have been used, which were described in detail elsewhere [5–11] and have not been given here. Furthermore, the PI cross section from an initial state $i$ to a final state $f$ has been calculated as follows

$$\sigma_{if}^{PI} = 4\pi a_0^2 \frac{df_{if}}{de},$$

(1)

where $\alpha$ is the fine structure constant, $a_0$ is the Bohr radius, and $df_{if}/de$ is the oscillator strength density, which can be written as [5]

$$\frac{df_{if}}{de} = \frac{\pi c}{2(L + 1)\omega^2} |\langle N^{-1}(P_f J_f M_f), \epsilon \kappa; N^N(P_i J_i M_i) | \tilde{O}^{(L)}(\epsilon_{\kappa}) | N^N(P_i J_i M_i) \rangle|^2.$$

(2)

To include relaxation effects [12,13], which are caused by the rearrangement of the electron density due to the absorption of a photon in PI processes, two individual MCDF calculations for the initial and final states are carried out. At the same time, the overlap integrals, which are caused by the non-orthogonality of two sets of electron orbitals, have been included in the evaluation of the many-electron transition matrix elements [14,15].

In this work, the photoionization cross sections of the following main and shake-up processes have been studied

$$h\nu + Fe^{15+}(1s^22s^22p^63s) \rightarrow Fe^{16+}(1s2s^22p^6ns) + e^-$$

$$Fe^{16+}(1s2s^22p^6ns) + e^-$$

$$Fe^{16+}(1s^22s^22p^5ns) + e^-$$

$$Fe^{16+}(1s^22s^22p^5np) + e^-$$

(3)

where $n_s = 3$ and $n_p = 2$ correspond the main PI processes, $n_s = 4$ and $n_p = 3$ correspond the accompanied shake-up processes.

3. Results and Discussions
3.1. Ionization energies
In Table 1, we partially present some ionization energies of the PI processes (main and shake-up) mentioned; also some available theoretical and experimental results are collected as comparison. From the table, we can see that the present calculations are in good agreement with both the theoretical [4,16] and experimental results [17], and the relative error is less than 0.2%.

3.2. PI cross sections
In Figure 1, the PI cross sections of the 2p electron are plotted as function of photon energy. For comparison, the existing calculations by Inal et al [4] from the $1s^22s^22p^63s$ to the $1s^22s^22p^53s$ are also included. It shows that the present results are in good agreement with the calculations of Inal et al. Again, the cross sections of the shake-up process from the $1s^22s^22p^63s$ to the $1s^22s^22p^54s$ are much smaller than the main PI process, but it is bigger than the cases of the removal of the 1s and 2s electrons, which are not shown any more in this paper.
Table 1. Ionization energies for several selected main and shake-up photoionization processes of Fe$^{15+}$ (in a.u.).

| Initial state | Final state | This work | Ref. [4] | Ref. [16] | Ref. [17] |
|---------------|-------------|-----------|----------|-----------|-----------|
| (1s$^2$3s$^2$) | (1s$^2$4s$^2$) | 281.023   | 290.383  |           |           |
| (2s$^2$3s$^2$) | (2s$^2$4s$^2$) | 49.559    | 58.774   |           |           |
| (2p$^2$)$^1$ | (2p$^2$)$^0$  | 44.652    | 44.669   | 44.695   |           |
| (2p$^2$)$^0$  | (2p$^2$)$^1$  | 45.045    | 45.070   | 45.093   |           |
| (1s$^2$2s$^2$2p$^6$3s$^2$) | (1s$^2$2s$^2$2p$^6$3s) | 53.839 | 53.910 |           |           |
| (1s$^2$2s$^2$2p$^6$3s) | (2p$^2$)$^1$ | 54.279 | 54.350 |           |           |
| (2p$^2$)$^0$  | (2p$^2$)$^1$  | 18.007    | 17.980   | 17.978   |           |
| (2p$^2$)$^1$ | (2p$^2$)$^0$  | 45.824    | 45.919   | 45.970   | 46.036    |
| (2p$^2$)$^0$  | (2p$^2$)$^1$  | 45.925    | 45.988   | 46.193   | 46.237    |
| (2p$^2$)$^1$ | (2p$^2$)$^0$  | 45.382    | 45.925   | 45.988   | 46.313    |
| (2p$^2$)$^0$  | (2p$^2$)$^1$  | 46.267    | 46.977   | 46.924   |           |

In Figure 2, the PI cross sections of the 3s electron are shown further. It can be seen that in the 2p shake-up process there is always a maximum at the region of 245 ∼ 300 a.u. in each process. To our knowledge, such a situation has not been noticed before for other similar systems.

4. Conclusion
In summary, the ionization energies and the PI cross sections for both the main and shake-up processes of the Na-like iron ion have been calculated systematically using the MCDF method including the effects of orbital relaxation and some important configuration interactions.

It is found that for the higher charged Fe$^{15+}$, the cross sections from the shake-up processes are smaller by 2–3 orders of magnitude than those from the main PI processes. But shake-up processes occur more easily for PI of outer shell electrons as opposed to inner shell electrons. This is quite similar to the conclusion of Kupliauskienè [18] for the PI of the excited states in Li, Na and K atoms. In addition, an enhanced feature is noticed for the 2p to 3p shake-up accompanied by the PI of the 3s electron. It should be interesting to do some further studies for other atomic and ionic systems.

Acknowledgments
This work has been supported by the National Natural Science Foundation of China (Grant Nos. 10376026, 10434100), the Foundation of China/Ireland Science and Technology Collaboration Research (Grant No. CI-2004-07), the Foundation of the Center of Theoretical Nuclear Physics, National Laboratory of Heavy Ion Accelerator of Lanzhou. The authors thank Lynn Gaynor and Paddy Hayden from UCD of Ireland for their help.
Figure 1. The PI cross sections of the 2p electron. Solid line, dashed line, dotted line and dashdotted line represent \((2p_{3/2}^{-1}3s)^2\), \((2p_{3/2}^{-1}3s)^1\), \((2p_{1/2}^{-1}3s)^0\) and \((2p_{1/2}^{-1}3s)^1\) in turn; □, ○, △ and ▽ are the calculations of Inal et al[4] for \((2p_{3/2}^{-1}3s)^2\), \((2p_{3/2}^{-1}3s)^1\), \((2p_{1/2}^{-1}3s)^0\) and \((2p_{1/2}^{-1}3s)^1\); similar symbols are also used for the corresponding shake-up processes in the inset.

Figure 2. The PI cross sections of the 3s electron. Solid line is for the final ionic state \(2p^61S_0\); in the inset, the basipetal curves represent \((2p_{1/2}1p_{3/2}3s)^2\), \((2p_{3/2}1p_{3/2}3s)^3\), \((2p_{3/2}1p_{3/2}3s)^2\), \((2p_{3/2}1p_{3/2}3s)^1\), \((2p_{1/2}1p_{3/2}3s)^1\), \((2p_{3/2}1p_{3/2}3s)^2\), \((2p_{3/2}1p_{3/2}3s)^1\) in turn.

References

[1] Moribayashi K, Kagawa T and Kim D E 2006 Journal of Plasma and Fusion Research Series 7 233
[2] Dong C Z, Kato T, Fritzsche S and Koike F 2006 Mon. Not. Roy. Astron. Soc. 369 1735
[3] Brown G V, Beiersdorfer P, Liedahl D A, Widmann K and Kahn. S M 1998 Astrophys. J. 502 1015
[4] Inal M K, Surzhykov A and Fritzsche S 2005 Phys. Rev. A 72 042720
[5] Ding X B, Xie L Y and Jiang J private communication
[6] Parpia F A, Fischer C F and Grant I P 1996 Comput. Phys. Commun. 94 249
[7] Fritzsche S 2001 J. Electron Spectroscopy and Related Phenomena 114-116 1155
[8] Grant I P, McKenzie B J, Norrington P H, Mayers D F and Pyper N C 1980 Comput. Phys. Commun. 21 207
[9] Dyall K G, Grant I P, Johnson C T, Parpia F A and Plummer E P 1989 Comput. Phys. Commun. 55 425
[10] Zhang H L, Sampson D H and Mohanty A K 1989 Phys. Rev. A 40 616
[11] Syty P, Sienkiewicz J E and Fritzsche S 2003 Rad. Phys. Chem. 68 301
[12] Dong C Z, Xie L Y, Zhou X X, Ma X W and Fritzsche S 2003 Hyperfine Interactions 146/147 161
[13] Dong C Z and Fritzsche S 2005 Phys. Rev. A 72 012507
[14] Fritzsche S, Fischer C F and Dong C Z 2000 Comput. Phys. Commun. 124 340
[15] Löwdin P O 1955 Phys. Rev. 97 1474
[16] Ralchenko Yu, Kramida A E and Reader J 2006 NIST Atomic Spectra Database http://physics.nist.gov/PhysRefData/ASD/index.html
[17] Gregory D C, Wang L J, Meyer F W and Rinn K 1987 Phys. Rev. A 35 3256
[18] Kupliauskienė A 1996 Physica Scripta 53 149