A&A manuscript no.
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02.01.3, 02.01.4

ASTRONOMY
AND
ASTROPHYSICS
26.9.1995

Analytic fits for partial photoionization cross sections*

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Received date; accepted date

Abstract. We present a compact, uniform and complete set of analytic fits to the partial Hartree-Dirac-Slater photoionization cross sections for the ground state shells of all atoms and ions of elements from H to Zn ($Z \leq 30$). Comparison with experiment and theory demonstrates generally high accuracy of the fits up to energies of 100 keV.

Key words: atomic data – atomic processes

1. Introduction

Photoionization cross sections of atoms and ions are required for constructing theoretical models of many objects, from planetary nebulae to active galactic nuclei and intergalactic medium. In an earlier paper (Verner et al. 1993, hereafter Paper I) we presented the Hartree-Dirac-Slater (HDS) calculations and analytic fits for the partial photoionization cross sections of atoms and ions for all subshells nl of the ground state species. The calculations embodied all neutral atoms from He to Zn and about 70% of ions of elements with atomic number $Z \leq 30$. The calculated cross sections were fitted by an analytic formula based on the approximate criterion of similarity (Kamrukov et al. 1983) of the photoionization cross sections for different atoms and ions. In Paper I, we performed also the secondary fitting of the fit parameters along Z and N (number of electrons) for the atomic species separated into several groups. This enables us now to calculate the fit parameters of the photoionization cross sections of the species omitted in the initial HDS computations.

2. Fits to the photoionization cross sections

In this paper we present a uniform, compact and complete set of the fit parameters to the cross sections for all subshells of atoms and ions of the elements under study. The partial photoionization cross sections $\sigma_{nl}(E)$ will be described by the fitting formula:

$$\sigma_{nl}(E) = \sigma_0\, F(E/E_0) \;\; \mathrm{Mb},$$
$$F(y) = \left[(y-1)^2 + y_{\rm w}^2\right] y^{-Q} \left(1+\sqrt{(y/y_{\rm a})}\right)^{-P}, \qquad (1)$$

where n is the principal quantum number of the shell, l =0, 1, 2 (or s, p, d) is the subshell orbital quantum number, E is the photon energy in eV, $y = E/E_0$; σ_0, E_0, $y_{\rm w}$, $y_{\rm a}$ and P are the fit parameters, and $Q = 5.5 + l - 0.5P$. As a rule, the parameters P, $y_{\rm w}$ and $y_{\rm a}$ vary smoothly over atomic species for a fixed subshell nl. Accordingly, the cross section shape is described by a nearly universal function $F(y)$. This reflects a useful criterion of similarity of the photoionization cross sections (Kamrukov et al. 1983). Two other fit parameters, σ_0 and E_0, rescale the function $F(y)$ for a given cross section. The rescaling is especially simple in logarithmic variables, $\log \sigma_{nl}$ against $\log E$: σ_0 shifts the universal curve $\log F$ along the cross section axis, while E_0 shifts the curve along the energy axis.

The explicit form of $F(y)$ given by Eq. 1 was proposed in Paper I. The form appears to be very accurate for most cases under study. All the parameters of $F(y)$ have a simple physical meaning. The $F(y)$-curve possesses a resonant-like dip of width $y_{\rm w}$ at $y \approx 1$ (for small $y_{\rm w}$). For higher y ($1 \ll y \ll y_{\rm a}$), $F(y)$ decreases with y as $F(y) \propto y^{-Q}$. Thus P defines the power-law index, and $y_{\rm a}$ determines the upper boundary of y for this power-law regime (that is realized provided $y_{\rm a} \gg 1$). Finally, when $y \gg y_{\rm a}$ our formula reproduces the well-known (e.g., Bethe & Salpeter 1957) non-relativistic asymptote $\sigma_{nl}(E) \propto E^{-3.5-l}$ for high energies. In addition to each set of the fit parameters, one should specify the threshold energy $E_{\rm th}$. In many cases, the latter is higher than the energy of the resonant dip, so that the dip does not appear in the actual cross section. However in some cases (mostly, for the outer shells of neutrals), $E_{\rm th}$ is lower or comparable to the dip position. This allows us to describe the sophisticated behaviour of the cross section curve just above the threshold in these cases. The advantage of the proposed fit is that it is not related directly to the cross section parameters at the threshold (see Paper I for details).

Equation 1 allows us to describe correctly the background photoionization cross sections near the threshold, at intermediate energies, and at high non-relativistic energies. The fit parameters have been taken from Paper I for the species with the calculated HDS cross sections (75% of data) or calculated from the the secondary fits of Paper I for non-hydrogenic species omitted from the HDS calculations (23% of data). As compared to Paper I, we have improved the 1s-shell fits for He I and Li I by including new high energy cross sections in the fitting. We have found that the 1s-shell photoionization cross sections for Li II in Paper I were calculated with the photoelectron wavefunction corresponding to erroneous electron energy.

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*Table 1 is available in electronic form: see the Editorial in A&AS 1994, Vol. 103, No. 1

This resulted in the overestimation of the cross section near the photoionization threshold by a factor of 1.5 although the overestimation factor decreased with photon energy. In the present paper, we give the fit for the correct Li II cross section. Using Eq. (1), we have also fitted the hydrogen-like cross sections (2% of data) calculated from the analytic expression (see, e.g., Bethe & Salpeter 1957).

In addition to the fit parameters, we present also the ionization threshold energies. For the outer subshells, we list the experimental ionization energies taken from Kelly (1987), Sugar & Corliss (1985) and Moore (1970). For the inner subshells of neutral atoms, we present the experimental energies from Sevier (1979). This does not violate the fit self-consistency, since the fits are not based on the threshold values. For the inner subshells of ions, we list the theoretical ionization energies from Paper I. All the fit parameters and ionization energies are given in Table 1. The columns are:

Z	–	atomic number
N	–	number of electrons
S	–	subshell
$E_{\rm th}$, eV	–	subshell ionization threshold energy
E_0, σ_0, $y_{\rm a}$, P, $y_{\rm w}$	–	fit parameters

The rms relative error of the hydrogen-like fit is $\delta_{\rm av} = 0.0019$ for 21 photon energy points placed logarithmically equidistant from the threshold energy $E = E_{\rm th}$ to $100E_{\rm th}$, with the maximum error $\delta_{\rm max} = 0.0044$ at the threshold. The fitting accuracy for the non-hydrogenic species evaluated from comparison with the calculated HDS cross sections is also rather good. The rms relative errors averaged over all the atomic species involved are within 0.7% for the $1s$, $2s$, $2p$, $3s$ and $3p$ subshells, and within 2.3% for the $3d$ and $4s$ subshells (see Paper I for details). Below we compare our analytic fits with other theoretical calculations and experimental data.

3. Comparison of the fits with experiment and theory

We have made extensive comparisons of the fits with experimental and theoretical data available. The cross sections have been measured mostly for the neutral atoms (see Samson et al. 1991 for a recent review of absolute atomic photoionization cross sections). Compilations of experimental and theoretical data for all atoms with $Z = 1 - 94$ are given by Henke et al. (1982) at $E = 30 - 9887$ eV and by Veigele (1973) at $E = 1 - 1000$ keV. The theoretical Hartree-Slater total photoionization cross sections for the atoms and ions with $Z \leq 30$ at $E = 5 - 5000$ eV are given in tabular form by Reilman & Manson (1979; hereafter RM). The recent Opacity Project (OP) calculations (Seaton et al. 1992) give, in particular, the cross sections for the ground state of atoms and ions of elements with $Z \leq 14$ and $Z = 16$, 18, 20, 26. The OP calculations are based on the high level methods of atomic physics such as the R-matrix method (Burke et al. 1971) that reproduces many autoionization resonances near the ionization thresholds.

For all neutral atoms, we have compared the photoionization cross sections obtained from the present analytic fits with those tabulated by Henke et al. (1982) and Veigele (1973), and with the published experimental data of Angel & Samson (O I, 1988), Samson & Angel (N I, 1990), Samson et al. (Cl I, 1986; Ne I, Ar I, 1991), Bizau et al. (Ca I, 1987), Hudson & Carter (Li I, Na I, 1967), Mehlman et al. (Li I, 1982), Krause et al. (Mn I, 1984), Jimenez-Mier et al. (Mn I, 1989), Parthasaradhi et al. (Ti I, Ni I, 1988), West & Marr (He I, Ne I, Ar I, 1976), Marr & West (He I, Ne I, Ar I, 1976), Cantú et al. (C I, 1981), Kohl & Parkinson (Al I, 1973), and Roig (Al I, 1975). We have also made a comparison with all the OP ground state cross sections available through the TOPbase 0.6 database (Cunto et al. 1993), and with all the data tabulated by RM. The general conclusions are the following:

1. The present fits summed over subshells are generally in a very good agreement with the total cross sections from RM. This is not a surprise, since our analytic formula fits accurately the HDS cross sections, and RM use the same (Hartree-Slater) method for calculating the photoionization cross sections at non-relativistic photon energies. We have found some omissions in the RM data. For S VIII, RM do not add the contribution from the outer $2p$-shell to the total cross section. Thus, for S VIII RM give the partial $2s$-shell cross section instead of the total one at all energies from the first threshold to the K-shell edge at 2700 eV. RM apparently assume that V II, Co II and Ni II possess $4s$ electrons. However the ground state electronic configurations of these ions are non-standard. Consequently the RM cross sections are inaccurate at $E \lesssim 80$ eV for V II, at $E \lesssim 130$ eV for Co II, and at $E \lesssim 160$ eV for Ni II. Moreover the RM data are inaccurate at $E < 330$ eV for Ar V, at $80 < E < 540$ eV for P III, and at $E > 3400$ eV for Li I and Li II. Excluding these cases from the comparison, we get an rms deviation of our fits from the RM data (averaged over all species) less than 0.03.
2. The present fits do not reproduce the resonance structures. However they are in a fairly good agreement with the OP and the experimental background cross sections. The agreement begins to deteriorate near the thresholds of the outer shells of neutral and low-ionized atoms. Note that the main goal of the OP is to give reliable data required for opacity calculations. The major efforts of the OP collaboration are to get highly accurate photoionization cross sections at low energies. In the meantime, the OP database TOPbase 0.6 gives photoionization cross sections with simple power-law tails at high energies. Comparison with experiment (Fig. 1a-b) shows that these tails are much less accurate than the present analytic fits. The high-energy cross sections provided by the TOPbase 0.6 database appear to be inaccurate for the neutral atoms as well as for ions (Fig. 1c-d). Moreover, the OP calculations do not include inner shell ionization.
3. The present fits agree very well with the cross sections from Henke et al. (1982) and Veigele (1973) which lie far from the thresholds of the outer shells. The agreement remains good as long as $E \lesssim 100$ keV, i.e. as long as the ejected photoelectron is non-relativistic. This is provided by the correct non-relativistic asymptote of Eq. (1).

These conclusions are in accord with the expected accuracy of the HDS method, which should be accurate for multicharged ions, for the deep shells of neutral and low-ionized atoms, and also far from the thresholds of the outer shells of the neutral and low-ionized atoms. The method may give significant errors near the thresholds of the outer shells of the neutral and low-ionized atoms where the correlation effects and the effects of atomic shell rearrangement during the photoionization process are important (Amusia 1990).

We have also compared our fits with the fits to the K-shell (i.e., $1s$) photoionization cross sections given by Daltabuit & Cox (1972). The latter fits are frequently used in astrophysical computer codes. These fits give errors of about 30% at the thresholds, $E = E_{\rm th}$. The errors decrease between $E = E_{\rm th}$ and $1.5 E_{\rm th}$ but grow noticeably with increasing E, since the fitting formula of Daltabuit & Cox (1972) does not reproduce the proper high-energy asymptote. At high energies, the fits of Daltabuit & Cox (1972) give cross sections which are different from experiment by large factors, whereas our fits are in error by a few percent only. The more accurate Seaton's formula used by Daltabuit & Cox (1972) for the H-like and He-like ions gives errors within $2-3\%$ in the energy range from once the threshold energy to $1.5E_{\rm th}$ and more than 10% at twice the threshold energy, and it gives cross sections which are different from experiment by large factors at high energies.

As an illustration, Figs. 2a-c and 3a-c compare the present fits with experiment and theory for two astrophysically important elements, N ($Z = 7$) and Fe ($Z = 26$). Both elements are taken in three ionization stages: neutral, intermediate, and high ionization.

4. Conclusions

Comparisons with experiment and theory show the high accuracy of the present fits for the partial photoionization cross sections of the ground states of atoms and ions up to energies of 100 keV. The cross sections used for fitting are less accurate at very low energies just above ionization thresholds of the outer shells of neutral and low-ionized atoms. The fits can be used, for instance, in computer codes which calculate the plasma ionization state. Note that the inner shell ionization may lead to subsequent ejection of Auger electrons. The probabilities of Auger processes after the photoionization from inner shells of all elements with $Z \leq 30$ are listed by Kaastra & Mewe (1993).

Acknowledgements. DAV is grateful to the Netherlands Organization for Pure Research (NWO) for financial support through the visitor programs, and to the Leids Kerkhoven-Bosscha Fonds for travel support. We acknowledge the use of the TOPbase 0.6 database through the Centre de Données Astronomiques de Strasbourg. We wish to thank J. Kaastra for providing us with the tables of Reilman & Manson in electronic form, and for helpful discussions. We are grateful to M. Trzhaskovskaya for recalculating the photoionization cross sections of He I, Li I and Li II.

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Figure captions

Fig. 1a-d. Total photoionization cross section (solid line) from the present fit as compared with theoretical calculations of the Opacity Project (dotted line) and Reilman & Manson 1979 (crosses), and with experimental data of Angel & Samson 1988 (circles) and West & Marr 1976 (triangles): **a** O I, **b** Ne I, **c** Si II, **d** Ca VI.

Fig. 2a-c. Total photoionization cross section (solid line) from the present fit as compared with the K-shell fits of Daltabuit & Cox 1972 (dashed line), with theoretical calculations of Reilman & Manson 1979 (crosses) and the Opacity Project (dotted line), with experimental data of Samson & Angel 1990 (triangles) and with the compilation of Veigele 1973 (circles): **a** N I, **b** N III, **c** N VI.

Fig. 3a-c. Total photoionization cross section (solid line) and the $3d$-shell cross section (dash–dotted line) from the present fits as compared with theoretical calculations of Reilman & Manson 1979 (crosses) and the Opacity Project (dotted line), and with experimental data from the compilations of Henke et al. 1982 (triangles) and Veigele 1973 (circles): **a** Fe I, **b** Fe IV, **c** Fe XXIV.

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