Photo-Ionization of Light Atoms at Intermediate Energies

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Abstract

The photoionization cross sections are important parameters in the determination of the ionization structure of cosmic gas subjected to ultraviolet and x-ray radiation. We present a set of analytic fits to the Hartree-Dirac-Slater photoionization cross sections for the ground state shell of elements (He, Li, Be, N & O). Comparison with experiment and theory demonstrates generally high accuracy of the fits up to energies of 200 eV.

1. Introduction

In recent publications\cite{1,2}, a universal shape function for cross sections of ionization by charged particle impact has been established. Here, we show how an analogous shape function for multiple ionization by photon can be constructed along the same line.

The last fifteen years or so have seen intensive effort, both theoretically\cite{3-5} and experimentally\cite{6,7}, in the study of three and four-body Coulomb problem found in the photoionization of helium and lithium atoms.

Subsequently, interest is growing in moving beyond the photoionization of (He) and (Li). More complex targets such as (Be), have been examined by the time-dependent close-coupling technique\cite{5} and other methods\cite{8,9}. These have been supported by experimental measurements of the total photoionization cross section of (Be)\cite{10}, in the near threshold. Another complex systems has been studied by Pattard\cite{11} using an analytical parametrization formula. This represents a much more difficult problem than the photoionization of the mentioned atoms, since the motion of the electrons must be treated equally\cite{5}.

Still, calculations of cross sections by \textit{ab initio} methods are far from trivial, and quickly become unmanageable going to more complicated systems or processes involving three or more electrons. It is for these reasons that simple semi-empirical formula for the description of cross sections are as interesting today as they were 20 or 30 years\cite{11}.
For the practitioner they may be the only available hint of what to expect when designing a new experiment. For the theorist, they may be the most simple and straightforward way to express simple physical principles without hiding them behind sometimes excessive algebra or numerics\(^\text{[11]}\).

2. Theory

In this paper we present analytic fits to the photoionization cross section \(\sigma(E)\), for the ground states of light atoms in question using the Hartree-Dirac-Slater method, by fitting formula\(^\text{[12]}\):

\[
\sigma(E) = \sigma_s F(y) \quad \text{Mb}
\]
\[
F(y) = [(x - 1)^2 + y_w^2]y^{0.5p-5.5}(1 + \frac{y}{y_w})^{-p}
\]
\[
x = \frac{E}{E_a} - y_a
\]
\[
y = \sqrt{x^2 + y_1^2}
\]

Where \((E)\) is refers to the photo energy in (eV), and \(\sigma_s, E_s, y_w, y_a, y_1, y_a\) and \(p\) are the fit parameters, \((1\text{Mb}=10^{-18}\ \text{cm}^2)\). All the fitting parameters and experimental ionization threshold energy \((E_{th})\) taken from Verner et al.\(^\text{[13]}\) are listed in table(1).

<table>
<thead>
<tr>
<th>atom</th>
<th>(\sigma_s (\text{Mb}))</th>
<th>(E_s (\text{eV}))</th>
<th>(E_a (\text{eV}))</th>
<th>(p)</th>
<th>(y_w)</th>
<th>(y_a)</th>
<th>(y_s)</th>
<th>(y_1)</th>
</tr>
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<tbody>
<tr>
<td>He</td>
<td>949.2</td>
<td>13.61</td>
<td>24.59</td>
<td>3.188</td>
<td>2.039</td>
<td>1.469</td>
<td>0.4434</td>
<td>2.136</td>
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<tr>
<td>Li</td>
<td>62.45</td>
<td>3.107</td>
<td>5.392</td>
<td>4.895</td>
<td>0.0</td>
<td>15.01</td>
<td>0.0</td>
<td>0.0</td>
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<tr>
<td>Be</td>
<td>2.932+5*</td>
<td>9.539</td>
<td>9.323</td>
<td>10.52</td>
<td>0.3655</td>
<td>0.4301</td>
<td>8.278-4</td>
<td>0.01269</td>
</tr>
<tr>
<td>N</td>
<td>823.5</td>
<td>4.034</td>
<td>14.53</td>
<td>3.928</td>
<td>0.09097</td>
<td>80.33</td>
<td>0.8598</td>
<td>2.325</td>
</tr>
<tr>
<td>O</td>
<td>1745</td>
<td>1.24</td>
<td>13.62</td>
<td>17.64</td>
<td>0.07589</td>
<td>3.784</td>
<td>8.698</td>
<td>0.1271</td>
</tr>
</tbody>
</table>

*2.932+5 denotes \(2.932 \times 10^5\)
Yan et al.\textsuperscript{[3]} constructed cross sections formula for atoms and show that their accuracy can be controlled by requiring that they be consistent with oscillator strength moment sum rules. The differential oscillator strength \( \frac{df}{d\varepsilon} \) is related to the photoionization cross section \( \sigma(E) \) by \textsuperscript{[3]}:

\[
\sigma(E) = 4.03 \frac{df}{d\varepsilon} \; Mb \quad \text{(5)}
\]

Where \( E = I + \varepsilon \); \( (I) \) the ionization potential, and \( \varepsilon \) is the energy of the ejected electron.

Whereas \( \frac{df}{d\varepsilon} \) have the expression \textsuperscript{[3]}:

\[
\frac{df}{d\varepsilon} \approx \frac{2^{1/2} Z^2 S(k)}{\pi} E^{-7/2} \quad \text{(6)}
\]

Where, \( (Z) \) is the atomic number, and \( S(k) \) defined as the oscillator strength moment.

\[
S(k) = \sum_n (E_0 - E_n)^k f_n + \int_0^\infty (I + \varepsilon)^k \frac{df}{d\varepsilon} d\varepsilon \quad \text{(7)}
\]

Where \( E_0, E_n \) are the eigenvalues of the initial and final state, respectively. \( f_n \) is the electric dipole absorption oscillator strength.

A method of analytical parameterization had proposed by Pattard\textsuperscript{[11]} provides an excellent description for cross sections of atoms ionized by photons, and introduced by:

\[
\sigma(E) = \sigma_M \chi^\alpha \left( \frac{\alpha + 7/2}{\alpha \chi + 7/2} \right)^{(\alpha+1)} \quad \text{(8)}
\]

Where \( (\chi = \frac{E_{\varepsilon}}{E_M}) \), \( (\alpha) \) is the Wannier exponent, \( (E_{\varepsilon}) \) is the excess energy, and \( (E_M), (\sigma_M) \) are the position and height of the cross section maximum, respectively.

### 3. Results and Discussion

Photoionization cross sections of atoms are required for constructing theoretical models of many objects, from planetary nebulae to active galactic nuclei and intergalactic medium.

Equation(1) allows us to describe correctly the background photoionization cross sections near the threshold, at intermediate energies. The advantage of the proposed fit is that it is not related directly to the cross section parameters at the threshold.

In fig.(1) the present work (P.W.) of the photoionization cross sections for (He, Li and Be)-atoms, where for He-atom we compare the data we calculate with the theoretical data of Yan et al.\textsuperscript{[3]} and the measurements of Samson et al.\textsuperscript{[6]}, for Li-atom we compare our results with the data of Yan et al.\textsuperscript{[3]} and the measurements are not available to this atom in the range we take it to our knowledge. Finally the results of Be-atom compared with the data of Berrington et al.\textsuperscript{[14]} and the experimental measurements of Wehlitz and Whitfield\textsuperscript{[10]}. In fig.(2) we compare our data of (N and O)-atoms with the asymptotic calculations of Pattard\textsuperscript{[11]}, and the experimental measurements of Samson & Ange\textsuperscript{[15]} and angel & Samson\textsuperscript{[16]}, respectively. Our results gave a very good agreement with the theoretical and experimental data which had compared with, for the most atoms under study.
In figure(2) Pattard data of photoionization cross section for (N) & (O) showed no match with the present work and the experimental data for the range (50-70) eV, and we are not responsible for this behavior. The cross sections used for fitting are less accurate at very low energies just above ionization threshold of the outer shell of neutral atoms. This fitting provides an excellent description of the respective cross sections in cases where indirect processes (excitation-autoionization) do not have to be taken into account. In our method, we denote rely on any perturbation expansion to describe interaction of the atom and the electromagnetic field. This interaction is included into theory from the beginning. We would like to emphasize the accuracy of the present results for the photoionization cross sections which, we believe, is on the level of a fraction of a percent. Although only limited range of a selected photon energies were reported in the paper. These results might serve as an accurate data base and find their use in various astrophysics and atomic physics applications.

Figure(1): Photoionization Cross Section vs. Photon Energy for (He, Li and Be)-atoms
References


التأين الضوئي للذرات الخفيفة عند الطاقات المتوسطة
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الخلاصة
تعد المقاطع العرضية للتتأين الضوئي من المعاملات المهمة في تكريب التأين لغاز الكون الالتفاح بالاشعة السينية والاشعة فوق البنفسجية. تم في هذا البحث مجموعه من التصحيحات التحليلية لمقاطع التأين الضوئي العرضية لـ هارتي-ديراك-سليتر لقشرة الحالة الأرضية للعناصر الخفيفة (الهيليوم، الليثيوم، البريليوم، النايتروجين و الأوكسجين). اظهرت مقارنات النتائج التي تمت بين حساباتنا والقيم العملية والنظرية الأخرى دقة جيدة من التوافق العام لقيم الطاقات ونهاية 000 الكترون فولت.