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DWBA calculation of positron impact ionization of argon

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Abstract
The ionization of the 3p and 3s orbitals of argon by 200 eV incident positrons is studied with the DWBA approximation. Our TDCS results for the 3p orbital ionization are found to be in good agreement with recent CDW-EIS data.

1. Introduction

Triple differential cross sections for electron and positron impact single ionization of argon remains a formidable theoretical and computational challenge.

Positron experiments measuring TDCS are very new. In 1998 the University College London group measured TDCS in the forward direction for H_2 [1] and more recently the Missouri University of Science and Technology group obtained the full variation of TDCS with the ejected electron angles for argon [2]. The accuracy of the positron impact TDCS experiments is much smaller than in some of the recent electron impact TDCS experiments [3].

Theoretical work for positron impact TDCS in H_2 employed the 3C model [4-6]. This work managed to confirm the presence of the experimentally observed Electron Capture in the Continuum (ECC) peak. Theory and experiment disagreed in the position of the EEC peak.

For argon it is expected the need for theoretical models which contain the distortion and the screening of the positron and ejected electron wave functions. In the electron impact case the following theoretical models were employed: the distorted-wave Born approximation (DWBA) [7], the extension of DWBA and 3C models to 3DWBA [8], the Continuum Distorted Wave - Eikonal Initial State (CDW-EIS) model [9] and the distorted wave Born plus R matrix (RM2) model [10]. In spite of the high level of sophistication in some of these models the current status of agreement between theory and experiment in the electron impact case is not satisfactory [9].

Very recently the CDW-EIS model was applied to the calculation of TDCS for positron impact ionization of the 3p orbital of argon [2]. The theoretical variation of TDCS with the ejected electron angles was compared with the experimental data. In this paper we study the same phenomenon employing a DWBA model.

2. Theory

The DWBA approximation is described very well in a number of papers, such as the one by Kheifets et al [11]. For relatively slow projectiles the distorting and screening effects on the continuum electron and positron states are very important and most of our work was dedicated to accounting for these effects.

For the ejected electron continuum states we included the attractive Hartree-Fock static potential of Ar+ and a Furness-McCarthy (FM) exchange potential. In this work we assumed that the exchange is triplet for all bound electrons. For the scattered positron continuum states there will be no exchange with the bound electrons, and the Ar+ static potential changes its sign relative to the electron case. For the incident positron continuum states we included the Hartree-Fock static potential of Ar, plus the target polarization potential.

We found that the convergence of the partial waves contributions was slow. In the orbital angular momentum expansions we needed to include 10 ejected electron continuum states and 50 incident positron continuum states.

In this work we considered the post-collision interaction (PCI) between the scattered positron and the ejected electron through a Gamow-type factor [12]. This factor lowers the TDCS in the electron impact case and raises them in the positron impact case.

3. Results and discussion

Figure 1 presents our results for positron impact ionization of the 3p and 3s orbitals of argon. We compare them with the recent CDW-EIS data of [2] for the 3p orbital ionization. To match the CDW-EIS results our DWBA data were divided by 1.447.

Figure 1 shows that the agreement between two theoretical models in the 3p orbital case. Unlike in the electron impact case, for positron impact ionization of argon the variation of TDCS with the ejected electron angles is very smooth showing a single binary peak at around 50 degrees and a recoil peak at around 220 degrees. The DWBA peaks are at slightly smaller angles than the CDW-EIS peaks. Also it is interesting that the 3p and 3s ionization TDCS have the peaks at the same angles.

A comparison with the experimental results can be made only after the theoretical results are convoluted over the experimental parameters. This work was done for the CDW-EIS 3p ionization data and it demonstrated that the convolution shifts the binary peak to 67 degrees and the recoil peak to 247 degrees, in quite good agreement with the experimental data.

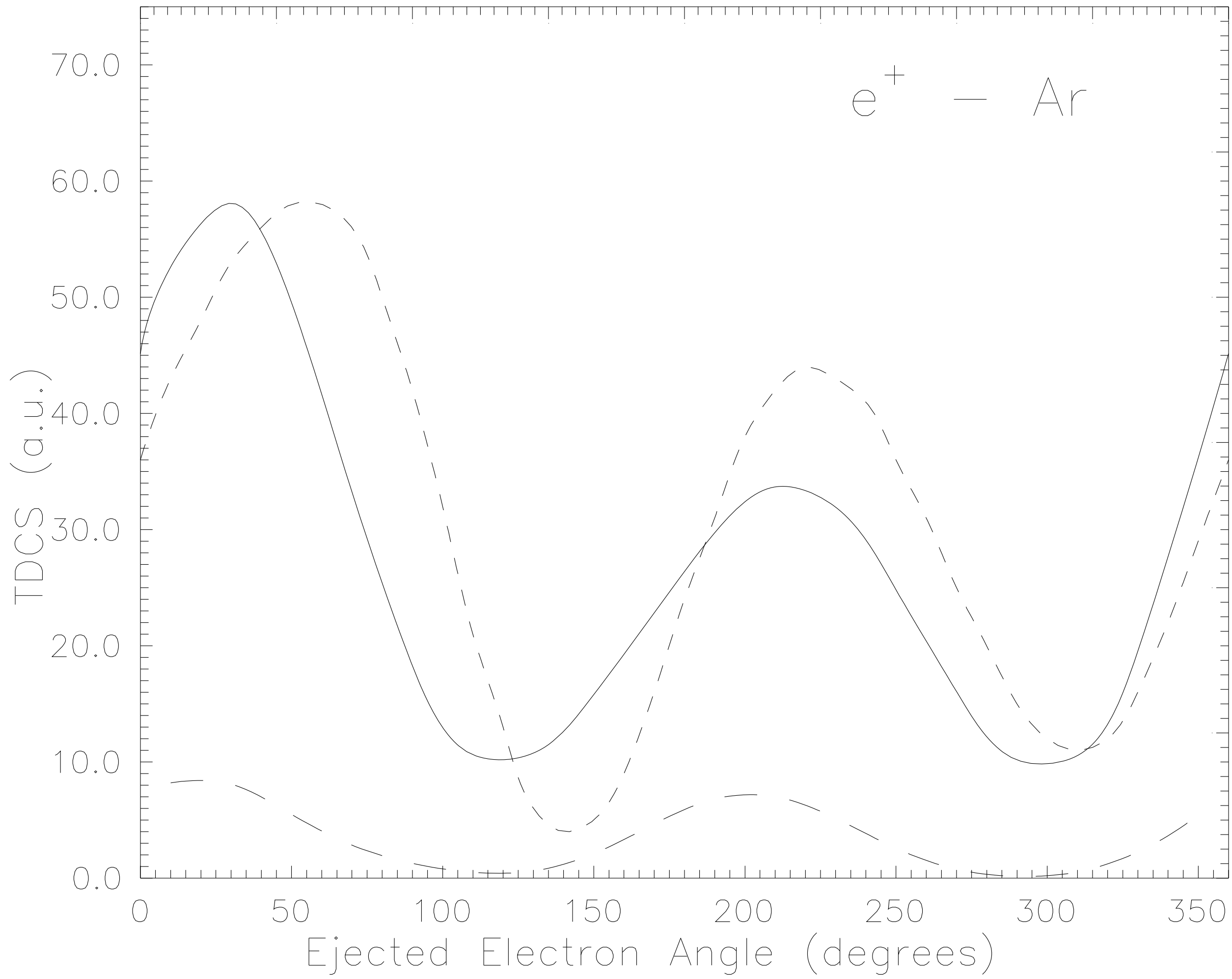

Figure 1. TDCS in atomic units for coplanar 200 eV positron impact ionization of the 3p and 3s shells of argon as a function of the ejected electron angles. The positron was scattered at 3 degrees and the ejected electron had 5.4 eV. For the 3p ionization the solid line corresponds to our DWBA calculation and the dashed line to the CDW-EIS calculations [2]. The long dashed curve corresponds to our DWBA data for the 3s ionization. Our DWBA data were divided by a factor of 1.447 to match the CDW-EIS results.

4. Conclusions

Our work shows that the DWBA model produces the same variation of TDCS with the ejected electron angle as the CDW-EIS model for the positron impact ionization of 3p orbital of argon. Our DWBA model included a complete account of the screening and distortion effects in the representation of the positron and ejected electron continuum states and an inclusion of the PCI effect.

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