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Effect of orthogonalization on total ionization cross sections by electron impact: application to small molecules

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Abstract. Total ionization cross sections by electron impact are calculated for H₂O, NH₃ and CH₄ molecules by using an improved first Born approximation which has been previously applied for atomic targets by Bartlett and Stelbovics [P.L. Bartlett, A.T. Stelbovics, Phys. Rev. A **66**, 012707 (2002)]. In this model a full orthogonalization of the final state to the initial state has been performed to evaluate the cross sections. One center wave functions are employed to describe the molecular orbitals. It is shown that the results obtained in the present model are immensely improved when compared with the first Born model without orthogonalization. Furthermore, an overall agreement is also observed when a comparison is made with the experimental data.

1 Introduction

Differential and total cross sections for the ionization of atoms and molecules by electron impact provide fundamental data in a wide range of applications such as plasma physics, fusion experiments and also in living matter [2–6]. Besides their strategic applications, investigations of molecular targets constitute effectively a challenging task for theorists because of their multicenter character. Theoretical investigations of ionization of molecules remain thus an open problem even in the case of first Born approximation. In fact, many theoretical models have been widely applied to atoms [7–11] in contrast to molecules where only a few models exist and are applied especially to small molecules [12–17]. On the other hand, total cross sections for molecular targets are more extensive in literature than the differential ones. Semi empirical studies of molecules have been used to estimate cross sections for molecules using various additive rules [18,19] which generally overestimate total cross sections. A semi empirical approach, referred to as the BEB model, is currently known to reproduce quite well the cross sections for a large variety of small molecules [20–22]. These theories provide only total and singly differential cross sections and are unable to describe the detailed aspect of the ion-

ization process. More recently, full quantum mechanical models have also been applied to molecules to calculate total and all multiply differential cross sections using a method like the FBA-CW [23,24] which represents a first Born approach where the ejected particle is represented by a Coulomb wave. These models were able to correctly reproduce experimental triple differential cross section in several regions even at a low impact energy. Nevertheless these models provide total cross sections which overestimate experiments like other first order models. The M3DW model [25], where the final state is represented by a 3-body distorted-wave, is currently the most sophisticated used approach. This rather complicated numerical model generally provides results in good agreement with experiments [26] but can lead to large discrepancies as in the ionization of the tetrahydrofuran [27]. However, this model has never been applied for the calculation of total cross section. Recently a multicenter distorted wave method has been developed and applied successfully for the single ionization of water molecule [28] but not for total cross section.

We examine here a first order model (FBA-CW) which is often used to calculate ionization cross sections of molecules by electron impact. It is well-known that first order models generally overestimate total cross sections at low impact energy. So one has to include second Born terms to improve the results. For atoms second Born

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calculations can be performed but for molecules the numerical situation becomes more complicated because of additional three integrations to average over Euler angles.

We present in the present work an improved model based upon the FBA-CW where the Coulomb wave representing the final state is orthogonalized to all occupied molecular initial states of the target. In fact this model (FBA-OCW) has been inspired by the work of Bartlett and Stelbovics [1] who applied it to atoms. It provided consistently good agreement with experiments for several atomic targets. It is worth noting that the notion of orthogonalization has recently been introduced to study the fragmentation of HDO^+ molecular ions produced by electron impact ionization [29].

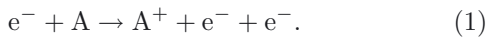
The molecular orbitals of the target are sometimes described by single center Slater-type wave functions [30–32] to avoid multicenter calculations. The accuracy of these single center molecular targets has been formerly examined while investigating molecular structures in electron momentum studies [24]. The calculated momentum profiles exhibited shapes in good agreement with experiments. The description of the targets used here can thus be considered to be reasonably accurate for calculating ionization cross sections.

The present paper is organized as follows: in Section 2 we outline the theory used to describe the ionization process. In Section 3, our results are discussed and compared with experiments. Finally, a conclusion is drawn in Section 4.

Atomic units are used throughout unless otherwise indicated.

2 Theory

The electron-impact single ionization of a molecular target A can be schematized by:



In the first Born approximation the fourfold differential cross section (4DCS) corresponding to a particular orientation of the molecule defined by Euler angles (α, β, γ) is given by:

$$\sigma^{(4)}(\alpha; \beta; \gamma) = \frac{d^4\sigma(\alpha; \beta; \gamma)}{d\Omega_{\text{Euler}}d\Omega_s d\Omega_e dE_e} = \frac{k_s k_e}{k_i} |T_{if}|^2, \quad (2)$$

where $d\Omega_{\text{Euler}} = \sin\beta d\alpha d\beta d\gamma$.

The lesser multiply differential and total cross sections are then obtained by successive integrations over $d\Omega_e$, $d\Omega_s$ and dE_e where $d\Omega_s$ and $d\Omega_e$ are the elements of solid angles corresponding to the scattered and the ejected electrons respectively while dE_e represents the energy interval of the ejected electron. \vec{k}_i , \vec{k}_s , and \vec{k}_e denote respectively the momentum of the incident, scattered and ejected electron, and are required to fulfil the conservation law

$$\frac{k_i^2}{2} = \frac{k_s^2}{2} + \frac{k_e^2}{2} + I_i, \quad (3)$$

where I_i is the ionization energy. The matrix element M is given by:

$$T_{if} = \frac{1}{2\pi} \langle \Psi_f | V | \Psi_i \rangle \quad (4)$$

and represents the transition from the initial state Ψ_i to the final state Ψ_f . V represents the interaction between the incident electron and the target, and is written as:

$$V = - \sum_{j=1}^M \frac{Z_j}{|\vec{r}_0 - \vec{R}_j|} + \sum_{i=1}^{i=N} \frac{1}{|\vec{r}_0 - \vec{r}_i|} \quad (5)$$

where N is the number of bound electrons, Z_j the charge of each nuclei and \vec{r}_i is the position of the i th bound electron of the target with respect to the center of the molecule. M is the number of nuclei constituting the molecule and \vec{R}_j their positions with respect to the center of mass of the molecule. In the present case the considered molecules are of type XH_n , the center of the molecule is located on the heavy atom X as indicated by Moccia [30–32]. The distance between the center of the molecule and the incoming electron is r_0 .

Moreover, by using the well-known frozen-core approximation and the single particle picture we reduce this N -electron problem to a one active electron problem. In this case the matrix element can be rewritten as

$$T_{if} = \frac{1}{2\pi} \langle \Phi_f(\vec{k}_s, \vec{k}_e, \vec{r}_0, \vec{r}_1) | \frac{1}{r_{01}} - \frac{1}{r_0} | \Phi_i(\vec{k}_i, \vec{r}_0, \vec{r}_1) \rangle \quad (6)$$

where \vec{r}_1 represents the position of the bound electron with respect to the center of the molecule while r_{01} is the distance between the projectile and the bound electron.

The triple differential cross section (TDCS) is obtained by integrating over the Euler angles due to the random orientation of the molecule in gaseous state:

$$\sigma^{(3)} = \frac{1}{8\pi^2} \int \sigma^{(4)} d\Omega_{\text{Euler}}. \quad (7)$$

2.1 The initial state description

In the single particle picture the initial state is written as:

$$\Phi_f(\vec{k}_i, \vec{r}_0, \vec{r}_1) = \varphi_p(\vec{k}_i, \vec{r}_0) \varphi_i(\vec{r}_1) \quad (8)$$

where $\varphi_p(\vec{k}_i, \vec{r}_0)$ is the plane wave describing the incident electron. All the individual bound electrons are represented by linear combinations of single center wave function of Moccia [30–32] and are written as:

$$\varphi_i(\vec{r}) = \sum_{k=1}^{N_i} a_{ik} \phi_{n_{ik} l_{ik} m_{ik}}^{\varepsilon_{ik}}(\vec{r}) \quad (9)$$

where N_i is the number of trial functions used in the construction of the i th molecular orbital and a_{ik} are the weights of each component. The trial Slater-type functions are taken to be:

$$\phi_{n_{ik} l_{ik} m_{ik}}^{\varepsilon_{ik}}(\vec{r}) = R_{n_{ik}}^{\varepsilon_{ik}}(r) S_{l_{ik}}^{m_{ik}}(\Omega). \quad (10)$$

The radial part $R_{n_{ik}}^{\varepsilon_{ik}}(r)$ may be given by the usual radial Slater-type functions such as $b_{n_{ik}} r^{n_{ik}-1} \exp(-\varepsilon_{ik} r)$, where $b_{n_{ik}}$ is the normalization constant while $S_{l_{ik}}^{m_{ik}}(\Omega)$ are the so called real spherical harmonics [33] expressed as:

$$\begin{cases} S_l^m(\Omega) = \left(\frac{m}{2|m|}\right)^{\frac{1}{2}} \\ \times \left\{ Y_l^{-|m|}(\Omega) + (-1)^m \left(\frac{m}{|m|}\right) Y_l^{|m|}(\Omega) \right\} & m \neq 0 \\ S_l^m(\Omega) = Y_l^m(\Omega) & m = 0. \end{cases} \quad (11)$$

2.2 The final state description

In the single particle picture the final state is given by:

$$\Phi_f(\vec{k}_s, \vec{k}_e, \vec{r}_0, \vec{r}_1) = \varphi_p(\vec{k}_s, \vec{r}_0) \varphi_c(\vec{k}_e, \vec{r}_1) \quad (12)$$

where $\varphi_p(\vec{k}_s, \vec{r}_0)$ and $\varphi_c(\vec{k}_e, \vec{r}_1)$ are a plane wave and a Coulomb wave describing the scattered and ejected electron respectively. The Coulomb wave is described by the following

$$\begin{aligned} \varphi_c(\vec{k}_e, \vec{r}) &= \frac{\exp(i\vec{k}_e \cdot \vec{r})}{(2\pi)^{3/2}} \\ &\times {}_1F_1\left(-i\frac{Z}{k_e}, 1, -i\left(\vec{k}_e \cdot \vec{r} + k_e r\right)\right) \\ &\times \exp\left(\frac{\pi Z}{2k_e}\right) \Gamma\left(1 + i\frac{Z}{k_e}\right). \end{aligned} \quad (13)$$

When equation (12) in combination with (13) represents the final state our model is called the FBA-CW model. This model constitutes a first Born theory which overestimates the total cross section. It is well known that non first order approaches like BBK [34] or second Born [35] are capable of improving the cross sections at low impact energies. However, these models require generally long time of computation and the situation becomes formidable when one deals with the molecules considered in this work. We present here an alternative method to calculate total cross sections for some molecules thanks to an improved first order model. In fact the model is inspired by a work applied previously by Bartlett and Stelbovics [1] for atoms. In this model, the final state is fully orthogonalized to the initial state. More explicitly, in our single particle picture the Coulomb wave describing the ejected electron is chosen to be orthogonal to all occupied molecular orbitals.

We would like to remind that the Coulomb wave given by equation (13) is not orthogonal to the molecular orbitals of Moccia given by equation (5). So we have chosen the final state such that the Coulomb wave is orthogonal to the initial state. The fully orthogonalized Coulomb wave is hence given by:

$$\varphi_c^\perp(\vec{k}_e, \vec{r}) = \varphi_c(\vec{k}_e, \vec{r}) - \sum_i \varphi_i(\vec{r}) \langle \varphi_i | \varphi_c \rangle \quad (14)$$

where $\varphi_c(\vec{k}_e, r)$ and $\varphi_i(\vec{r})$ refer respectively to the non-orthogonalized Coulomb wave and denote the molecular orbitals describing the target. As stated by Bartlett and Stelbovics, relation (14) is valid only if the orbitals form an orthonormal set. This requirement is satisfied for the molecular description of Moccia [30–32] used here.

The new model, called FBA-OCW (first order approximation with an orthogonalized Coulomb wave), is used to perform calculations for three molecules, namely, H₂O, CH₄ and NH₃. This model is able to provide results for the fully differential as well as the total cross section. Furthermore, the matrix elements calculations are carried out analytically [36] in almost all cases enabling considerable economy of computation time.

3 Results and discussion

We have calculated the total cross section (TCS) for single ionization of some molecules in their ground states by electron impact. These cross sections have been obtained on integrating the TDCS given by equation (7) over the scattering and ejection angles as well as the ejection energy successively. An improved first order model with orthogonalization of the final state to the initial state (FBA-OCW) has been used to calculate TCS's. In particular H₂O, NH₃ and CH₄ molecules have been considered. These molecules consist of ten electrons but they have different geometries. In addition to this difference they are composed of different numbers of atoms.

The goal of the present investigation is to study the effect of orthogonalization on the calculation of the cross sections of these molecules. We therefore apply the FBA-OCW model to calculate total ionization cross sections for the cited targets, and compare the results with the first Born model without orthogonalization (FBA-CW) and available experiments.

First of all let's look at the case of atomic Neon which has already been investigated [1] and where the TCS's obtained with FBA-CW and FBA-OCW are displayed for incident energies from threshold to 5 keV. This atom consists of ten electrons like molecular targets under investigation in this work.

We observe in Figure 1 that the results are greatly improved with the use of the orthogonalized model FBA-OCW and agree quite well with experiments in all regions. The calculations agree very well with the data even at low impact energy where generally first order models fail. The peak is also well reproduced in the FBA-OCW. The cross sections corresponding to the non-orthogonalized model FBA-CW considerably overestimate the experiments at low impact energy as it was expected. We can conclude that the effect of the orthogonalization is extremely important in reproducing the amplitude especially in the peak region, the position of the maximum being kept unchanged.

We now consider the case of some small molecules, e.g., H₂O, NH₃ and CH₄. From the practical point of view, these molecules are of great interest in several domains, for example, H₂O in living matter, and NH₃ and CH₄ in

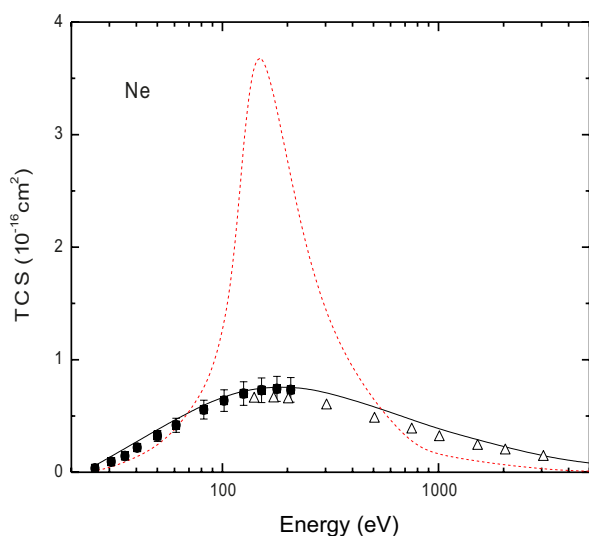


Fig. 1. Comparison of the measured data with our theoretical total cross sections versus incident energy with the FBA-OCW (solid line) and FBA-CW (dashed line) in the case of Neon. The data are taken from several sources: Sorokin et al. [37] (up triangles) and Wetzel et al. [38] (full squares).

astrophysics. As it was stated above, accurate single center wave functions, whose accuracy has been checked by using electron momentum spectroscopy technique, have been used for these molecules reducing the problem to atomic calculations. In each case we display TCS's corresponding to the orthogonalized model (FBA-OCW) as well as to the non orthogonalized one (FBA-CW) simultaneously for comparison.

The water molecule is first investigated. We use the single center description of Moccia for the five occupied orbitals of H_2O in its ground state: $1a_1$, $2a_1$, $1b_2$, $3a_1$ and $1b_1$. As the inner orbital $1a_1$ is strongly bound (-558.277 eV), its contribution will be neglected. The ionization energies corresponding to the orbitals $2a_1$, $1b_2$, $3a_1$ and $1b_1$ are respectively 32.2, 18.6, 14.7 and 12.6 eV. The total cross section of the ionization of the molecule in its ground state is obtained by summing the contribution of the individual molecular orbitals representing the structure of the target. Before displaying the total cross section, we present in Figure 2 the results representing the contribution of each orbital in order to check the effect of the orthogonalization separately. It is seen that the TCS decreases when orthogonalization is applied. The inner orbital $2a_1$ is the most sensitive to the orthogonalization, the amplitude is practically divided by four while for the other orbitals the decrease is less important.

In Figure 3 we show the TCS for the ionization of H_2O in an incident energy range from threshold to 5 keV. It is seen that calculations without orthogonalization (dashed line) largely overestimate the experiments at low impact energy especially in the peak region. When orthogonalization is used, the results are considerably improved. At low impact energy our theoretical results reproduce very well the data and the amplitude is quite well reproduced when compared with experiments. The peak is also well located.

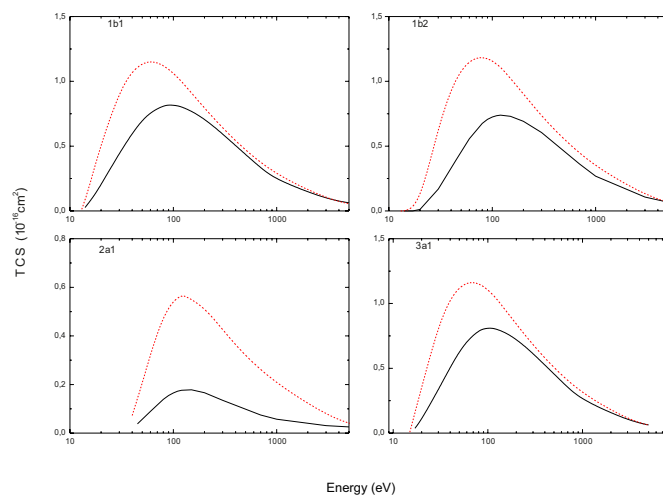


Fig. 2. Comparison between the theoretical total cross sections versus incident energy with the FBA-OCW (solid line) and FBA-CW (dashed line) in the case of H_2O . The comparison is made for the four individual molecular orbitals $1b_1$, $1b_2$, $2a_1$ and $3a_1$.

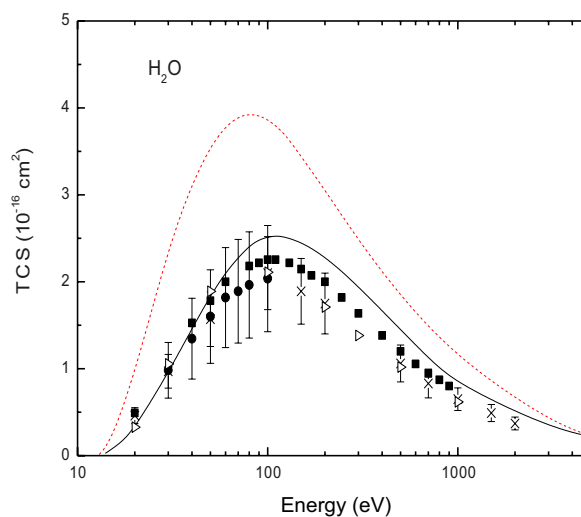


Fig. 3. Comparison of the measured data with our theoretical total cross sections versus incident energy with the FBA-OCW (solid line) and FBA-CW (dashed line) in the case of H_2O . The data are taken from several sources: Shutten et al. [39] (solid circles), Djuric et al. [40] (solid squares), Khare and Meath [41] (open triangles) and Straub et al. [42] (crosses).

At high energy the two models converge and provide similar results.

For NH_3 , the TCS is displayed in Figure 4 and compared with experiments. Here the outer molecular orbitals $2a_1$, $3a_1$ and $1e$ corresponding to ionization energies 30.5 eV, 11.3 eV and 16.5 eV, respectively have been investigated. We further observe that orthogonalization causes a lot of improvement. The amplitude is substantially reduced and results are quite close to experiments. In particular, at low impact energy the present calculations are in excellent agreement with experimental data. In the vicinity of the maximum, the experiments are

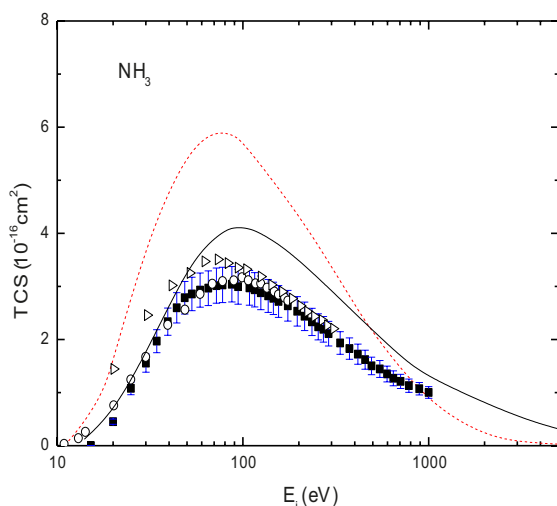


Fig. 4. Comparison of the measured data with our theoretical total cross sections versus incident energy with the FBA-OCW (solid line) and FBA-CW (dashed line) in the case of NH_3 . The data are taken from several sources: Rao and Srivastava [43] (solid squares), Djuric et al. [44] (open up triangles) and Crowe and McConkey [45] (open circles).

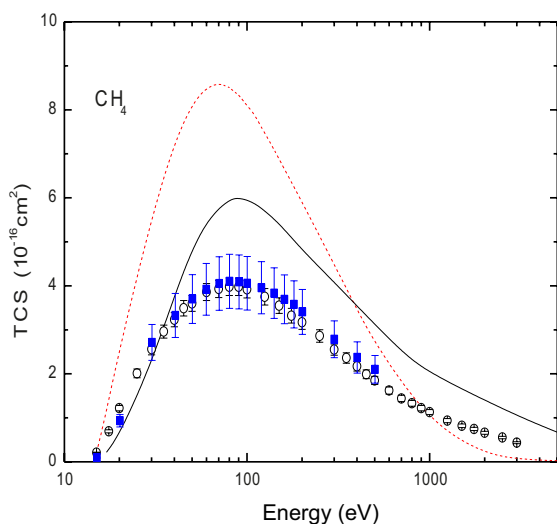


Fig. 5. Comparison of the measured data with our theoretical total cross sections versus incident energy with the FBA-OCW (solid line) and FBA-CW (dashed line) in the case of CH_4 . The data are taken from several sources: Nishimura and Tawara [46] (solid squares) and Orient and Srivastava [47] (open circles).

still improved but the data are somewhat overestimated. At high energies the results corresponding to the FBA-CW model fall more rapidly and the experiments are well reproduced. We can state that the overall shape of the TCS agrees rather well with experimental data for NH_3 when orthogonalization is applied.

In Figure 5 we present our results for CH_4 molecule, where $2a_1$ and $1t_2$ (corresponding to ionization energies 25.7 eV and 14.25 eV) have been treated. The calculations still agree very well with experiments at low energies. The TCS for FBA-OCW model falls more rapidly to

zero and agrees better with experiments when compared with non-orthogonalization results. The amplitude weakly overestimates the data in the peak region and the maximum is well located.

In summary, we can state that our first order model FBA-OCW provides TCS results which improve the calculations considerably and agree quite well with experiments. Results are in excellent agreement with experiments at low impact energies. The peak is well reproduced for H_2O but remains weakly overestimated for NH_3 and CH_4 . Nevertheless it is observed that the model reproduces the general shape of the TCS in most regions.

4 Conclusion

We have presented an improved first Born model (FBA-OCW) to calculate total ionization cross sections for some small molecules by electron impact. This model consists of orthogonalizing the final state to all occupied initial states which are represented by single center molecular orbitals. It shows substantial improvement over the traditional first Born model without orthogonalization (FBA-CW) which overestimates the TCS at low impact energies. The FBA-OCW is capable of reproducing the amplitude at low incident energy highlighting an overall good agreement with experiments with the peaks somewhat reasonably reproduced and well located. The agreement is found to be better for H_2O while for NH_3 and CH_4 the peaks are weakly overestimated.

We plan to apply the model for larger molecular targets like the strategic DNA molecules whose interest has grown during the last few years in view of their importance in radiotherapy, for example. To date, several theoretical and experimental investigations have been successfully accomplished at the triple differential cross section level [48–50]. However, theoretical calculations of total cross sections are still to be reported in spite of the availability of experimental data [51].

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