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Double ionization of neon by electron impact: use of correlated wave functions*

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Abstract. A model including correlation both in the initial state and in the final state is applied to the case of the double ionization of neon. The results of our model are compared to the available experimental data performed at high incident energy. Fully (fivefold) differential cross sections (FDCS) have been studied by applying the first Born approximation. Four ion states of Ne^{++}, which are not resolved in the experiments, have been included in our calculation.

1 Introduction

The double ionization of an atom is one of the fundamental processes to understand the different mechanisms leading to energy deposition by radiation in matter. Three mechanisms are involved in the double ionization by electron impact: the shake-off (SO), the two-step 1 (TS1) and the two-step 2 (TS2). The SO mechanism is a single interaction between the incident electron and one target electron. This target electron is then ejected. The first ionization is followed by a relaxation process due to the sudden change of potential that may be responsible for a second ejection. The TS1 mechanism consists of a first interaction between the incident electron and one target electron as in the SO mechanism. It leads to a first ejected electron that interacts with another target electron and ejects it. The TS2 mechanism takes into account two interactions between the incident electron and the target. The study of this second-order process (TS2) requires the second Born approximation. Schröter et al. [1] have performed measurements of FDCS on neon at high incident energy (5582.6 eV). Since the incident electron is very fast, we can apply the first Born approximation and neglect the TS2 mechanism because Jones and Madison [2] show that the 6C model (which describes the scattered electron and the two ejected electrons in the field of the ion on equal footing) practically gives the same result than the 3C model (it is a first Born approximation) for an incident energy of 5599 eV in the case of the double ionization of helium. Moreover Grin et al. [3] and Kheifets [4] find that the differences between the results given by the second Born approximation and those given by the first Born approximation are weak for this high incident energy. In recent years, a large number of models have been developed for the double ionization of helium by electron impact [5–19] at high incident energy. It is not the case for the double ionization of neon as, up to now, only one model has been applied [20]. In this paper, Dal Cappello et al. [20] used a correlated wave function to describe the ground state and an approximation of the 3C model [21] to study the double ionization of neon performed at high incident energy [1]. In this case the three final ion states (^{3}P, ^{1}D and ^{1}S) of $Ne^{++}(2p^4)$ have been investigated. We decide to include in this study the double ionization of neon $2s^{-1}2p^{-1}{}^3$P state because Schröter et al. [1] suggest a possible contribution of this ion state due to the low energy resolution used in the channel detecting the scattered electron (20 eV). We moreover employ the 3C wave function which has the correct asymptotic behaviour when all interparticle distances are large. This model was only applied for the double ionization of helium [5–7] and water [22]. In the first case, it was shown that the 3C model (by using high correlated wave functions for the initial state) was able to give a good agreement with the experiments of Lahmam-Bennani et al. [23] and Taouil et al. [24] exactly for the same kinematics: a high incident energy of 5599 eV and the two ejected electrons having identical energies (10 eV). In the second case, the initial state of the water molecule was described by a Hartree-Fock wave function [22]. We may assume that such a model (3C for the final state and correlated wave function for the initial state) can be applied for the double ionization of neon.

The aim of the present work is to apply this sophisticated model in order to describe the available experimental data on neon [1].

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The structure of the paper is as follows. In Section 2 we outline the theory employed in the present work. Numerical results are compared and discussed to the available experiments in Section 3. Conclusions are summarized in Section 4.

Atomic units are used throughout unless otherwise indicated.

2 Theory

We study the collision between an incident electron and the neon atom in its ground state Ne $(2p^6)^1$S:

$$e^- + \mathrm{Ne} \longrightarrow e^- + e^- + e^- + \mathrm{Ne}^{++}, \tag{1}$$

for which the ion state $\mathrm{Ne}^{++}(2p^4)$ is in its ground state ^{3}P or in its excited states ^{1}D and ^{1}S. The momenta of the incident, scattered, and ejected electrons are denoted by $\vec{k}_i$, $\vec{k}_s$, $\vec{k}_1$ and, $\vec{k}_2$ respectively, and fulfil the conservation law:

$$\frac{k_i^2}{2} = \frac{k_s^2}{2} + \frac{k_1^2}{2} + \frac{k_2^2}{2} + I^{++}, \tag{2}$$

where $I^{++} = 62.6$ eV represents the energy necessary to eject two electrons from the neon atom (for the ground state of $\mathrm{Ne}^{++}(2p^4)(^3\mathrm{P})$, 65.3 eV for the excited ion state $\mathrm{Ne}^{++}(2p^4)(^1\mathrm{D})$, and 69.3 eV for the other excited state $\mathrm{Ne}^{++}(2p^4)(^1\mathrm{S})$).

The scattering plane is defined by $\vec{k}_i$ and $\vec{k}_s$. A coplanar geometry means that the two (slow) ejected electrons (10 eV each one) are into the scattering plane. The momentum transfer is defined by $\vec{K} = \vec{k}_i - \vec{k}_s$.

Since the projectile is very fast, electron energies for incident and scattered electrons are 5582.6 eV and 5500 eV, respectively, we use plane waves to describe it. So we arrive at standard first Born approximation of this collision problem. The FDCS may be written [25]:

$$\frac{d^5\sigma}{d\Omega_s d\Omega_1 d\Omega_2 dE_1 dE_2} = \frac{k_s k_1 k_2}{k_i} \sum_{j=1}^{j=15} \left| f_{B1}^j \right|^2, \tag{3}$$

where f_{B1}^j denotes the amplitude of the first Born term. The summation over the index j means that we consider in LS coupling the 15 possible ion final states corresponding to the 15 possibilities of leaving two electrons in the $2p^6$ outer shell of the neon atom (nine of them for the ion state $\mathrm{Ne}^{++}(2p^4)(^3\mathrm{P})$, five for the ion state $\mathrm{Ne}^{++}(2p^4)(^1\mathrm{D})$ and one for the ion state $\mathrm{Ne}^{++}(2p^4)(^1\mathrm{S})$).

This first Born term may be written as:

$$f_{B1}^j = -\frac{1}{2\pi} \left\langle e^{i\vec{k}_s\vec{r}_0} \Psi_f^j \left(\vec{k}_1, \vec{k}_2; \vec{r}_1, \ldots, \vec{r}_{10}\right) \right| - \frac{10}{r_0} + \sum_{i=1}^{i=10} \frac{1}{r_{0i}} \left| e^{i\vec{k}_i\vec{r}_0} \Psi_i \left(\vec{r}_1, \ldots, \vec{r}_{10}\right) \right\rangle, \tag{4}$$

where $\Psi_i(\vec{r}_1, \ldots, \vec{r}_{10})$ is the wave function for the ground state of the neon atom and $\Psi_f^j(\vec{k}_1, \vec{k}_2; \vec{r}_1, \ldots, \vec{r}_{10})$ that of the final state (two ejected electrons and the ion Ne^{++}). In the above expressions $\vec{r}_0$ is the coordinate of the incident electron, $\vec{r}_1, \ldots, \vec{r}_{10}$ refer to the coordinates of the initially bound electrons, and $\vec{r}_{0i} = |\vec{r}_0 - \vec{r}_i|$. In equation (4), it is assumed that the exchange between the fast incident (and scattered) electron and the target electron is neglected.

The integration over the projectile coordinate $\vec{r}_0$ can be performed analytically using the Bethe relation to obtain:

$$f_{B1}^j = -\frac{2}{K^2} \left\langle \Psi_f^j \left(\vec{k}_1, \vec{k}_2; \vec{r}_1, \ldots, \vec{r}_{10}\right) \right| - 10 + \sum_{i=1}^{i=10} e^{i\vec{K}.\vec{r}_i} \left| \Psi_i \left(\vec{r}_1, \ldots, \vec{r}_{10}\right) \right\rangle. \tag{5}$$

In order to examine the importance of the correlations in the initial state, the following two different wave functions will be examined: the Roothaan-Hartree-Fock wave function of Clementi and Roetti [26] which is a single Slater determinant:

$$\Psi_i \left(\vec{r}_1, \ldots, \vec{r}_{10}\right) = |1s1\bar{s}2s2\bar{s}2p_0 2\bar{p}_0 2p_1 2\bar{p}_1 2p_{-1} 2\bar{p}_{-1}| \tag{6}$$

(the notation p means that we consider a spin orbital which depends of (r, θ, φ) with a spin up and $\bar{p}$ means a spin down) and a correlated wave function calculated by superposition of configurations [27] which includes three terms: $3s^2, 3p^2$ and $3d^2$. The correlation energy is –0.16162 au which corresponds to 40% of the exact correlation energy (–0.3917 au) [28].

Now, assuming that the two electrons which will be ejected after the collision have the coordinates $\vec{r}_1$ and $\vec{r}_2$, it is easy to show that (after integration over $\vec{r}_3, \ldots, \vec{r}_{10}$):

$$\left\langle \Psi_f^j \left(\vec{r}_3, \ldots, \vec{r}_{10}\right) \right| - \frac{10}{r_0} + \sum_{i=1}^{i=10} \frac{1}{r_{0i}} \left| \Psi_i \left(\vec{r}_3, \ldots, \vec{r}_{10}\right) \right\rangle = -\frac{2}{r_0} + \frac{1}{r_{01}} + \frac{1}{r_{02}} + \sum_{m=1}^{m=8} \exp\left(-a_m r_0\right) \times \left[\frac{A_m}{r_0} + B_m + C_m r_0 + D_m {r_0}^2 + E_m r_0^3 \right], \tag{7}$$

where $A_m B_m$, $C_m D_m$, E_m and a_m are obtained from the Roothaan-Hartree-Fock wave function of Clementi and Roetti ($E_m = 0$) or from the correlated wave function calculated by superposition of configurations ($E_m \neq 0$).

The small contribution due to the term $\sum_{m=1}^{m=8} \exp(-a_m r_0) \left[\frac{A_m}{r_0} + B_m + C_m r_0 + D_m {r_0}^2 + E_m r_0^3 \right]$ is usually neglected. Finally, we are able to reduce the N-electron-target problem to a problem of two active electrons (these two electrons being ejected after the collision) [29,30] and we obtain:

$$f_{B1}^j = -\frac{2}{K^2} \left\langle \Psi_f \left(\vec{k}_1, \vec{k}_2; \vec{r}_1, \vec{r}_2\right) \right| - 2 + e^{i\vec{K}.\vec{r}_1} + e^{i\vec{K}.\vec{r}_2} \left| \Psi_i^j \left(\vec{r}_1, \vec{r}_2\right) \right\rangle, \tag{8}$$

Table 1.

j	States	M_L	M_S	$\Psi_i^j(\vec{r}_1,\vec{r}_2)$
1	^{3}P	1	1	$\lvert 2p_1 2p_0\rvert$
2	^{3}P	1	−1	$\lvert 2\bar{p}_1 2\bar{p}_0\rvert$
3	^{3}P	0	1	$\lvert 2p_1 2p_{-1}\rvert$
4	^{3}P	0	−1	$\lvert 2\bar{p}_1 2\bar{p}_{-1}\rvert$
5	^{3}P	−1	1	$\lvert 2p_{-1} 2p_0\rvert$
6	^{3}P	−1	−1	$\lvert 2\bar{p}_{-1} 2\bar{p}_0\rvert$
7	^{3}P	1	0	$\frac{1}{\sqrt{2}}(\lvert 2p_1 2\bar{p}_0\rvert + \lvert 2\bar{p}_1 2p_0\rvert)$
8	^{3}P	0	0	$\frac{1}{\sqrt{2}}(\lvert 2p_1 2\bar{p}_{-1}\rvert + \lvert 2\bar{p}_1 2p_{-1}\rvert)$
9	^{3}P	−1	0	$\frac{1}{\sqrt{2}}(\lvert 2p_{-1} 2\bar{p}_0\rvert + \lvert 2\bar{p}_{-1} 2p_0\rvert)$
10	^{1}D	2	0	$\lvert 2p_1 2\bar{p}_1\rvert$
11	^{1}D	−2	0	$\lvert 2p_{-1} 2\bar{p}_{-1}\rvert$
12	^{1}D	1	0	$\frac{1}{\sqrt{2}}(\lvert 2p_1 2\bar{p}_0\rvert - \lvert 2\bar{p}_1 2p_0\rvert)$
13	^{1}D	−1	0	$\frac{1}{\sqrt{2}}(\lvert 2p_0 2\bar{p}_{-1}\rvert - \lvert 2\bar{p}_0 2p_{-1}\rvert)$
14	^{1}D	0	0	$\frac{1}{\sqrt{6}}(\lvert 2p_1 2\bar{p}_{-1}\rvert - \lvert 2\bar{p}_1 2p_{-1}\rvert + 2\lvert 2p_0 2\bar{p}_0\rvert)$
15	^{1}S	0	0	$\frac{1}{\sqrt{3}}(-\lvert 2p_1 2\bar{p}_{-1}\rvert + \lvert 2\bar{p}_1 2p_{-1}\rvert + \lvert 2p_0 2\bar{p}_0\rvert)$

Table 2.

m	States	M_L	M_S	$\Psi_{i,sp}^m(\vec{r}_1,\vec{r}_2)$
1	^{3}P	0	1	$\lvert 2s 2p_0\rvert$
2	^{3}P	0	−1	$\lvert 2\bar{s} 2\bar{p}_0\rvert$
3	^{3}P	1	1	$\lvert 2s 2p_1\rvert$
4	^{3}P	1	−1	$\lvert 2\bar{s} 2\bar{p}_1\rvert$
5	^{3}P	−1	1	$\lvert 2s 2p_{-1}\rvert$
6	^{3}P	−1	−1	$\lvert 2\bar{s} 2\bar{p}_{-1}\rvert$
7	^{3}P	0	0	$\frac{1}{\sqrt{2}}(\lvert 2s 2\bar{p}_0\rvert + \lvert 2\bar{s} 2p_0\rvert)$
8	^{3}P	1	0	$\frac{1}{\sqrt{2}}(\lvert 2s 2\bar{p}_1\rvert + \lvert 2\bar{s} 2p_1\rvert)$
9	^{3}P	−1	0	$\frac{1}{\sqrt{2}}(\lvert 2s 2\bar{p}_{-1}\rvert + \lvert 2\bar{s} 2p_{-1}\rvert)$

where $\Psi_i^j(\vec{r}_1,\vec{r}_2)$ represents a Slater determinant which is an eigenfunction for the operators L^2 and S^2. The eigenfunctions are shown in Table 1.

Then, if we consider a possible contribution of the ion state $Ne^{++}(2s^1 2p^5)(^3P)$ whose threshold is 87.8 eV [1], the FDCS may be written as:

$$\frac{d^5\sigma_{sp}}{d\Omega_s d\Omega_1 d\Omega_2 dE_1 dE_2} = \frac{k_s k_1 k_2}{k_i} \sum_{m=1}^{m=9} \left|f_{B1}^m\right|^2, \qquad (9)$$

where f_{B1}^m denotes the amplitude of the first Born term and the summation over the index m means that we consider in LS coupling the 9 possible ion final states corresponding to a part of the 12 possibilities of leaving two electrons in the $2s^2 2p^6$ shells of the neon atom (nine of them for the ion state $Ne^{++}(2s^1 2p^5)(^3P)$ and the three other for the ion state $Ne^{++}(2s^1 2p^5)(^1P)$) which is neglected here because the corresponding threshold is too high. By using the Bethe relation, the frozen-core approximation and reducing the N-electron-target problem to a problem of two active electrons we obtain:

$$f_{B1}^m = -\frac{2}{K^2}\left\langle \Psi_f\left(\vec{k}_1,\vec{k}_2;\vec{r}_1,\vec{r}_2\right)\right| - 2 + e^{i\vec{K}.\vec{r}_1} + e^{i\vec{K}.\vec{r}_2}\left|\Psi_{i,sp}^m\left(\vec{r}_1,\vec{r}_2\right)\right\rangle, \qquad (10)$$

where $\Psi_{i,sp}^m(\vec{r}_1,\vec{r}_2)$ represents a Slater determinant which is an eigenfunction for the operators L^2 and S^2. The eigenfunctions are shown in Table 2.

The wave function for the final state is the well-known 3C which satisfies the Coulomb boundary conditions exactly in the asymptotic region for two ejected electrons

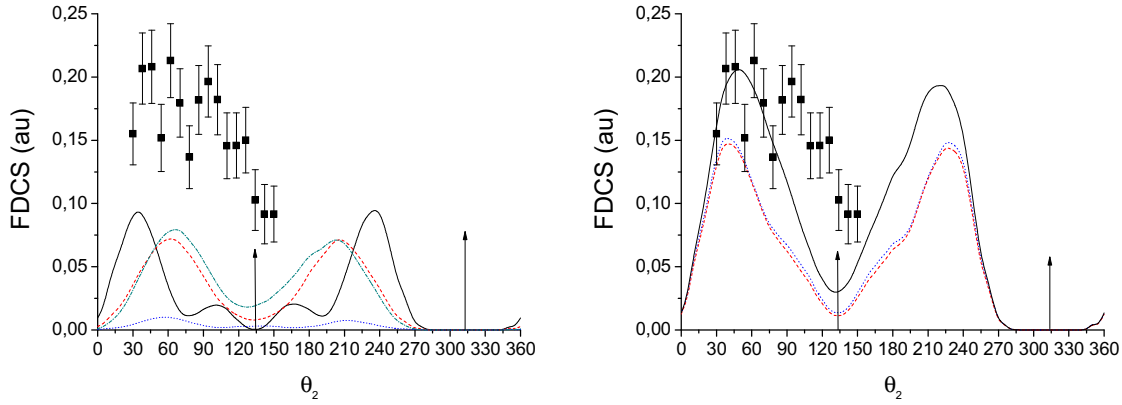

Fig. 1. (a) Five differential cross section (FDCS) for the double ionization of neon by 5582.6 eV electron impact. Electron energies are 5500 eV and 10 eV, respectively, for scattered and ejected electrons. The scattering angle is $\theta_s = 0.45°$. The first ejected electron is detected along the momentum-transfer direction ($\theta_1 = 314°$), while the second is detected at variable angles. The results of the 3C model for the ^{3}P ion state are represented by a full line, those for the ^{1}D ion state by a dashed line, those for the ^{1}S ion state by a dotted line and those for the ion state $Ne^{++}(2s^1 2p^5)^3$P by a dash-dotted line. The experiments of Schröter et al. [1] are represented by squares. The arrows indicate the direction of the momentum transfer ($\pm\vec{K}$). (b) Same as (a) but the results of the 3C model (with the correlated initial-state wave function) for all the contributions of the ion states are represented by a full line, those for $^3\mathrm{P} + {}^1\mathrm{D} + {}^1\mathrm{S}$ ion states (with the correlated initial-state wave function) by a dashed line, those for the $^3\mathrm{P} + {}^1\mathrm{D} + {}^1\mathrm{S}$ ion states (with the Roothan-Hartree-Fock initial-state wave function) by a dotted line.

in the field of a nucleus of charge Z [31,32]:

$$\Psi_f\left(\vec{k}_1,\vec{k}_2;\vec{r}_1,\vec{r}_2\right) = \frac{1}{\sqrt{2}}\left[\varphi\left(\vec{k}_1,\vec{r}_1\right)\varphi\left(\vec{k}_2,\vec{r}_2\right) \pm\varphi\left(\vec{k}_1,\vec{r}_2\right)\varphi\left(\vec{k}_2,\vec{r}_1\right)\right] \times C\left(\alpha_{12},\vec{k}_{12},\vec{r}_{12}\right), \quad (11)$$

where the coulomb wave is given by:

$$\varphi\left(\vec{k},\vec{r}\right) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{r}} C\left(\alpha,\vec{k},\vec{r}\right), \quad (12)$$

and the distorting factor by:

$$C\left(\alpha,\vec{k},\vec{r}\right) = e^{-\pi\alpha/2}\Gamma\left(1-i\alpha\right){}_1F_1 \times\left(i\alpha,1,-i\left(\vec{k}\cdot\vec{r}+kr\right)\right), \quad (13)$$

with $\alpha_i = -\frac{Z}{k_i}$, $\alpha_{12} = \frac{1}{2k_{12}}$, $\vec{k}_{12} = \frac{\vec{k}_1-\vec{k}_2}{2}$ and $Z = 2$.

The sign + corresponds to a final state wave function which is symmetrical for the space part (for ^{1}D and ^{1}S) and the sign – for the other case (^{3}P). We use the double Fourier transform scheme [33] which allows us to reduce a six-dimensional integral to a three-dimensional one. We have checked our results with those given by the method developed by Joulakian et al. [5] and Brauner et al. [32] which reduces the six-dimensional integral to a two-dimensional one but needs many derivates [34].

3 Results and discussion

We study the double ionization of neon for high incident energy (5582.6 eV), low scattering angle (0.45°) and slow ejected electrons (10 eV). We compare our present theoretical results with the relative experimental data of Schröter et al. [1].

We select some typical situations:

- One electron is ejected along the direction of the momentum transfer (it corresponds here to 314° and 134°). This is an important case because if the symmetry around the momentum transfer is destroyed [27] it usually means that the second Born approximation [3] must be taken into account.
- One electron is ejected either 110°, or 150° or 330°. These particular choices allow us to see what happens when one electron is detected between 0° and the direction of $-\vec{K}$, between $-\vec{K}$ and $+\vec{K}$ and finally between $+\vec{K}$ and 360°. In these situations, the direction of the momentum transfer generally plays no important role.

In Figure 1, we study the situation where one electron is ejected along the momentum-transfer direction. The experimental data present three maxima: a first one around $\theta_1 = 45°$, a second one around $\theta_1 = 62°$ and a third one around $\theta_1 = 95°$. Figure 1a shows the contribution of each residual state (^{3}P, ^{1}D or ^{1}S). The maximum around $\theta_1 = 95°$ is not reproduced by the theory. The first maximum ($\theta_1 = 45°$) is partially reproduced by our model including the contribution of the ^{3}P residual state. A better agreement is found when our model includes the sum over the contributions of the three final ion states. The second maximum ($\theta_1 = 62°$) is reproduced by our model if we include the contribution of the ^{1}D ion state or those of the ^{1}S ion state. Now, if we consider the contribution of the $2s^1 2p^5 {}^3$P ion state there is no improvement except for the minimum at 134°. This contribution increases

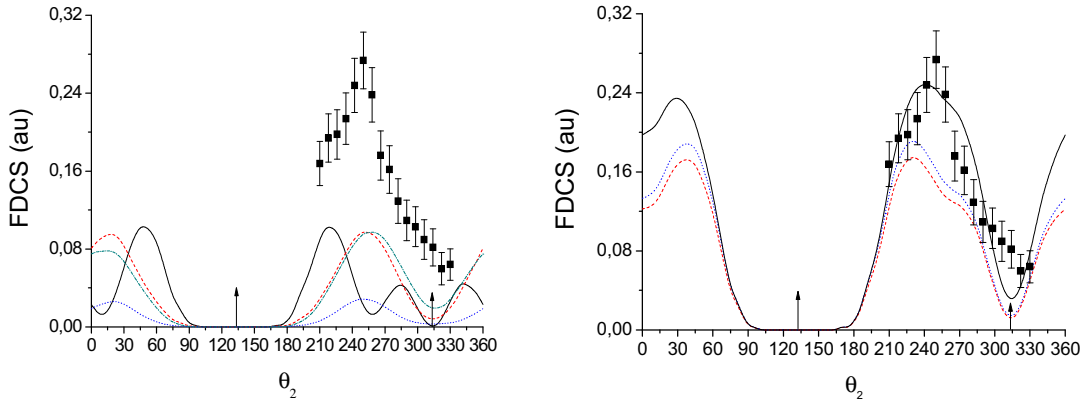

Fig. 2. (a) Same as Figure 1a but the first ejected electron is detected along the opposite momentum-transfer direction ($\theta_1 = 134°$). (b) Same as Figure 1b but the first ejected electron is detected along the opposite momentum-transfer direction ($\theta_1 = 134°$).

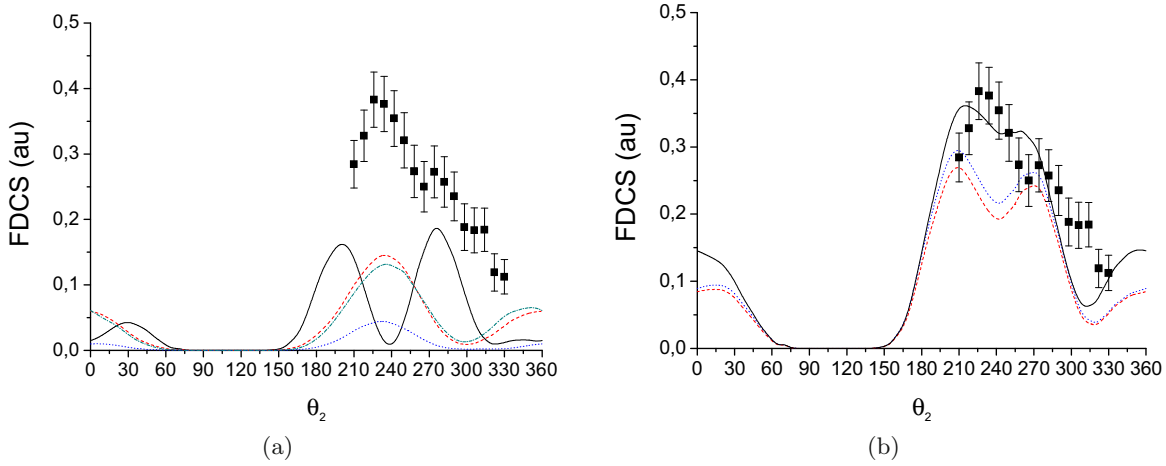

Fig. 3. (a) Same as Figure 1a but the first ejected electron is detected at $\theta_1 = 110°$. (b) Same as Figure 1b but the first ejected electron is detected at $\theta_1 = 110°$.

the amplitude of this minimum which better corresponds to the experimental data (Fig. 1b). We notice that our theoretical results are not symmetric around the momentum transfer. It is an expected result since the energy necessary to ionize two times the neon atom is different. The momentum transfer has a different direction for each final ion state. Figure 1b shows that the results given by the correlated initial-state wave function are close to those given by the Roothan-Hartree-Fock wave function.

Figures 2a and 2b display the FDCS's when one electron is ejected along the opposite momentum-transfer: $\theta_1 = 134°$. The experiments exhibit a maximum at $\theta_1 = 250°$. The FDCS for a ^{3}P ion state presents four maxima: $\theta_1 = 45°$, $\theta_1 = 220°$, $\theta_1 = 285°$ and $\theta_1 = 340°$. The FDCS for a ^{1}D or for a ^{1}S ion state exhibits two maxima around 60° and 250°. The FDCS which corresponds to the contribution of the $(2s^1 2p^5)^3$P ion state gives two maxima at 15° and 260° (Fig. 2a). Here it is necessary to consider the sum of these contributions: the theoretical results obtained by summing the four contributions of the final ion states give now a peak close to those observed in the experiments: $\theta_1 = 242°$ (Fig. 2b). Schröter et al. [1] write that the accuracy of the measurements of the angle is 8° and we can consider that the agreement between experiment and theory is relatively good. We notice that the contribution of the $(2s^1 2p^5)^3$P ion state is here necessary to get a relative good agreement. The contribution due to the correlation in the initial state is yet weak (Fig. 2b).

Figures 3a and 3b present a comparison between experiments and theory for $\theta_1 = 110°$. We notice a first maximum around $\theta_1 = 226°$ and a second one around 274°. In Figure 3a the contribution of the final ion state ^{3}P shows two maxima: one close to 200° and another around 275°. The other contributions (^{1}D and ^{1}S ion states) exhibit a maximum at 235°. The contribution of the $(2s^1 2p^5)^3$P ion state must be added (Fig. 3b) and finally the agreement

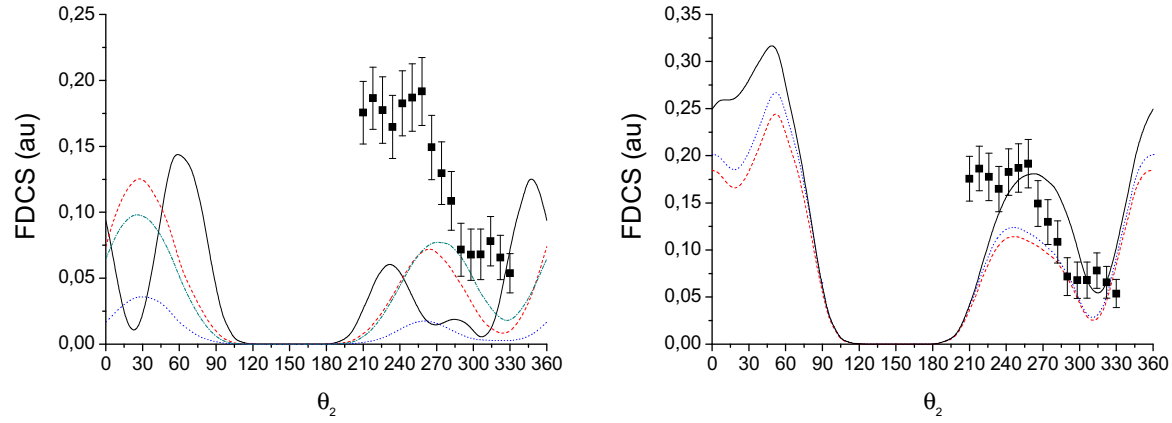

Fig. 4. (a) Same as Figure 1a but the first ejected electron is detected at $\theta_1 = 150°$. (b) Same as Figure 1b but the first ejected electron is detected at $\theta_1 = 150°$.

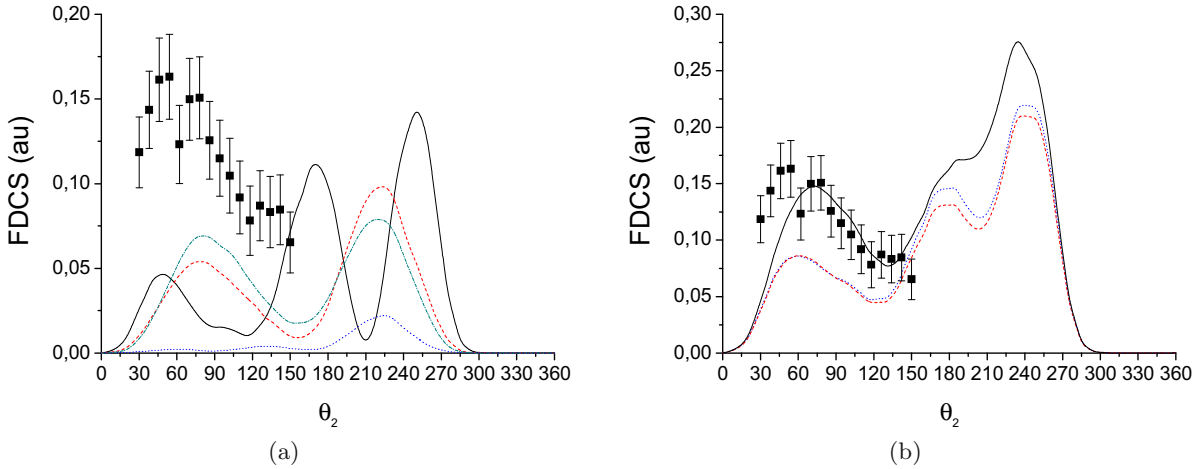

Fig. 5. (a) Same as Figure 1a but the first ejected electron is detected at $\theta_1 = 330°$. (b) Same as Figure 1b but the first ejected electron is detected at $\theta_1 = 330°$.

between theory and experiment is relatively good. We notice a new time that the contribution due to the correlation in the initial state is weak.

Figures 4a and 4b show a comparison between experiments and theory for $\theta_1 = 150°$. We notice two maxima at $\theta_1 = 218°$ and $\theta_1 = 258°$. In Figure 4a the contribution of the final ion state ^{3}P presents three maxima: $\theta_1 = 60°$, $\theta_1 = 230°$ and $\theta_1 = 345°$. The other contributions (^{1}D and ^{1}S) exhibit two maxima at 27° and 262°. The contribution of the $2s^12p^{5\,3}$P ion state gives two maxima close to those found previously ($\theta_1 = 25°$ and $\theta_1 = 270°$). The theory is not able to reproduce the first maximum at $\theta_1 = 218°$ but gives a moderate agreement for the other experimental data: the second maximum at $\theta_1 = 258°$ is well reproduced when we take into account for all the contributions of the ion states (Fig. 4b).

Figures 5a and 5b are drawn for $\theta_1 = 330°$. The experimental data present three maxima: at $\theta_1 = 54°$, $\theta_1 = 76°$ and $\theta_1 = 126°$. In Figure 5a the contribution of the final ion state ^{3}P presents three maxima too: $\theta_1 = 50°$, $\theta_1 = 170°$ and $\theta_1 = 250°$. The FDCS with the contribution of the ^{1}D ion final state has two maxima at 75° and 225°. For the ^{1}S ion state we notice three other maxima: two weak maxima at 60° and 135° and a stronger maximum at 225°. The contribution of the $2s^12p^{5\,3}$P ion state gives two maxima close to those found previously ($\theta_1 = 80°$ and $\theta_1 = 220°$). The theory is here able to reproduce the main part of the experimental data (Fig. 5b).

4 Conclusion

We have calculated FDCS's for electron-impact double ionization of neon for high incident energy and low ejection energies. In this calculation, we have used the first Born approximation and correlated wave functions for the initial and final states of the target. The initial state is described by a correlated wave function calculated by superposition of configurations. For the final state (the two ejected electrons in the field of the ion) we have adopted

the 3C model. We have also studied the contributions from the $^3P^1D$ and ^1S states of the residual ions separately. As suggested in [1], we include the contribution of the ion state $Ne^{++}(2s^12p^5)^3P$. We point out that the correlation in the initial state plays no important role here. This result was previously found by Dal Cappello et al. [26] by using an approximation of the 3C model. Nevertheless, we notice that a different result for the double ionization of argon and krypton was found [26]. We show that all the contributions of the ion states are often necessary to explain the general behaviour of experiments. Some disagreements between experiment and theory remain. We think that our correlated wave function could be improved and that the two ejected electrons could be described by distorted waves instead of coulomb waves in a 3C model.

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References

1. C. Schröter, B. El Marji, A. Lahmam-Bennani, A. Duguet, M. Lecas, L. Spielberger, J. Phys. B **31**, 131 (1998)
2. S. Jones, D.H. Madison, Phys. Rev. Lett. **91**, 073201 (2003)
3. M. Grin, C. Dal Cappello, R. El Mkhanter, J. Rasch, J. Phys. B **33**, 131 (2000)
4. A.S. Kheifets, Phys. Rev. A **69**, 032712 (2004)
5. B. Joulakian, C. Dal Cappello, M. Brauner, J. Phys. B **25**, 2863 (1992)
6. B. Joulakian, C. Dal Cappello, Phys. Rev. A **47**, 3788 (1993)
7. J. Berakdar, H. Klar, J. Phys. B **26**, 4219 (1993)
8. A. Kheifets, I. Bray, A. Lahmam-Bennani, A. Duguet, I. Taouil, J. Phys. B **32**, 5047 (1999)
9. A. Kheifets, I. Bray, J. Berakdar, C. Dal Cappello, J. Phys. B **35**, L15 (2002)
10. V.Serov, V. Derbov, B. Joulakian, S. Vinitsky, Phys. Rev. A **75**, 012715 (2007)
11. M.J. Ambrosio, F.D. Colavecchia, G. Gasaneo, D.M. Mitnik, L.U. Ancarani, J. Phys. B **48**, 055204 (2015)
12. G. Gasaneo, L.U. Ancarani, D.M. Mitnik, J.M. Randazzo, A.L. Frapiccini, F.D. Colavecchia, Adv. Quantum Chem. **67**, 153 (2013)
13. L.U. Ancarani, T. Montagnese, C. Dal Cappello, Phys. Rev. A **70** 012701 (2003)
14. L.U. Ancarani, C. Dal Cappello, J. Electron Spectrosc. Relat. Phenom. **161** 22 (2007)
15. A.S. Kheifets, I. Bray, Phys. Rev. A **69**, 050701 (R) (2004)
16. J. Berakdar, Phys. Rev. Lett. **85**, 4036 (2000)
17. S.A. Zaytsev, V.A. Knyr, Yu.V. Popov, Phys. At. Nucl. **70**, 676 (2007)
18. A.W. Malcherek, J.S. Briggs, J. Phys. B **30**, 4419 (1997)
19. J.R. Götz, M. Walter, J.S. Briggs, J. Phys. B **36**, L77 (2003)
20. C. Dal Cappello, H. Hda, A.C. Roy, Phys. Rev. A **51**, 3735 (1995)
21. C. Dal Cappello, B. Joulakian, J. Langlois, J. Phys. **3**, 125 (1993)
22. I. Kada, A. Mansouri, C. Dal Cappello, P.A. Hervieux, A.C. Roy, J. Phys. B **42**, 025201 (2009)
23. A. Lahmam-Bennani, I. Taouil, A. Duguet, M. Lecas, L. Avaldi, J. Berakdar, Phys. Rev. A **59**, 3548 (1999).
24. I. Taouil, A. Lahmam-Bennani, A. Duguet, M. Lecas, L. Avaldi, Phys. Rev. Lett. **81**, 4600 (1998)
25. R. El Mkhanter, C. Dal Cappello, A. Lahmam-Bennani, Y. Popov, J. Phys. B **29**, 1101 (1996)
26. E. Clementi, C. Roetti, At. Data Nucl. Data Tables **14**, 177 (1974)
27. C. Dal Cappello, J. Langlois, M.C. Dal Cappello, B. Joulakian, A. Lahmam-Bennani, A. Duguet, R. Tweed, Z. Phys. D **23**, 389 (1992)
28. E.R. Davidson, S.A. Hagstrom, J.S. Chakravorty, Phys. Rev. A **44**, 7071 (1991)
29. H. Hda, C. Dal Cappello, J. Langlois, Z. Phys. D **29**, 25 (1994)
30. J.W. Cooper, R.W. van Boeyen, J. Phys. B **37**, L77 (2004)
31. M. Brauner, H. Klar, J.S. Briggs, Z. Phys. D **11**, 257 (1989)
32. M. Brauner, H. Klar, J.S. Briggs, J. Phys. B **22**, 2265 (1989)
33. M.A. Kornberg, J.E. Miraglia, Phys. Rev. A **48** 3714 (1989)
34. C. Dal Cappello, F. Menas, S. Houamer, Yu.V. Popov, A.C. Roy, J. Phys. B **48**, 205201 (2015)