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Double Ionization of Molecular Hydrogen by Fast Electron Impact

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Abstract. We propose a theoretical model of the double ionization of homonuclear diatomic targets by fast electron impact. By application of two-effective-center continuum waves to describe the ejected electrons in the exit channel and by use of Nordsieck-type integrals, an expression has been obtained by an analytical treatment for the five-fold differential cross section, the relevant quantity to describe the kinematically complete collisions in the coplanar geometry. The correlate motion of the ejected electrons is taken into account by means of adequate Sommerfeld parameters.

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Key words: Hydrogen, collision, ionization, analytical method.

1 Introduction

Ionization of atoms and molecules by electron impact is one of the fundamental processes of atomic physics, whose comprehension becomes important in many domains such as plasma physics and nuclear fusion devices [1]. In particular, the study of kinematically complete double ionization experiments by electron impact provides a straightforward and powerful tool to understand the role of the electron-correlation effects as well as the projectile-target interaction during the collision process.

The first theoretical studies of double ionization of atoms by electron impact by Byron and Joachain [2], Smirnov *et al.* [3] and Neudatchin *et al.* [4] appealed for experiments, which were carried out several years later by Lahmam-Bennani *et al.* [5, 6]. However, the development of kinematically complete double ionization experiments by electron impact rapidly turned out to be very challenging. On the one hand, the need for using triple-coincidence techniques, to detect energies and angles of the electrons produced

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by the reaction, is a serious experimental limitation. On the other hand, an additional complication for measurements arises from the low intensity of the double ionization cross section.

Nevertheless, the technical advances achieved in the area of high sensitivity detection and the emergence over the last few years of a new generation of sophisticated spectrometers [7–9] have renewed the interest for the experimental study of double ionization by electron impact [10].

From the theoretical point view, only few models have been proposed to describe kinematically complete double ionization on atomic targets [11, 12]. In the case of diatomic targets, the description of the continuum electrons in the field of two Coulomb or distorted centers is much more difficult. The use of the solutions of the two-center Schrödinger equation in prolate spheroidal coordinates to determine the multiply differential cross section results with such computational difficulties that their direct application turns out rapidly to a purely numerical problem relevant to the computer science field.

In the present study, we propose a theoretical model of the double ionization of homonuclear diatomic molecules by fast electron impact. A two-effective-center approach (TEC), which has shown to successfully reproduce experiments on molecular hydrogen targets [13, 14], is applied to describe the ejected electrons in the exit channel. By use of Nordsieck-type integrals [15] and dynamic Sommerfeld parameters [16], an expression has been obtained by an analytical approach for the fivefold differential cross section (5DCS), which is the relevant quantity to describe the kinematically complete collisions in the coplanar geometry. As an illustration of our theoretical treatment, we present 5DCS results for the double ionization of H_2 at an incident energy of 1099 eV and under symmetric kinematics for the two ejected electrons, which have an identical energy of 10 eV. For the sake of comparison with the (e,3e) experimental results for helium reported in Ref. [10], both the so-called *fixed ejected angle* and *symmetric geometry* modes are investigated in this work.

Atomic units are used throughout unless otherwise stated.

2 Theory

Let us consider the dissociative double ionization reaction of the hydrogen molecule in its electronic ground state by electron impact, i.e.,

$$e^- + H_2(^1\Sigma_g^+) \rightarrow 3e^- + H^+ + H^+. \tag{2.1}$$

The collision is described in the laboratory system, whose origin coincides with the center of mass of the molecular hydrogen target, and the longitudinal z-axis is chosen parallel to the direction of the wave vector $\mathbf{k}_i$ of the incident electron. In the case of fast electron impact collisions where the TEC approximation is valid (typically of the order of several

keV), the collision time is much smaller than the periods of the nuclear motions. In addition, the experiments of coincidence spectroscopy which have been performed so far are characterized by a low-energy resolution. Consequently, the ionization process can be considered, to a good approximation, as a pure electronic transition occurring at fixed equilibrium internuclear distance, $\boldsymbol{\rho}_0$, of the $X\ ^1\Sigma_g^+$ electronic state of H_2 [17].

Though recent ionization experiments carried out on diatomic targets have shown to successfully discriminate the initial orientation of the molecular target [18], the use of the cold target recoil ion momentum spectroscopy techniques (COLTRIMS) in the present full collision is for the moment unrealistic. Indeed, a quadruple coincidence would be required to record only those events where three electrons and one proton would be detected. As a consequence, we consider that the distribution of the directions of the internuclear vector $\boldsymbol{\rho}$ is isotropic and an average over all possible orientations is performed. The fivefold differential cross section, which describe the kinematically complete collisions in the coplanar geometry, is then given by the expression

$$\sigma^{(5)} = \frac{d^5\sigma}{d\Omega_s d\Omega_1 d\Omega_2 d(k_1^2/2) d(k_2^2/2)} \tag{2.2a}$$

$$\cong \frac{1}{4\pi}(2\pi)^4 \frac{k_s k_1 k_2}{k_i} \int d\Omega_\rho \left| t_{fi}^e(\boldsymbol{\rho}_0) \right|^2, \tag{2.2b}$$

where Ω_ρ, Ω_s, Ω_1 and Ω_2 denote, respectively, the solid angles corresponding to the internuclear axis $\boldsymbol{\rho}$, $\mathbf{k}_s$, $\mathbf{k}_1$ and $\mathbf{k}_2$, the last three being the wave vectors of the scattered electron and both emitted electrons labeled by 1 and 2, respectively. In Eq. (2.2b), the electronic transition matrix element, in a first order of the Born series, reads

$$t_{fi}^e(\boldsymbol{\rho}_0) = < \Psi_f^- | V_i | \Psi_i >, \tag{2.3}$$

where Ψ_f^- and Ψ_i represent the electronic wave functions of the whole system in its final and initial states, respectively. Recent studies of the double ionization process by electron impact show that the first Born approximation is valid for electrons with high translational energies [19, 20]. The interaction potential between the impinging electron and the target in the entrance channel is then given by

$$V_i = -\frac{1}{R_a} - \frac{1}{R_b} + \frac{1}{r_{1p}} + \frac{1}{r_{2p}}, \tag{2.4}$$

with the different position vectors defined in Fig. 1.

The initial wave function is expressed as a product of a plane wave describing the fast incident electron by a non-perturbed wave function representing the ground state of the molecular target, i.e.,

$$\Psi_i = \frac{e^{i\mathbf{k}_i.\mathbf{R}}}{(2\pi)^{\frac{3}{2}}} \Phi_i(r_1, r_2, \rho), \tag{2.5}$$

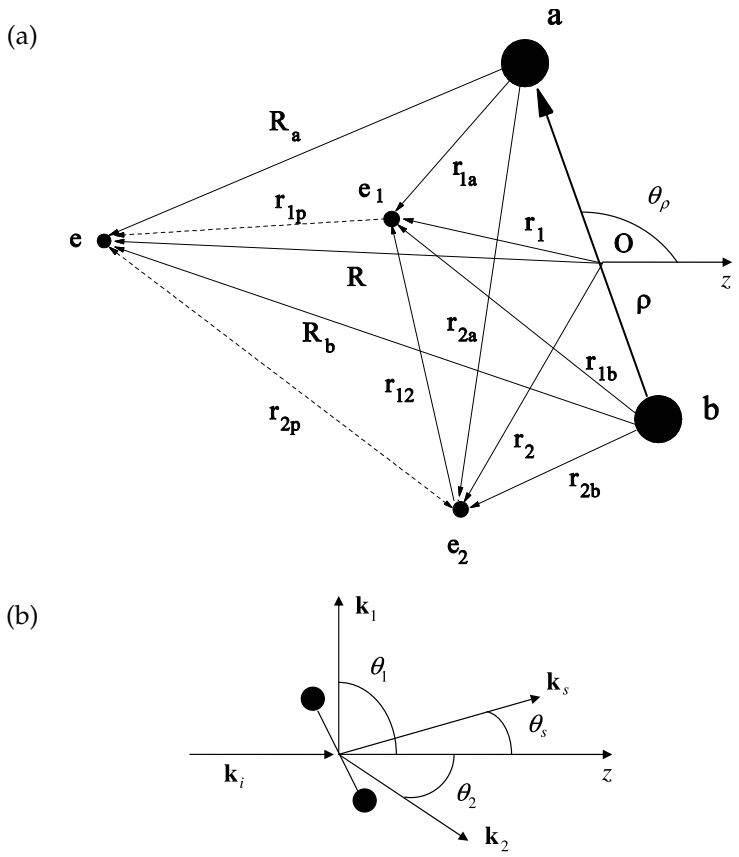

Figure 1: (a) The different position vectors of the incident and bound electrons with respect to the two nuclei a and b. (b) Schematic diagram for the (e,3e) collision.

where Φ_i is the variational Heitler-London type wave function given by Wang [21]

$$\Phi_i = \frac{\alpha^3}{\pi\sqrt{2(1+S^2)}}\left(e^{-\alpha r_{1a}}e^{-\alpha r_{2b}}+e^{-\alpha r_{1b}}e^{-\alpha r_{2a}}\right), \tag{2.6}$$

with $\alpha=1.166$ for the equilibrium distance $\rho_0=1.406$. S denotes the usual overlap integral between the atomic orbitals [22].

As a first approximation, the final state wave function of the system can be expressed as the product of a plane wave representing the fast scattered electron, as in preceding calculations on atomic targets [23], times a BBK-type wave function [24], i.e.,

$$\Psi_f^- = \frac{e^{i(\mathbf{k}_s.\mathbf{R})}}{(2\pi)^{3/2}}\frac{1}{\sqrt{2}}\left[\frac{e^{i(\mathbf{k}_1.\mathbf{r}_1+\mathbf{k}_2.\mathbf{r}_2)}}{(2\pi)^3}\chi(\mathbf{r}_1,\mathbf{k}_1,\beta_1)\chi(\mathbf{r}_2,\mathbf{k}_2,\beta_2)\chi(\mathbf{r}_{12},\mathbf{k}_{12},\beta_{12})+\chi_{\rm xc}\right], \tag{2.7}$$

where $\chi_{\rm xc}$ denotes the wave function obtained by exchanging electrons 1 and 2 (the exchange with the scattered electron is neglected), β_1, β_2 and β_{12} are the Sommerfeld pa-

rameters, $\mathbf{k}_{12}=(\mathbf{k}_1-\mathbf{k}_2)/2$ and the Coulomb distortion factors χ are given by

$$\chi(\mathbf{r},\mathbf{k},\beta)=e^{-\frac{\pi\beta}{2}}\Gamma(1-i\beta)_1F_1[i\beta,1;-i(kr+\mathbf{k}.\mathbf{r})]. \tag{2.8}$$

In Eq. (2.7), the correlate motion of both ejected electrons is taken into account by the introduction of the new Sommerfeld parameters for any geometry case given by Zhang [16]

$$\beta_1=-\frac{Z-[2k_{12}k_1^2/(k_1+k_2)^3][\frac{1}{4}(3+\cos^2[4\xi(k_2)])]^2}{k_1}, \tag{2.9a}$$

$$\beta_2=-\frac{Z-[2k_{12}k_2^2/(k_1+k_2)^3][\frac{1}{4}(3+\cos^2[4\xi(k_1)])]^2}{k_2}, \tag{2.9b}$$

$$\beta_{12}=\frac{1-[4k_{12}^2/(k_1+k_2)^3][\frac{k_1}{4}(3+\cos^2[4\xi(k_2)])+\frac{k_2}{4}(3+\cos^2[4\xi(k_1)])]^2}{2k_{12}}, \tag{2.9c}$$

with

$$\xi(k)=\arccos\left\{\frac{k}{\sqrt{k_1^2+k_2^2}}\right\}. \tag{2.10}$$

The charge of the dissociating target is chosen to satisfy the correct boundary condition, i.e., $Z=2$ in Eqs. (2.9a) and (2.9b).

However, since the BBK treatment has not yet found a suitable closed form for molecular targets, the Coulomb factor accounting for the interaction between both ejected electrons in Eq. (2.7) is simply approximated by [12]

$$\chi(\mathbf{r}_{12},\mathbf{k}_{12},\beta_{12})\approx e^{-\frac{\pi\beta_{12}}{2}}\Gamma(1-i\beta_{12}). \tag{2.11}$$

In the spirit of the TEC approximation, which rests on the assumption that the ionization mechanism occurs at the vicinity of both nuclei, and using Eq. (2.11), the final wave function can be readily rewritten as

$$\Psi_f^-=\frac{e^{i(\mathbf{k}_s.\mathbf{R})}}{(2\pi)^{3/2}}\frac{1}{\sqrt{2}}\left[\frac{e^{i(\mathbf{k}_1.\mathbf{r}_1+\mathbf{k}_2.\mathbf{r}_2)}}{(2\pi)^3}e^{-\frac{\pi\beta_{12}}{2}}\Gamma(1-i\beta_{12})\chi(\mathbf{r}_{1j},\mathbf{k}_1,\beta_1)\chi(\mathbf{r}_{2k},\mathbf{k}_2,\beta_2)+\chi_{\rm xc}\right], \tag{2.12}$$

with the condition $(j,k\in\{a,b\},\ j\neq k)$, i.e., the two ejected electrons are ionized from different nuclei. The choice of the nuclear center to be used in the calculation of t_{fi}^e is merely dictated by the presence of the terms $\exp(-\alpha r_{la})$ or $\exp(-\alpha r_{lb})$, with $l=1,2$, in the integrands when the wave function given by Eq. (2.6) is chosen. Further details on the TEC approximation are given in [13].

By substitution of Eqs. (2.4), (2.5) and (2.12) in Eq. (2.3) and after some algebra, the 5DCS given by Eq. (2.2b) can be written in the closed form

$$\sigma^{(5)}\cong\mathcal{N}\int d\Omega_\rho\Big|\sum_{i,j=1;i\neq j}^{2}\cos\left[\frac{\boldsymbol{\rho}}{2}.(\mathbf{k}_j-\mathbf{k}_i-\mathbf{K})\right]I(\mathbf{k}_i,\mathbf{k}_i,\beta_i,\alpha)$$
$$\left\{-I(\mathbf{k}_j,\mathbf{k}_j,\beta_j,\alpha)+I(\mathbf{k}_j,\mathbf{k}_j-\mathbf{K},\beta_j,\alpha)\right\}\Big|^2, \tag{2.13}$$

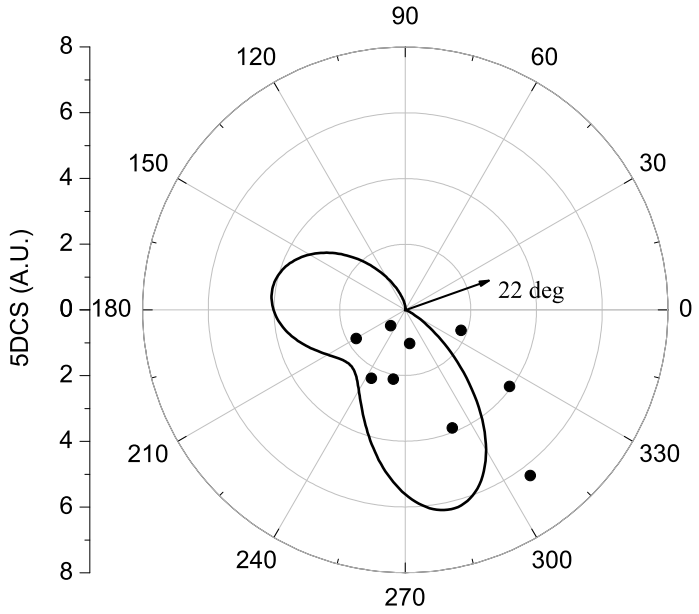

Figure 2: Fivefold differential cross sections (5DCS) for the double ionization in coplanar geometry of molecular hydrogen (solid line: theoretical results) and helium targets (full circles: experimental data). The impact energy is set to $E_i = 1099$ eV, with a the momentum transfer $K = 0.45$ ($\theta_s = 1.1^\circ$), and the two ejected electrons have equal energies $E_1 = E_2 = 10$ eV. In the *fixed ejected angle* mode considered, the ejection angle of the electron labeled 1 is fixed at $\theta_1 = 22.0^\circ$, and the angular distribution of electron 2 is sampled onto the complete plane.

where $\mathbf{K} = \mathbf{k}_i - \mathbf{k}_s$ is the momentum transferred, $\mathcal{N}$ is a constant and I are the simplified Nordsieck-type integrals [15]

$$I(\mathbf{k}_i, \mathbf{k}_j, \beta, \alpha) = \int d\mathbf{r}\, e^{-i\mathbf{k}_j.\mathbf{r}} \times {}_1F_1[-i\beta, 1; i(k_i r + \mathbf{k}_i.\mathbf{r})] e^{-\alpha r}, \tag{2.14}$$

which in our case have a simple analytical expression.

3 Results and discussion

The fivefold differential cross sections (5DCS) calculated using Eq. (2.13) are shown in Figs. 2-5. Since, to our knowledge, no such experiments have been reported yet on diatomic targets, a qualitative comparison is made with recent measurements of cross sections on helium targets [10]. As the correlate motion of the two ejected electrons is taken into account only in an approximate way (cf. Eq. (2.11)), our results are relative. They are arbitrarily chosen to be renormalized to the experimental data on He, made absolute by use of scaling factors to reproduce the theoretical convergent close-coupling calculations of the 5DCS on helium targets [25].

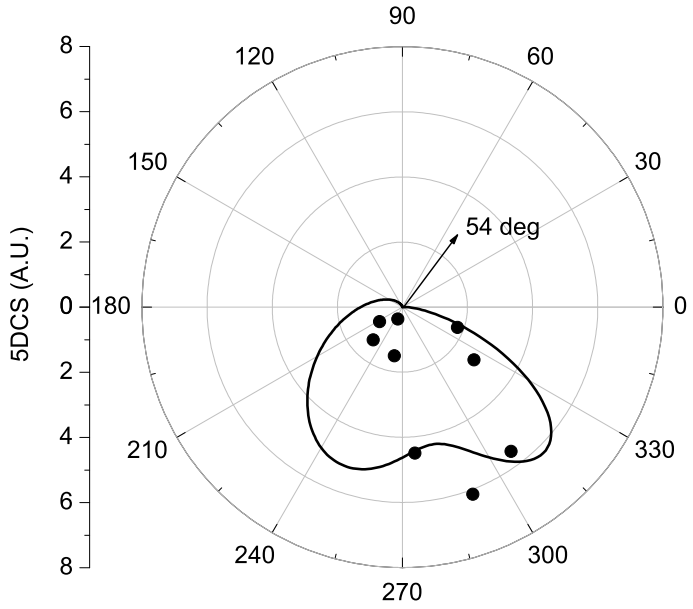

Figure 3: Same as Fig. 2 for a fixed ejected angle value $\theta_s = 54.0^\circ$.

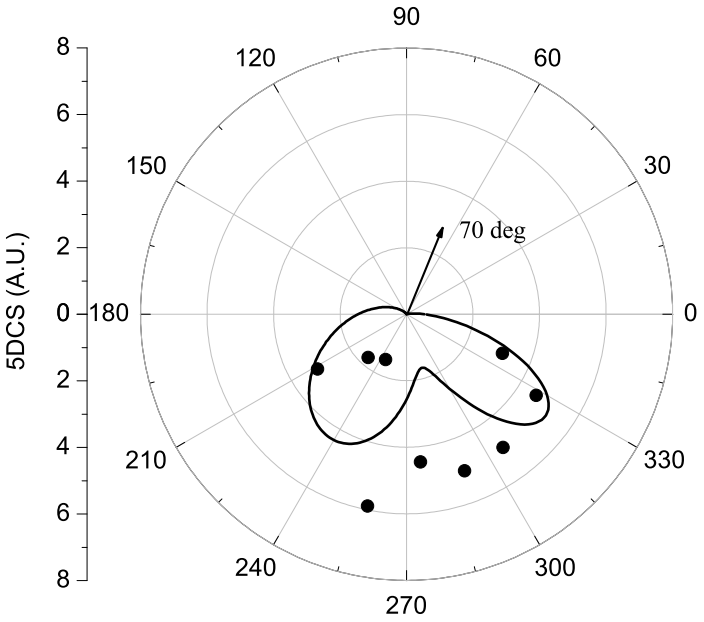

Figure 4: Same as Fig. 2 for a fixed ejected angle value $\theta_s = 70.0^\circ$.

Throughout this study, the same kinematical conditions as in Ref. [10] are used, i.e., the impact energy of the monokinetic electron beam is set to $E_i = 1099$ eV, while the fast scattered electrons are detected with an energy $E_s = 1000$ eV at a fixed angle, $\theta_s = 1.10^\circ$, with respect to the reference direction of the incident beam. The momentum transfer resulting is oriented with an angle $\theta_K = -21.6^\circ$ and has a relatively small value, $K = 0.45$ a.u.

The ejected electrons have both an identical energy of $E_1 = E_2 = 10$ eV and their angular distributions are investigated under both the so-called *fixed ejected angle* and *symmetric geometry* modes. In the first detection mode, the ejection direction of one electron is chosen fixed, while the distribution of the second one is sampled onto the complete plane. In the *symmetric geometry* mode, on the other hand, both ionized electrons emerge symmetrically with respect to the incident beam direction.

3.1 Fixed ejected angle mode

Figs. 2-4 show the calculated and measured 5DCS for molecular hydrogen and helium targets, respectively, at the fixed ejection angle values, $\theta_{\rm fix} = 22.0^\circ$, 54.0° and 70.0°.

In the three situations considered, a general two-lobe structure appears in the angular distribution of the second ejected electron. Parallel emission is forbidden due to the Pauli principle and the Coulomb repulsion between the two electrons. Though the 5DCS corresponding to the collisions on both molecular hydrogen and helium targets exhibit such a feature, a noticeable difference is observed in both cases with respect to the type of minimum between the two lobes. In fact, in the case of helium targets, practically a node separates the lobes while for the double ionization reaction on molecular hydrogen targets, the 5DCS only shows a minimum more or less pronounced. The finite intensity of the deep minimum observed for *back-to-back* emission in the atomic case was attributed to non-dipolar contributions [10]. In the molecular case, the minimum appears shifted with respect to the back-to-back emission.

Moreover, important shifts are to be noted between the ejection angular distributions for the case of helium and hydrogen targets. For instance, in the case of molecular hydrogen, the main lobe in the *forward* half-plane (i.e., for $-90^\circ < \theta < +90^\circ$) is rotated backwards by $\sim 25^\circ$ for $\theta_{\rm fix} = 22.0^\circ$ (Fig. 2) and forward by $\sim 20^\circ$ for $\theta_{\rm fix} = 54.0^\circ$ (Fig. 3) and $\sim 25^\circ$ for $\theta_{\rm fix} = 70.0^\circ$ (Fig. 4). The scarcity of experimental data for the lobe in the *backward* half-plane ($+90^\circ < \theta < +270^\circ$) would make any comparison with our calculations unreliable.

Finally, one can notice the different intensity ratios of the two lobes between experiments on helium and the present theoretical calculations on molecular hydrogen. In particular, the lobes for the case of experiments on helium are much more dissimilar in intensity than for molecular hydrogen. For $\theta_{\rm fix} = 22.0^\circ$, the intensity ratio of the forward half-plane lobe by the backward one is just ~ 1.5 in the case of our calculations, though it reaches ~ 2.5 for experiments on helium. This difference increases substantially for $\theta_{\rm fix} = 54.0^\circ$, where these ratios are ~ 1.2 and ~ 4.0, respectively.

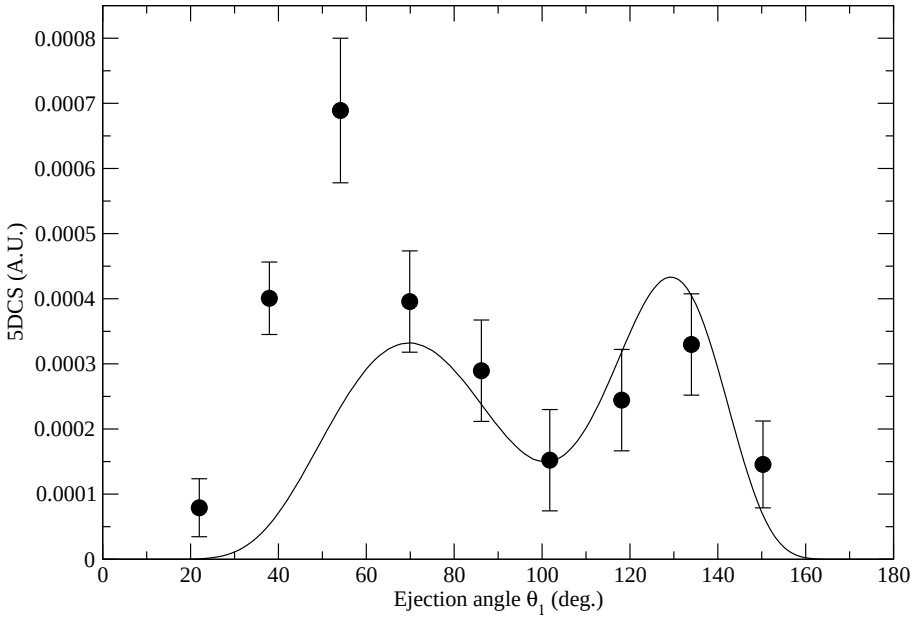

Figure 5: 5DCS for the double ionization in coplanar geometry of molecular hydrogen (solid line: theoretical results) and helium targets (full circles: experimental data), in the *symmetric geometry* mode; both ejected electrons emerge with symmetric angles with respect to the incident beam direction, i.e., $\theta_1 = -\theta_2$.

3.2 Symmetric geometry mode

In Fig. 5, the theoretical 5DCS for molecular hydrogen and the measurements for helium targets are represented for the symmetric geometry mode, where the ionized electrons emerge symmetrically on both sides of the incident electron beam, i.e., $\theta_1 = -\theta_2$. Due to the symmetry of the problem, the ejection angle θ_1 can be arbitrarily chosen to describe the range 0° to 180°, without any loss of generality.

As in the case of the fixed ejected angle mode, both the theoretical and the measured 5DCS show a two lobe structure. The angular distribution calculated for H_2 is reminiscent of the experimental shape obtained for He, specially for the backward half-plane lobe for $+90^\circ < \theta_1 < +180^\circ$, with a maximum at approximately 130°. Nevertheless, for the forward peak in the region $0^\circ < \theta_1 < +90^\circ$, a shift amounting to up to $\sim 20^\circ$ is observed between the maximum of our calculations, at $\theta_1 \sim 70^\circ$, and the experimental one, at $\theta_1 \sim 50^\circ$. Although this may illustrate the different nature of the targets, a possible explanation for this shift may be found in the limitation of our model which rests on the first-order Born series. In fact, in the same way as for single-ionization reactions [26], second-order effects strongly characterize the angular distributions of the ejected electrons in the symmetric geometry. The presence of this shift may also be attributed most likely to the approximation used to describe the Coulomb repulsion of both ejected electrons in the final channel. The intensity ratios of the forward/backward scattering lobes are ~ 0.8 and ~ 2.0 for molecular hydrogen and helium targets, respectively.

4 Conclusions

Theoretical fivefold differential cross sections have been presented for the double ionization of molecular hydrogen by fast electron impact, in the coplanar geometry, with equal energy sharing of the two ejected electrons. The results, obtained by extension of the analytical two-effective-center (TEC) approach for single-ionization reactions, have been compared to experimental data available under the same kinematics on double ionization of helium targets. The two detection modes investigated, i.e., the fixed ejected angle mode and the symmetric geometry mode, have revealed a general two lobe structure for both types of targets, for the angular ranges considered. However, qualitative differences are observed with respect to the intensity ratios of the lobes, the nature of the minimum separating the two peaks and the positions of the maxima. In particular, the important shift between the experimental and theoretical maxima of the forward lobe may be attributed mainly to higher-order effects, which are not taken into account in the present theoretical treatment, and to the approximate description of the Coulomb repulsion between both ejected electrons.

In a forthcoming work we propose to calculate the second-order term of the Born series and to introduce the dynamic correlation between the two slow ionized electrons by means of a more complete BBK-type description, as indicated in Eq. (2.7), which has recently shown to significantly improve the agreement between theory and experiment for the single-ionization reaction of molecular hydrogen by electron impact [27].

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