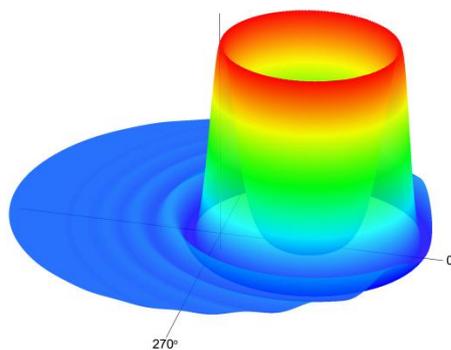


"Babeş-Bolyai" University Cluj-Napoca
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PHD THESIS SUMMARY

INTERFERENCE EFFECTS IN THE IONIZATION OF DIATOMIC MOLECULES



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Keywords

Interference effects

Ionization

Scattering

Diatomic molecule

Differential cross section

Introduction

The size of the molecular systems, as well as the range of forces, are very small and can not be measured directly. Therefore, scattering is very important in the study of atomic systems. A lot of information has been obtained about atoms, atomic nuclei, and elementary particles, through scattering experiments. For the interpretation of experimental results the theoretical description of the observed phenomenon is very important, as well as the performed calculations, which are usually very difficult, even with high-performance computers.

The wave property of the electrons has been known since 1924, but its consequences on the ionization of diatomic molecules by charged projectiles were first observed and described only in 2001 by N. Stolterfoht et al. [1]. Before that, in general, the collision of molecules with electrons, ions or photons was described by the so-called additivity rule [2], neglecting the coherence between waves associated with ejected electrons by different atoms of the molecule. Stolterfoht et al. have measured the double-differential cross section ratio, depending on electron velocity and ejection angle. In order to observe interference effects, they divided the molecular section obtained with two independent atomic sections. The oscillations observed in the cross section ratio – the ratio between the molecular cross section and the sum of the atomic cross sections – as a function of the electron velocity, have proved to be a clear evidence of the interference.

The two nuclei of the diatomic molecules are at a distance of the order \AA , which is comparable to the wavelength of the electrons. These nuclei can be conceived as two coherent sources of electrons. The coherent waves emitted near the nuclei of the molecule interfere in the spectrum of the emitted electron. Interference effects have been observed in the case of the random orientation of the target molecules.

Stolterfoht et al. have built a theoretical model, but they failed to explain the oscillation dependence on the ejection angle of the electron. They have compared their results with the experimental ones [1]. The relatively good correspondence between theory and experiment has aroused interest for research in the field.

Shortly after the publication of these results, in 2002, Nagy et al. [3] have made a theoretical description of this effect. They revealed the oscillation dependency of the cross section ratio of the

electron ejection angle and found almost complete disappearance of oscillations in case of perpendicular ejection. Their results have been experimentally confirmed by Stolterfoht et al. [4].

At the same time, other experiments have confirmed the interference effects in the ionization of homonuclear diatomic molecules: for H_2 [5-12] and larger molecules [13-16], by various projectiles – proton, C^{6+} , F^{9+} , Kr^{33+} , Kr^{34+} – with high energy, followed by several theoretical descriptions [17-26]. Recently the HeH^+ heteronuclear diatomic molecular ion [27, 28] has been studied – where the electron ejection of the two atoms is asymmetrical – as well as other, more complex molecules, for example H_2O [29], where the effect is more complicated than in the case of diatomic molecules. However, despite the huge amount of work, some aspects of the interference have not been clarified – for example, frequency doubling and the discrepancy between experiment and theory, at perpendicular ejection.

The present thesis contains four chapters. In the first chapter, we have presented the most important experiments which confirmed the wave property of the particles, the general theory of the cross sections [30-32], the time-dependent perturbation theory [30-32] and the single electron transitions, induced by the impact of charged particles. In the second chapter we have presented the first experimental and theoretical results of the interference effects in the ionization of the hydrogen molecule by ionic impact, and an analytical analysis of the interference effects. In the third chapter, we have presented a theoretical study for the ionization of the HeH^+ heteronuclear molecular ion by fast protons. We have generalized the analytical model used successfully to describe the interference effects in the H_2 molecule by Nagy [3] and applied it to study the interference effects in the ionization of the HeH^+ molecular ion. The study of heteronuclear diatomic molecules is interesting, when the ejection of the electrons compared to the two atoms is not symmetrical. In order to describe the emission of the electron, the semi-classical approximation has been applied, according to which the projectile was approached with classical physics formulas and it has been hypothesized that its trajectory is linear, due to the high projectile energy. By contrast, the target electrons have been treated with the formalisms of quantum mechanics, and the interaction between the projectile and the target particle, as a perturbation because the projectile influences the quantum state of the target. Finally we have identified the interference structures, we have analyzed the observed oscillations in the differential cross section ratio, depending on the ejected electron velocity for different ejection angles, and we have compared our results with those of Tachino [27, 28] and with results obtained for the hydrogen molecule with the method of [3]. Our results have been published [33] and presented at conferences [34, 35].

In the last chapter, we have presented a new theoretical model to describe the ionization process of the H_2 homonuclear molecule by impact with charged projectiles. We have analyzed

the deficiencies of the previous model and we have made substantial changes in order to obtain more precise results. Thus, we have achieved a more accurate theoretical description of the ionization process by the ionic impact. In this new model, as well as in the previous one, we used the independent electron approximation and the first-order perturbation theory, but with a much more precise description of the final state. In the previous model the final wave function of the electron is actually a plane wave, and in this model, it is approximated by coulombic waves centered on the two nuclei of the H_2 molecule. These significant changes have led to a more precise formula of the molecular differential cross section which depends only on atomic amplitude. As expected, a more accurate description of the final state and of the impact parameters has led to better results. We have compared our results with experimental data and with the results of other models, including the results of the previous model, and we have analyzed the causes of these differences. Our results have been published [36] and presented at conferences [37, 38].

The purpose of our research was the study and deep understanding of the interference phenomena in the ionization of diatomic molecules, by charged particles, the creation of a more developed theoretical model, which could provide a better understanding of the interference phenomena and effects, as well to obtain more accurate results compared to other theoretical models. With the present results, we will contribute to a deeper understanding of the interference effects in the ionization of homo- and heteronuclear molecules.

1. Theory

In the first part of this chapter we have presented the main experiments that demonstrated de Broglie's hypothesis, namely, the wave property of the particles (mainly of the electron): the Ramsauer-Townsend effect, the experiments of G. P. Thomson (1927), Davisson and Germer (1927), and Feynman, performed by R. Bach (2013).

In the second part of this chapter, we have presented the time-dependent scattering theory, relevant to our study, from the definition of the cross sections, through time-dependent perturbation theory, to the approach of atom ionization by the impact of charged-particles.

This chapter is based on references [39-54].

2. Observation and description of interference effects in the ionization of the hydrogen molecule

In the ionizations induced by charged particles, special attention has been given to the most simple diatomic target molecule, the H_2 molecule [53]. Due to the fact that its nuclei are identical, the ionization of the molecule causes coherent waves and as a consequence, interference occurs. However, until 2001 interference effects have not been observed in the spectra of electrons emitted by molecules due to ionization by fast ions. In 2001 Stolterfoht et al. conducted an experiment [1], using Kr^{34+} ions with the energy of 60 MeV/u, which was directed to a H_2 gas target. They measured the double differential cross section in the electron emission for different ejection angles and then divided the result by the double of the independent hydrogen atom's cross section. They noticed that the effective cross section ratio varies depending on the ejected electron velocity, and realized that this is the clear evidence of the interference effects. It is worth mentioning that interference effects have been observed in the random orientation of the H_2 target molecules.

Following the experimental results, Stolterfoht et al. have built a theoretical model to describe the interference effects in the ionization of the H_2 molecule, and have made calculations and comparisons between theoretical and experimental results. They have found that interference effects can be observed by the representation of the differential cross section ratio as a function of the ejected electron velocity.

In this chapter, we have presented and interpreted the first experimental and theoretical results of Stolterfoht. Although he failed to explain the dependence of oscillations on the ejection angle of the electron, the relatively good correspondence between theory and experiment, has raised interest for research in the field.

Shortly after the publication of these results, in 2002 Nagy et al. [3] presented a theoretical description of this effect. They predicted the dependence of the cross section ratio's oscillations on the electron ejection angle and observed the almost total disappearance of the oscillations at perpendicular ejection. The results were experimentally confirmed in 2003 by Stolterfoht et al. [4]. We presented the theoretical description of the interference effects in the ionization of the hydrogen molecule by fast ions of L. Nagy et al. [3].

3. Interference effects in the ionization of heteronuclear molecules

In order to understand in detail the interference effects observed in the ionization of molecules, it is interesting the study of the heteronuclear diatomic molecules, when the ejection of electrons in the vicinity of the two atoms is not symmetrical.

In the present paper we have generalized the analytic model for H_2 of L. Nagy [3] and applied it for the study of the interference effects in the ionization of HeH^+ molecular ion – a heteronuclear molecule with two electrons – by proton impact. Tachino et al. [27, 28] have performed theoretical calculations to study the ionization of the HeH^+ heteronuclear molecule. We have compared our results with those of Tachino et al. [28] and those for the hydrogen molecule, with the results of L. Nagy et al. [3]. We analyzed the observed oscillations in the differential cross section ratio according to the ejected electron velocity for different ejection angles.

3.1. Theoretical description

Given the high velocity of the projectile, for the ionization of the HeH^+ heteronuclear molecular ion, we apply the semi-classical approximation, considering that the trajectory of the projectile is rectilinear. The direction of the z axis coincides with the direction of the projectile, which moves with velocity v_p . The origin of the coordinate system is taken at the distance χD ($0 < \chi < 1$) from the He nucleus, and, respectively at the distance from $(1 - \chi)D$ from the H nucleus.

The initial state of the active electron in the heteronuclear molecule is described by a linear combination of two 1s type hydrogen atomic orbitals centered on each of the nuclei. By noting with α_1 and α_2 the effective charges of the He and H atoms, the initial wave function of the active electron is:

$$\Psi_i(\mathbf{r}, \mathbf{D}) = c_1 e^{-\alpha_1 |r + \chi \mathbf{D}|} + c_2 e^{-\alpha_2 |r - (1 - \chi) \mathbf{D}|}, \quad (3.1)$$

where the coefficients c_1 and c_2 give the contributions of the atomic orbitals to the molecular orbital for He and H atoms. We approximate the final wave function with the corresponding plane wave function:

$$\Psi_k(\mathbf{r}) \approx (2\pi)^{-3/2} e^{i\mathbf{k}\mathbf{r}}, \quad (3.2)$$

where \mathbf{k} is the momentum of the ejected electron.

The first-order transition amplitude for a projectile having the electric charge Z_p and the impact parameter b , for a given orientation of the molecular axis $\hat{\mathbf{D}}$ and for the ejected electron's momentum \mathbf{k} , can be written as:

$$a(b, \hat{\mathbf{D}}) = \frac{iZ_p}{v_p} \int_{-\infty}^{\infty} dz e^{iqz} \left\langle \Psi_k(\mathbf{r}) \left| \frac{1}{|\mathbf{r} - \mathbf{R}|} \right| \Psi_i(\mathbf{r}, \mathbf{D}) \right\rangle, \quad (3.3)$$

where q is the minimum momentum transfer to the electron, whereas \mathbf{r} and \mathbf{R} are the position vectors of the active electron and respectively, of the projectile.

The transition amplitude was calculated using the Bethe integral to describe the potential. In our calculations, we used the approximation for fast electrons, and thus considered only the high velocity electrons.

Since the transition probability for an impact parameter b and a $\hat{\mathbf{D}}$ -direction of the molecular axis is equal to the square of the transition amplitude's modulus, we have shown that the first one is expressed with the following formula:

$$w(b, \hat{\mathbf{D}}) = \frac{8}{\pi} \frac{Z_p^2}{v_p^2 k^4} \left[c_1^2 \frac{\alpha_1^2}{\gamma_1^2} (b_+ K_1(b_+ \gamma_1))^2 + c_2^2 \frac{\alpha_2^2}{\gamma_2^2} (b_- K_1(b_- \gamma_2))^2 + c_1 c_2 \frac{\alpha_1 \alpha_2}{\gamma_1 \gamma_2} b_+ b_- K_1(b_+ \gamma_1) K_1(b_- \gamma_2) (e^{-i(k_{\parallel} - q)D_{\parallel}} + e^{+i(k_{\parallel} - q)D_{\parallel}}) \right], \quad (3.4)$$

where

$$\gamma_{1,2} = [\alpha_{1,2}^2 + (q - k_{\parallel})^2]^{1/2}, \quad (3.5)$$

and b_+ and b_- are the impact parameters relative to the two nuclei; k_{\parallel} and D_{\parallel} are the parallel components of the final momentum of the electron \mathbf{k} , respectively of the \mathbf{D} internuclear distance, relative to the z axis.

The relationship (3.4) depends not only on the impact parameter but also on the orientation of the molecular axes. For the comparison with the experiment, the probability has to be averaged over all possible molecular orientations:

$$w(b) = \frac{1}{4\pi} \int d\varphi_D \int \sin \theta_D d\theta_D w(b, \hat{\mathbf{D}}). \quad (3.6)$$

The differential cross section is obtained by integrating the probability over the impact parameter:

$$\frac{d\sigma}{d\Omega_k dk} = 2\pi \int bw(b)db. \quad (3.7)$$

The integrations (3.6) and (3.7) must be calculated numerically.

If we average only the interference factor

$$e^{-i(k_{\parallel}-q)D_{\parallel}} + e^{+i(k_{\parallel}-q)D_{\parallel}}, \quad (3.8)$$

after the orientation of the molecular axis, and *assuming* that the other variations of the equation (3.4) are insignificant, the transition probability and the differential cross section results:

$$w(b) = c(b) + g(b) \frac{\sin[(k_{\parallel} - q)D]}{(k_{\parallel} - q)D} \quad (3.9)$$

$$\frac{d\sigma}{d\Omega_k dk} = C + G \frac{\sin[(k_{\parallel} - q)D]}{(k_{\parallel} - q)D}. \quad (3.10)$$

Relations (3.9) and (3.10) are similar to those obtained by L. Nagy et al. [3].

3.2. Results and discussions

As Stolterfoht [1] had pointed out, interference cannot be observed in the differential cross section but can be demonstrated by calculating the differential cross section ratio.

We made calculations for the ionization of the HeH^+ molecular ion by proton impact, for three different projectile energies: 1 MeV/u, 13.7 MeV/u, and 100 MeV/u. We have analyzed the cross sections as a function of the ejected electron momentum, for four ejection angles: 0° , 30° , 90° and 150° . We performed the calculations taking into consideration the origin both in the geometric and in the mass center of the molecule. The calculations have shown that the results obtained do not depend on the value of χ , namely the choice of the origin position.

In order to show the interference effects, we calculated the differential cross section ratio and studied its dependence from the momentum and the ejection angle of the electron, and compared our results with those of Tachino et al. [28]. In figures 3.1-3 we represented the cross section ratio for three different proton energies and four electron ejection angles. Our results show oscillations in the cross section ratio and are in good agreement with those obtained by Tachino et al. [28].

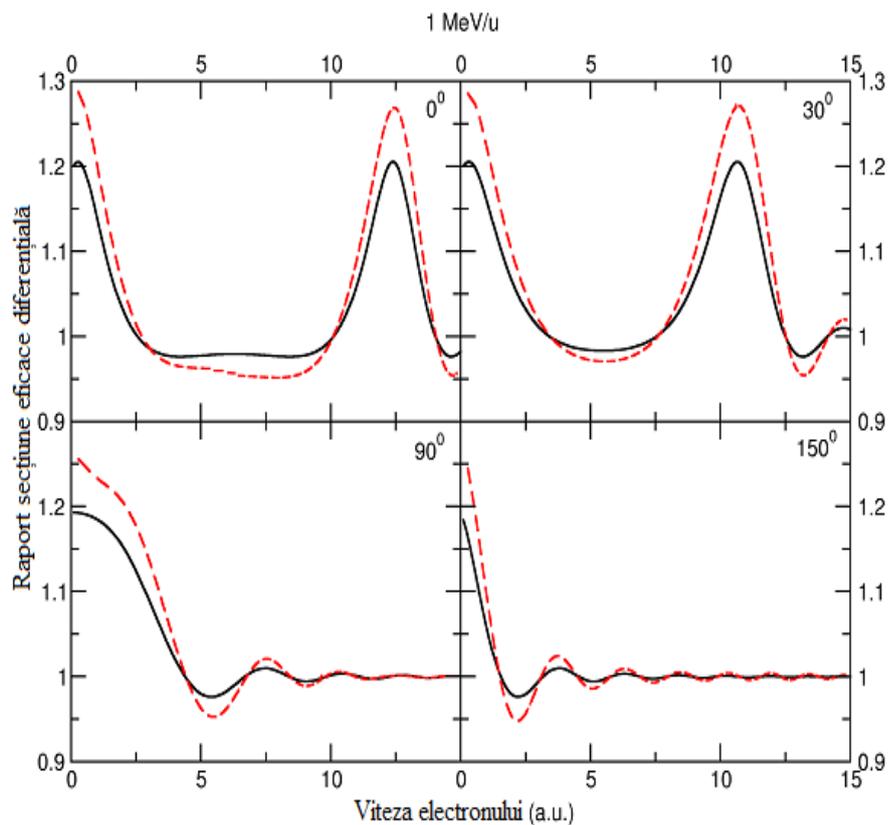


Figure 3.1. Differential cross section ratios as a function of the ejected electron velocity, in case of ionization of the HeH^+ by 1 MeV/u proton, for different electron ejection angles. Solid lines (—) represents our results, and dashed lines (- -) are the results of Tachino et al. [28].

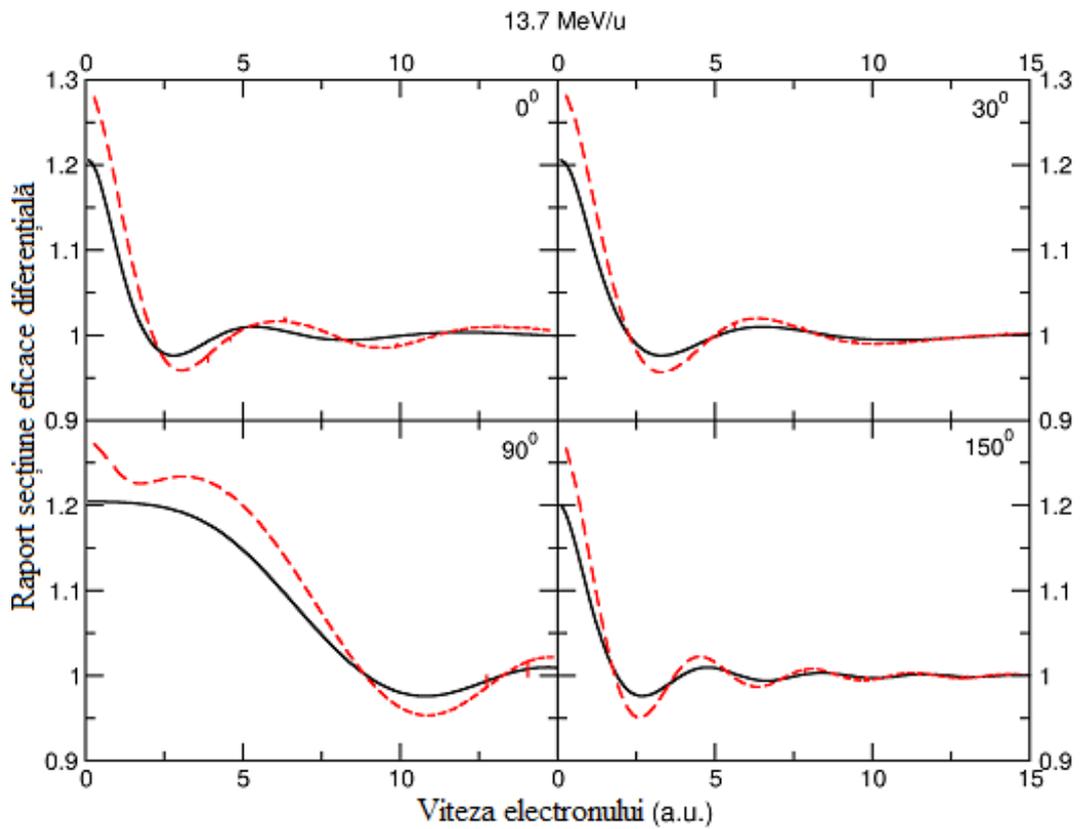


Figure 3.2. Same as in Figure 3.1, but the proton energy is 13.7 MeV/u.

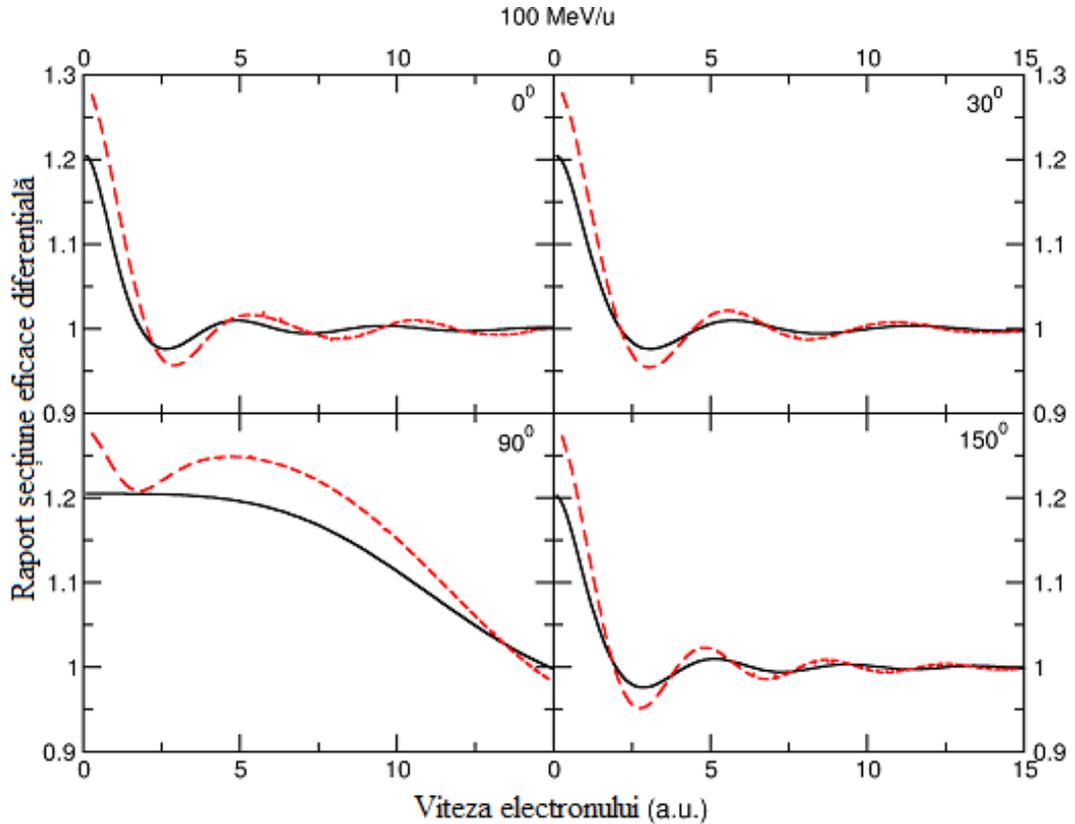


Figure 3.3. Same as in Figure 3.1, but the proton energy is 100 MeV/u.

Figures 3.4-6 show the polar representation of the cross section ratio depending on the momentum of the ejected electron, as a radial coordinate, and on the ejection angle for three different projectile energies. In case of impact with a 1 MeV/u projectile (figure 3.4), the main peak with the circular shape can be fully observed, because the radius of the binary circle is 12.54 a.u. and the highest momentum in the graphics is 15 a.u. At higher proton energy the radius of the binary circle increases. In figures 3.5 and 3.6 the binary peak is only partially visible because the radius of the binary circle is 46.77 a.u. in case of projectiles with energy 13.7 MeV/u and 125.47 a.u. for 100 MeV/u. In figures 3.5-6 we can observe secondary oscillations both inside and outside the binary peak circle, and at the same time that the value of the binary maximum does not depend on the ejection angle of the electron.

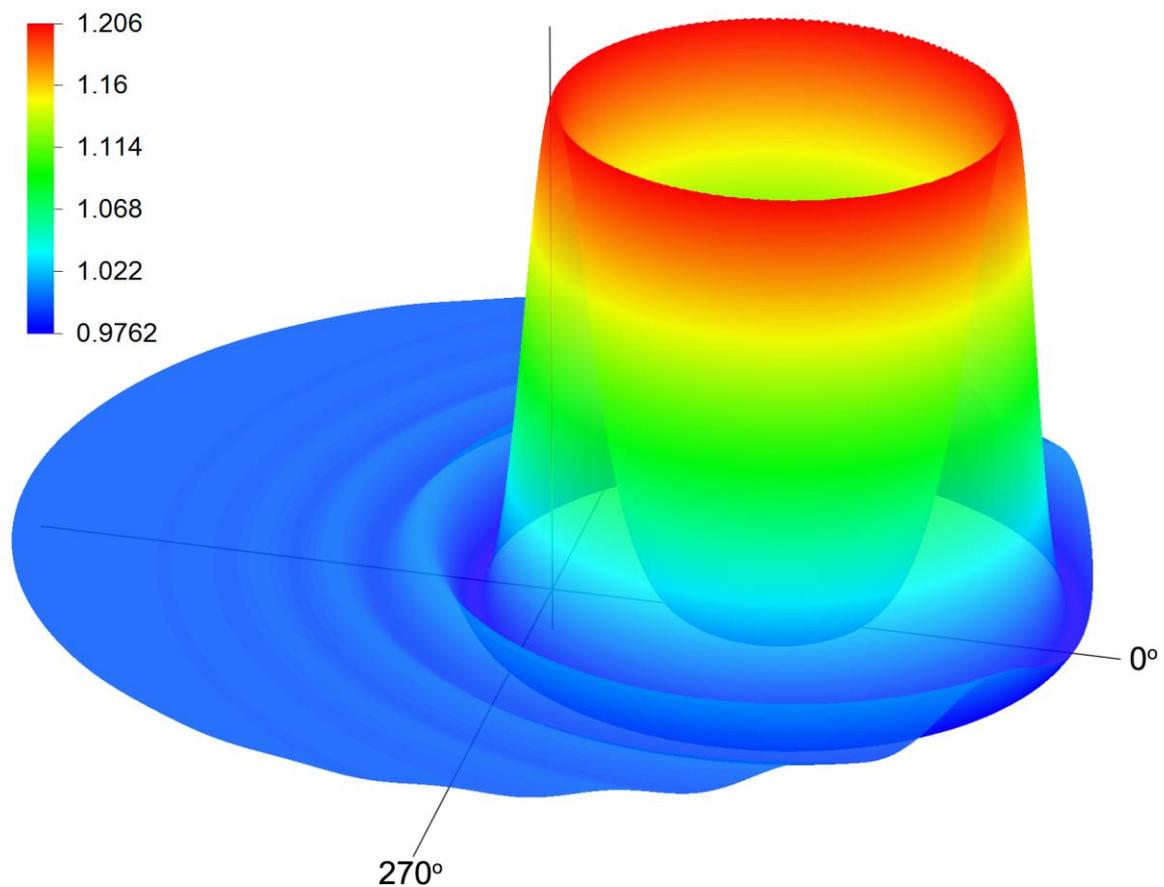


Figure 3.4. Differential cross section ratio, as a function of the ejected electron velocity and ejection angle, where the velocity is used as radial coordinate, in the ionization of the HeH^+ by 1 MeV/u proton. The maximum value of the electron velocity is 15 a.u.

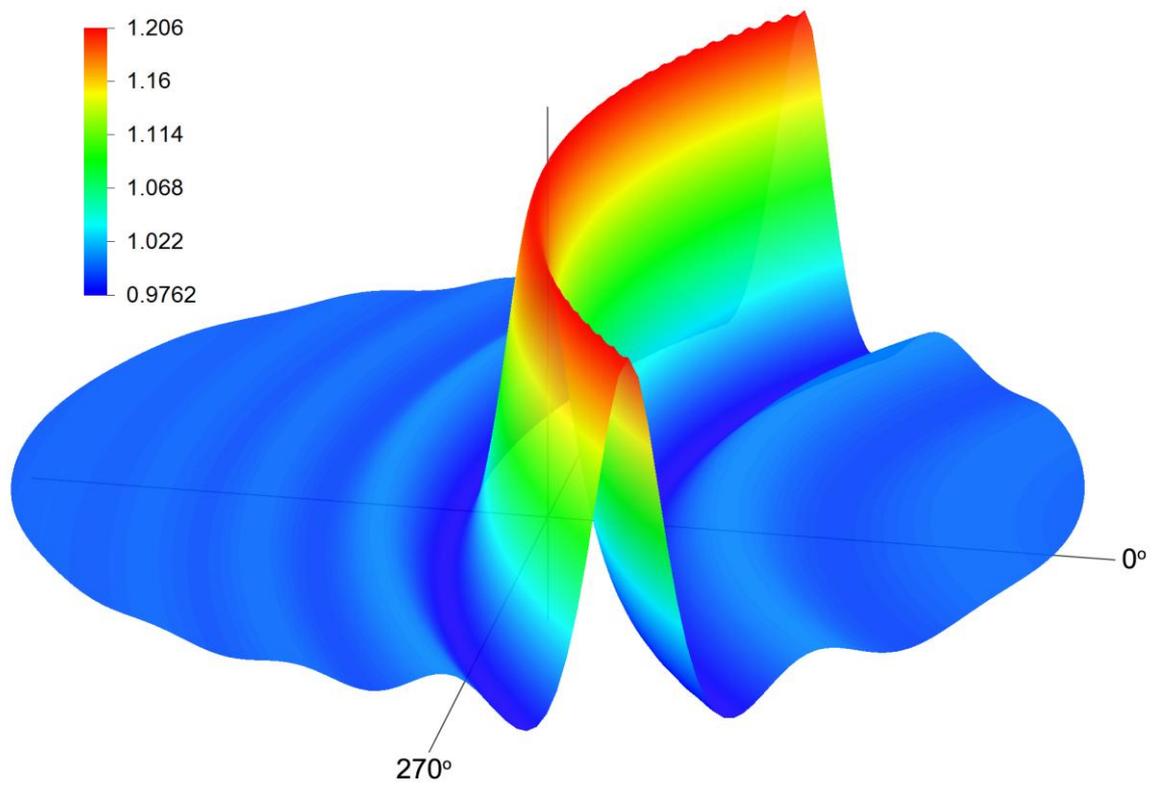


Figure 3.5. Same as 3.4, but the energy of the proton is 13.7 MeV/u.

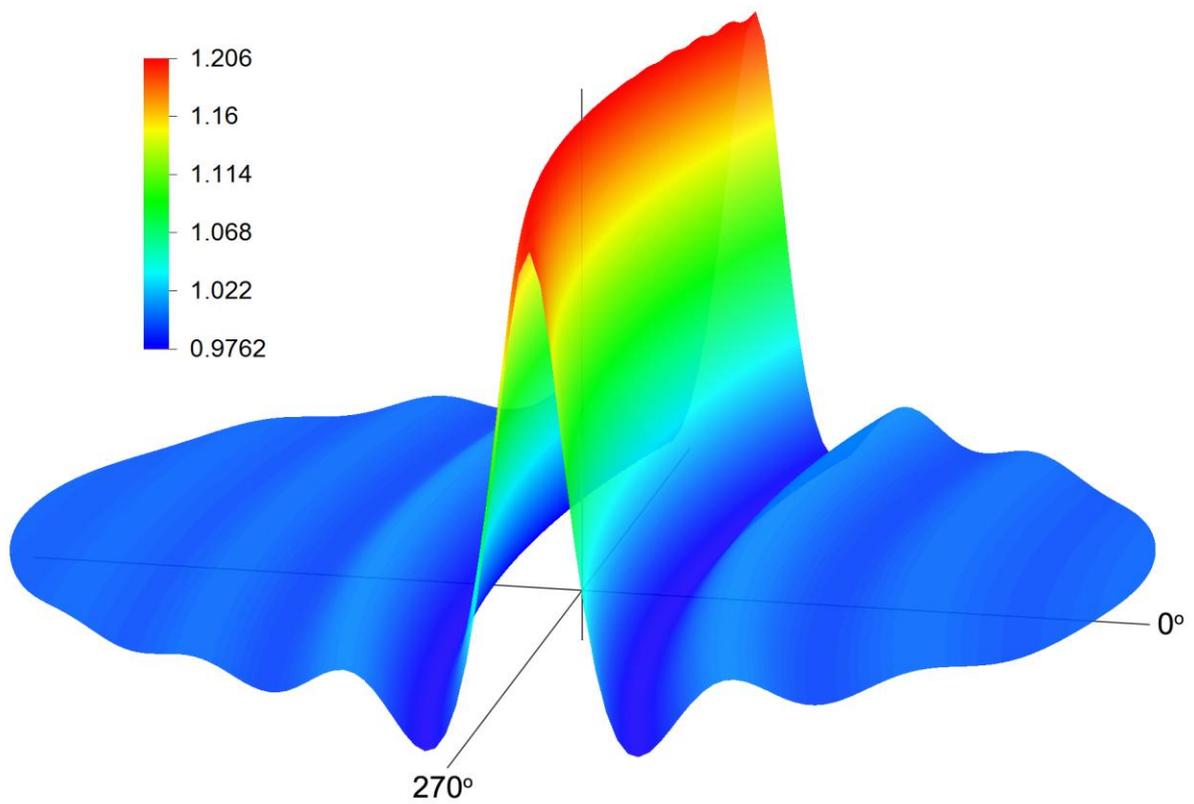


Figure 3.6. Same as 3.4, but the energy of the proton is 100 MeV/u.

We have compared the cross section ratio of the heteronuclear molecule HeH^+ to that of the H_2 homonuclear molecule (figures 3.7-9). The amplitude of the oscillations is less than for the H_2 homonuclear molecule, calculated by the method [3]. This is normal, because the electron density is much higher around the helium nucleus than around the proton, and the interference effects between waves with different amplitudes are less pronounced than for waves with equal amplitudes.

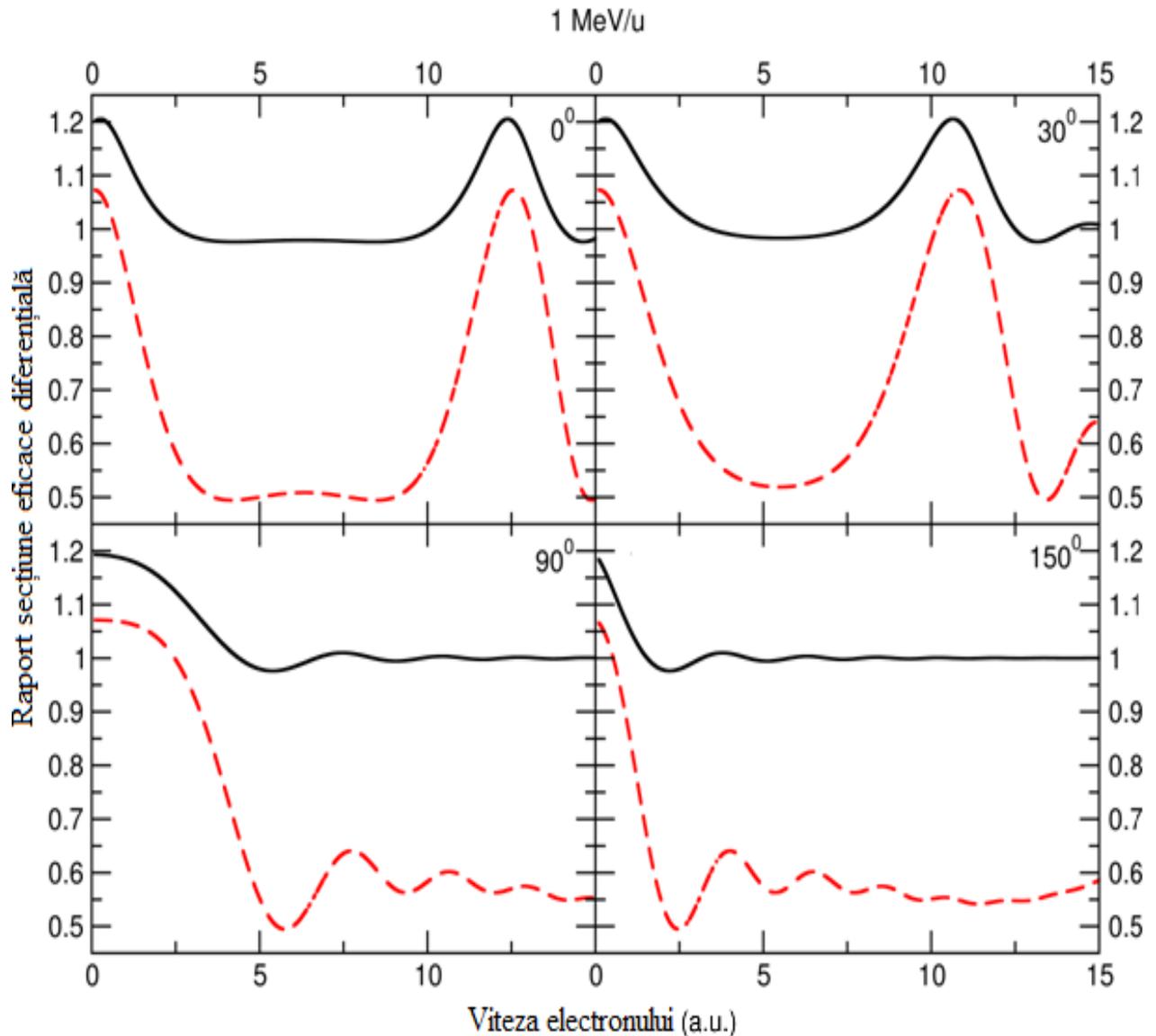


Figure 3.7. Differential cross section ratios as a function of the electron velocity and ejection angle, in case of ionization by proton impact, with energy 1 MeV/u. The solid lines (-) represent our results for the ionization of the heteronuclear molecular ion HeH^+ . The red, dashed lines (- -) are the results for the H_2 molecule.

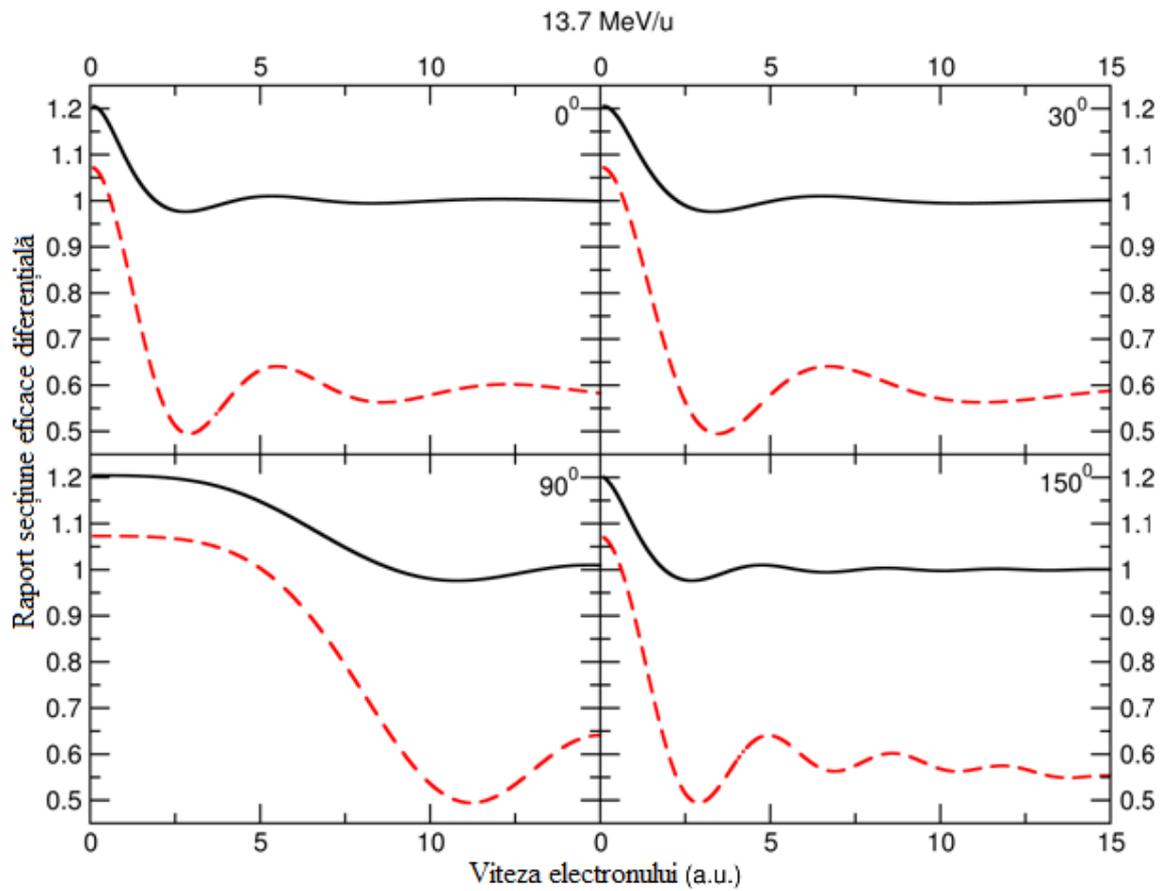


Figure 3.8. Same as figure 3.7, but the energy of the proton is 13.7 MeV/u.

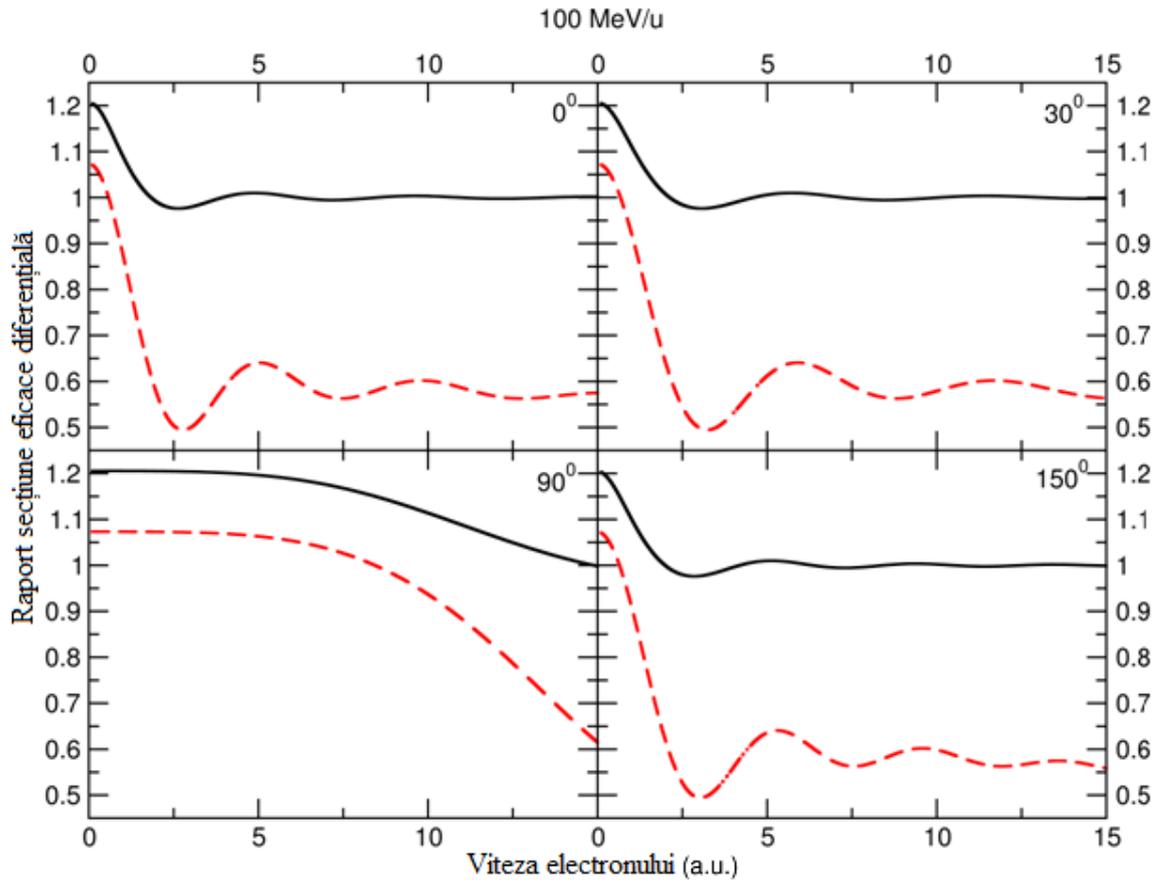


Figure 3.9. Same as figure 3.7, but the energy of the proton is 100 MeV/u.

3.3 Conclusions

We have performed a theoretic investigation of the interference effects in the ionization of the HeH^+ molecular ion, using the previously developed model of L. Nagy for the H_2 molecule [3], generalized now for heteronuclear molecules. Interference effects have been highlighted by representing the differential cross section ratio, as a function of the ejected electron's velocity. Both the principal and the secondary maximums can be calculated and can be well observed on our graphics. Our results are in very good agreement with the results of Tachino et al. [28]. We have compared our results with those for the H_2 homonuclear molecule, and, as expected, the oscillations on the heteronuclear molecule were less pronounced than on the homonuclear molecule.

4. Interference effects in the ionization of the H₂ molecule by fast ion impact.

Comparison of different models

In this chapter we will present a more advanced theoretical model, compared to the previous, based on plane waves (PW), used to study the interference effects in the ionization of the HeH⁺ heteronuclear molecule. In the previous model, the final wave function of the electron is a plane wave, but in this model, it is improved by coulombic waves, centered on the two nuclei of the H₂ molecule. After these significant changes, we achieved a more precise theoretical description of the ionization process due to the ionic impact. In order to describe the interference effects, another group has applied a different theoretical model, called CDW-EIS (Continuum Distorted Wave – Eikonal Initial State), performing calculations for the same phenomenon [18, 19]. They have achieved similar results for the differential cross section, cross section ratio and for the oscillations of the cross section ratio.

Some aspects of interference caused by ionic impact have not been clarified, for example, the discrepancy between theory and experiment at the 90° ejection angle, or doubling the frequency [7], and so on.

With the present formulation, we will contribute to a deeper understanding of the interference phenomena in the ionization of diatomic molecules by fast ions. We will compare our results with those of the PW and CDW-EIS models, along with those obtained by the analytical formula, and finally, we will analyze the cause of the differences.

4.1. Theoretical description

We use the first-order perturbation approximation, considering that the energy of the projectile is much higher compared to the energy of the interaction. The origin of the coordinate system is chosen in the center of the molecule. We consider only one active electron. \mathbf{R} is the distance from the origin to the projectile, \mathbf{r} is the position of the active electron, and \mathbf{r}_+ and \mathbf{r}_- are the distances from the nuclei to the electron.

The initial state of the molecule is approximated as a linear combination of two $1s$ hydrogen atomic orbitals

$$\psi_i(\mathbf{r}, \mathbf{D}) = N \left(e^{-\alpha|r-\frac{\mathbf{D}}{2}|} + e^{-\alpha|r+\frac{\mathbf{D}}{2}|} \right). \quad (4.1)$$

Inserting the last relationship (4.1) into the formula (3.3), the transition amplitude may be split into two terms:

$$a(\mathbf{b}, \hat{\mathbf{D}}) = a_+(\mathbf{b}, \hat{\mathbf{D}}) + a_-(\mathbf{b}, \hat{\mathbf{D}}), \quad (4.2)$$

where

$$a_{\pm}(\mathbf{b}, \hat{\mathbf{D}}) = \frac{iZ_p}{v} \int_{-\infty}^{\infty} dz e^{iqz} \left\langle \psi_k(\mathbf{r}) \left| \frac{1}{|\mathbf{r} - \mathbf{R}|} \right| \psi_H(\mathbf{r}_{\pm}) \right\rangle, \quad (4.3)$$

are the transition amplitudes of the two atoms in the molecule, where

$$\psi_H(\mathbf{r}_{\pm}) = N e^{-\alpha r_{\pm}}. \quad (4.4)$$

Replacing

$$\mathbf{r}_{\pm} = \mathbf{r} \pm \frac{\mathbf{D}}{2} \quad (4.5)$$

into the relationship (3.2), we obtain the final wave function, in coordinate systems centered on each nucleus

$$\psi_k^*(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} e^{-ikr_{\pm}} e^{\pm ik\frac{D}{2}} = \psi_k^*(\mathbf{r}_{\pm}) e^{\pm ik\frac{D}{2}}. \quad (4.6)$$

In the relationship of the amplitude (4.3), the z coordinate is considered from the center of the molecule. We note with z_{\pm} the coordinates of the nuclei

$$z_{\pm} = z \pm \frac{D_{\parallel}}{2}, \quad (4.7)$$

thus,

$$a_{\pm}(\mathbf{b}, \hat{\mathbf{D}}) = e^{\pm i k \frac{D}{2}} e^{\mp i q \frac{D_{\parallel}}{2}} \frac{i Z_p}{v} \int_{-\infty}^{\infty} dz_{\pm} e^{i q z_{\pm}} \left\langle \Psi_k(\mathbf{r}_{\pm}) \left| \frac{1}{|\mathbf{r}_{\pm} - \mathbf{R}_{\pm}|} \right| \Psi_H(\mathbf{r}_{\pm}) \right\rangle, \quad (4.8)$$

where \mathbf{R}_{\pm} refers to the distances measured from the projectile to the two nuclei.

The impact parameters to the two nuclei are

$$\mathbf{b}_{\pm} = \mathbf{b} \pm \frac{\mathbf{D}_{\perp}}{2}, \quad (4.9)$$

thus, the transition amplitudes of the two atoms,

$$a_H(\mathbf{b}_{\pm}, \mathbf{D}) = \frac{i Z_p}{v} \int_{-\infty}^{\infty} dz_{\pm} e^{i q z_{\pm}} \left\langle \Psi_k(\mathbf{r}_{\pm}) \left| \frac{1}{|\mathbf{r}_{\pm} - \mathbf{R}_{\pm}|} \right| \Psi_H(\mathbf{r}_{\pm}) \right\rangle. \quad (4.10)$$

Using relationships (4.8) and (4.10), the transition amplitudes become

$$a_{\pm}(\mathbf{b}, \hat{\mathbf{D}}) = e^{\pm i [(k_{\parallel} - q) \frac{D_{\parallel}}{2} + \mathbf{k}_{\perp} \frac{\mathbf{D}_{\perp}}{2}]} a_H(\mathbf{b}_{\pm}, \mathbf{D}). \quad (4.11)$$

The differential cross section for a certain orientation of the molecular axis is obtained by integrating the transition probability – which is the square of the modulus of the transition amplitude – over the impact parameter. Considering the sum

$$e^{i[(k_{\parallel} - q)D_{\parallel} + \mathbf{k}_{\perp} \mathbf{D}_{\perp}]} + e^{-i[(k_{\parallel} - q)D_{\parallel} + \mathbf{k}_{\perp} \mathbf{D}_{\perp}]} = 2 \cos[(k_{\parallel} - q)D_{\parallel} + \mathbf{k}_{\perp} \mathbf{D}_{\perp}], \quad (4.12)$$

we obtain the differential cross section

$$\frac{d^2 \sigma(\hat{\mathbf{D}})}{d\Omega_k dk} = 2 \frac{d^2 \sigma_H}{d\Omega_k dk} + 2 \cos[(k_{\parallel} - q)D_{\parallel} + \mathbf{k}_{\perp} \mathbf{D}_{\perp}] \int d\mathbf{b} a_H^*(\mathbf{b}_+, \mathbf{D}) \cdot a_H(\mathbf{b}_-, \mathbf{D}). \quad (4.13)$$

The first term of the above equation stands for the atomic differential cross section. The second one may be interpreted as *interference term*, due to coherent electron emission from the two atoms. The cosine factor from the (4.13) equation resembles the one from (3.8), obtained by analytic calculation, with the difference that in the first one in the argument of the cosine function the $\mathbf{k}_{\perp} \mathbf{D}_{\perp}$ component also appears. In the averaging procedure of the cross section over the orientation of the molecular axis, this term of perpendicular components tends to cancel out, however, this cancellation is not accurate.

For a comparison with the experiment, the (4.13) differential cross section should be averaged over the molecular orientation

$$\frac{d^2\sigma}{d\Omega_k dk} = \frac{1}{4\pi} \int \frac{d^2\sigma(\hat{\mathbf{D}})}{d\Omega_k dk} d\hat{\mathbf{D}}. \quad (4.14)$$

Considering that the term

$$\frac{d^2\sigma_{int}(\hat{\mathbf{D}})}{d\Omega_k dk} = \int d\mathbf{b} a_H^*(\mathbf{b}_+, \mathbf{D}) \cdot a_H(\mathbf{b}_-, \mathbf{D}) \quad (4.15)$$

has a weak dependence on the orientation of the molecular axis, and the term with the perpendicular components in the cosine function argument is canceled in integration over φ_D , for the molecular differential cross section we obtain the analytical formula

$$\frac{d^2\sigma_{analytic}}{d\Omega_k dk} = 2 \frac{d^2\sigma_H}{d\Omega_k dk} \left\{ 1 + G_0 \frac{\sin(k_{\parallel} - q)D_{\parallel}}{(k_{\parallel} - q)D_{\parallel}} \right\}. \quad (4.16)$$

Dividing the equation (4.16) with the double of the atomic differential cross section, we obtain the analytical formula of the differential cross section ratio

$$R = 1 + G_0 \frac{\sin(k_{\parallel} - q)D_{\parallel}}{(k_{\parallel} - q)D_{\parallel}}. \quad (4.17)$$

In the following, we will examine the validity of this hypothesis.

4.2. Results and discussions in the ionization of the H₂ molecule by F⁹⁺, Kr³³⁺ and Kr³⁴⁺ projectiles

We have performed calculations for the differential cross section and for the differential cross section ratio, in the ionization of the H₂ molecule, by Kr³³⁺ projectiles, with the energy of 68 MeV/u, Kr³⁴⁺ of 60 MeV/u and F⁹⁺ of 5 MeV/u, for various ejection angles. We compared our results with those obtained by plane waves approximation – PW model, based on the numerical integration of ionization probabilities over the impact parameter and the molecular orientation, presented in [3] – with CDW-EIS calculations [18, 19], and with results, using the analytical formula (4.17).

In figure 4.1 we have shown differential cross sections for ejection angles of 30° (left) and 150° (right), as a function of the ejected electron's energy. We compared our results with those of the PW model [3], the CDW-EIS calculations [18, 19] and the experimental data [1].

In our model, where we use a two-center final wave function (4.6), located in the two nuclei of the hydrogen molecule, we describe the final state more precisely than the PW model used for the H₂ [3], but in the previous chapter also, for the HeH⁺ molecular ion. As expected, the current, more accurate description of the final state lead to results in agreement with experimental data and are more precise than those of the PW model. We concluded that for large ejection angles, theory overestimates the experimental values [1]. Likewise, with the exception of small energies, the cross section values of our model are higher for both ejection angles than those of the PW model.

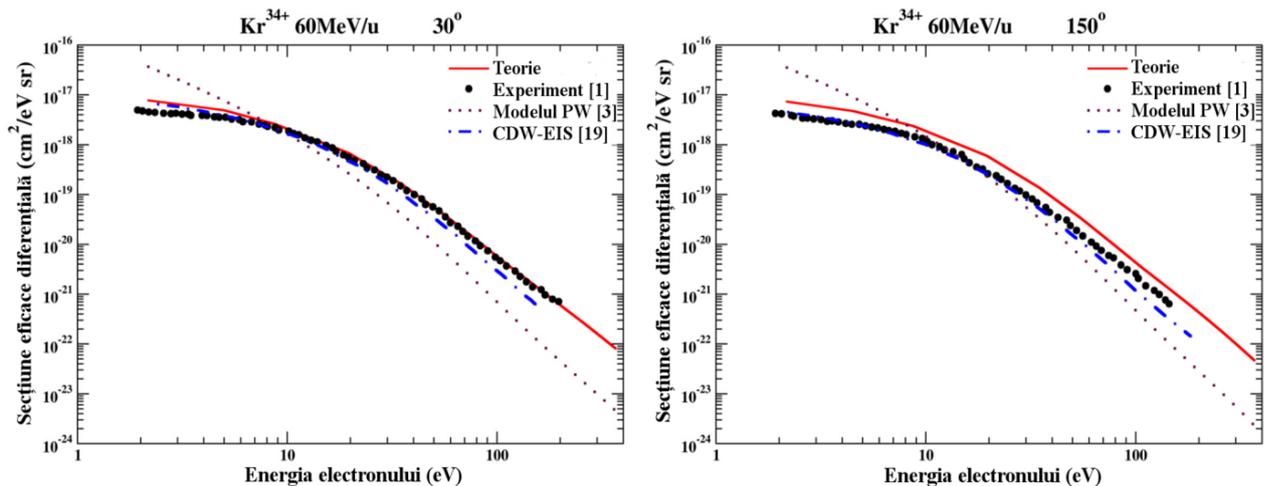


Figure 4.1 – Doubly differential cross sections for the ionization of H₂ by fast Kr³⁴⁺ ions, for different ejection angles. Our results are compared to the PW [3] and CDW-EIS [19] models, as well as to the experimental data [1].

In figure 4.2 we presented the differential cross section ratio, which was obtained by dividing the equation (4.14) with twice of the effective atomic cross section, as a function of the ejected electron's velocity. We compared our results with the experimental data [1, 4], with the PW model [3], with CDW-EIS calculations [18, 19] and with the calculations obtained by the analytical formula given by the equation (4.17). In this equation, the G_0 factor is a constant, the value of which we chose to be 0.4, in order to match the experimental data [1, 4].

Similar to the differential cross sections, the values of the ratios are always higher than those obtained by the PW model. Regarding the frequency of the oscillations, their value is slightly higher, compared to the PW model, and much higher than those given by the analytical formula. (4.17).

It can be observed that for velocities under 1.5 a.u. there is a discrepancy between theoretical and experimental results. The explanation of this difference is that in this velocity-range – as shown in [20] - the scattering of electrons on nuclei becomes important, and we have not included these effects in our theoretical model. Likewise, electron correlation is important in the two-electron system of the H_2 molecule, which can influence the cross section ratio for small velocities. [56].

In case of electron velocities above 1.5 a.u, for ejection angles of 30° and 150° , but especially in the first case, the results are in agreement with experimental data [1], and CDW-EIS [18] calculations. At 150° ejection angle, the agreement is very good with the CDW-EIS [19] results, but both have lower frequency than the oscillation of the experimental data [4].

For ejection around 90° angle – the second and third panel of figure 4.2 – there is a larger discrepancy between our model and the CDW-EIS calculations [19]. The most important result of this approach can be observed at these ejection angles, but especially at 90° , where the analytical formula and the PW model give a constant ratio, in the studied velocity range, and the CDW-EIS ratio shows a monotonic tendency, increasing with velocity, while our model, surprisingly, reproduces a part of the secondary oscillations observed in the experiment, for both ejection angles. In order to investigate the origin of this surprising behavior, starting from the equation (4.13), without the oscillating cosine factor

$$\frac{d^2\sigma(\widehat{\mathbf{D}})}{d\Omega_k dk} = 2 \left[\frac{d^2\sigma_H}{d\Omega_k dk} + \int d\mathbf{b} a_H^*(\mathbf{b}_+, \mathbf{D}) \cdot a_H(\mathbf{b}_-, \mathbf{D}) \right], \quad (4.18)$$

we calculated the cross section ratio

$$R' = 1 + \left(\frac{d^2\sigma_{int}}{d\Omega_k dk} \right) / \left(\frac{d^2\sigma_{2H}}{d\Omega_k dk} \right), \quad (4.19)$$

where $\frac{d^2\sigma_{int}}{d\Omega_k dk}$ is the expression (4.15) averaged over the orientation of the molecular axis.

In figure 4.2 it may be observed that the ratio, without the cosine factor (4.19), is oscillating, not only for perpendicular ejection but for 60° angle, too. If we also take into account the effect of the cosine factor, we are lead to more complex oscillations of the cross section ratio as a function of the ejected electron's velocity, observed mostly for perpendicular ejection, but also for 60°, which means, that the "constant" G_0 in the equation (4.17) behaves in an oscillatory manner, and the assumption that equation (4.15) has a weak dependence on molecular orientation is not valid. Thus, oscillation is governed not only by the sinus function but is also modulated by the factor G_0 .

The causes of these additional oscillations due to the interference between the electron waves emitted from the vicinity of the two nuclei can be:

1. The difference of phases $\mathbf{kD} = k_{\parallel}D_{\parallel} + k_{\perp}D_{\perp}$, originating from the equation (4.6), which expresses the difference of distances between the nuclei and the detector, and/or
2. The parallel momentum-transfer qD_{\parallel} , coming from the equation (4.7) and represents the different time moments for the momentum-transfer to the electron in the vicinity of the two nuclei, due to the fact that the projectile reaches one of the nuclei with $\Delta t = \frac{D_{\parallel}}{v_p}$ later.

Thus,

$$qD_{\parallel} = \frac{E_i + \frac{k^2}{2}}{v_p} D_{\parallel} = \left(E_i + \frac{k^2}{2} \right) \Delta t. \quad (4.20)$$

On the other hand, the perpendicular momentum-transfer, qD_{\perp} , comes from the equation (4.9) and does not influence the cosine factor in the equation (4.13). This is responsible only for the different phases of the amplitudes and influences the behavior of the integral (4.15).

Summing up the above, we can state that the oscillations driven by the cosine factor of the equation (4.13) are modulated, due to the different phases of amplitudes related to the perpendicular momentum transfer to the electron from the vicinity of the two nuclei.

Since we did not introduce the electron scattering on the nuclei of the H₂ molecule in our model, our description is of first-order. For more precise results and for a deeper understanding of the interference effects, the rescattering of the electron must be taken into consideration. This second-order effect was modeled previously [7].

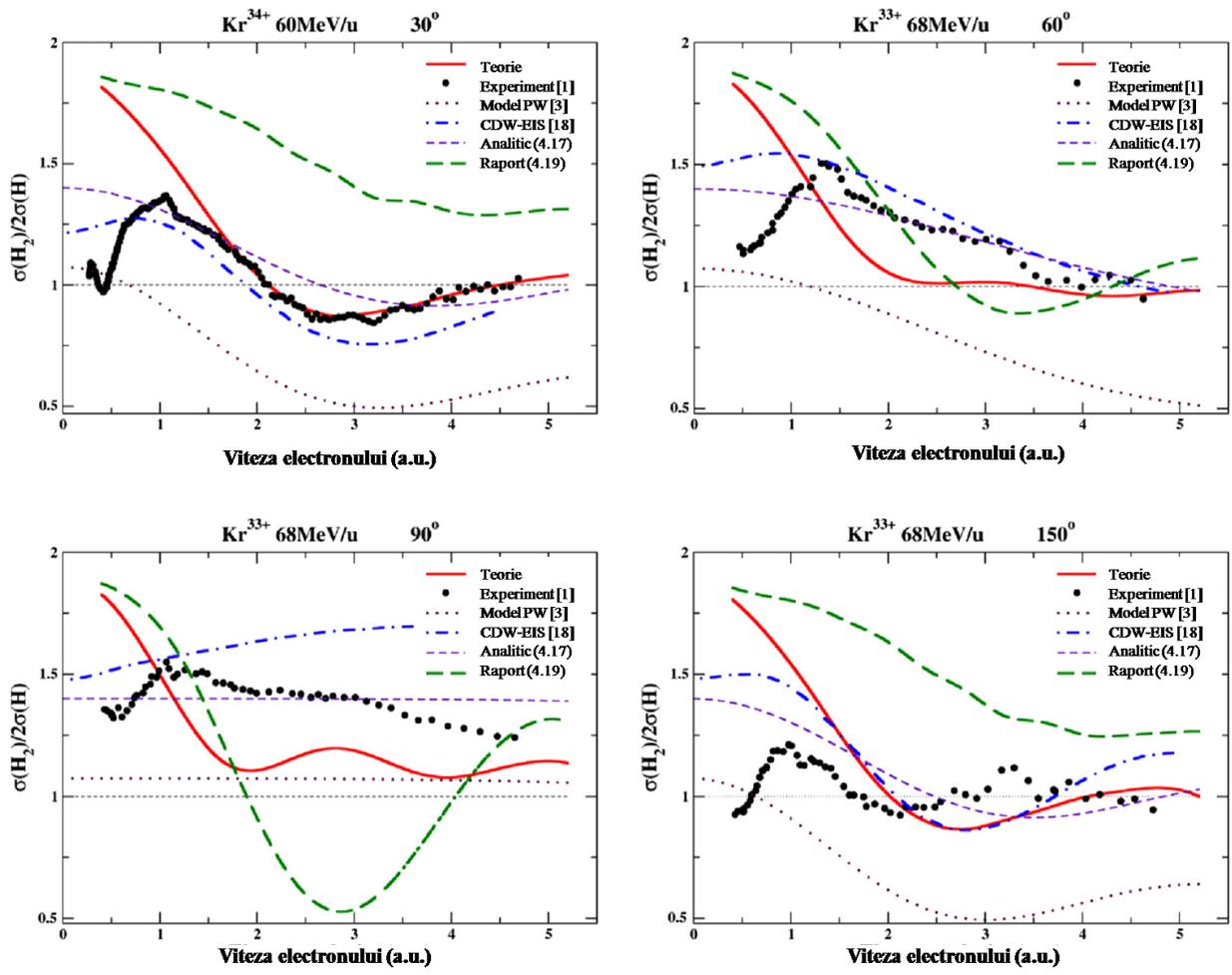


Figure 4.2. H_2 and $2H$ cross-section ratios in the ionization by fast Kr^{33+} and Kr^{34+} ions for different ejection angles, as a function of electron velocity. Our results are compared with the experimental data [1], with PW [3], CDW-EIS [18], and analytical models (4.17), as well as with the ratio of the equation (4.19).

In figures 4.3 and 4.4 we compared the results of this model with a set of experimental data for projectiles F^{9+} , with energy 5 MeV/u [11]. In figure 4.3 we represented the double differential cross sections for the ionization of the H_2 molecule and for two effective H atoms, along with the experimental results for H_2 [11], as a function of the ejected electron energy. Figure 4.3 shows that theoretical results for the molecule are in good agreement with the experimental ones, especially for small angles, with the exception of small energies. For large angles, above 30° , the theoretical results exceed the experimental ones. However, it is more important that interference effects are obvious for all angles, especially for small energies, where we can notice the difference between the $2H$ total atomic differential cross sections and that of the H_2 molecule.

In figure 4.4 we compared the results of the theoretical ratio of the differential cross section with experimental results [11], with the CDW-EIS [11] and analytical (4.17) models, as well as with the ratio of equation (4.19), as a function of the electron velocity, for the same ejection

angles as in the case of the previous figure, for the impact of fast F^{9+} projectiles, with 5 MeV/u energy.

For 30° and 150° angles, oscillations show a similar tendency, as it can be seen in figure 4.2, for the same angles, and are in good agreement with experimental data [11], and with CDW-EIS [11] results. We observed that the frequency of the oscillations increases in case of angles larger than 90° , as presented in fig. 4.2, the fact also confirmed by the analytical formula (4.17). Compared to the CDW-EIS model [11] and to the analytical formula (4.17), the values of our theoretical model are smaller, compared to both, but, most importantly, our results are closer to the experimental ones [11], both in terms of the value of the cross section ratio and the frequency of the oscillations.

We can also observe that in the ionization with F^{9+} projectile, around the 90° ejection angle – more precisely from 60° to 120° – the ratio of our model oscillates, while the analytical ratio, outside the 120° ejection angle, does not present oscillations, having a constant value, or a monotonous decrease, within the velocity-range studied.

The ratio, without the cosine factor (4.19), has the same behavior as in the ionization with Kr^{33+} and Kr^{34+} projectiles (fig. 4.2): does not complicate the simple oscillations – for example, for ejection angles of 30° and 150° – but modulates the cosine factor from (4.13).

We must point out the fact that experimental values for 90° angle, and for electron velocity above 3 a.u. – especially for angles of 30° , 120° and 150° – have large errors. For this reason, comparison with the experiment – primarily for these ejection angles – is not very conclusive.

Taking into account the values of the cross section ratio of this model, it is clear that for velocities lower than 1 a.u., our first-order description cannot produce results in agreement with the experimental ones [11], without taking into account the correlation between electrons [56] and the second-order effects, mentioned earlier [20].

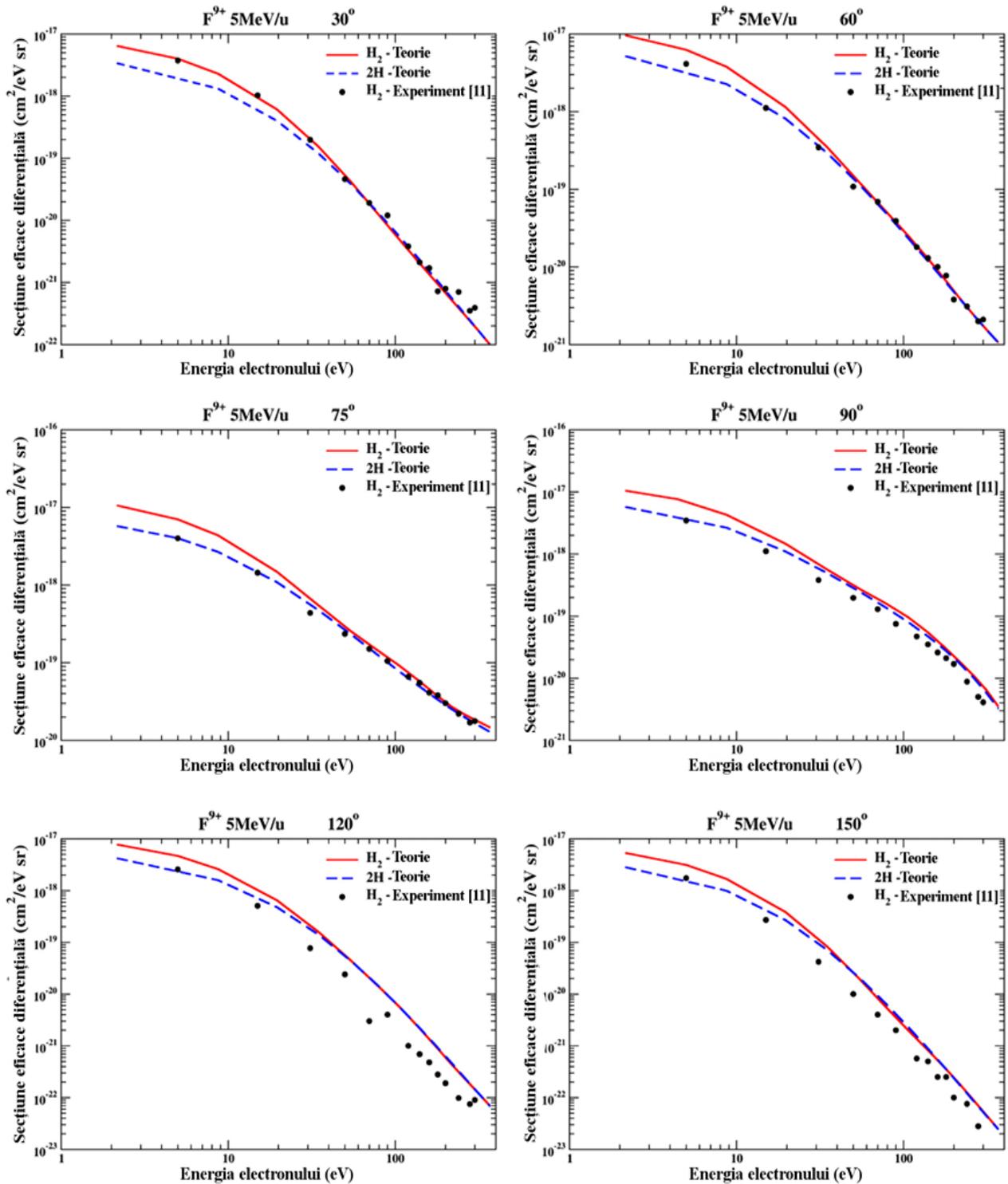


Figure 4.3. Doubly differential cross sections for the ionization of the H_2 molecule and two effective H atoms by F^{9+} ions, compared to the experimental data for the H_2 [11] molecule, for different ejection angles, as a function of electron energy.

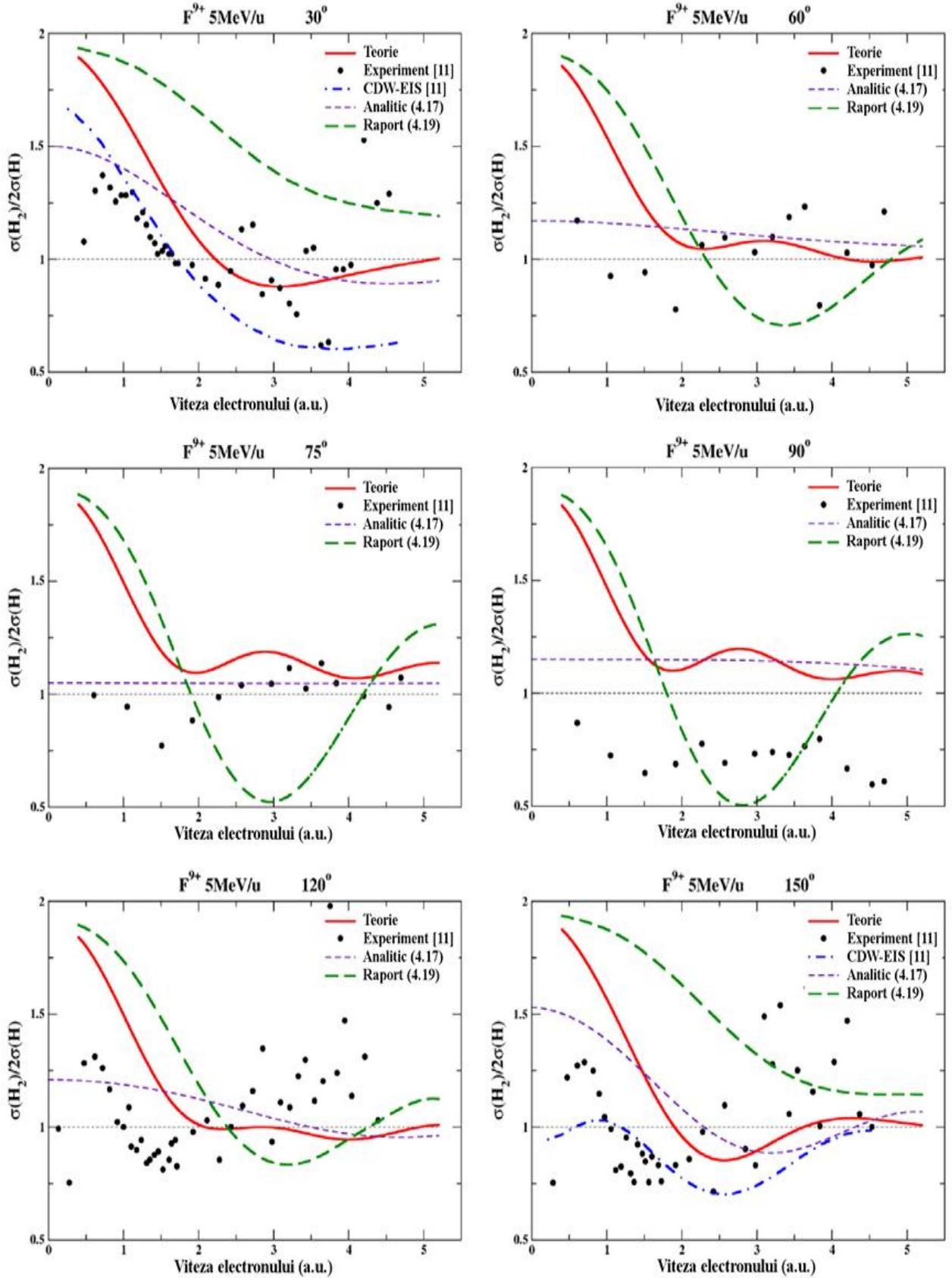


Figure 4.4. Same as Figure 4.2 but for F^{9+} projectiles with 5 MeV/u energy.

4.3. Conclusions

We have performed calculations for the ionization of the H_2 molecule by fast ion impact (F^{9+} , Kr^{33+} , and Kr^{34+}), focusing mainly on the interference effects, due to the two-center character of the target molecule. The results obtained for the differential cross sections are in good agreement with the experimental data [1, 11], mainly at low ejection angles.

We have highlighted the interference effects due to coherent electron emission in the vicinity of the two nuclei, by graphical representation of the differential cross section, as a function of the ejected electron energy (fig. 4.1 and 4.3), and of the cross section ratio, as a function of the electron velocity (fig. 4.2 and 4.4), for different ejection angles. The difference between the $2H$ atomic differential cross sections and of the hydrogen molecule, especially for lower energies, is the clear sign of the interference effects. These are much more evident from the point of view of the differential cross section ratio. Our results are in good agreement with the experimental data [1, 11] for velocities above 1.5 a.u.; for lower velocities, the correlation between electrons and second-order effects may be important. The oscillation frequency of the cross section ratio is higher than of the analytical ratio, and are in good agreement with the CDW-EIS [18, 19] results and with the experimental data [1, 11], for angles smaller than 90° .

The primary outcome of this approach can be observed for ejection angles between 60 - 120° , where the ratio of our model oscillates, while the analytical ratio (4.17), and the CDW-EIS [19] calculations do not present oscillations, having a constant value or a monotonous increase. These oscillations are also visible in experimental data [1, 11]. It is surprising that we obtain these secondary oscillations in a first-order approximation, while these were interpreted as a result of the rescattering of the ejected electron on the nuclei [7] and were attributed to the second-order effects. However, for a precise description for all secondary oscillations observed experimentally, second order effects also must be taken into account.

In order to understand the difference between the PW model, which we have applied in the previous chapter for the heteronuclear HeH^+ molecule, and our, more advanced theoretical model, used to investigate interference effects of the H_2 homonuclear molecule, it is advisable to compare the two models in the light of the obtained results.

In both models, we used a first-order and independent electron approximation, but with different final wave functions. In the PW model, the final wave function, given by the relationship (3.2), is a plane wave. In the other model, the final wave function is improved (4.6), with two centers, located in the nuclei of the H_2 molecule. These significant changes have led to a more precise formula of the molecular differential cross section (4.13). Comparisons performed between the two models, using Figures 4.1, reveal that not only the values of the differential cross section and of the differential cross section ratio but also the frequency of the oscillations are closer to the experimental data [1, 11] than the results of the PW model.

The PW model, which we applied for the HeH^+ molecular ion, we used the approximation for fast electrons, which allowed subsequent analytical evaluation of the theoretical results. Consequently, these results are valid only for relatively high-velocity electrons, therefore at low-velocity electrons the results of the PW model show errors. Figure 4.1 clearly shows that at low electron energies, the results of our model compared to the PW model are more precise.

In conclusion, we can note that the better description of the final state – as expected – has led to more accurate results. According to the above, we can affirm that our theoretical model used to describe the interference effects for the H_2 molecule is more precise than the PW model, which we applied for the heteronuclear molecular ion.

Final conclusions

In the present thesis, we have studied and presented the interference effects in the ionization of homonuclear and heteronuclear diatomic molecules, by fast ion impact for different emission angles of the electrons. Oscillations caused by the bi-centric character of the diatomic molecules can be observed in the differential cross section ratio, as a function of the electron velocity.

For the description of the electron emission, we applied the semi-classical approximation, according to which the projectile was approached with classical physics formulas and the target electrons with formalisms of quantum mechanics. We considered that the interaction between the projectile and the target particle is a perturbation, and thus we calculated the differential cross section.

We have presented two theoretical models: one for the HeH^+ heteronuclear molecular ion and the other one for the H_2 homonuclear molecule. In the first case, for the HeH^+ molecule, we have applied the model developed for the hydrogen molecule by Nagy [3]. We have identified the interference effects by representing the differential cross section ratio, as a function of the ejected electron's velocity. Our results agree with those of Tachino [28], both in terms of value and of the frequency and amplitude of the oscillations. We have also compared our results with those of the H_2 homonuclear molecule of Nagy [3]. Our results show an agreement in the frequency of oscillations, but - as expected - the amplitudes of the heteronuclear molecule are smaller than of the homonuclear one.

In the second part of our research, we developed a new, more advanced theoretical model with a more precise description of the final state, for the presentation of the interference effects in the ionization of the hydrogen molecules by the ionic impact. The changes made have determined a more precise formula of the molecular differential cross section. We performed calculations for the ionization of the H_2 molecule, for impact with fast F^{9+} , Kr^{33+} , and Kr^{34+} ions, mainly focusing on the interference effects, due to the two-center character of the target. As expected, our results are in good agreement with experimental data and with the results of other theoretical models. The most important result of this model is for the emission near the 90°

angle. While other models show an almost total suppression of oscillations, our model reproduces partly these oscillations, which can be seen in the experimental results. We have obtained these oscillations in a first-order approximation, although so far it has been assumed that these are the consequences of the rescattering of the ejected electron on the nuclei [7], namely they were assigned to the second-order effects. However, for a precise description of all secondary, experimentally observed oscillations, second-order effects should also be considered.

We compared the results of the two models along with the experimental data [1, 11], for the H_2 molecule. The results of our more advanced model are closer to the experimental ones, than those of the first model [3], both for the differential cross section and for the differential cross section ratio. In the first model, where the approximation for fast electrons was used, according to which only electrons with relatively high velocities were considered, the results for velocities under 1.5 a.u. are imprecise. At these energies, the results of our more advanced model are more precise, but, in the same time, differ from the experimental ones, because of the second-order effects - which at small energies become more important - have not been taken into account. Of course, for more precise results, these effects have to be taken into consideration.

With these results, we will contribute to a deeper understanding of the interference effects in the ionization of homo-, and heteronuclear diatomic molecules.

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