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Nuclear Instruments and Methods in Physics Research B 233 (2005) 293–297

NIM B
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Interference effects in the differential ionization cross-section of H_2 by H^+ impact

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Available online 24 May 2005

Abstract

Interference effects occurring in the ionization of H_2 by proton impact, observed experimentally by Hossain et al. [Nucl. Instr. and Meth. B 205 (2003) 484] are investigated theoretically. Model calculations are presented also for the additional oscillatory pattern characterized by frequency doubling that has been observed recently by Stolterfoht et al. [Phys. Rev. A 69 (2004) 012701]. In the model the ejected electron rescatters on the two nuclei of H_2, producing the additional oscillations.

PACS: 34.50.Fa

Keywords: Ionization; Hydrogen molecule; Interference effect

In the last few years there have been reported numerous experimental and theoretical studies of the interference effects occurring in the ionization of the hydrogen molecule. It has been observed that the $\sigma(H_2)/2\sigma(H)$ cross-section ratio has an oscillatory character as a function of the velocity of the ejected electron. These oscillations are similar to those of the Young-type two-slit experiment, in this case the sources of the coherent emission being the two nuclei of the hydrogen molecule. The effect was first predicted by Cohen and Fano [1] for the photoionization. Stolterfoht et al. reported experimental results for Kr^{34+} [2], Kr^{33+} [3] projectiles on H_2 target, while Hossain et al. used H^+ projectile in their experiments for the same target [4,5]. Several theoretical investigations have been dealing with the interference effects in the electron ejection from the hydrogen molecule by heavy-ion impact [6,8,7] and photoionization [9,10]. Recently Stolterfoht et al. observed an additional oscillating pattern characterized by a frequency doubling [11].

The present paper provides theoretical results for the interference effects observed in the

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0168-583X/$ - see front matter © 2005 Published by Elsevier B.V.
doi:10.1016/j.nimb.2005.03.124

differential ionization cross-section of the hydrogen molecule by proton impact. The same theory is used as in our previous paper [6]. The calculations are based on the impact parameter formulation. In our previous paper we calculated the transition amplitude using first-order perturbation theory, and approximated the final state by a plane wave. Thus we have reproduced theoretically the presence of the interference pattern in the ionization of the hydrogen molecule by fast charged projectiles, and have predicted its dependence on the ejection angle. However, there are some features observed in the experiments that remained unexplained by our first-order calculations. One of these features is the frequency doubling mentioned above. We assume that the higher frequency oscillations can be explained by taking into account the two-center character of the final-state wavefunction. In this work we calculated a second-order transition amplitude in order to examine this assumption. This amplitude physically describes a two-step (double scattering) process. In the first step one of the electrons of H_2 is ejected by the projectile–electron interaction. In the second step the ejected electron rescatters on the two nuclei of H_2, approximating the two-center feature of the exact continuum wavefunction.

In the following we investigate the double scattering of the electron in detail. First, the electron undergoes a transition from the initial state (the ground state of the H_2) $\Psi_i(\mathbf{r}, D)$, caused by the interaction $V(t')$ with the fast charged projectile, to an intermediate state. Second, it is scattered by the nuclei via the interaction with the two nuclei, W, going to the final state $\Psi_{\mathbf{k}}(\mathbf{r})$. As explained in [12] the second-order amplitude may be written as follows

$$a^{(2)} = -\frac{\pi}{v_{\rm p}} \int K \,\mathrm{d}\widehat{\mathbf{K}} \int_{-\infty}^{+\infty} \mathrm{d}Z \langle \Psi_{\mathbf{k}} \mid W \mid \Psi_{\mathbf{K}} \rangle \mathrm{e}^{\mathrm{i}qZ} \langle \Psi_{\mathbf{K}} \mid V(Z) \mid \Psi_i \rangle. \tag{1}$$

Here $v_{\rm p}$ is the velocity of the projectile, $Z = v_{\rm p}t$, $q = (E_k - E_i)/v_{\rm p}$. $\mathbf{K}$ and $\mathbf{k}$ are the momenta of the electron in the intermediate and final state, respectively. In our model the latter states, $\Psi_{\mathbf{K}}$ and $\Psi_{\mathbf{k}}$, are approximated by plane waves. The initial state of the electron is taken as a linear combination of two hydrogenlike 1s atomic orbitals:

$$\Psi_i(\mathbf{r}) = N(\mathrm{e}^{-\alpha r_a} + \mathrm{e}^{-\alpha r_b}) \tag{2}$$

with N denoting a normalization factor, α the effective charge. r_a and r_b are the distances between the electron and the two nuclei of the hydrogen molecule

$$\mathbf{r_a} = \mathbf{r} + \frac{\mathbf{D}}{2}, \qquad \mathbf{r_b} = \mathbf{r} - \frac{\mathbf{D}}{2}, \tag{3}$$

$\mathbf{D}$ being the vector associated to the internuclear distance.

The interaction of the ejected electron with the nuclei can be written as

$$W = -\frac{1}{r_a} - \frac{1}{r_b}. \tag{4}$$

In order to avoid divergence due to the use of plane waves, the Coulomb potential is replaced by a Yukawa potential

$$W = -\frac{\mathrm{e}^{-\eta r_a}}{r_a} - \frac{\mathrm{e}^{-\eta r_b}}{r_b}. \tag{5}$$

Introducing (5) into expression (1) and calculating the matrix element of W, one obtains

$$a^{(2)} = \frac{1}{\pi v_{\rm p}} \int K \,\mathrm{d}\widehat{\mathbf{K}} \frac{\cos[(\mathbf{K}-\mathbf{k})\mathbf{D}/2]}{|\mathbf{K}-\mathbf{k}|^2 + \eta^2} \times \int_{-\infty}^{+\infty} \mathrm{d}Z \,\mathrm{e}^{\mathrm{i}qZ} \langle \Psi_{\mathbf{K}} \mid V(Z) \mid \Psi_i \rangle. \tag{6}$$

The evaluation of the matrix element of the projectile–electron interaction $V(Z)$ is done using the peaking approximation [6,13] valid for large values of k. The integration along the projectile trajectory is performed as in [6].

The expression for the second-order amplitude (6) is similar to the first-order amplitude $a^{(1)}$ obtained in [6], but we have in addition an integral over the angles of the intermediate-state momentum $\widehat{\mathbf{K}}$ and the oscillating factor

$$\frac{\cos(\mathbf{QD}/2)}{\mathbf{Q}^2 + \eta^2} \tag{7}$$

with $\mathbf{Q} = \mathbf{k} - \mathbf{K}$, the momentum transfer at the rescattering. The integral of the first-order amplitude

$$\int_{-\infty}^{+\infty} \mathrm{d}Z \,\mathrm{e}^{\mathrm{i}qZ} \langle \Psi_{\mathbf{K}} \mid V(Z) \mid \Psi_i \rangle \tag{8}$$

is modulated by this factor, leading to the additional higher frequency oscillations. In general, through second-order, the transition probability may be written as $|a^{(1)} + a^{(2)}|^2 = |a^{(1)}|^2 + |a^{(2)}|^2 + 2\mathrm{Re}(a^{(1)*}a^{(2)})$, the last being the interference term. In the present calculation we have assumed that the first and second-order amplitudes are 90° out of phase. This assumption can be justified by approximating the integral (8) with its value at the maximum of the factor (7), i.e. $\mathbf{K} = \mathbf{k}$. In this case the phase difference between $a^{(1)}$ and $a^{(2)}$ is 90° , and the interference term is zero.

In order to compare our theoretical results with the experimental ones we have performed the calculations for 1, 3 and 5 MeV H^+ projectile energy, and for various electron ejection angles. In the calculations we have used $\eta = 1$. We note here that decreasing the value of η, the first maximum of the $\sigma(H_2)/2\sigma(H)$ cross-section ratio increases.

In Figs. 1–3 we have presented the ratios of cross-sections obtained for the hydrogen molecule and two independent hydrogen atoms as a function of the ejected electron velocity. The sum of the second- and first-order results along the first-order results and the experimental data are shown for three different projectile energies and for 30°, 60°, 90° and 150° ejection angles [4,5]. As is seen, the inclusion of the second-order amplitude in the calculations enhances the cross-section ratio at small electron velocities. Furthermore, for angles other than 90° the second-order results show higher frequency oscillations.

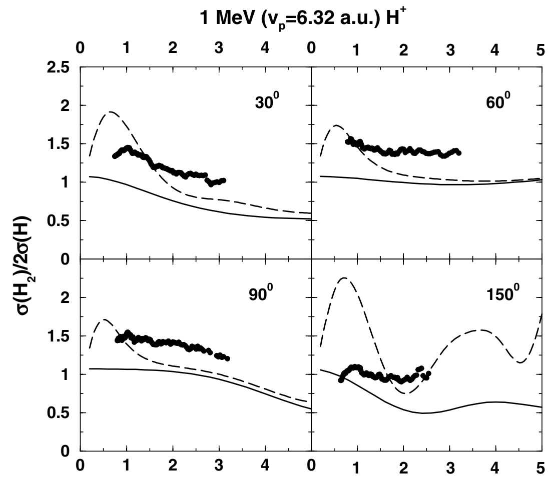

Fig. 1. $\sigma(H_2)/2\sigma(H)$ cross-section ratios as a function of the ejected electron velocity for ionization of H_2 by 1 MeV protons at 30°, 60°, 90° and 150° electron ejection angles. Solid lines represent first-order results, dashed lines the sum of first- and second-order results, and dots stand for the experimental data [5].

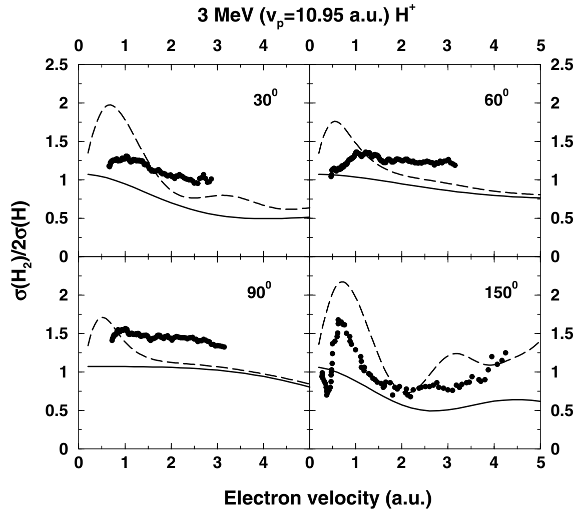

Fig. 2. The same as Fig. 1, but for 3 MeV potons. The experimental data are from [5] for 30°, 60° and 90° ejection angle, and from [4] for 150°.

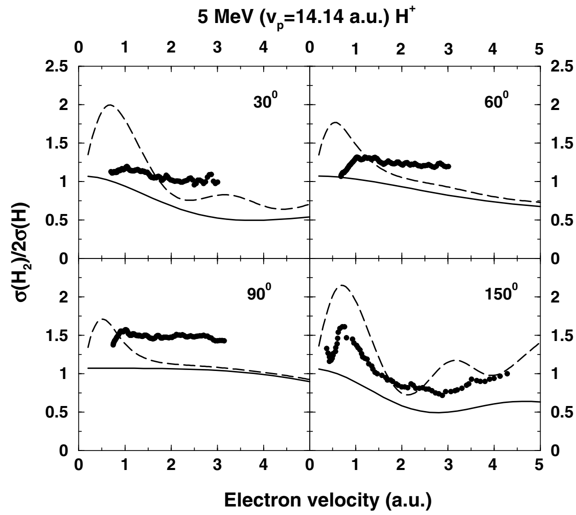

Fig. 3. The same as Fig. 2, but for 5 MeV protons.

The dependence of the calculated first-order ratios on the electron velocity is similar to that of the experimental ones. However, comparison with the experiment is not conclusive. Except for 150° ejection angle at 3 and 5 MeV projectile energy, the experiments do not show the characteristic oscillations that can be seen for other projectiles [2,3]. Experimental points for higher velocities are missing, and only part of the oscillations can be observed. Furthermore, the 'experimental' ratio is calculated using the experimental data for molecules, while the theoretical ones were calculated for atoms. This procedure may shift the absolute value of these ratios, as we have discussed in our previous paper [6]. From the comparison with these experimental data it is not clear the improvement of the results when using the second-order theory.

Our second-order model in its present stage seems to overestimate the cross-section ratios. A possible reason for that is the use of perturbational method, instead of using correct, two-center final wavefunctions. Our goal at this step was to give an analytic description of the features observed, and not exact quantitative predictions. Our method leads to an additional oscillation with doubled frequency relative to the first-order one at 0°. The frequency of the oscillations does not agree with the experimental findings.

The $\sigma(H_2)/2\sigma(H)$ cross-section ratio depends on the projectile velocity through the minimum momentum transfer $q = \Delta E/v_p$. In order to evidence this dependence, in Fig. 4 we have plotted the cross-section ratio calculated in first-order for various electron ejection angles, and for 6.32, 10.95 and 14.14 a.u. projectile velocities (corresponding to 1, 3 and 5 MeV proton energies, respectively).

The differential cross-section ratios as a function of the perpendicular and parallel component of the ejected electron velocity relative to the projectile trajectory are plotted in Fig. 5. One can see a sharp maximum of the cross-section ratio on the place of the binary encounter peak (for $k_{\|} = q$, $k_{\|}$ being the parallel component relative to the projectile trajectory of the ejected electron momentum, see Eq. (22) in [6]).

In conclusion we can say that our theoretical model reproduces the interference effects in the differential ionization cross-section for for proton impact. The dependence of the interference pattern on the projectile velocity has been investigated. The second-order calculations reproduces qualitatively

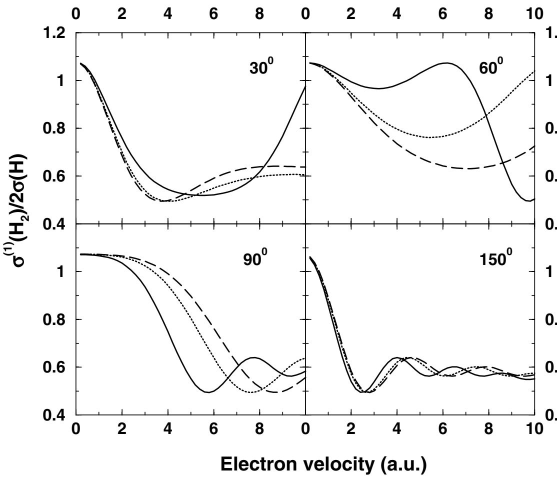

Fig. 4. First-order theoretical results for $\sigma(H_2)/2\sigma(H)$ cross-section ratios as a function of the ejected electron velocity for ionization of H_2 at 30°, 60°, 90° and 150° electron ejection angles. Solid lines represent results for 1 MeV protons, dotted lines for 3 MeV protons, and dashed lines for 5 MeV protons.

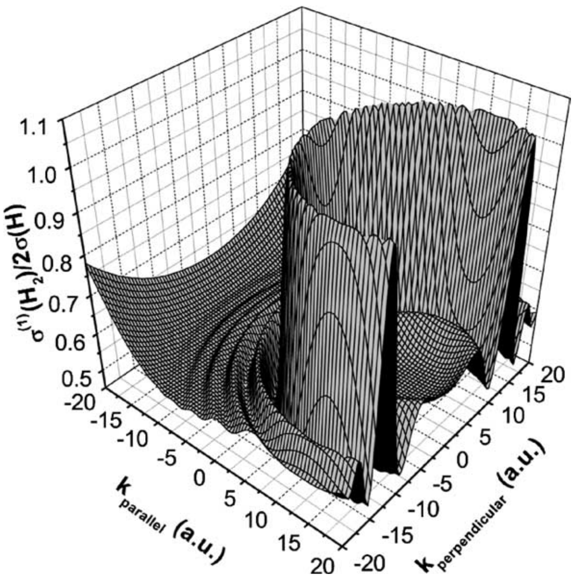

Fig. 5. First-order theoretical results for $\sigma(H_2)/2\sigma(H)$ cross-section ratios as a function of the perpendicular and parallel component of the ejected electron velocity relative to the projectile beam for ionization of H_2 by 5 MeV protons.

the enhancement of the cross-section ratio at low electron velocities, and the appearance of additional, higher frequency oscillations relative to the first-order predictions. Quantitative agreement needs improvement.

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