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$(e,2e)$ ionization of $H_2{}^+$ by fast electron impact: Application of the exact nonrelativistic two-center continuum wave

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The multiply differential cross section of the dissociative ionization of $H_2{}^+$ by fast (2 keV) electron impact is determined theoretically using a two-center continuum wave function constructed using the exact solutions of the separable two-center Schrödinger equation in prolate spheroidal coordinates for the slow (50 eV) ejected electron. The comparison of the results to those obtained by approximate approaches, like those using an effective center Coulomb wave or Pluvinage-type two-center wave or the wave packet evolution approach, shows the limits of these approximate methods. Additionally, the variation of the sevenfold differential cross section, which corresponds to the ionization of aligned molecules, reveals interesting mechanisms and gives some insight into the optimal conditions for the dissociative ionization of more complex diatomic targets.

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I. INTRODUCTION

The dissociative ionization of diatomic molecules is the object of growing interest, especially in the domain of atomic collisions, because of the rapid development of a variety of coincidence detection techniques [1–5]. These techniques measure the momenta of the emerging fragments, such as the residual ions and the electrons, and deduce by coincidence counting the corresponding multiply differential cross sections. Studying these cross sections can deliver precious information about the electronic structure, the mechanism of the fragmentation process, and the influence of the molecular alignment.

In the particular domain of $(e,2e)$ collisions, which corresponds to ionization by electron impact with coincidence detection of the two emerging electrons, diatomic targets are less frequently studied than atomic ones [6], especially in the theoretical domain, in spite of the fact that gases exist naturally in diatomic molecular form. This can be explained by the fact that theoretically the construction of a wave describing a free electron in the field of two fixed centers is a somewhat difficult task. Usually, the description of the ejected slow electron is realized by one-center continuum wave functions in the form of partial wave development [7–9] or of a closed Coulomb wave judiciously centered [10,11] on the center of the diatomic molecule or on the nuclei.

The simple $(e,2e)$ ionization of $H_2{}^+$ is one of the rare experimental situations, with (γ,e) on $H_2{}^+$, where a free electron with measurable wave vector $\mathbf{k}_e$ is found in the field of two positively charged nuclei which can reasonably be considered as fixed. From this point of view this unique physical situation can serve as an excellent test for different theoretical models concerning this basic problem. In the past, many attempts have been made to find a proper approximation for the description of this electron. Joulakian *et al.* [12] used an approximate wave function inspired by the Pluvinage model [13] constructed as the product of two Coulomb functions centered on the nuclei. Serov *et al.* [14], on the other hand, followed a completely different method by numerically solving the Schrödinger equation with a wave packet evolution approach. The fact that for the Coulomb potential the two-center Schrödinger equation is separable in prolate spheroidal coordinates [15–17], and thus gives exact analytical or numerical solutions, is very rarely exploited in real physical situations involving two-center continuum electrons [18]. To our knowledge, in simple $(e,2e)$ ionization, the partial wave development in prolate spheroidal exact solutions for the description of the slow ejected electron in the field of two fixed nuclei has not yet been realized. The aim of our paper is to determine and study the multiply differential cross section of this process, see the limits of the validity of the other existing approximate models, and explore physically interesting situations for experimental applications.

In what follows we will present briefly our numerical approach to the basic two-center Schrödinger equation in prolate spheroidal coordinates; then we will introduce our partial wave development into the transition matrix element of the $(e,2e)$ ionization of aligned $H_2{}^+$ systems. In Sec. V we will compare the variation of the sevenfold differential cross section obtained by these exact solutions to recent results cited above.

II. THE TWO-CENTER PROBLEM

We begin this section by presenting the solution of the Schrödinger equation of an electron in the field of two fixed Coulomb centers:

$$(\hat{H}_0 - E)\psi(\mathbf{r}) = 0 \tag{1}$$

with

$$\hat{H}_0 = -\frac{1}{2}\Delta_{\mathbf{r}} - \frac{Z_a}{|\mathbf{r}-\mathbf{R}/2|} - \frac{Z_b}{|\mathbf{r}+\mathbf{R}/2|}. \tag{2}$$

The wave function of the two-center problem with charges Z_a and Z_b separated by a distance R can be factored into the form [17,19]

$$\psi_{Eml}(\xi,\eta,\varphi) = T_{ml}(c,\xi)S_{ml}(c,\eta)\frac{\exp(im\varphi)}{\sqrt{2\pi}} \tag{3}$$

where $\xi \in [1,\infty)$, $\eta \in [-1,-1]$, and $\varphi \in [0,2\pi)$ are the prolate spheroidal coordinates. We put the charge Z_a in the left focus $(\xi=1, \eta=-1)$ and the charge Z_b in the right focus $(\xi=1, \eta=1)$. The functions $T_{ml}(c,\xi)$ and $S_{ml}(c,\eta)$ are solutions of the following system of equations obtained by the separation of the two-center Hamiltonian:

$$\left[\frac{d}{d\xi}(\xi^2-1)\frac{d}{d\xi} + RZ_+\xi - \frac{m^2}{\xi^2-1} + c^2\xi^2 + A\right] \times T_{ml}(c,\xi) = 0, \tag{4}$$

$$\left[\frac{d}{d\eta}(1-\eta^2)\frac{d}{d\eta} + RZ_-\eta - \frac{m^2}{1-\eta^2} - c^2\eta^2 - A\right] \times S_{ml}(c,\eta) = 0. \tag{5}$$

Here, $c = \sqrt{ER^2/2}$, m is the eigenvalue of the projection of the angular momentum operator on the internuclear axis $\mathbf{R}$, and $A = -\lambda - (R^2/2)E$ represents the eigenvalue of the constant of separation. The integer l identifies the eigenvalues λ of the angular operator. These eigenvalues tend to $l(l+1)$ for $\mathbf{R} \to \mathbf{0}$. Finally, $Z_+ = Z_a + Z_b$ and $Z_- = Z_b - Z_a$.

We suppose that $|T_{ml}(c,1)| < +\infty$, $|S_{ml}(c,\pm 1)| < +\infty$, and express the asymptotic behavior for $\xi \to +\infty$ of the function $T_{ml}(c,\xi)$ in the form

$$T_{ml}(c,\xi) \to \frac{1}{c\xi}\sin\left(c\xi + \frac{a}{2c}\ln(2c\xi) - \frac{l\pi}{2} + \delta_{ml}\right), \tag{6}$$

where $a = RZ_+$ and δ_{ml} is the phase shift of the radial function.

III. NUMERICAL SOLUTION OF THE SPHEROIDAL EQUATIONS

We begin by the following transformation [20,23] in Eq. (4):

$$Y(\eta) = (1-\eta^2)S_{ml}(c,\eta),$$

which permits us to write

$$\left[(1-\eta^2)\frac{d^2}{d\eta^2} + 2\eta\frac{d}{d\eta} + \frac{2(1+\eta^2)}{1-\eta^2} + RZ_-\eta - \frac{m^2}{1-\eta^2} - c^2\eta^2 - A\right]Y(\eta) = 0, \tag{7}$$

with the new boundary conditions

$$Y(-1) = 0, \quad Y(1) = 0, \tag{8}$$

and the normalization condition

$$\int_{-1}^{1} Y^2(\eta)d\eta - 1 = 0. \tag{9}$$

For a given value of the energy E we can find the numerical value of A. We solve Eqs. (7)–(9) for the quasiangle function $Y(\eta)$ and A by using the continuous analog of the Newton method and a finite-difference scheme of fourth order.

Similarly, we apply in Eq. (5) the following transformation [20]:

$$X(\xi) = (\xi-1)T_{ml}(c,\xi),$$

and write for $X(\xi)$ the equation

$$\left[(\xi^2-1)\frac{d^2}{d\xi^2} - 2\xi\frac{d}{d\xi} + \frac{2}{\xi-1} + RZ_+\xi - \frac{m^2}{\xi^2-1} + c^2\xi^2 + A\right]X(\xi) = 0, \tag{10}$$

with the new boundary condition

$$X(1) = 0 \tag{11}$$

and the asymptotic

$$X(\xi) \to \frac{1}{c}\sin\left(c\xi + \frac{a}{2c}\ln(2c\xi) - \frac{l\pi}{2} + \delta\right), \quad \xi \to +\infty. \tag{12}$$

Using the modified analog of the Newton method [21] we look for $\xi_{max} \gg 2\pi/c$ such that

$$X(\xi_{max}) = 0 \tag{13}$$

for a given value E^* of the energy. We begin with $E^{(0)}$, which may be different from the given value $E^* > 0$, and fix the point $\xi_{max}^{(0)}$ such that $X(\xi_{max}^{(0)}) = 0$. To close the system we introduce the artificial normalization condition

$$\int_1^{\xi_{max}} X^2(\xi)d\xi=1. \tag{14}$$

The eigenvalue problem Eqs. (10)–(14) is solved with the help of the continuous analog of the Newton method and a finite-difference scheme of fourth order. The next approximation is calculated by the relation

$$\xi_{max}^{(1)}=\xi_{max}^{(0)}+\frac{\Delta E^{(0)}}{E^*}\xi_{max}^{(0)},$$

$$\xi_{max}^{(k+1)}=\frac{\xi^{(k)}\Delta E^{(k)}-\xi^{(k-1)}\Delta E^{(k-1)}}{\Delta E^{(k)}-\Delta E^{(k-1)}},$$

where $\Delta E^{(k)}=E^{(k)}-E^*$. The iteration process is stopped when $|E-E^*|<\varepsilon$, the desired precision.

The phase δ_{ml} is calculated by the formula

$$\delta_{ml}(\xi_{max})=\pi j-\left(c\xi_{max}+\frac{a}{2c}\ln(2c\xi_{max})-\frac{l\pi}{2}\right),$$

where j is even for $X(\xi_{max}-h)<0,\ h\ll 2\pi/c$, or odd for $X(\xi_{max}-h)>0$. The magnitude of j is chosen so as to keep the phase δ in the interval $[0,2\pi)$. Taking into account the asymptotic correction $\Delta\delta$,

$$\Delta\delta_{ml}(\xi_{max})=\sum_{i=2}^{\infty}\frac{w_i}{i-1}\left(\frac{1}{\xi_{max}}\right)^{i-1},$$

with w_i the coefficients of the expansion of the potential $V^{1/2}(\xi)$ [22],

$$V^{1/2}(\xi)=\sum_{i=0}^{\infty}w_i\left(\frac{1}{\xi}\right)^i,$$

$$V(\xi)=\frac{A}{\xi^2-1}+\frac{RZ_+\xi}{\xi^2-1}+\frac{ER^2}{2}\frac{\xi^2}{\xi^2-1}+\frac{1-m^2}{(\xi^2-1)^2},$$

in power series, we obtain the value of the phase

$$\delta_{ml}=\delta_{ml}(\xi_{max})+\Delta\delta_{ml}(\xi_{max}).$$

IV. THE MULTIPLY DIFFERENTIAL CROSS SECTION OF IMPACT IONIZATION OF $H_2{}^+$

We start from the usual expression for the amplitude of transition between an initial and final state given by the first term of the Born series in which the fast incident and scattered electrons are described by plane waves:

$$f_{fi}(\mathbf{K},\Omega_R)=-\frac{1}{2\pi}\int d\mathbf{r}_0\int d\mathbf{r}\Psi_f^*(\mathbf{r})\times\exp(i\mathbf{K}\cdot\mathbf{r}_0)\frac{1}{|\mathbf{r}-\mathbf{r}_0|}\Psi_i(\mathbf{r}). \tag{15}$$

The direction of the quantization axis of the diatomic molecule is defined by the polar θ_R and the azimuthal φ_R angles designated in compact notation by the solid angle Ω_R with respect to the laboratory frame of reference. $\mathbf{K}=\mathbf{k}_i-\mathbf{k}_s$ defines the momentum transfer, with $\mathbf{k}_i$ and $\mathbf{k}_s$ the wave vectors of the incident and scattered electrons, respectively. Integrating over the coordinates of the fast incident electron $\mathbf{r}_0$ by application of the relation

$$\int\frac{d\mathbf{r}_0}{|\mathbf{r}-\mathbf{r}_0|}\exp(i\mathbf{K}\cdot\mathbf{r}_0)=\frac{4\pi}{K^2}\exp(i\mathbf{K}\cdot\mathbf{r}), \tag{16}$$

we obtain

$$f_{fi}(\mathbf{K},\Omega_R)=-\frac{2}{K^2}\int d\mathbf{r}\Psi_f^*(\mathbf{r})\exp(i\mathbf{K}\cdot\mathbf{r})\Psi_i(\mathbf{r}). \tag{17}$$

Here $\Psi_i(\mathbf{r})$ represents the wave function of the molecular electron in its initial bound state. $\Psi_f(\mathbf{r})=\Psi^-_{\mathbf{k}_e}(\mathbf{r})$, on the other hand, represents the wave function of the ejected electron having wave vector $\mathbf{k}_e$. Now $\Psi^-_{\mathbf{k}_e}(\mathbf{r})$ is a solution of Eq. (1) with Coulomb wave asymptotics at $r\to\infty$,

$$\Psi^-_{\mathbf{k}_e}(\mathbf{r})\ \to(2\pi)^{-3/2}\times\exp\left\{i\mathbf{k}_e\cdot\mathbf{r}-\frac{iZ_+}{k_e}\ln(k_er+\mathbf{k}_e\cdot\mathbf{r})\right\}. \tag{18}$$

The construction of $\Psi^-_{\mathbf{k}_e}(\mathbf{r})$ and $\exp(i\mathbf{K}\cdot\mathbf{r})$ in spheroidal coordinates with the above solutions of the separable Schrödinger equation will be done in the following way. We introduce first the spheroidal harmonics which will be given like spherical harmonics in the form

$$\Upsilon_{lm}(c,\theta,\varphi)=S_{ml}(c,\cos\theta)\frac{\exp(im\varphi)}{\sqrt{2\pi}}. \tag{19}$$

With this definition $\Upsilon_{lm}(c\to 0,\theta,\varphi)=Y_{lm}(\theta,\varphi)$. The expansion of the plane wave [19] can be written as

$$\exp(i\mathbf{K}\cdot\mathbf{r})=4\pi\sum_{m=-\infty}^{\infty}\sum_{l=|m|}^{\infty}\Upsilon^*_{lm}(c_0,\theta_{KR},\varphi_{KR})\times i^l\Upsilon_{lm}(c_0,\theta,\varphi)je_{ml}(c_0,\xi). \tag{20}$$

Here θ_{KR} and φ_{KR} are the angles between the molecular axis and the direction of $\mathbf{K}$, and $c_0=KR/2$. $S_{ml}(c_0,\eta)$ and $je_{ml}(c_0,\xi)$ are, respectively, solutions of the quasiangular and quasiradial equations for $Z_b=Z_a=0$ having the asymptotic behavior

$$je_{ml}(c,\xi\to\infty)=\frac{1}{c\xi}\sin\left(c\xi-\frac{\pi}{2}l\right). \tag{21}$$

Similarly,

$$\Psi^-_{\mathbf{k}_e}(\mathbf{r})=(2\pi)^{-3/2}4\pi\sum_{m=-\infty}^{\infty}\sum_{l=|m|}^{\infty}\Upsilon^*_{lm}(c_e,\theta_{eR},\varphi_{eR})$$

$$\times i^{l}e^{-i\delta_{ml}}\Upsilon_{lm}(c_e,\theta,\varphi)T_{ml}(c_e,\xi), \tag{22}$$

where $c_e=k_eR/2$, and θ_{eR} and φ_{eR} give the direction of $\mathbf{k}_e$ in the molecular coordinate system whose Z axis coincides with the internuclear axis. Here $T_{ml}(c_e,\xi)$ are solutions of the quasiradial equation for an electron in the field of two nuclei with $Z_a=Z_b=1$ and they satisfy the asymptotic condition (6). The initial state wave function representing the fundamental $1\sigma_g$ state of $\mathrm{H_2}^+$ will also be given by the solution of the above Schrödinger equation for the equilibrium distance corresponding to $R=2$ a.u.:

$$\Phi_{1\sigma_g}(\mathbf{r})=\frac{1}{\sqrt{2\pi}}\phi_{1\sigma_g}(\xi)S_{00}(c_b,\eta). \tag{23}$$

Now the above wave functions are defined in the molecular frame with the quantization z axis on the internuclear axis of the molecular target, whose direction in the laboratory frame is given by $\Omega_R(\theta_R,\varphi_R)$. In what follows we will choose the laboratory frame of reference such that its z axis coincides with the direction of incidence, i.e., $\mathbf{k}_i$, and the xOz plane with that formed by the two vectors $\mathbf{k}_s$ and $\mathbf{k}_i$. Performing the necessary rotational transformations on the wave vectors, we can write the scattering amplitude for a given Ω_R as

$$f(\mathbf{K},\mathbf{k}_e,\Omega_R)=-\frac{2}{K^2}\langle\Psi^-_{\mathbf{k}_e}|\exp(i\mathbf{K}\cdot\mathbf{r})|\Phi_{1\sigma_g}\rangle. \tag{24}$$

Replacing the different terms by their expressions (22) and (20) we can write Eq. (24) in terms of sums of products of one-dimensional integrals:

$$f(\mathbf{K},\mathbf{k}_e,\Omega_R)=-\frac{8}{K^2}\sum_{m=-\infty}^{\infty}\sum_{l=|m|}^{\infty}\sum_{l'=|m|}^{\infty}\Upsilon^*_{lm}(c_e,\theta_{eR},\varphi_{eR})$$
$$\times\Upsilon^*_{l'-m}(c_0,\theta_{KR},\varphi_{KR})i^{l'-l}e^{i\delta_{ml}}A_{mll'}, \tag{25}$$

with

$$A_{mll'}=\frac{R^3}{8}\int_1^\infty\int_{-1}^{1}(\xi^2-\eta^2)d\xi d\eta\, Q(\xi)P(\eta), \tag{26}$$

where

$$Q(\xi)=T_{ml}(c_e,\xi)je_{ml'}(c_0,\xi)\phi_{1\sigma_g}(\xi),$$

$$P(\eta)=S_{ml}(c_e,\eta)S_{ml'}(c_0,\eta)S_{00}(c_b,\eta).$$

Finally, the multiply differential cross section of the ionization of $\mathrm{H_2}^+$ by a fast electron for given incidence and ejection energy values E_i and E_e, respectively, and for given directions of the scattering $\Omega_s(\theta_s,\varphi_s)$, ejection $\Omega_e(\theta_e,\varphi_e)$, and molecular alignment $\Omega_R(\theta_R,\varphi_R)$, is given by

$$\sigma(E_i,E_e,\Omega_R,\Omega_s,\Omega_e)=\frac{k_ek_s}{k_i}|f(\mathbf{k}_i-\mathbf{k}_s,\mathbf{k}_e,\Omega_R)|^2. \tag{27}$$

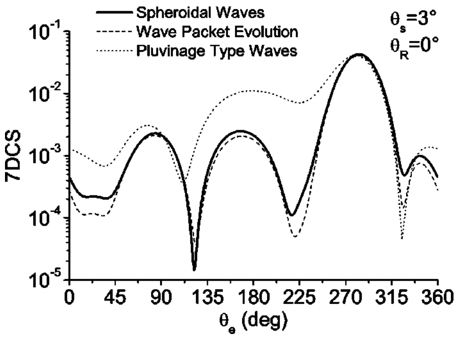

FIG. 1. Sevenfold differential cross section (7DCS) versus ejection angle θ_e for fixed scattering and molecular axis angles $\theta_s=3°$ and $\theta_R=0°$, calculated by different methods: present approach (solid line), WPE approach (dashed line), and PTCC approach with two-parametric variational bound state (dotted line).

V. RESULTS

In what follows we will consider situations where the internuclear axis and the directions of incidence, scattering, and ejection are all in the same plane. For comparison with recent results we will fix the energy value of the ejected electron to 50 eV, and that of the incident electron to 2 keV, for which its description by a plane wave is justified. Before using our procedure on $\mathrm{H_2}^+$, we verified it for zero nuclear charge, i.e., by considering $Z_a=Z_b=0$ in the calculation of the final state spheroidal functions. In this case the final state wave function can be given simply be a plane wave, rendering the determination of the transition amplitude in Eq. (24) very simple. Once we obtained the same numerical values by our procedure and the analytical formula, we could pass to the comparison of our results for a real physical situation $Z_a=Z_b=1$ to those obtained by the wave packet evolution (WPE) approach [14], which gives very reliable results in the case of small scattering angles, and to those obtained by a Pluvinage-type two-center Coulomb (PTTC) wave function [12]. Now in Figs. 1 and 2 we present, for fixed orientations of the internuclear axis $\varphi_R=0°$, $\theta_R=0°$ and 90°, respectively, the variation of the sevenfold differential cross section of the $(e,2e)$ ionization of H_2^+ in terms of the ejection angle defined with respect to the incidence direction in the case of a small scattering angle $\theta_s=3°$. We see that our results reproduce with quite good fidelity those of [14]. The small differences should be attributed to the approximation made

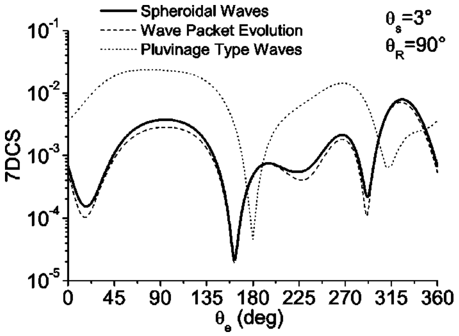

FIG. 2. The same as in Fig. 1 for molecular angle $\theta_R=90°$.

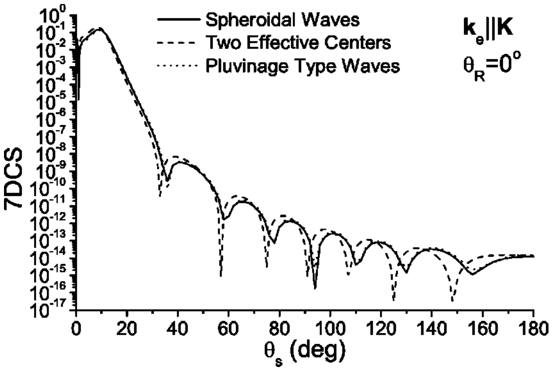

FIG. 3. Sevenfold differential cross section versus scattering angle θ_s for $\mathbf{k}_e \| \mathbf{K}$ for given molecular axis direction angle $\theta_R = 0°$: present approach (solid line), TEC approximation with one-parametric variational bound state (dashed line), and PTCC method (dotted line).

in the latter in the determination of the modulus of the momentum transfer. The agreement between these two completely different approaches, one based on the direct approximated numerical solution of the Schrödinger equation (WPE), and the present work employing an approach based on the determination of the transition matrix elements using the first term of the Born series with the exact (numerical) solutions of the two-center problem, shows as expected that the first term of the Born series that we are considering is the dominant part of this series. The comparison with the results of the PTTC method shows that good agreement is obtained only for ejection directions near the momentum transfer direction in the case $\theta_R = 0°$. This can be explained by the fact that, in contrast to the present work, the initial and final state wave functions used in [12] are not solutions of the same Hamiltonian.

We consider next in Figs. 3 and 4 the variation of the 7DCS for a fixed direction of the molecular axis $\theta_R = 0°$ and 90°, respectively, in terms of the scattering angle. In this case we compare our results to those of the PTTC method and the two-effective-centers (TEC) approximation. We see that in this case our results reproduce the same structures due to the two-center effect of the problem, which creates optical-type interferences. This shows first the feasibility of our calculations for very large momentum transfer and second that these interference structures (whose shape depends on the energy of the incident electron, the direction of the internuclear axis, and the distance between the two scattering centers) seem to be common to all types of physical processes involving two-center targets [24]. Now an eventual experimental reproduction of these minima and the structure of their distribution might be a very efficient method for the determination of the alignment of two-center targets and the incident energy of collision.

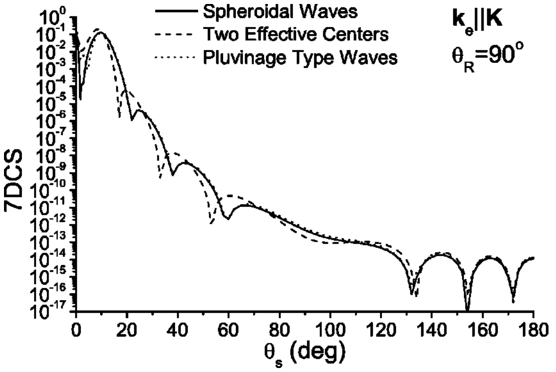

FIG. 4. The same as in Fig. 3 for molecular angle $\theta_R = 90°$.

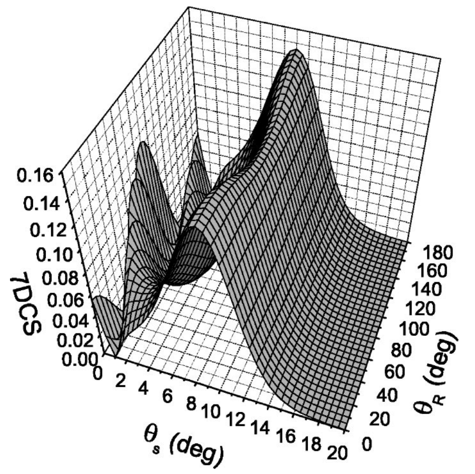

FIG. 5. Sevenfold differential cross section for ejection in the momentum transfer direction $\mathbf{k}_e \| \mathbf{K}$ versus scattering angle θ_s and molecular axis direction angle θ_R.

In Fig. 5 we present the variation of the 7DCS in terms of the orientation of the molecule θ_R and the scattering angle θ_s simultaneously. The ejection direction here is taken parallel to that of the momentum transfer, which itself (the direction) varies but very slowly with θ_s. We consider the domain of θ_s between 0° and 20°. For intermediate values of θ_s, we are in what we call the Bethe ridge region, where the momentum transfer is relatively large (>1 a.u.) and where the maximum 7DCS is obtained at zero recoil momentum of the target, for situations where the momentum transfer is equal and parallel to the momentum of the ejected electron. Now the Bethe ridge is found at $\theta_s = 9°$ for the given energy values. It is interesting to see that as expected the 7DCS is not

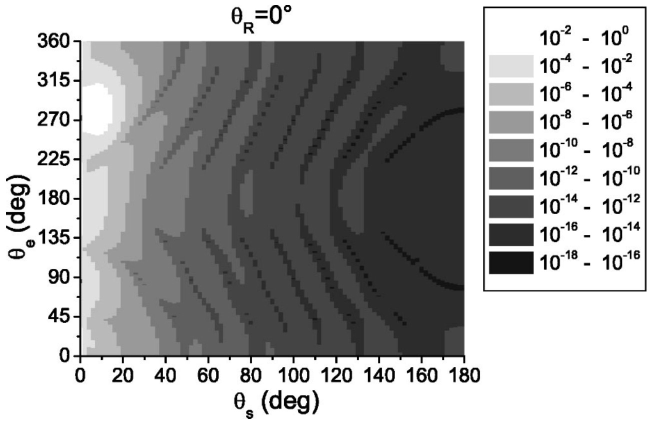

FIG. 6. Sevenfold differential cross section versus two angles θ_s and θ_e for given molecular angle $\theta_R = 0°$.

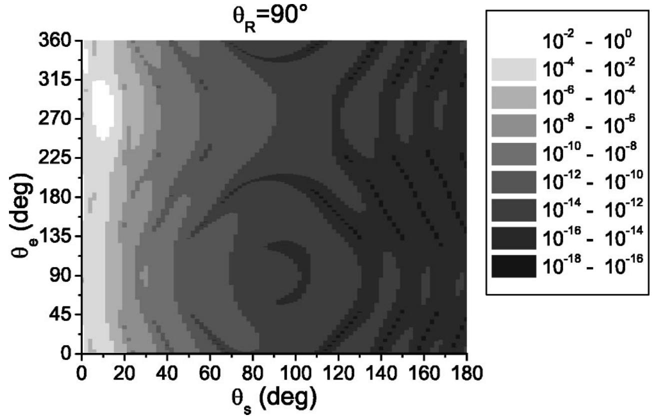

FIG. 7. The same as in Fig. 6 for $\theta_R = 90°$.

very sensitive to the variation of the orientation of the molecule θ_R. This can be explained by the fact that in the Bethe ridge region the collision between the incident and target electrons is frontal [6] and the shape of the rest of the target has only a small effect on the result of the collision. We can nevertheless observe that the maximum does not occur at constant θ_s. This means that the zero of the recoil momentum of the center of mass of the molecule is not, as in the atomic case, the most favorable situation for ionization in the momentum transfer direction.

In Figs. 6 and 7 we present a gray scale map of the 7DCS for a fixed direction of the molecular axis $\theta_R = 0°$ and 90°, respectively, in terms of the ejection and scattering angles. The regularity of the structures that one observes in these figures shows that our calculations do not have accidentally divergent points. More, the shape of the structure shows in a clear way the alignment of the molecule and the energy of the impact. These two pieces of information could be very valuable in the case of other dissociative ionization experiments on more complex diatomic targets.

VI. CONCLUSION

We have presented our procedure for the determination of the sevenfold differential cross section of the simple $(e,2e)$ ionization of H_2^+ using the exact numerical two-center wave functions for the bound and continuum states in the construction of the necessary partial wave development in the first term of the Born series of the transition matrix element. The comparison of our results to those obtained by the wave packet evolution method and using Pluvinage-type two-center continuum wave functions shows the feasibility of this type of calculation and confirms the results of the WPE method for small scattering angles. For large scattering angles our results reproduce the optical structures obtained by the PTTC approach. These structures seem to be independent of the wave functions used and common to all types of collision process on diatomic targets. Our work opens the way for wider application in other processes, like electron capture and photoionization on more complex diatomic systems, of the spheroidal waves developed in this work.

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