

Two-effective center approximation for the single ionization of molecular hydrogen by fast electron impact

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The triple differential cross section (3DCS) for the $(e,2e)$ ionization of diatomic hydrogen is determined using the first-order transition matrix element of the Born series. A two-effective center continuum wave function which takes into account the diatomic character of the target is introduced to describe the ejected electron in the exit channel. Vertical transitions from the equilibrium position of the $^1\Sigma_g^+$ ground electronic state of the target to the $^2\Sigma_g^+$ ground electronic state of the residual H_2^+ are considered for relatively high incident electron energy values (~ 4 keV). This approach, which needs relatively small computational efforts to apply it to other diatomic systems, produces results that are in good agreement with existing experimental data. The influence on 3DCS of the screening of the nuclear charges produced by the residual bound electron in the exit channel is studied.

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I. INTRODUCTION

The $(e,2e)$ ionization by electron impact, which consists in coincidence detection of the scattered and ejected electrons, is a powerful means for the study of the electronic structure of atoms, molecules, and clusters. It permits one to find the favorable kinematical conditions and thus understand the mechanisms of the ionization by electron impact [1]. Theoretically, the principal task in the study of this process consists of the determination of the multiply differential cross section which demands an appropriate description of the continuum states of the incident, scattered, and ejected electrons and their mutual interactions. In the case of atomic targets, this difficulty is overcome by the use of solutions corresponding to one center potentials (Coulomb or distorted).

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 Schrodinger equation in prolate spheroidal coordinates [2] to determine the multiply differential cross section ends up with such computational difficulties that their application, for the moment, is unrealistic.

In the past, either very simple descriptions, like plane waves [3,4], or somewhat complicated descriptions employing approximate orthogonalized one-center Coulomb waves [5,6] were used. Another description to the continuum considers the interaction of the ejected electron with the residual ionized target through a static-exchange potential evaluated in the frozen-core Hartree-Fock approximation [6].

In this paper, we present results concerning the triple differential cross section obtained by the application of a two-effective center continuum wave in the exit channel having a closed form, which takes into account the diatomic structure and the influence of the bound electron, and gives results, with relatively small computational efforts, which are in

good agreement with experimental data.

Concerning the rotational and vibrational aspects of the diatomic problem, we have admitted that the ionization process is a vertical transition between the ground level (electronic, vibrational, and rotational) of the neutral target (here H_2) to one of the vibrational and rotational states of the lowest electronic state of the residual ion (here H_2^+). Now, as the rotational and vibrational levels are very close to each other, the energy resolutions of the existing experimental setups ($0.5 \text{ eV} \leq \Delta E \leq 4 \text{ eV}$) (see in [1]) are for the moment not sufficient to distinguish between them. Theoretically, this is overcome by applying the closure relation on the rotational and vibrational levels of the residual ion as proposed by Iijima *et al.* [7] for the electron scattering problem.

We have recently studied in detail [8,9] the influence of the initial and final vibrational states on the triple differential cross section of H_2 , D_2 , and T_2 molecules using a first-order Born approximation. The general conclusion from these previous works [3,8,9] following the procedure proposed by Iijima *et al.* [7] for low-energy resolution is that the introduction of the diatomic vibrational effects could be important only in high-energy resolution experiments ($\Delta E \leq 0.1 \text{ eV}$), which have not been performed so far. Atomic units will be used except otherwise stated.

II. THEORY

The $(e,2e)$ process for a H_2 molecular target is described in a laboratory frame, the z axis of which is parallel to the wave vector \mathbf{k}_i of the incident electron. The origin is fixed on the center of mass of the target. Coordinates are defined in Fig. 1 with $\boldsymbol{\rho}$ the internuclear vector and \mathbf{R} and \mathbf{r}_j ($j=1,2$) the positions of the impinging electron and the j th-target electron, respectively.

We consider high-impact energy values (\sim few keV) and assume vertical transitions (i.e., constant $\boldsymbol{\rho}$) from the $^1\Sigma_g^+$

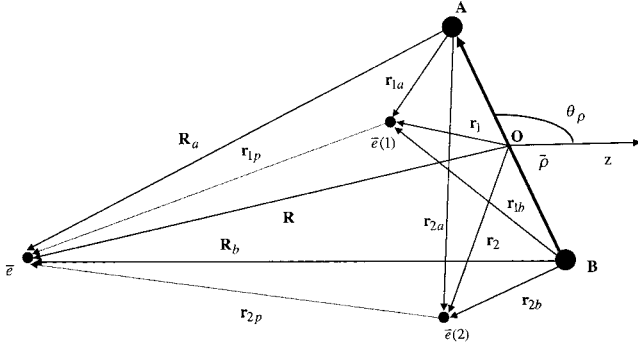


FIG. 1. Coordinates used in the text.

ground electronic state of the target to the $2\Sigma_g^+$ ground electronic state of the residual H_2^+ . We admit that for experiments with low-energy resolution, the ionization process can be considered as a pure electronic transition (see Ref. [9]) as the closure relation can be applied over all possible final rotational and vibrational states. Also, as the target molecules in the considered experiments are not oriented, and all directions of internuclear vector ρ are equally probable, we average over all possible molecular orientations [9] and the triple differential cross section can be written as

$$\begin{aligned} \sigma^{(3)} &= \frac{d^3\sigma}{d\Omega_e d\Omega_s d(k_s^2/2)} \\ &= \frac{1}{4\pi} (2\pi)^4 \frac{k_e k_s}{k_i} \int d\Omega_\rho \int d\rho |v_i|^2 |t_{fi}^e(\rho)|^2, \end{aligned} \quad (1)$$

where $t_{fi}^e(\rho)$ is the electronic transition matrix element and v_i the initial vibrational wave function. Ω_ρ , Ω_e , and Ω_s denote, respectively, the solid angles corresponding to ρ , \mathbf{k}_e , and \mathbf{k}_s , the last two being the wave vectors of the ejected and scattered electrons, respectively. However, assuming that $t_{fi}^e(\rho)$ depends weakly with ρ , Eq. (1) can be approximated by the expression

$$\sigma^{(3)} \cong \frac{ds^3\sigma}{d\Omega_e d\Omega_s d(k_s^2/2)} = \frac{1}{4\pi} (2\pi)^4 \frac{k_e k_s}{k_i} \int d\Omega_\rho |t_{fi}^e(\rho_0)|^2 \quad (2)$$

with ρ_0 the equilibrium internuclear distance of the molecular target. For the highly asymmetric geometries studied here, where the scattered electron is much more energetic than the ejected one, the exchange and capture terms that the antisymmetrization of the wave functions produces in the expression of the transition matrix element are negligible (see Ref. [10]). Only the direct term, in which the coordinates \mathbf{R} of the incident electron are attributed to the scattered electrons, should be taken into account. Under this condition, the transition matrix within the first-order Born approximation reads

$$t_{fi}^e(\rho) = \sqrt{2} \langle \Psi_f^-(\rho, \mathbf{R}, \mathbf{r}_1, \mathbf{r}_2) | V | \Psi_i(\rho, \mathbf{R}, \mathbf{r}_1, \mathbf{r}_2) \rangle, \quad (3)$$

where integrations run over the coordinates \mathbf{R} , \mathbf{r}_1 , and \mathbf{r}_2 of all the electrons. V represents the interaction of the incident electron with the target in the entrance channel given by (see Fig. 1)

$$V = -\frac{Z}{R_a} - \frac{Z}{R_b} + \frac{1}{r_{1p}} + \frac{1}{r_{2p}} \quad (4)$$

with $Z=1$ representing the nuclear charges. The energy values E_i , E_s , and E_e of the incident, scattered, and ejected electrons, respectively, satisfy the energy conservation equation:

$$E_i = I^+ + E_e + E_s \quad (5)$$

with I^+ representing the ionization potential at the equilibrium position of the target.

A. The choice of the initial wave function

The initial wave function has for high incident energy values the form

$$\Psi_i = \frac{e^{i\mathbf{k}_i \cdot \mathbf{R}}}{(2\pi)^{3/2}} \Phi_{1\Sigma_g^+}(\rho, \mathbf{r}_1, \mathbf{r}_2), \quad (6)$$

where, $\Phi_{1\Sigma_g^+}(\rho, \mathbf{r}_1, \mathbf{r}_2)$, the initial molecular bound state, is described by a Heitler–London type wave function

$$\Phi_{1\Sigma_g^+}(\rho, \mathbf{r}_1, \mathbf{r}_2) = N^{\text{HL}}(\rho) \{ e^{-\alpha r_{1a}} e^{-\alpha r_{2b}} + e^{-\alpha r_{1b}} e^{-\alpha r_{2a}} \} \quad (7)$$

with the variational parameter $\alpha = 1.1694$ for an equilibrium internuclear distance $\rho = 1.435$, or by a Wallis type wave function [11]

$$\begin{aligned} \Phi_{1\Sigma_g^+}(\rho, \mathbf{r}_1, \mathbf{r}_2) &= N^{\text{W}}(\rho) [e^{-\kappa r_{1a}} e^{-\mu r_{2b}} + e^{-\kappa r_{1b}} e^{-\mu r_{2a}} \\ &+ e^{-\mu r_{1a}} e^{-\kappa r_{2b}} + e^{-\mu r_{1b}} e^{-\kappa r_{2a}} \\ &+ \lambda (e^{-\kappa r_{1a}} e^{-\mu r_{2a}} + e^{-\kappa r_{1b}} e^{-\mu r_{2b}} \\ &+ e^{-\mu r_{1a}} e^{-\kappa r_{2a}} + e^{-\mu r_{1b}} e^{-\kappa r_{2b}})] \end{aligned} \quad (8)$$

with three variational parameters $\kappa = 1.4$, $\mu = 1.0$, and $\lambda = 0.2584$ for an equilibrium internuclear distance $\rho = 1.40$. $N^{\text{HL}}(\rho)$ and $N^{\text{W}}(\rho)$ represent the respective normalization factors. Wave functions corresponding to bound electrons can be improved by increasing the variational parameters or using more elaborate correlated wave functions (see Refs. [12] and [13]).

B. The choice of the final wave function

As the scattered electron is supposed to move with a relatively high energy (few keV), the final wave function in the exit channel is given by

$$\Psi_f^- = \frac{e^{i\mathbf{k}_s \cdot \mathbf{R}}}{(2\pi)^{3/2}} \Phi_{1s\sigma_g}(\mathbf{r}_2, \rho) \xi_C(\mathbf{k}_e, \mathbf{r}_1). \quad (9)$$

The function $\xi_C(\mathbf{k}_e, \mathbf{r}_1)$ describes one of the target electrons in a continuum state (we suppose that the electron 1 is ionized without any loss of generality in the modelization employed) and $\Phi_{1s\sigma_g}(\mathbf{r}_2, \rho)$ represents the final nondissociative bound state of the residual H_2^+ ion. In our case, we have chosen a linear combination of atomic orbitals (LCAO) type wave function,

$$\Phi_{1s\sigma_g}(\mathbf{r}_2, \rho) = M(\rho) \{e^{-\beta r_{2a}} + e^{-\beta r_{2b}}\} \quad (10)$$

with $\beta = 1.3918$ for the above-given internuclear distances corresponding to the chosen initial bound states, and $M(\rho)$ the normalization factor.

We can at this stage perform the integration over the coordinates \mathbf{R} of the incident electron by using the relation

$$\int \frac{e^{i\mathbf{K}\cdot\mathbf{R}}}{|\mathbf{R}-\mathbf{a}|} dR = \frac{4\pi e^{i\mathbf{k}\cdot\mathbf{a}}}{K^2} \quad (11)$$

and write the transition matrix element Eq. (3) in the form

$$t_{ji}^e(\boldsymbol{\rho}) = \frac{1}{\sqrt{2}\pi K^2} \langle \Phi_{1s\sigma_g}(\mathbf{r}_2, \rho) \xi_C(\mathbf{k}_e, \mathbf{r}_1) | -Z e^{i\mathbf{K}\cdot\boldsymbol{\rho}^2} \times (1 + e^{-i\mathbf{K}\cdot\boldsymbol{\rho}} + e^{i\mathbf{K}\cdot\mathbf{r}_1} + e^{i\mathbf{K}\cdot\mathbf{r}_2} | \Phi_{1\sigma_g^+}(\rho, \mathbf{r}_1, \mathbf{r}_2) \rangle. \quad (12)$$

Here $\mathbf{K} = \mathbf{k}_i - \mathbf{k}_s$, represents the momentum transfer.

1. The two-center approximation to the continuum

Exact solutions of the final continuum wave function for slow ejected electrons can be obtained using prolate spheroidal coordinates (see [2]). However, their application is extremely cumbersome and unrealistic at the present. So, one has to employ some judicious approximations to represent the final continuum wave function. In a previous work [14], we have proposed for the $(e, 2e)$ ionization of H_2^+ , where no bound electron is left in the final state, a two center continuum function (TCC) in the form of a product of a plane wave with two continuum factors associated with the interaction between the ionized electron and each one of the molecular nuclei given by

$$\xi_C(\mathbf{k}_e, \mathbf{r}) = \frac{e^{i\mathbf{k}_e \cdot \mathbf{r}}}{(2\pi)^{3/2}} C(\mathbf{k}_e, \mathbf{r}_a) C(\mathbf{k}_e, \mathbf{r}_b), \quad (13)$$

where \mathbf{r}_a (\mathbf{r}_b) is the position of the electron with respect to the nucleus a (b) and

$$C(\mathbf{k}_e, \mathbf{r}_j) = e^{-\pi\gamma/2} \Gamma(1 - i\gamma) {}_1F_1(i\gamma, 1; -i(k_e r_j + \mathbf{k}_e \cdot \mathbf{r}_j)) \quad (14)$$

with $j = a, b$ and $\gamma = -Z/k_e$. In this way, the action of the molecular nuclei on the ejected electron is considered on equal footing. Moreover, the orthonormalization in a box condition

$$\langle \xi_C(\mathbf{k}_e, \mathbf{r}) | \xi_C(\mathbf{k}'_e, \mathbf{r}) \rangle = \delta(\mathbf{k}_e - \mathbf{k}'_e) \quad (15)$$

is satisfied. This representation [Eq. (13)] of the two center continuum can be considered as the renormalized zero-order term of the approximate continuum solution recently presented by Gassaneo *et al.* [15] for the three-body Coulomb problem with two heavy particles and one light particle.

In the case of H_2 , the application of the TCC approximation is not appropriate as it ignores completely the presence of the bound electron in the exit channel. However, we use this model to evaluate the influence of the bound electron in that channel by comparison with other theoretical models that take into account its presence. In order to calculate the TCC transition matrix element given by Eq. (12), we employ a peaking approximation previously introduced to study single electron capture by impact of bare ions on molecular H_2 [16]. In the peaking approximation one uses the fact that the bound state of the diatomic system presents separate peaks at $r_{1a} \cong 0$ and $r_{1b} \cong 0$. So, one can approximate the continuum factor $C(\mathbf{k}_e, \mathbf{r}_{1b})$ by $C(\mathbf{k}_e, \boldsymbol{\rho})$ when the peak around $r_{1a} \cong 0$ is involved in the integrals (as $\mathbf{r}_{1b} = \boldsymbol{\rho} + \mathbf{r}_{1a}$). In the same way, $C(\mathbf{k}_e, \mathbf{r}_{1a})$ can be approximated by $C(\mathbf{k}_e, -\boldsymbol{\rho})$ when the peak around $r_{1b} \cong 0$ appears in the integrand. It is clear that as a consequence of its initial distribution the electron is ionized preferably from regions close to the molecular centers (nuclei).

2. The two-effective center approximation to the continuum

In a more realistic description of the $e + \text{H}_2 \rightarrow 2e + \text{H}_2^+$ reaction, as above indicated, the interaction between molecular electrons in the exit channel cannot be ignored. As the electron is ionized preferably from the proximities of each one of the nuclei, we assume that the residual electron screens the other nucleus. Starting from the TCC model, and supposing that the nucleus is completely screened, the integral corresponding to the transition matrix element can be calculated considering two different effective center continuum factors. In such a case, we take $\gamma = 0$ in the factor $C(\mathbf{k}_e, \mathbf{r}_{1b})$ [$C(\mathbf{k}_e, \mathbf{r}_{1a})$] of Eq. (13) when the peak of the initial bound wave function around $r_{1a} \cong 0$ ($r_{1b} \cong 0$) appears in the integrand of Eq. (12), which is equivalent to considering $C(\mathbf{k}_e, \mathbf{r}_{1b}) = 1$ [$C(\mathbf{k}_e, \mathbf{r}_{1a}) = 1$]. In this way, $\xi_C(\mathbf{k}_e, \mathbf{r})$ reduces to

$$\xi_C(\mathbf{k}_e, \mathbf{r}) = \frac{e^{i\mathbf{k}_e \cdot \mathbf{r}}}{(2\pi)^{3/2}} C(\mathbf{k}_e, r_j); \quad j = a, b. \quad (16)$$

The choice of the center a or b for $\xi_C(\mathbf{k}_e, \mathbf{r})$ will be dictated by the exponential terms of the initial state of the ejected electron present in the transition matrix element. We call this theoretical model the ‘‘two-effective center’’ (TEC) approximation because one or the other target nucleus must be considered separately in the description of the continuum state of the ionized electron, according to the prescription given above. It verifies the correct asymptotic conditions in the exit channel associated with the ejected electron-residual target interaction because at sufficiently large distances the ionized electron will feel an effective Coulomb center of charge unity. This is not the case of TCC for H_2 .

Moreover, it is important to note that the use of a basis of exponential functions to describe the initial state and continuum factors to describe the final one, both centered on the same nuclei, results in transition matrix elements given in closed analytical forms.

III. RESULTS AND DISCUSSIONS

Various theoretical models have been previously considered to guide the existing experimental efforts and give the optimal conditions for simple ionization of H_2 which are in general performed for coplanar asymmetric geometries [17]. Among them, a plane-wave impulse model (PWIA) [18] and an approximated first-Born treatment (SOP) [19]. In PWIA all unbound electrons are represented by plane waves and in SOP the ejected electron-residual target wave function is introduced by using the closure relation and the corresponding Born operator is truncated in the second order of a time representation series. These methods show agreement with experimental 3DCS in the Bethe ridge region but fail to describe existing measurements for other kinematical conditions. Results obtained with a factorized first-Born–Coulomb wave, fixed-nuclei, model were presented both in the Coulomb-wave velocity (CWVA) and Coulomb-wavelength (CWLA) forms [6,17]. The CWLA and CWVA forms reproduce successfully the experimental data for various angular distributions and different energetic conditions (see Figs. 2 and 3). In these models, the restricted Hartree–Fock wave function of Cade and Wahl [20] which is constructed from 12 Slater-type orbitals centered at each nucleus is used to represent the H_2 initial state and the ejected electron is described by an orthogonalized Coulomb wave. Coulomb wave and plane-wave functions defined in the bond midpoint are developed in partial waves to make possible the numerical calculation of 3DCS. The final wave function represents the ejected electron-residual target continuum corresponding to asymptotic distances. The discrepancy between the 3DCS's in length and velocity forms shown in the figures have been essentially attributed to the use of the frozen-core Hartree–Fock approximation and the neglect of the electron correlation [6].

To compare our results with the corresponding ones of the above works, we present in Figs. 2(a)–2(c) the variation of the 3DCS as a function of the ejection angle θ_e for an incident energy $E_i=4087$ eV and ejection energy $E_e=20$ eV. The scattering angle takes the values $\theta_s=1^\circ$, 1.5° , and 3° , respectively. Now the results obtained by the above-described TEC model using a Heitler–London-type wave function to represent the H_2 -bound initial state [see Eq. (7)] is situated between the curves corresponding to the length (CWLA) and velocity (CWVA) forms of Zurales *et al.* [6] in the region of the binary encounter peak, but overestimates the recoil peak for $\theta_s=1^\circ$. For this scattering angle (as well as for $\theta_s=1.5^\circ$ and 3°) the best agreement with experiments is obtained with CWLA. As the scattering angle increases (closer encounters) the agreement of our TEC results with experiments improves. Experimental uncertainties in absolute scale are of the order of 10% (see Ref. [17] for details). Present TCC calculations, also shown in the figures, obtained

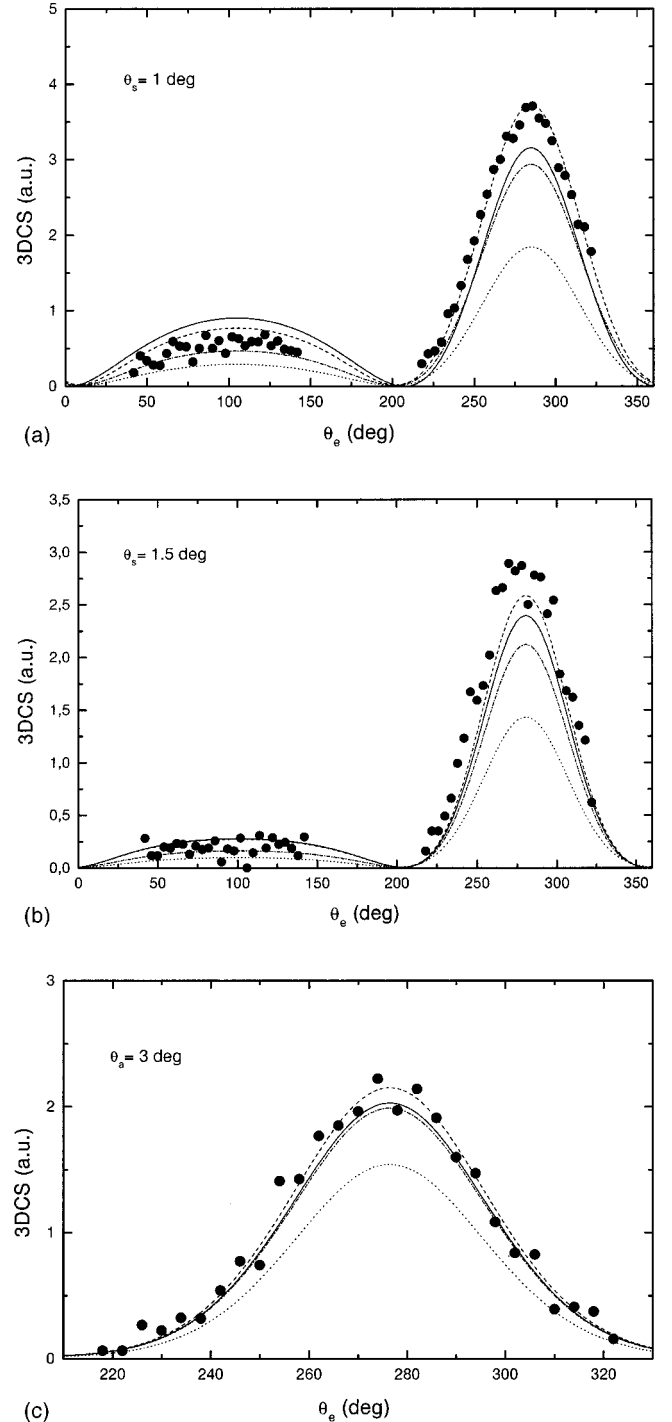


FIG. 2. Triple differential cross section as a function of the ejection angle θ_e , for $E_i=4087$ eV and $E_e=20$ eV. Scattering angles $\theta_s=1^\circ$, 1.5° , and 3° for (a), (b), and (c), respectively. Theoretical calculations are TEC, full line; TCC, dotted line; CWLA, dashed line; and CWVA, dot-dashed line. Experimental data [17] are indicated by dots.

using the same initial wave function as TEC show only a qualitative agreement with experimental data. The differences between TCC and both TEC and CWLA results give an estimation of the influence on 3DCS of the screening of the molecular nuclei produced by the residual bound electron

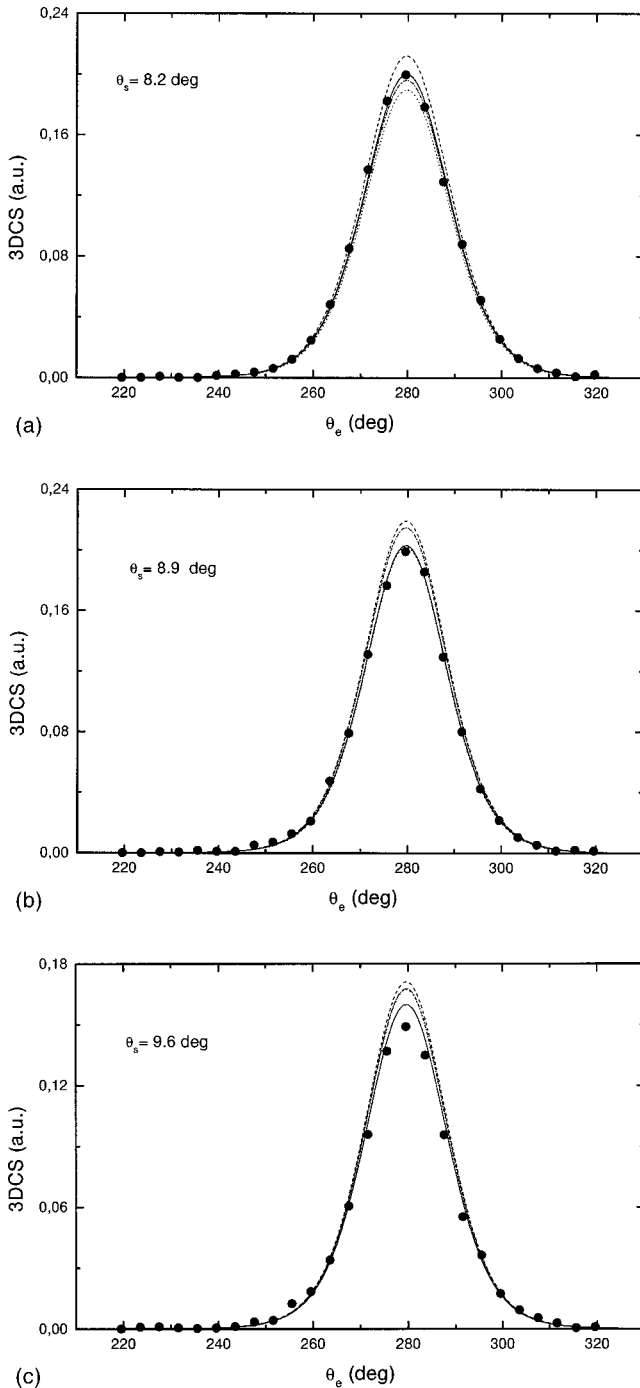


FIG. 3. Same notation as in Fig. 2 but for $E_i=4168$ eV and $E_e=100$ eV. Scattering angles are $\theta_s=8.2^\circ$, 8.9° , and 9.6° for (a), (b), and (c), respectively.

during the reaction (see Sec. II). This effect should diminish as the ejection energy increases, because the ionization process should be expected to become less sensitive to the representation of the continuum state of the emitted electron. In particular, this behavior is observed in the Bethe region around $\theta_s \cong 8.9^\circ$, shown in Figs. 3(a)–3(c) for $\theta_s=8.2^\circ$, 8.9° , and 9.6° , respectively. Here the energy values are $E_i=4168$ eV and $E_e=100$ eV. A closer agreement than in the cases previously considered is obtained for the 3DCS evalu-

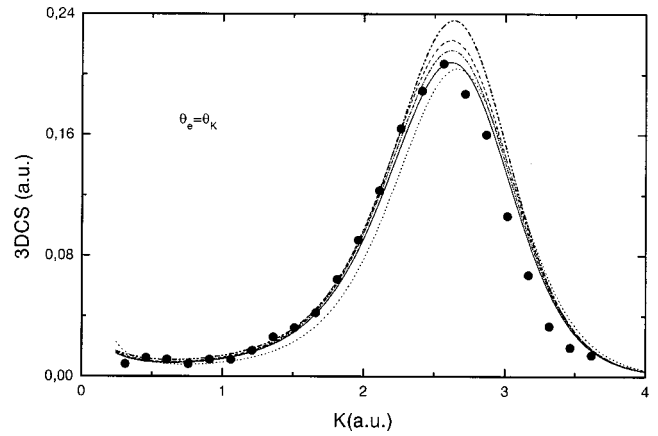


FIG. 4. Triple differential cross section as a function of momentum transfer K with the same notation as in Fig. 3. The ejection angle is chosen such as $\theta_e = \theta_K$. TEC calculations using Heitler–London- or Wallis-type initial bound wave functions are given by the full line or double dot-dashed line curves, respectively.

ated using the TEC and TCC models. It shows the fact that the screening produced by the bound electron plays a minor role as the ejection energy increases. Now, the present TEC model gives a very good agreement with experimental data. By comparison to results obtained by TEC at lower ejection energies (see Fig. 2), one is tempted to assume that it is enough to describe the continuum in the proximities of the nuclei for close collision encounters (i.e., high ejection energies).

In Fig. 4, the binary-3DCS ($\theta_e = \theta_K$; with θ_K the azimuthal angle subtended by the momentum transfer \mathbf{K}) is shown as a function of the modulus of the momentum transfer K , for $E_i=4168$ eV and $E_e=100$ eV. A very good representation of experimental data is obtained using the TEC approximation calculated with an initial-Heitler–London-type wave function. TEC results employing a Wallis-type wave function [see Eq. (8)] to represent the initial molecular bound state are included to estimate the role played by the representation of the initial state. The most important difference between both theoretical curves (approximately 14%) appears at the maximum of the 3DCS and decreases for other K values. A similar effect (not shown in here) is also obtained for 3DCS presented in Fig. 3 as a function of the ejection angle. At the region of the binary encounter peak (BEP) calculations using Heitler–London- or Wallis-type wave functions present a discrepancy of the order of 13%. This discrepancy diminishes as the ejection angle deviates from the BEP region. It should be noted that ionic terms are included in the Wallis-type wave function. So, it could be considered to be in contradiction with the hypothesis used to deduce the TEC approximation, where it is assumed that the nonejected electron screens the nucleus from which ionization does not take place. CWLA, CWVA, and TCC results are also included in the figure for further comparison.

IV. CONCLUSIONS

The two-effective center (TEC) model has been introduced in the first-order Born approximation to study the

($e,2e$) reaction for the case of neutral diatomic H_2 targets. This model takes into account the diatomic molecular structure in the wave function corresponding to the ejected electron in the exit channel. Our approximation, which ends up with integrals whose analytical determination is made by the use of Nordsieck integrals [21] in contrast to the difficulties arising with the use of other approximations, produces results which are in good general agreement with existing experimental data. The role played by the screening of the nucleus charges produced by the residual target electron in the exit channel has been estimated. The relative success of the TEC model motivates us to employ our procedure for other more complex diatomic systems like N_2 , where molecular orbitals can be constructed from a linear combination of atomic orbitals in a self-consistent field (MOLCAOSCF)

[22]. This method has been shown to be useful in studying ionization of molecular targets by impact of fast ions [23].

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