Ionization of molecular hydrogen by proton impact. II. Two-electron processes

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Cross sections for double ionization and ionization plus excitation of H_2 by high-energy protons are calculated as a function of the orientation of the H_2 internuclear axis. Only the contributions of the double-collision process have been included. The ground state of H_2 is described by Heitler-London-type wave functions, and the molecular orbitals for the excited states of H_2^+ are constructed from atomic functions. The results have been compared with the data of Edwards *et al.* [Phys. Rev. A **42**, 1367 (1990); **44**, 797 (1991); Nucl. Instrum. Methods Phys. Res. B **53**, 472 (1991)] and Ezell *et al.* [Nucl. Instrum. Methods Phys. Res. B **56/57**, 292 (1991)]. The theoretical and measured cross sections have the same magnitude for double ionization. For the excitation of the $2p\sigma_u$, $2p\pi_u$, and $2s\sigma_g$ states, the calculated cross sections are much lower than the measured ones.

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I. INTRODUCTION

Cross sections for two-electron processes that occur during collisions of fast charged projectiles with H_2 were recently reported by Edwards and co-workers [1–3]. These processes included double ionization and the excitation of the $2p\sigma_u$, $2p\pi_u$, and $2s\sigma_g$ states of H_2^+. The production of these dissociative states was analyzed [1–3] at specified angles of the molecular axis relative to the beam direction.

The calculation of cross sections of the two-electron processes as a function of molecular orientation is extremely complicated. Even the accurate calculations of double-ionization cross sections for a He target require great effort [4]. Due to the two-center character of the molecular wave functions, the specification of the proper initial and final electronic states is more difficult than the definition of the corresponding states for the He atom. Therefore, to keep the task in a manageable form, we are forced to introduce a number of approximations.

When a fast projectile interacts with a H_2 molecule, various interactions can produce two-electron transitions. In this paper we restrict ourselves to the study of the double-collision mechanism when the projectile interacts separately with each electron to produce the final state. No electron correlation is involved. Neglecting the contributions, which involve a single projectile-electron interaction plus some electron correlation effect, we are unable to reproduce the dependence of the cross sections on the sign of the projectile charge [5]. As the omission of these terms might influence the magnitude of the cross sections, our calculated values cannot be accepted as accurate. Our aim is to obtain information about the importance of the double-collision mechanism in the production of the investigated channels.

II. THEORETICAL FRAMEWORK

We calculate the cross sections of the two-electron processes in the independent-electron model [6] which is formulated within the framework of the semiclassical (SCA) approximation [7]. We keep the assumptions and notations introduced in the first part of our work [8]. The classical trajectory is approximated by a straight line. We take the center of mass of the two protons as the origin of the coordinate system, with the z axis in the direction of incidence and the vector $\mathbf{R}_0$ of the molecular axis in the xz plane. We use atomic units.

The ground state g of the H_2 target is described by Heitler-London [9] and Shull-Ebbing [10] wave functions. In these wave functions $\mathbf{R}_0$ has a fixed value and they are written in the form

$$\Phi_g = N_g(R_0,\zeta)[\exp(-\zeta r_{a1}-\zeta r_{b2}) + \exp(-\zeta r_{a2}-\zeta r_{b1})] , \quad (1)$$

$N_g(R_0,\zeta)$ is a normalization constant. r_{ai} and r_{bi} denote the distances of the ith electron, $i=1,2$, from the atomic centers a and b, respectively,

$$\mathbf{r}_{ai} = \mathbf{r}_i - \frac{\mathbf{R}_0}{2} \quad (2a)$$

$$\mathbf{r}_{bi} = \mathbf{r}_i + \frac{\mathbf{R}_0}{2} . \quad (2b)$$

A. Double ionization

The final state f of the target is a product of the wave functions $\phi_{\mathbf{k}_i}(\mathbf{r}_i)$ of the two ejected electrons

$$\Phi_f = \phi_{\mathbf{k}_1}(\mathbf{r}_1)\phi_{\mathbf{k}_2}(\mathbf{r}_2) , \quad (3)$$

where $\mathbf{k}_i$ are the wave-number vectors of the continuum electrons. The partial-wave expansions of $\phi_{\mathbf{k}_i}(\mathbf{r}_i)$ have the form

$$\phi_{\mathbf{k}_i}(\mathbf{r}_i) = \sum_{l_f} i^{l_f}\exp(i\sigma_{l_f})R_{l_f}(k_i r_i) \times \sum_{m_f} Y_{l_f m_f}(\hat{\mathbf{k}}_i)Y^*_{l_f m_f}(\hat{\mathbf{r}}_i) . \quad (4)$$

Here we approximate the radial wave function $R_{l_f}(k_i r_i)$ as

$$R_{l_f}(k_i r_i)=\left[\frac{2}{\pi}\right]^{1/2}\frac{1}{k_i r_i}F_{l_f}\left[-\frac{Z_{\text{eff}}}{k_i},k_i r_i\right] . \tag{5}$$

the Coulomb function $F_{l_f}(-Z_{\text{eff}}/k,k_i r_i)$ describes the motion in the field of an effective charge Z_{eff} positioned in the center of mass of the two target protons. In the wave function of the slower ejected electron the value $Z_{\text{eff}}=2$, for the faster electron $Z_{\text{eff}}=1$ were applied.

The double-ionization cross section at molecular orientation $\hat{\mathbf{R}}_0$ can be obtained by integrating the square of the transition amplitude $a(\mathbf{B},\mathbf{k}_1,\mathbf{k}_2,\mathbf{R}_0)^{2+}$ over the momenta of the two continuum electrons, the impact parameter B, and the azimuthal angle φ_B of the projectile

$$\frac{d\sigma^{2+}(\hat{\mathbf{R}}_0)}{d\hat{\mathbf{R}}_0}=\int d\mathbf{k}_1 d\mathbf{k}_2 \times\int_0^\infty dB\, B\int_0^{2\pi}d\varphi_B|a(\mathbf{B},\mathbf{k}_1,\mathbf{k}_2,\mathbf{R}_0)^{2+}|^2 . \tag{6}$$

In the case of a straight-line trajectory of a projectile with velocity v, $a(\mathbf{B},\mathbf{k}_1,\mathbf{k}_2,\mathbf{R}_0)^{2+}$ can be calculated as a double integral along the trajectory

$$a(\mathbf{B},\mathbf{k}_1,\mathbf{k}_2,\mathbf{R}_0)^{2+}=\frac{-1}{v^2}\int_{-\infty}^{\infty}dZ_1\exp\left[i\frac{\Delta E_1}{v}Z_1\right]\int_{-\infty}^{\infty}dZ_2\exp\left[i\frac{\Delta E_2}{v}Z_2\right]W(\mathbf{B},Z_1,Z_2,\mathbf{R}_0,\mathbf{k}_1,\mathbf{k}_2) . \tag{7}$$

Here ΔE_i is the energy transfer to electron i defined as the sum of the binding energy and the kinetic energy of the continuum electron.

$$\Delta E_i=\frac{k_i^2}{2}+\varepsilon_i . \tag{8}$$

We have assumed that $\varepsilon_1=\varepsilon_2=25.3$ eV that is the binding energy difference between the two-proton system with a distance R_0 and the ground state of the H_2 molecule [13] is equally distributed between the two ejected electrons.

If the initial state is a product of two single-electron wave functions, then in Eq. (7) $W(\mathbf{B},Z_1,Z_2,\mathbf{R}_0,\mathbf{k}_1,\mathbf{k}_2)$ can be written as a product of two projectile-electron Coulomb matrix elements taken between the initial bound and the final continuum electron states. However, our initial molecular wave function has a more complicated form. Using Eq. (1), W may be expressed as a sum of two products,

$$W(\mathbf{B},Z_1,Z_2,\mathbf{R}_0,\mathbf{k}_1,\mathbf{k}_2)=N_g(R_0,\zeta)Z_p^2\left[\left\langle\phi_{\mathbf{k}_1}(\mathbf{r}_1)\left|\frac{1}{|\mathbf{r}_1-\mathbf{R}_1|}\right|\exp(-\zeta r_{a1})\right\rangle\left\langle\phi_{\mathbf{k}_2}(\mathbf{r}_2)\left|\frac{1}{|\mathbf{r}_2-\mathbf{R}_2|}\right|\exp(-\zeta r_{b2})\right\rangle + \left\langle\phi_{\mathbf{k}_1}(\mathbf{r}_1)\left|\frac{1}{|\mathbf{r}_1-\mathbf{R}_1|}\right|\exp(-\zeta r_{b1})\right\rangle\left\langle\phi_{\mathbf{k}_2}(\mathbf{r}_2)\left|\frac{1}{|\mathbf{r}_2-\mathbf{R}_2|}\right|\exp(-\zeta r_{a2})\right\rangle\right] . \tag{9}$$

Here Z_p is the charge of the projectile, $R_i=(B^2+Z_i^2)^{1/2}$. Let us expand the exponential factors of the molecular wave function in terms of the Legendre polynominals

$$\exp(-\zeta r_{ai})=\sum_{l_g}c_{l_g}(r_i,R_0)P_{l_g}(\cos\omega_i) , \tag{10a}$$

$$\exp(-\zeta r_{bi})=\sum_{l_g}d_{l_g}(r_i,R_0)P_{l_g}(\cos\omega_i) . \tag{10b}$$

Here ω_i is the angle between the vectors $\mathbf{r}_i$ and $\mathbf{R}_0$. Taking into account Eqs. (2a) and (2b) we get

$$d_{l_g}(r_i,R_0)=(-1)^{l_g}c_{l_g}(r_i,R_0) . \tag{11}$$

Using Eqs. (10) and (11) the expression (9) may be written in a more compact form

$$W(\mathbf{B},Z_1,Z_2,\mathbf{R}_0,\mathbf{k}_1,\mathbf{k}_2)=N_g(R_0,\zeta)Z_p^2\sum_{l_g,L_g}[1+(-1)^{l_g+L_g}]\left\langle\phi_{\mathbf{k}_1}(\mathbf{r}_1)\left|\frac{1}{|\mathbf{r}_1-\mathbf{R}_1|}\right|c_{l_g}(r_1,R_0)P_{l_g}(\cos\omega_1)\right\rangle \times\left\langle\phi_{\mathbf{k}_2}(\mathbf{r}_2)\left|\frac{1}{|\mathbf{r}_2-\mathbf{R}_2|}\right|c_{L_g}(r_2,R_0)P_{L_g}(\cos\omega_2)\right\rangle . \tag{12}$$

Lower-case indices and upper-case indices relate to the electron of wave number $\mathbf{k}_1$ and $\mathbf{k}_2$, respectively. Applying this representation, the transition amplitude (7) will be expressed as

$$a(\mathbf{B},\mathbf{k}_1,\mathbf{k}_2,\mathbf{R}_0)^{2+}=\frac{-N_b(R_0,\xi)Z_p^2}{v^2}\sum_{l_gL_g}[1+(-1)^{l_g+L_g}]X_{l_g}(\mathbf{k}_1,\mathbf{B},\mathbf{R}_0)X_{L_g}(\mathbf{k}_2,\mathbf{B},\mathbf{R}_0)\ . \tag{13}$$

Following the steps in the derivation of the transition matrix element given in Ref. [8], $X_{l_g}(\mathbf{k}_i,\mathbf{B},\mathbf{R}_0)$ has the form

$$X_{l_g}(\mathbf{k}_i,\mathbf{B},\mathbf{R}_0)=(4\pi)^{3/2}\sum_{l_fl_c}\frac{i^{-l_f}\exp(-i\sigma_{l_f})}{[(2l_f+1)(2l_c+1)(2l_g+1)]^{1/2}}(l_c0l_g0|l_f0)$$
$$\times\sum_{m_f,m_c,m_g}(l_cm_cl_gm_g|l_fm_f)Y_{l_gm_g}(\hat{\mathbf{R}}_0)Y^*_{l_fm_f}(\hat{\mathbf{k}}_i)\exp(im_c\varphi_B)G^{m_c}_{l_fl_cl_g}(k_i,B,R_0)\ . \tag{14}$$

Here we have introduced the notation

$$G^{m_c}_{l_fl_cl_g}(k_i,B,R_0)=\int_{-\infty}^{\infty}dZ\exp\left[i\frac{\Delta E_i}{v}Z\right]Y_{l_cm_c}(\hat{\mathbf{R}})\exp(-im_c\varphi_B)\int_0^{\infty}dr\,r^2R_{l_f}(k_ir)\frac{r_<^{l_c}}{r_>^{l_c+1}}c_{l_g}(r,R_0)\ . \tag{15}$$

Now squaring $a(\mathbf{B},\mathbf{k}_1,\mathbf{k}_2,\mathbf{R}_0)^{2+}$, integrating over B, φ_B, $\mathbf{k}_1$, and $\mathbf{k}_2$ we obtain at incident proton energy E the differential cross section of double ionization as a function of the direction of the molecular axis $\hat{\mathbf{R}}_0$. Decomposing the product of the four spherical harmonics having the same argument and summing up over the magnetic quantum numbers we obtain

$$\frac{d\sigma(\mathbf{R}_0,E)^{2+}}{d\hat{\mathbf{R}}_0}=2\pi(4\pi)^3\left[\frac{Z_p^2N_g}{v^2}\right]^2\sum_L A_L^{2+}P_L(\cos\theta_{R_0})\ , \tag{16}$$

where the Legendre coefficients A_L^{2+} have the form

$$A_L^{2+}=\sum_{l_gl_g'L_gL_g'}[1+(-1)^{l_g+L_g}][1+(1-1)^{l_g'+L_g'}]$$
$$\times\sum_{l_cl_c'L_cL_c'}\sum_{l_fL_f}\sum_{L_aL_b}(-1)^{l_f+L_f-l_c-L_c}\frac{[(2L_a+1)(2L_b+1)]^{1/2}}{(2l_c'+1)(2L_c'+1)}(l_c0l_g0|l_f0)(l_c'0l_g'0|l_f0)$$
$$\times(L_c0L_g0|L_f0)(L_c'0L_g'0|L_f0)(l_g0l_g'0|L_a0)(L_g0L_g'0|L_b0)$$
$$\times(L_a0L_b0|L0)\begin{Bmatrix}l_c & l_g & l_f\\ l_g' & l_c' & L_a\end{Bmatrix}\begin{Bmatrix}L_c & L_g & L_f\\ L_g' & L_c' & L_b\end{Bmatrix}$$
$$\times\sum_{m_cm_c'M_c}(l_cm_cL_am_c'-m_c|l_c'm_c')(L_cM_cL_bm_c-m_c'|L_c'm_c-m_c'+M_c)$$
$$\times(L_am_c'-m_cL_bm_c-m_c'|L0)$$
$$\times\int_0^{\infty}dB\,B\int_0^{\infty}k_1^2dk_1G^{m_c}_{l_fl_cl_g}(k_1,B,R_0)G^{m_c'*}_{l_fl_c'l_g'}(k_1,B,R_0)$$
$$\times\int_0^{\infty}k_2^2dk_2G^{M_c}_{L_fL_cL_g}(k_2,B,R_0)G^{m_c-m_c'+M_c*}_{L_fL_c'L_g'}(k_2,B,R_0)\ . \tag{17}$$

Here $\begin{Bmatrix}l_1 & l_2 & l_3\\ l_4 & l_5 & l_6\end{Bmatrix}$ denotes a $6j$ symbol.

B. Ionization plus excitation

We have performed calculations for the production of the $2p\sigma_u$, $2s\sigma_g$, and $2p\pi_u$ excited states of the H_2^+ molecule. Here the final state is a product of the wave functions of the excited H_2^{+*} molecule ion and of the ejected electron of wave-number vector $\mathbf{k}$

$$\Phi_f=\phi_{\mathbf{k}}(\mathbf{r}_1)\psi_f(\mathbf{r}_2)\ . \tag{18}$$

The molecular orbitals for the excited states are constructed from atomic functions [11]

$$2p\sigma_u:\ \psi_f(\mathbf{r})=\exp(-r_a)-\exp(-r_b)\ , \tag{19}$$

$$2s\sigma_g:\ \psi_f(\mathbf{r})=(2-r_a)\exp\left[-\frac{r_a}{3}\right]+(2-r_b)\exp\left[-\frac{r_b}{2}\right]\ , \tag{20}$$

$$2p\pi_u:\ \psi_f(\mathbf{r})=r_a\exp\left[-\frac{r_a}{2}\right]Y_{1m_g}(\hat{\mathbf{r}}'_a)+r_b\exp\left[-\frac{r_b}{2}\right]Y_{1m_g}(\hat{\mathbf{r}}'_b)\ . \tag{21}$$

For the $2p\pi_u$ state $m_g=\pm1$ because it is constructed from π orbitals. $\hat{\mathbf{r}}'_a$ and $\hat{\mathbf{r}}'_b$ are defined in the molecular frame. Since the velocity of the projectile is high, in $\psi_f(\mathbf{r})$ R_0 has the same value as was used for the ground state of H_2. The wave functions (19)–(21), which approximate the molecular orbitals as a linear combination of atomic orbitals, may provide a not-too-bad wave function at internuclear separation $R_0\sim1.4$.

The ionization plus excitation cross section at molecular orientation $\hat{\mathbf{R}}_0$ can be obtained by integrating the square of the transition amplitude $a(\mathbf{B},\mathbf{k},\hat{\mathbf{R}}_0)^{+*}$ over B, φ_B, and the momentum $\mathbf{k}$ of the ejected electron

$$\frac{d\sigma^{+*}(\hat{\mathbf{R}}_0)}{d\hat{\mathbf{R}}_0}=2\int d\mathbf{k}\int_0^\infty dB\,B\int_0^{2\pi}d\varphi_B|a(\mathbf{B},\mathbf{k},\hat{\mathbf{R}}_0)^{+*}|^2\ . \tag{22}$$

We calculate $|a(\mathbf{B},\mathbf{k},\hat{\mathbf{R}}_0)^{+*}|^2$, following closely the derivation in Eqs. (7)–(17). In the case of the $2p\sigma_u$ and $2s\sigma_g$ states, with the final-state wave functions (19) and (20), the coefficients $d_l(r,R_0)$ of the Legendre expansion are

$$\psi_f(\mathbf{r})\exp(-r_b)=\sum_l d_l(r,R_0)P_l(\cos\omega)\ , \tag{23}$$

where ω is the angle between $\mathbf{r}$ and $\mathbf{R}_0$. As for the $2p\pi_u$ state in Eq. (21) the spherical harmonic depends on the vector $\mathbf{r}'_a=\mathbf{r}'-\hat{\mathbf{z}}'R_0/2$ defined in the molecular frame. $\mathbf{r}'_a\,Y_{1m_g}(\mathbf{r}'_a)$ can be expanded as

$$r'_aY_{1m_g}(\hat{\mathbf{r}}'_a)=rY_{1m_g}(\hat{\mathbf{r}}')+\frac{R_0}{2}Y_{1m_g}(\hat{\mathbf{z}}')\delta_{0m_g}\ . \tag{24}$$

See, for example, the textbook [12]. Since $m_g=\pm1$, the second term of the sum on the right-hand side of this equation is zero. $Y_{1m_g}(\hat{\mathbf{r}}')$ is expanded in terms of spherical harmonics that depend on vectors measured in the frame of the collision

$$Y_{1m_g}(\hat{\mathbf{r}}')=\sum_m Y_{1m}(\hat{\mathbf{r}})D^1_{mm_g}(0,\theta_{R_0},0)\ . \tag{25}$$

Here the Wigner D function $D^{1*}_{mm_g}(0,\theta_{R_0},0)$ depends on the angle between the z axis and the vector of the molecular axis. The $d_l(r,R_0)$ coefficients for the $2p\pi_u$ states are defined by the expansion

$$\left[\exp\left[-\frac{r_a}{2}\right]+\exp\left[-\frac{r_b}{2}\right]\right]\exp(-r_b)=\sum_l d_l(r,R_0)P_l(\cos\omega)\ . \tag{26}$$

Further we introduce the notation

$$F^M_{lL}(B,R_0)=\int_{-\infty}^{\infty}dZ\exp\left[i\frac{\Delta E_s}{v}Z\right]Y^*_{LM}(\hat{\mathbf{R}})\times\exp(-iM\varphi_B)\times\int_0^\infty dr\,r^2\frac{r_<^L}{r_>^{L+1}}d_l(r,R_0)\ , \tag{27}$$

where s refers to the $2p\sigma_u$, $2s\sigma_g$, and $2p\pi_u$ final channels. The transferred energies for the excitation of the $2p\sigma_u$, $2s\sigma_g$, and $2p\pi_u$ states have been taken as $\Delta E_{2p\sigma_u}=0.67$, $\Delta E_{2s\sigma_g}=0.91$, and $\Delta E_{2p\pi_u}=0.84$, respectively. These values were extracted from the potential curves of Sharp [13] at internuclear distance $R_0\sim1.4$. The cross section of the production of the ionization plus excitation final states may be expressed as

$$\frac{d\sigma(\hat{\mathbf{R}}_0,E)^{+s}}{d\hat{\mathbf{R}}_0}=(4\pi)^5\left[\frac{Z_pN_s}{v^2}\right]^2\sum_L A_L^{+s}P_L(\cos\theta_{R_0})\ , \tag{28}$$

N_s contains the normalization constants of the initial and final states. With the functions defined in Eqs. (15) and (27) A_L^{+s} reads

$$\begin{aligned}A_L^{+s}=&\sum_{l_f,L_g,L}\ \sum_{l_c,l'_c,l_g,l'_g}\ \sum_{L_f,L'_f}\ \sum_{L_c,L'_c}(-1)^{l_f-l'_c}\left[\frac{2L+1}{(2l_c+1)(2l'_c+1)^2(2L_c+1)^3(2L'_c+1)^3}\right]^{1/2}M^{L_cL'_c}_{L_fL'_f}\\&\times(l_c0l_g0|l_f0)(l'_c0l'_g0|l_f0)(l_g0l'_g0|L_g0)(L0L_g0|k0)\\&\times[1+j(-1)^{l_g+L_f}][1+j(-1)^{l'_g+L'_f}]\begin{Bmatrix}l_c & l_g & l_f\\ l'_g & l'_c & L\end{Bmatrix}\\&\times\sum_{m_c,m'_c,M_c}(-1)^{M_c-m_c+m'_c}(l_cm_cLm'_c-m_c|l'_cm'_c)\\&\times(L_cM_cL'_c-M_c+m_c-m'_c|L_gm_c-m'_c)(Lm'_c-m_cL_gm_c-m'_c|k0)\\&\times\int_0^\infty dB\,BF^{M_f}_{L_fL_c}(B,R_0)F^{M_c-m_c+m'_c*}_{L'_fL'_c}(B,R_0)\\&\times\int_0^\infty k^2dkG^{m_c}_{l_fl_cl_g}(k,B,R_0)G^{m'_c*}_{l_fl'_cl'_g}(k,B,R_0)\ .\end{aligned} \tag{29}$$

Here $j=1$ for the $2p\sigma_u$, $2s\sigma_g$ and $j=-1$ for the $2p\sigma_u$ final states, respectively. $M_{L_fL_F}^{L_cL_c'}$ in Eq. (29) is defined for the σ and π final channels as

$$2p\sigma_u, 2s\sigma_g: \quad M_{L_fL_f'}^{L_cL_c'} = \delta_{L_fL_c}\delta_{L_f'L_c'}(L_f 0 L_f' 0 | L_g 0) , \tag{30a}$$

$$2p\pi_u: \quad M_{L_fL_f'}^{L_cL_c'} = -(10L_f 0|L_c 0)(10l_f' 0|L_c' 0) \times(11L_f 0|L_c 1)(11l_f' 0|L_c' 1)(11l_f' 0|L_c' 1) \times(L_c 1 L_c' -1|L_g 0) . \tag{30b}$$

III. RESULTS AND DISCUSSION

The cross sections for double ionization of H_2 are shown in Fig. 1 and 2. In Fig. 1 the cross sections of H_2 oriented at 90° relative to the projectile direction are presented as a function of the projectile energy. The difference between the experimental cross sections [1] induced by proton and equivelocity electrons cannot be explained by our simple model based on the double-collision mechanism only. Figure 1 shows that the curve calculated with Shull-Ebbing wave function fits well the experimental points for proton impact, and is lower by a factor of 2 than the data for electron bombardment. The same magnitude of the measured and calculated cross sections suggests that the double-collision mechanism gives the dominant contribution to the double-ionization process.

As for the dependence of the cross sections on the orientation of the molecular axis, Fig. 2 shows that the theoretical curve satisfactorily describes the data obtained with proton projectile. The difference between the angular distributions induced by protons and electrons offers a good motivation for future studies of interference effects due to the presence of different mechanisms. The remarkable dependence of the calculated cross sections on the target wave function suggests that the model might be improved by using more realistic H_2 wave functions, too.

For the ionization plus excitation cross sections the discrepancy between the measured and calculated cross

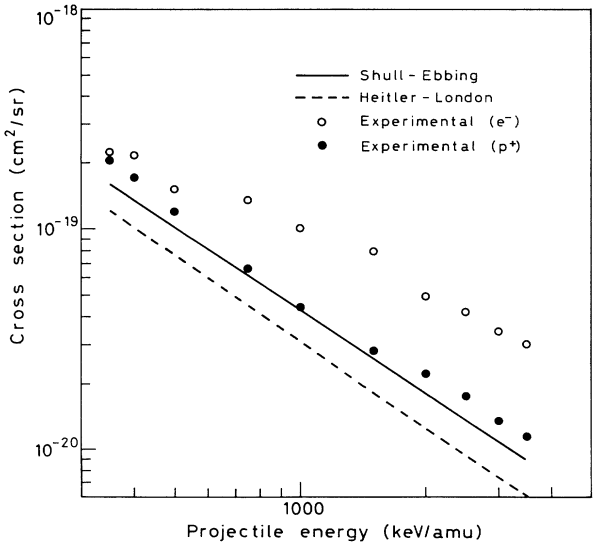

FIG. 1. Double-ionization cross sections of H_2 by electrons and protons oriented at 90° relative to the projectile direction as a function of the projectile energy. The data points were taken from Edwards *et al.* [1], the experimental errors are comparable with the extent of the symbols. The theoretical curves have been calculated by assuming the double-collision mechanism.

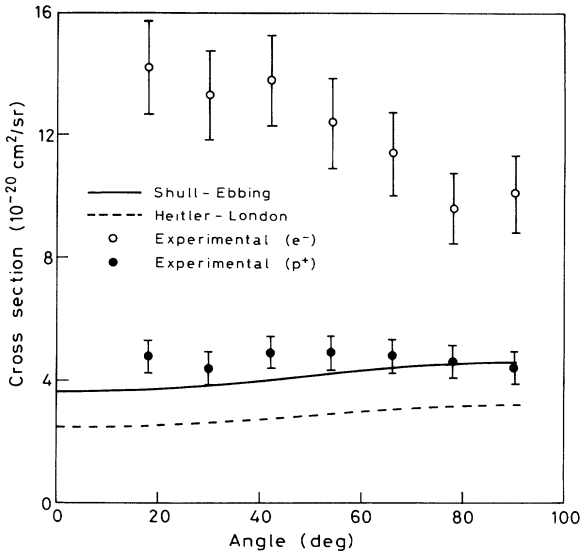

FIG. 2. Angular dependence of the double-ionization cross section on the orientation of the molecular axis relative to the projectile direction at 1 MeV/amu projectile energy. The experimental points are taken from Ezell *et al.* [3]. The theoretical curves have been calculated by assuming the double-collision mechanism.

For the ionization plus excitation cross sections the discrepancy between the measured and calculated cross

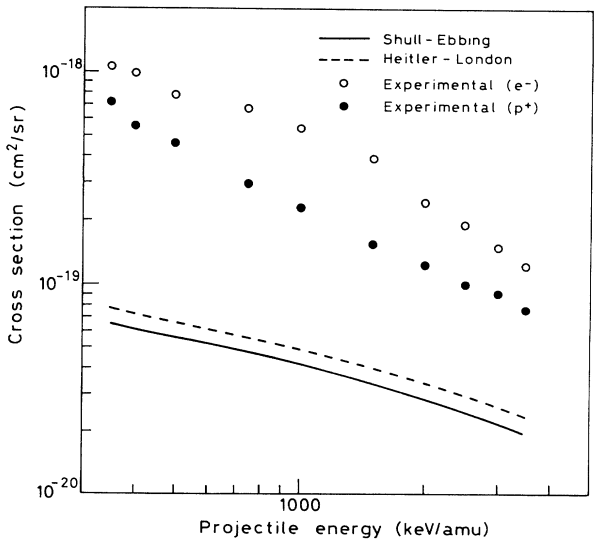

FIG. 3. The same as in Fig. 1 for ionization plus excitation to the $2p\sigma_u$ state.

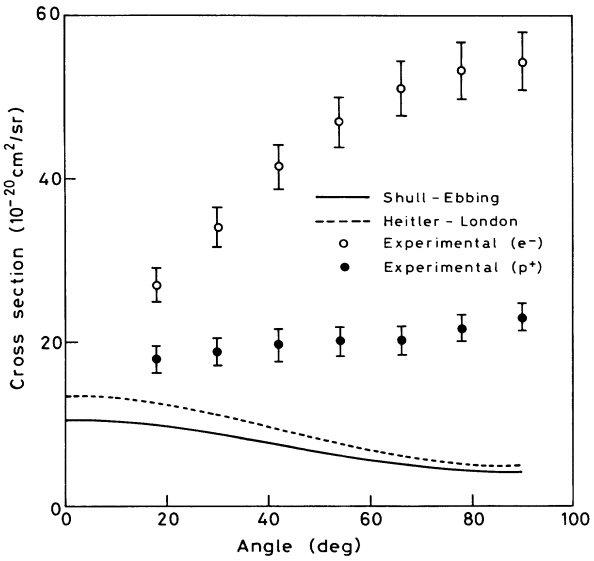

FIG. 4. The same as in Fig. 2 for ionization plus excitation to the $2p\sigma_u$ state. The experimental points are taken from Edwards *et al.* [2].

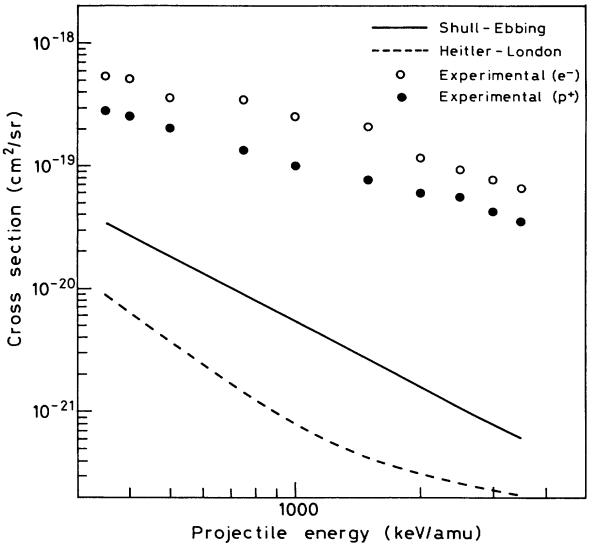

FIG. 5. The same as in Fig. 1 for ionization plus excitation to the $2s\sigma_g$ state.

sections is much higher. Comparing the experimental and theoretical cross sections of the production of the $2p\sigma_u$ state, presented in Figs. 3 and 4, we can see that the measured points are a factor of 5 higher than the calculated values and the calculated angular distribution does not follow the trend of the experimental data. Investigating the production of the $2s\sigma_g$ state, the theoretical values are roughly one-tenth of the measured ones, see Fig. 5. As far as the $2p\pi_u$ channel is concerned, the experimental cross sections of the $2p\pi_u$ final states are larger by 2–3 orders of magnitude than our calculated values.

The small values of the calculated cross section suggest that the double-collision mechanism does not give the dominant contribution to the amplitude of the ionization pulse excitation processes. The leading contribution might come from a mechanism where the projectile interacts with one electron removing it to the continuum and the second electron is excited to the molecular orbital by some electron-electron interaction process. Such a contribution could be included in the framework of the model relatively easily. A further task is to investigate how good the (19)–(21) wave functions are for approximation to the exact H_2^+ molecular orbitals.

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