Ionization of molecular hydrogen by proton impact. I. Single ionization

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Single-ionization cross sections of the proton-hydrogen molecule collision are calculated in semiclassical approximation by using atomic and Heitler-London-like two-center molecular wave functions for the ground state of H_2. In transition matrix elements, calculated with two-center wave functions, the factors depending on $|\mathbf{r} - \mathbf{R}_0/2|$ ($\mathbf{R}_0$ is the vector of the molecular axis) are expanded into Legendre series. The calculated total and differential cross sections are compared to the measured data, and their dependence on target wave functions is discussed. The success of the simple approach, which uses twice the cross sections calculated for the hydrogen atom, is explained with the dominance of monopole contributions in the expansion in $\mathbf{R}_0$. While for homonuclear diatomic molecules the differential cross sections could be well described by the additivity rule, for other molecules the validity of such approaches is questionable.

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INTRODUCTION

In many fields of research related to the interaction of radiation with matter, a good knowledge of the total and differential ionization cross sections is indispensable. Although, in general, the irradiated material is of complicated molecular structure, we have to rely on cross-section values measured mainly on atomic or simpler molecular targets. Usually when calculating cross sections we invoke the additivity rule. This approximates the molecular cross section with the sum of the cross sections of the constituent atoms that are considered free and uncorrelated.

In the case of the single ionization of H_2 molecules the sum of the calculated cross sections of H atoms (occasionally with binding energy modified so as to reproduce the ionization potential of the hydrogen molecule [1,2]) coincided reasonably well with the measured total cross sections above 80-keV incident proton energies. The differential electron-ejection cross sections were not in detailed agreement with experiment [3,4]; the largest discrepancy appeared at small ejection angles [5]. The calculations after the inclusion of the long-range proton-electron interaction reproduced the experimental values within their accuracy [6].

While for proton impact ionization the effect of the molecular structure seems to be unimportant, the two-center character of the H_2 wave function is relevant in the analysis of the elastic electron scattering [7] and the photoionization data [8]. Even at the ionization of a structured projectile colliding with the H_2 target, due to the spatial correlation of the two hydrogen atoms in the molecule, interference pattern should occur in the electron angular distribution [9].

In this paper we consider the question of why the additivity rule is so efficient for description of the proton impact ionization of the hydrogen molecule. To calculate the ionization amplitudes, we employ simple Heitler-London-type molecular wave functions for the ground state of H_2. The formalism, presented here, will also be applied in the paper [10] in order to calculate cross sections of the two-electron processes which depend on the orientation of the molecular axis. Such data have been published very recently be Edwards et al. [11].

MODEL

We calculate the ionization cross section within the framework of the semiclassical (SCA) approximation [12] where the projectile path is described classically. This classical trajectory is approximated by a straight line. Taking 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 $\mathbf{B}$ as a vector perpendicular to z and of length equal to the impact parameter, the straight-line orbit is $\mathbf{R}$ where

$$\mathbf{R} = \mathbf{B} + \mathbf{v}t . \tag{1}$$

Here $\mathbf{v}$ is the velocity of the proton and $t = 0$ is the time of closest approach.

The initial state g of H_2 is represented by a molecular wave function with a fixed $\mathbf{R}_0$ distance between the two protons. We have applied the wave functions of Heitler and London [13], and Shull and Ebbing [14] which can be written in the form

$$\Phi_g = N_g(R_0,\zeta)[\exp(-\zeta r_{a1} - \zeta r_{b2}) + \exp(-\zeta r_{a2} - \zeta r_{b1})] . \tag{2}$$

For the Heitler-London wave function $\zeta = 1$ and $R_0 = 1.51$, for the Shull-Ebbing wave function $\zeta = 1.165$ and $R_0 = 1.42$. We use atomic units throughout the paper. In the Shull-Ebbing wave function the atomic orbital centers are closer to each other than the nuclei, each center is shifted by $x = 0.055$. $N(R_0,\zeta)$ is a normalization constant. r_{ai} and r_{bi} denote the distances of the ith electron with position vectors $\mathbf{r}_i$, $i = 1,2$, from the atomic center a and b, respectively,

$$\mathbf{r}_{ai} = \mathbf{r}_i - \frac{\mathbf{R}_0}{2} ,$$

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

The final state Φ_f is a product of the continuum-electron wave function $\phi_{\mathbf{k}}(\mathbf{r}_1)$ and the bound-state wave function of the residual ion

$$\Phi_f = N_f(R_0, \zeta)[\exp(-\zeta r_{a2}) + \exp(-\zeta r_{b2})]\phi_{\mathbf{k}}(\mathbf{r}_1) , \qquad (3)$$

where $\mathbf{k}$ is the wave-number vector of the continuum electron. Since the velocity of the projectile is high, the final state of the residual ion is approximated by a H_2^+ wave function with the $\mathbf{R}_0$ vector of the initial H_2 state.

The total ionization cross section may be expressed by an integral of the transition probabilities $P(B)$ over the impact parameter

$$\sigma = \int_0^\infty dB \, BP(B) , \qquad (4)$$

where $P(B)$ is the integral of the squared transition amplitude $a(\mathbf{B}, \mathbf{k}, \mathbf{R}_0)$ over $\mathbf{k}$, the azimuthal angle φ_B of the projectile, and the direction of the molecular axis,

$$P(B) = 2 \int d\hat{\mathbf{R}}_0 \int d\mathbf{k} \int_0^{2\pi} d\varphi_B |a(\mathbf{B}, \mathbf{k}, \mathbf{R}_0)|^2 . \qquad (5)$$

The factor 2 reflects the presence of two target electrons in the same molecular orbit in the ground state of the target. For straight-line trajectories the transition amplitude can be calculated as an integral

$$a(\mathbf{B}, \mathbf{k}, \mathbf{R}_0) = -\frac{i}{v} \int_{-\infty}^\infty dZ \, V_{gf}(\mathbf{R}, \mathbf{R}_0)\exp\left[i\frac{\Delta E}{v}Z\right] . \qquad (6)$$

ΔE is the difference between the energies of the initial and final electronic states

$$\Delta E = \varepsilon + \frac{k^2}{2} \qquad (7)$$

where ε is the ionization potential of the H_2 molecule. The matrix element V_{gf} describes the Coulomb interaction of a projectile of charge Z_p with one of the electrons,

$$V_{gf}(\mathbf{R}, \mathbf{R}_0) = -Z_p \int d\mathbf{r}_1 d\mathbf{r}_2 \Phi_f^*(\mathbf{r}_1, \mathbf{r}_2, \mathbf{R}_0)$$

$$\times \frac{1}{|\mathbf{r}_1 - \mathbf{R}|}\Phi_g(\mathbf{r}_1, \mathbf{r}_2, \mathbf{R}_0) . \qquad (8)$$

Substituting the initial and final wave functions defined by Eqs. (2) and (3) into Eq. (8) and performing the integration over coordinate $\mathbf{r}_2$ the transition amplitude (6) may be expressed as

$$a(\mathbf{B}, \mathbf{k}, \mathbf{R}_0) = -\frac{i}{v} \frac{2Z_p N_g}{N_f} \int_{-\infty}^\infty dZ \exp\left[i\frac{\Delta E}{v}Z\right]\left\langle \phi_{\mathbf{k}}(\mathbf{r}_1) \left| \frac{1}{|\mathbf{r}_1 - \mathbf{R}|} \right| \exp\left[-\zeta\left|\mathbf{r}_1 - \frac{\mathbf{R}_0}{2}\right|\right] + \exp\left[-\zeta\left|\mathbf{r}_1 + \frac{\mathbf{R}_0}{2}\right|\right] \right\rangle . \qquad (9)$$

To evaluate the matrix element in the integrand we apply the partial-wave expansions of the continuum-electron wave function

$$\phi_{\mathbf{k}}(\mathbf{r}_1) = \sum_{l_f} i^{l_f}\exp(i\sigma_{l_f})R_{l_f}(kr_1)\sum_{m_f} Y_{l_f m_f}(\hat{\mathbf{k}})Y_{l_f m_f}^*(\hat{\mathbf{r}}_1) . $$

$$\qquad (10)$$

Here the radial wave function $R_{l_f}(kr_1)$ is taken as

$$R_{l_f}(kr_1) = \left[\frac{2}{\pi}\right]^{1/2}\frac{1}{kr_1}F_{l_f}\left[-\frac{1}{k}, kr_1\right] , \qquad (11)$$

that is the wave function of the continuum electron moving in the field of the residual H_2^+ molecular ion is approximated with the Coulomb function $F_{l_f}(-1/k, kr_1)$ which describes the motion in the field of a unit positive charge positioned in the center of mass of the two pro-

tons of the molecule. The Coulomb interaction in (9) is expanded into partial-wave series

$$\frac{1}{|\mathbf{r}_1 - \mathbf{R}|} = \sum_{l_c} \frac{r_<^{l_c}}{r_>^{l_c+1}} \frac{4\pi}{2l_c+1} \sum_{m_c} Y_{l_c m_c}(\hat{\mathbf{R}})Y_{l_c m_c}^*(\hat{\mathbf{r}}_1) . \qquad (12)$$

The target wave function which depends on the direction of the vector $\mathbf{R}_0$ of the molecular axis is expanded into a Legendre series

$$\exp\left[-\zeta\left|\mathbf{r}_1 - \frac{\mathbf{R}_0}{2}\right|\right] + \exp\left[-\zeta\left|\mathbf{r}_1 + \frac{\mathbf{R}_0}{2}\right|\right]$$

$$= \sum_{l_g} c_{l_g}(r_1, R_0)P_{l_g}(\cos\omega_1) , \qquad (13)$$

where ω_1 is the angle between the vectors $\mathbf{r}_1$ and $\mathbf{R}_0$. The expansion coefficients defined as

$$c_{l_g}(r_1, R_0) = \frac{2l_g+1}{2} \int_{-1}^1 dx \, P_{l_g}(x)\left\{\exp\left[-\zeta\left[r_1^2 + \frac{R_0^2}{4} - r_1 Rx\right]^{1/2}\right] + \exp\left[-\zeta\left[r_1^2 + \frac{R_0^2}{4} + r_1 Rx\right]^{1/2}\right]\right\} . \qquad (14)$$

Expressing the Legendre polynomials as a product of spherical harmonics

$$P_{l_g}(\cos\omega_1) = \frac{4\pi}{2l_g+1} \sum_{m_g} Y_{l_g m_g}(\hat{\mathbf{R}}_0)Y_{l_g m_g}^*(\hat{\mathbf{r}}_1) , \qquad (15)$$

the dependence on the direction $\hat{\mathbf{R}}_0$ of the molecular axis can be separated. For the homonuclear H_2 molecule, in Eq.

(13) only the coefficients with even l_g can be nonzero, since c_{l_g} for odd l_g is vanishing.

Substituting Eqs. (10)–(15) into Eq. (9) the transition amplitude may be represented as

$$a(\mathbf{B},\mathbf{k},\mathbf{R}_0) = -\frac{i(4\pi)^2}{v}\frac{Z_p N_g}{2N_f}\sum_{l_f,m_f}\sum_{l_c,m_c}\sum_{l_g,m_g}\frac{i^{-l_f}\exp(-i\sigma_{l_f})}{(2l_c+1)(2l_g+1)}Y_{l_g m_g}(\hat{\mathbf{R}}_0)Y^*_{l_f m_f}(\hat{\mathbf{k}})$$

$$\times\int d\hat{\mathbf{r}}_1 Y^*_{l_c m_c}(\hat{\mathbf{r}}_1)Y^*_{l_g m_g}(\hat{\mathbf{r}}_1)Y_{l_f m_f}(\hat{\mathbf{r}}_1)$$

$$\times\int_{-\infty}^{\infty}dZ\exp\left[i\frac{\Delta E}{v}Z\right]Y_{l_c m_c}(\hat{\mathbf{R}})$$

$$\times\int_0^{\infty}dr_1 r_1^2 R_{l_f}(kr_1)\frac{r_<^{l_c}}{r_>^{l_c+1}}c_{l_g}(r_1,R_0)\ . \tag{16}$$

Performing the integration over $\hat{\mathbf{r}}_1$

$$\int d\hat{\mathbf{r}}_1 Y^*_{l_c m_c}(\hat{\mathbf{r}}_1)Y^*_{l_g m_g}(\hat{\mathbf{r}}_1)Y_{l_f m_f}(\hat{\mathbf{r}}_1) = \left[\frac{(2l_c+1)(2l_g+1)}{4\pi(2l_f+1)}\right]^{1/2}(l_c 0 l_g 0|l_f 0)(l_c m_c l_g m_g|l_f m_f)\ . \tag{17}$$

See, for example, the textbook [15], where $(lml'm'|LM)$ denotes a Clebsch-Gordan coefficient and using the notations

$$\Gamma_{l_f l_c l_g}(k,R,R_0) = \int_0^{\infty}dr_1 r_1^2 R_{l_f}(kr_1)\frac{r_<^{l_c}}{r_>^{l_c+1}}c_{l_g}(r_1,R_0) \tag{18}$$

and

$$G^{m_c}_{l_f l_c l_g}(k,B,R_0) = \int_{-\infty}^{\infty}dZ\exp\left[i\frac{\Delta E}{v}Z\right]Y_{l_c m_c}(\hat{\mathbf{R}})\exp(-im_c\varphi_B)\Gamma_{l_f l_c l_g}(k,R,R_0) \tag{19}$$

we may express the transition amplitude as

$$a(\mathbf{B},\mathbf{k},\mathbf{R}_0) = -\frac{i(4\pi)^{3/2}}{v}\frac{Z_p N_g}{2N_f}\sum_{l_f l_c l_g}\frac{i^{-l_f}\exp(-i\sigma_{l_f})}{[(2l_f+1)(2l_c+1)(2l_g+1)]^{1/2}}(l_c 0 l_g 0|l_f 0)$$

$$\times\sum_{m_f,m_c,m_g}(l_c m_c l_g m_g|l_f m_f)Y_{l_g m_g}(\hat{\mathbf{R}}_0)Y^*_{l_f m_f}(\hat{\mathbf{k}})\exp(im_c\varphi_B)G^{m_c}_{l_f l_c l_g}(k,B,R_0)\ . \tag{20}$$

Taking the square of $a(\mathbf{B},\mathbf{k},\mathbf{R}_0)$ and integrating over B, φ_B, and $\hat{\mathbf{R}}_0$ and summing up over the magnetic quantum numbers we get at incident proton energy E the differential cross section of ionization as a function of $\mathbf{k}$,

$$\frac{d\sigma(\mathbf{k},E)}{d\mathbf{k}} = (4\pi)^3\left[\frac{Z_p N_g}{2N_f v}\right]^2\sum_{l_g,l_f,l_c}\sum_{l'_f,l'_c}(-1)^{l_c+l_g}\sum_L\left[\frac{(2L+1)(2l_f+1)}{(2l_g+1)(2l_c+1)(2l'_c+1)}\right]^{1/2}$$

$$\times(l_c 0 l_g 0|l_f 0)(l'_c 0 l_g 0|l'_f 0)(l_f 0 l'_f 0|L 0)\left\{\begin{matrix}l_f & l_c & l_g\\ l'_c & l'_f & L\end{matrix}\right\}P_L(\cos\theta_k)$$

$$\times\sum_{m_c}(l_c m_c L 0|l'_c m_c)\int_0^{\infty}dB\ B G^{m_c}_{l_f l_c l_g}(k,B,R_0)G^{m_c*}_{l'_f l'_c l_g}(k,B,R_0)\ . \tag{21}$$

Here $\left\{\begin{smallmatrix}l_f & l_c & l_g\\ l'_c & l'_f & L\end{smallmatrix}\right\}$ denotes a $6j$ symbol. The total cross section of ionization is obtained by integrating over the momenta $\mathbf{k}$ of the ejected electrons

$$\sigma(E) = (4\pi)^4\left[\frac{Z_p N_g}{2N_f v}\right]^2\sum_{l_f,l_c,l_g}\frac{1}{(2l_g+1)(2l_c+1)^2}(l_c 0 l_g 0|l_f 0)^2\sum_{m_c}\int_0^{\infty}k^2 dk\int_0^{\infty}dB\ B\ |G^{m_c}_{l_f l_c l_g}(k,B,R_0)|^2\ . \tag{22}$$

RESULTS AND DISCUSSION

We can compare the recommended ionization cross section of Rudd et al. [1] for a molecule and the sum of cross sections of the constituent atoms or smaller molecules, see Fig. 1. It is apparent, that, at least at high proton energies, the total cross section is well described by the additivity rule. We have analyzed this conclusion and the similar statement for differential cross sections of Ref. [5] within the framework of our model.

We have calculated the total cross sections of proton-H_2 molecule singly ionizing collisions in the projectile energy range from 100 to 3500 keV. The maximum partial wave for the continuum-electron wave function in the expansion (10) was taken as $l_f = 4$. The theoretical curves are compared with the recommended curve of Rudd et al. [1]. Figure 2 contains the calculated curves with Heitler-London [13] and Shull-Ebbing [14] and atomic wave functions. The latter curve is obtained as twice the cross sections calculated for hydrogen atom with binding energy 15.42 eV that reproduces the ionization potential of the hydrogen molecule. As Fig. 2 shows, all calculated cross sections are larger than the recommended ones [1].

As for calculations with atomic wave functions we should note that if we limit the maximum orbital momentum of the ejected electrons as $l_f = 1$ we have obtained an excellent agreement with the tabulated value of Hansteen, Johnsen, and Kocbach [16]. Taking into account the contribution of continuum electrons to maximum orbital momentum $l_f = 4$ the total cross sections increase about 20%. In fact, for electrons ejected with very low energy ejected electrons the $l_f \geq 2$ contributions are small, as discussed by Kocbach, Hansteen, and Gunder-
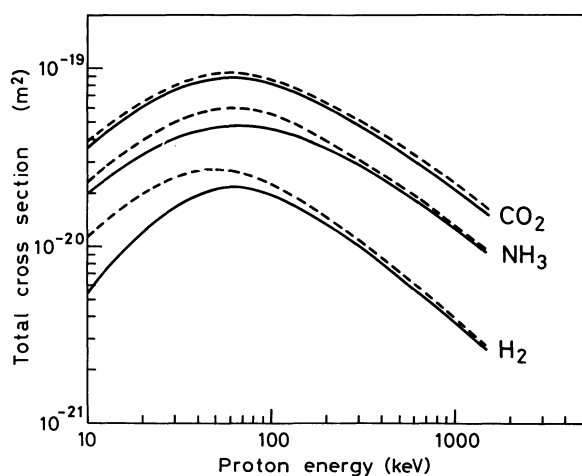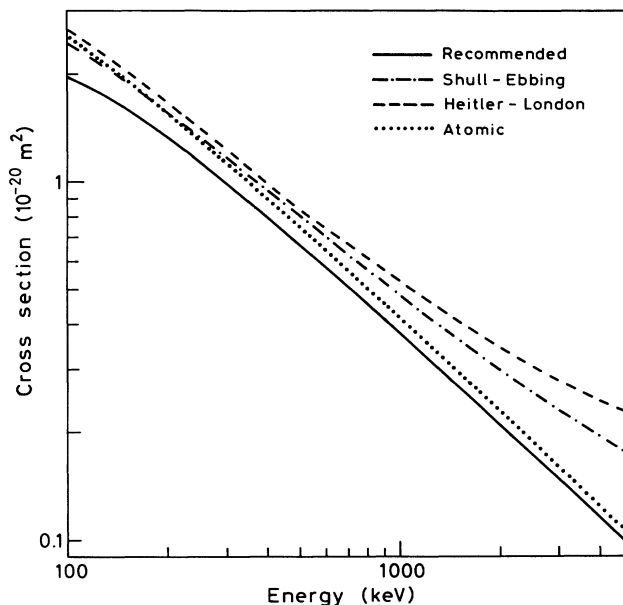

FIG. 2. Total single-ionization cross sections by H_2 by proton projectiles. The recommended curve is taken from the review of Rudd et al. [1].

sen [17]; see Fig. 3(a). Here the factors $\Gamma_{l_f l_c l_g}(k, R, R_0 = 0)$ defined by Eq. (18) are presented as a function of R for $l_g = 0$ and $l_f = l_c$. $\Gamma_{110}(k, R, R_0 = 0)$ is equal to the $G_{fg}^l(R)$ factor of Ref. [17]. At ~ 30 eV, which is the average value of the ejected electrons [18], the contributions with $l_f \geq 2$ are relevant, see Fig. 3(b), and the omission of these contributions leads to remarkable deviations in the total cross sections.

The cross sections with Heitler-London and Shull-Ebbing wave functions do not give such a good agreement with the recommended curve as is provided by the additivity rule. Only the results with Shull-Ebbing wave function at small projectile energies give slightly better cross sections than those with atomic wave function. With increasing proton energies the difference between the cross sections calculated with the additivity rule and the experimental curve becomes smaller. At the same time, these differences become larger for calculations with molecular wave functions.

Cross sections, obtained with molecular wave functions which provide lower ground-state energy for the H_2 molecule, are closer to the experimental values. Figure 2 shows that the curve with a Shull-Ebbing wave function that yields a binding energy $D = 3.93$ eV for the H_2 molecule fits the experiments significantly better than the one calculated with the simpler Heitler-London wave function with $D = 3.14$ eV. We have checked the validity of this statement for other simpler wave functions of Weinbaum [19], Hellman [20], and Coulson [21].

Anyway, we may not state that a perfect agreement with the experimental curve could be achieved by improving the molecular wave function of the target. The assumption formulated by Eq. (11), which means that the

FIG. 1. Total single-ionization cross sections of H_2, NH_3, and CO_2 targets by proton projectiles. The solid lines are the recommended curves of Rudd et al. [1]. The dotted lines are calculated as a sum of the constituent cross sections taken also from Rudd et al. [1] as follows: $\sigma(H_2) = 2\sigma(H)$, $\sigma(NH_3) = 0.5\sigma(N_2) + 1.5\sigma(H_2)$, and $\sigma(CO_2) = \sigma(CO) + 0.5\sigma(O_2)$.

molecular Coulomb wave function is approximated by a single-centered one, might cause serious errors, too.

To shed light on why the additivity rule is so successful, we compare the ways of the calculation with atomic and molecular wave functions. In the atomic limit the length of the molecular axis is zero; that is, $R_0 = 0$. Now
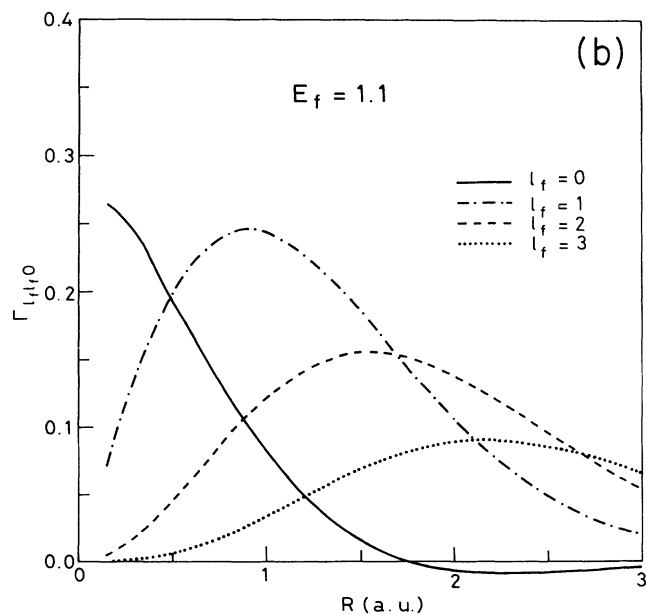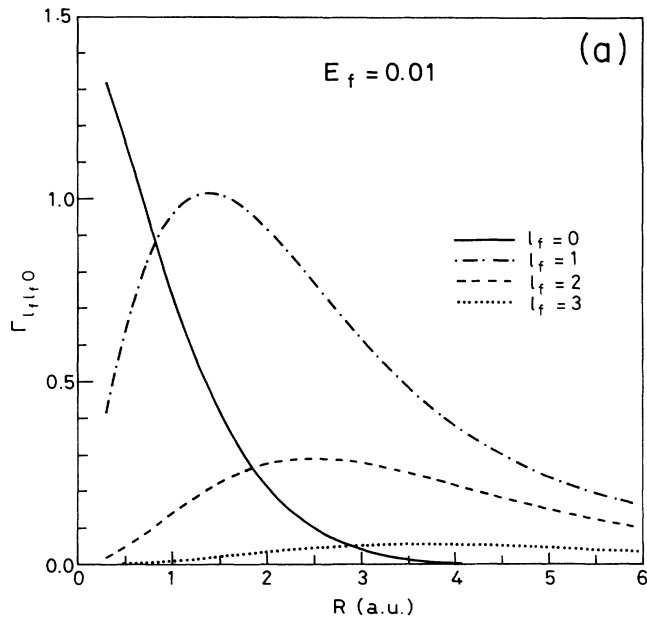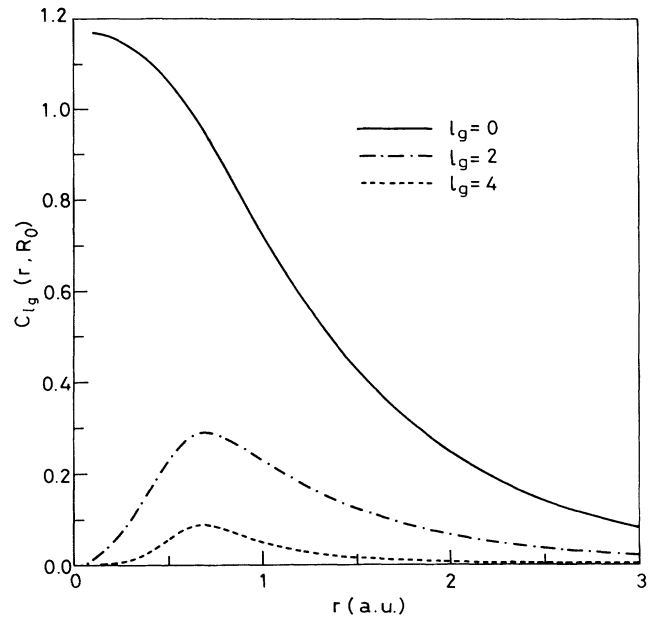

FIG. 4. The $c_{l_g}(r, R_0)$ coefficients of the Legendre expansion in Eq. (14) with $R_0 = 1.4$. $c_{2n+1}(r, R_0) = 0$ for homonuclear diatomic molecules.

in amplitude (16) the expansion coefficient is equal to the radial hydrogenic wave function; that is, $c_{l_g}(r_1, 0) = \delta_{l_g 0} 2 \exp(-r)$. In integral (14) for diatomic homonuclear molecules the $l_g = 0$ term is the dominant one, see Fig. 4, terms with $l_g > 0$ contribute only 2–3 %

FIG. 3. The factors $\Gamma_{l_f l_c l_g}(k, R, R_0)$ defined by Eq. (18) for $l_g = 0$ and $R_0 = 0$ for small (a) and average (b) energy values of the outgoing electrons.
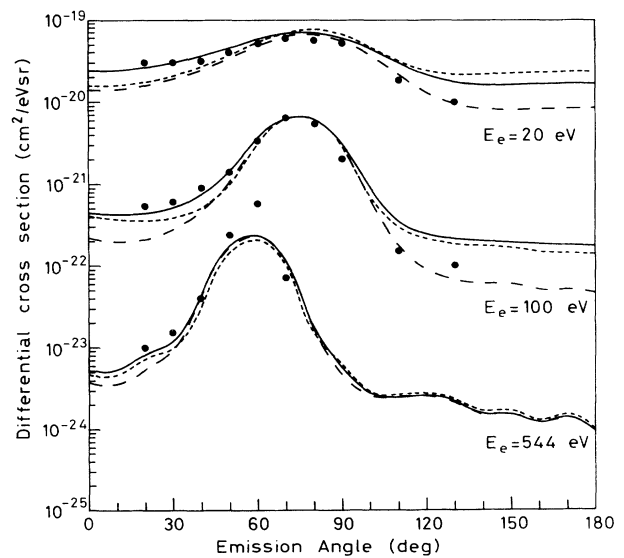

FIG. 5. Differential cross sections of electron emission from H_2 target by 1-MeV proton impact. The experimental values are taken from Toburen and Wilson [5]. The theoretical curves are calculated with Shull-Ebbing (solid line), atomic (long-dotted line), and Heitler-London (short-dotted line) wave functions.

to the total cross sections. As we have already mentioned, the term with $l_g = 1$ is zero. Therefore the values of the proton-H_2 cross sections which are calculated by using atomic wave functions are acceptable. For heteronuclear molecules the $l_g = 1$ term may be important and therefore the additivity rule may fail.

The differential cross sections as functions of the energies and angles of the ejected electrons are presented in Figs. 5 and 6. Calculating the differential cross sections for high-energy electrons, the partial waves up to $l_f = 8$ are taken into account. Generally at electron ejection angles less than 90° the cross sections with molecular wave functions are closer to the experimental points of Toburen and Wilson [5] than the curves obtained with the additivity rule. At angles larger than 90° we obtain an opposite tendency, but in this region more detailed measurements are needed.

CONCLUSIONS

The total and differential single-ionization cross sections of homonuclear diatomic molecules by proton impact may be well approximated as twice the atomic cross sections calculated with binding energy that reproduces the ionization potential of the molecule. For heteronuclear molecules the additivity rule may fail for the calculation of total and mainly for differential cross sections.
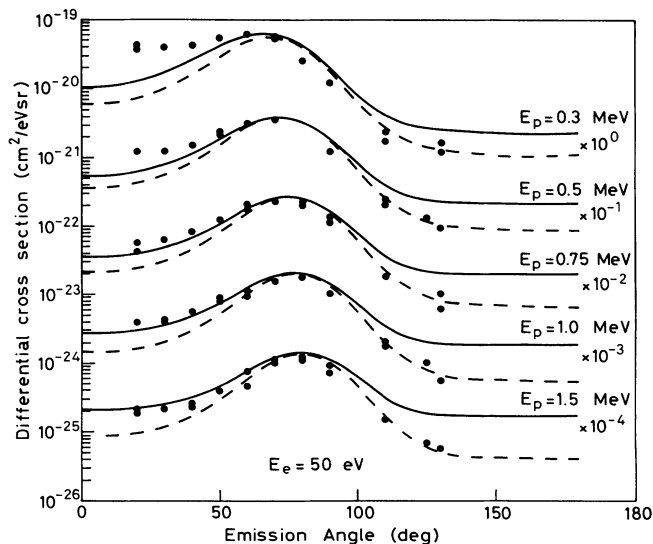

FIG. 6. Differential cross sections of emission 50-eV electrons from H_2 target by proton impact. The experimental values are taken from Toburen and Wilson [5]. The theoretical curves are calculated with Shull-Ebbing (solid line), and atomic (long-dotted line) wave functions.

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