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Distorted-wave models for single-electron capture from molecular targets by the impact of bare ions

S. E. Corchs and R. D. Rivarola*

Instituto de Física Rosario, Consejo Nacional de Investigaciones Científicas y Técnicas and Universidad Nacional de Rosario, Avenida Pellegrini 250, 2000 Rosario, Argentina

J. H. McGuire and Y. D. Wang

Department of Physics, Tulane University, New Orleans, Louisiana 70118

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Electron capture from diatomic molecular targets by the impact of bare ions is studied at high collision velocities. Different distorted-wave models, which take account of the long-range Coulombic behavior of perturbative potentials, are introduced here. Impact-parameter probabilities and single-differential cross sections, depending on the alignment of the intermolecular axis, are studied for $H^+ + H_2{}^+$ collisions. Interference patterns characteristic of scattering from the two molecular centers associated with each one of the nuclei of the target are obtained. Total cross sections, summed over all possible alignments of the intermolecular axis, are also calculated for the $H^+ + H_2$ system for which experimental data exist.

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I. INTRODUCTION

The present work deals with the study of single-electron capture from diatomic molecular targets by the impact of high-velocity bare ions. Interest in such reactions has recently been renewed experimentally. Cheng *et al.* [1], for example, have analyzed charge exchange to O^{8+} projectiles in coincidence with the alignment of the internuclear axis in H_2 targets. Following the pioneering work of Tuan and Gerjuoy [2], this type of reaction has recently been studied by Wang and co-workers [3,4] and Shingal and Lin [5]. Wang and McGuire [4] have used a two-effective-center Oppenheimer-Brinkmann-Kramers (OBK) approximation. Their calculations do reproduce some experimental interference patterns characteristic of scattering from molecular targets at fixed molecular orientation. The magnitude, however, is an order of magnitude larger than experiment.

In this paper we develop improved theoretical perturbative representations containing more physical information than the simplest OBK approximation. We have extended, to the case of molecular targets, two different theoretical approximations previously used for atomic targets: the first orders of the Bates series [6,7] (Ba1) and of the correct-boundary-conditions Born series [8] (B1B). For monoelectronic targets, such as $H_2{}^+$, the initial molecular wave function is represented as a linear combination of one center-single electron orbital (centered on each one of the nuclei of the target). In order to include the long-range behavior of the projectile-electron interaction, each orbital is distorted by an eikonal phase. These phases are evaluated as a function of the position of the projectile with respect to the nucleus where the orbital is centered. In the B1B approximation each phase is chosen with the electron fixed on the respective molecular nucleus, while in the Ba1 model the projectile-electron interaction is averaged over the corresponding one-center orbital. Thus it is expected that the Ba1 approximation may give a better description than B1B when the projectile distorts the molecule in the entry channel. In the exit channel the wave function describing the electron bound to the projectile is distorted by an eikonal phase that is related to the molecular *effective* center from which the electron is captured. This corresponds to describing the reaction as a scattering from two *effective* centers (each center associated with each one of the nuclei of the molecule) as done by Wang, McGuire, and Rivarola [3] for the OBK approximation. If we study capture from the effective center j (with $j=1,2,$), the final bound wave function is distorted by an eikonal phase that accounts for the interaction between the electron and the nucleus j, assuming the electron is placed on the projectile nucleus when the B1B approximation is calculated. For the Ba1 approximation the same interaction is averaged on the final bound wave function. These approximations are also extended to the dielectronic-target case.

In order to test the three above-cited models (OBK, B1B, and Ba1), we have calculated, within these approximations, probabilities (as a function of the impact parameter **B** taken with respect to the center of mass of the molecule) and single-differential cross sections (as a function of the polar angle formed between the internuclear molecular vector and the initial impact velocity vector) for electron capture from a molecular-ion $H_2{}^+$ by the impact of high-velocity protons. We have also calculated total cross sections for single charge transfer in $H^+ + H_2$ collisions so as to compare the theoretical results with the experimental data available. Atomic units are used unless otherwise stated.

II. THEORETICAL FORMULATION

A. Monoelectronic targets

Let us consider a bare nucleus of charge Z_P impacting on a diatomic molecule. In this section we treat the case of a monoelectronic target. Following Wang, McGuire, and Rivarola [3], we describe the molecule as a system containing two effective centers placed on each of its nuclei. As we are interested in impact-parameter probabilities, single-differential cross sections (as a function of the polar angle of the internuclear molecular vector), and total cross sections, we will use the fact, recently shown [9] by using an impact-parameter formulation, that the interaction between the projectile and the molecular nuclei can be excluded from the treatment. If rescattering between the molecular centers is neglected, the operator $\hat{T}_M$ corresponding to the molecular scattering can be written as

$$\hat{T}_M \cong \hat{T}_1 + \hat{T}_2 \ , \tag{1}$$

where $\hat{T}_j$ (with $j=1,2$) is the operator corresponding to the scattering with the effective center j.

Let us choose the center of mass of the target as the origin of the reference system. Since we study high-velocity collisions it is assumed that the internuclear molecular vector $\boldsymbol{\rho}$ remains frozen during the reaction. If $\mu = M_1/(M_1+M_2)$ (with M_j the nuclear mass of center j) and considering that $M_j \gg 1$, the effective center j is displaced from the reference origin by the vector $(\delta_{1j}-\mu)\boldsymbol{\rho}$. So it is easy to write the molecular T-matrix element T^M_{if} as [3]:

$$T^M_{if} = \sum_{j=1}^{2} T^j_{if} \exp\{-i(\delta_{1j}-\mu)\boldsymbol{\alpha}\cdot\boldsymbol{\rho}\} \ , \tag{2}$$

where T^j_{if} is the T-matrix element corresponding to the j effective center (seen from a reference frame placed on the nucleus of this center) and $\boldsymbol{\alpha}$ is the total momentum transfer.

Let us consider the case of an homonuclear molecule. The initial nonperturbed stationary wave function φ_i representing the molecule in a gerade state is chosen as

$$\varphi_i = N_i[\varphi_i^1 + \varphi_i^2] \ , \tag{3}$$

where φ_i^j $(j=1,2)$ is an effective electron orbital corresponding to the center j and N_i is the molecular normalization factor.

If φ_f is the final nonperturbed stationary wave function describing the electron bound to the projectile and assuming that $M_p, M_j \gg 1$ (with M_p the projectile mass), we calculate T^j_{if} in first-order approximation, so that

$$T^j_{ij} = \langle \chi^j_f | W^j_i | \chi^j_i \rangle \ , \tag{4}$$

where χ^j_i and χ^j_f are distorted wave functions of the form

$$\chi^j_i = N_i \varphi^j_i \exp\{i\mathbf{K}_i\cdot\mathbf{R}_j\} L^j_i(\mathbf{R}_j) \ , \tag{5}$$

$$\chi^j_f = \varphi_f \exp\{i\mathbf{K}_f\cdot\mathbf{R}_j\} L^j_f(\mathbf{R}_j) \ , \tag{6}$$

and W^j_i is the corresponding perturbative potential. In Eqs. (5) and (6), $\mathbf{K}_i = \mathbf{M}_P\mathbf{v}_i$ and $\mathbf{K}_f = (M_P+1)\mathbf{v}_f$ are the initial and final momenta, respectively, and $\mathbf{v}_i$ and $\mathbf{v}_f$ the initial and final velocities, respectively. Also, $\mathbf{R}_j$ is the position of the projectile with respect to the nucleus j and $L^j_i(\mathbf{R}_j)$ and $L^j_f(\mathbf{R}_j)$ represent the initial and final distortion factors, respectively. These factors are chosen in different forms. In the OBK model we have

$$L^j_i = L^j_f = 1 \ , \tag{7a}$$

$$W^j_i = -Z_P/s \ , \tag{7b}$$

where $\mathbf{s}$ is the position of the electron with respect to the projectile nucleus.

In the B1B model the factors take the form

$$L^j_i(R_j) = \exp\left\{ -i/v \int_{-\infty}^{z_j} dz'_j Z_P/R_j \right\} \tag{8a}$$

$$L^j_f(R_j) = \exp\left\{ i/v \int_{z_j}^{+\infty} dz'_j Z_j/R_j \right\} \ , \tag{8b}$$

$$W^j_i = -Z_P/s + Z_P/R_j \ , \tag{8c}$$

where Z_j is the nuclear charge of the center j and z_j is the component of $\mathbf{R}_j$ in the direction given by $\mathbf{v} \equiv \mathbf{v}_i \cong \mathbf{v}_f$. Finally, in the Ba1 approximation,

$$L^j_i(R_j) = \exp\left\{ -i/v \int_{-\infty}^{z_j} dz'_j \langle \varphi^j_i | Z_P/s | \varphi^j_i \rangle \right\} \ , \tag{9a}$$

$$L^j_f(R_j) = \exp\left\{ i/v \int_{z_j}^{+\infty} dz'_j \langle \varphi_f | Z_j/x_j | \varphi_f \rangle \right\} \ , \tag{9b}$$

$$W^j_i = -Z_P/s + \langle \varphi^j_i | Z_P/s | \varphi^j_i \rangle \ , \tag{9c}$$

with $\mathbf{x}_j$ the electron coordinate with respect to the nucleus j.

The B1B and Ba1 approximations may be also obtained from a molecular picture, where the initial distorted molecular wave function is chosen as

$$\xi_i = N_i(\varphi^1_i L^1_i + \varphi^2_i L^2_i)\exp\{i\mathbf{K}_i\cdot\mathbf{R}_i\} \tag{10a}$$

and the final distorted one as

$$\xi_f = \varphi_f L^1_f L^2_f \exp\{i\mathbf{K}_f\cdot\mathbf{R}_f\} \ , \tag{10b}$$

where $\mathbf{R}_i$ $(\mathbf{R}_f)$ is the initial (final) position vector of the projectile with respect to the center of mass of the target. The distorting factors L^j_i and L^j_f $(j=1,2)$ are taken as indicated in Eqs. (8) and (9), depending on whether the B1B or the Ba1 approximation is developed. We assume that the orbitals φ^j_i $(j=1,2)$ are chosen to satisfy the Schrödinger equation

$$\left[-\tfrac{1}{2}\nabla^2_{x_j} - \frac{Z^*_j}{x_j} + \frac{Z^{*2}_j}{2} \right] \varphi^j_i = 0 \ , \tag{11}$$

with Z^*_j $(j=1,2)$ the effective charge of the orbital φ^j_i. Then, the molecular T-matrix element will be given by the expression

$$\begin{aligned} T^M_{if} &= \langle \xi_f | H - E | \xi_i \rangle \\ &\cong N_i \sum_{j=1}^{2} \left\langle \xi_f \left| W^j_i - \frac{Z_1}{x_1} - \frac{Z_2}{x_2} + \frac{Z^*_j}{x_j} - \frac{Z^{*2}_j}{2} \right. \right. \\ &\qquad \left. \left. - \varepsilon_i 0 \right| \varphi^j_i L^j_i \exp\{i\mathbf{K}_i\cdot\mathbf{R}_i\} \right\rangle \ . \end{aligned} \tag{12}$$

In Eq. (12) H is the total Hamiltonian of the four-particle system given by

$$H=-\frac{1}{2M_P}\nabla^2_{R_i}-\tfrac{1}{2}\nabla^2_r-\frac{Z_1}{x_1}-\frac{Z_2}{x_2}-\frac{Z_p}{s} \tag{13}$$

and the total energy E is

$$E=\frac{K_i^2}{2M_p}+\varepsilon_i \ . \tag{14}$$

Also in Eq (12), ε_i is the molecular initial energy and $\mathbf{r}$ the electron coordinates with respect to the center of mass of the two molecular nuclei. As it is assumed that the molecular nuclei remain frozen during the collision, the corresponding internuclear potential has been excluded from H. Correspondingly, in the initial orbital energy ε_i this potential is also ignored.

In the initial asymptotic region we have $\mathbf{R}_1\rightarrow\mathbf{R}_i$, $\mathbf{R}_2\rightarrow\mathbf{R}_i$, and $\mathbf{s}\rightarrow\mathbf{R}_i$; so that

$$\lim_{|K_iR_i-\mathbf{K}_i\cdot\mathbf{R}_i|\rightarrow\infty}\xi_i=\zeta_i=N_i(\varphi_i^1+\varphi_i^2)\exp\{i\mathbf{K}_i\cdot\mathbf{R}_i\}\times\exp\{-iZ_P/v\ln(K_iR_i-\mathbf{K}_i\cdot\mathbf{R}_i)\}. \tag{15a}$$

In the same way, for the exit channel results,

$$\lim_{|K_fR_f-\mathbf{K}_f\cdot\mathbf{R}_f|\rightarrow\infty}\xi_f=\varphi_f\exp\{i\mathbf{K}_f\cdot\mathbf{R}_f\}\times\exp\{i(Z_1+Z_2)/v\ \ln(K_fR_f+\mathbf{K}_f\cdot\mathbf{R}_f)\}\ . \tag{15b}$$

In accord with (15a), we obtain the following asymptotic perturbation:

$$(H-E)\zeta_i=\left[-\frac{Z_P}{s}+\frac{Z_P}{R_i}\right]\zeta_i+N_i\exp\{i\mathbf{K}_i\cdot\mathbf{R}_i\}\exp\{-iZ_P/v\ \ln(K_iR_i-\mathbf{K}_i\cdot\mathbf{R}_i)\}\times\sum_{j=1}^{2}\left[-\frac{Z_1}{x_1}-\frac{Z_2}{x_2}+\frac{Z_j^*}{x_j}-\frac{Z_j^{*2}}{2}-\varepsilon_i\right]\varphi_i^j\ . \tag{16}$$

The terms in the sum in Eq. (16) are neglected when we represent the nonperturbed molecular wave function as a simple linear combination of one-center orbitals. If similar terms are neglected in Eq. (12), then T_{if}^M reads

$$T_{if}^M\cong N_i\sum_{j=1}^{2}\langle\xi_f|W_i^j|\varphi_i^jL_i^j\exp\{i\mathbf{K}_i\cdot\mathbf{R}_i\}\rangle\ . \tag{17}$$

From Eq. (16) we can note that the asymptotic perturbative potential is not Coulombic, so that ξ_i satisfies appropriate initial boundary conditions. The same condition results for the exit channel if ξ_f is chosen as in Eq. (10b).

If we want to obtain the two-effective-center model the influence of one molecular center on the other one must be neglected. This implies approximating L_f^2 and L_f^1 by unity in the first and second terms of Eq. (17), respectively. So, Eq. (2) is recovered. With this last approximation we have lost the Coulomb boundary condition corresponding to the exit channel.

At fixed alignment of the molecular axis corresponding to a solid angle Ω_p, the double-differential cross is given by

$$\frac{d\sigma}{d\Omega_pd\Omega}=\frac{M_P(M_P+1)}{4\pi^2}\frac{K_f}{K_i}|T_{if}^M|^2\ , \tag{18}$$

where Ω is the solid angle subtended by the projectile in the exit channel. The single-differential cross section $d\sigma/d(\cos\theta_p)$, as a function of the polar angle θ_p, is then obtained by integration over Ω and over the azimuthal angle ϕ_p of the internuclear axis.

In the impact-parameter picture, the position $\mathbf{R}$ of the projectile relative to the center of mass of the molecule is given by

$$\mathbf{R}=\mathbf{B}+\mathbf{v}t\ , \tag{19}$$

where $\mathbf{B}$ is the impact parameter. Using expression (2) the scattering amplitude $a_M(\mathbf{B})$ is obtained through the Fourier transform

$$a_M(\mathbf{B})=\frac{1}{v}\int\exp\{i\boldsymbol{\alpha}_\perp\cdot\mathbf{B}\}T_{if}^Md\boldsymbol{\alpha}_\perp\ , \tag{20}$$

where $\boldsymbol{\alpha}_\perp$ is the component of $\boldsymbol{\alpha}$ perpendicular to $\mathbf{v}$. Then, the scattering amplitude is given by [3]

$$a_M(\mathbf{B})=\sum_{j=1}^{2}a_j(\mathbf{B}_j)\exp\{-i(\delta_{1j}-\mu)\alpha_z\rho_z\}\ , \tag{21}$$

where $a_j(\mathbf{B}_j)$ is the transition amplitude corresponding to the effective center j [found by replacing T_{if}^M by T_{if}^j in Eq. (20)] and $\mathbf{B}_j$ represents the impact parameter referred to the same center. Also in Eq. (21), α_z and ρ_z are the components of $\boldsymbol{\alpha}$ and $\boldsymbol{\rho}$ in the direction of $\mathbf{v}$. Molecular-impact-parameter probabilities can be obtained by employing the following expression:

$$P_M(\mathbf{B})=|a_1(\mathbf{B}_1)|^2+|a_2(\mathbf{B}_2)|^2+2\,\mathrm{Re}(a_1^*a_2\exp\{i\alpha_z\rho_z\})\ . \tag{22}$$

B. Dielectronic targets

Let us now treat the case of dielectronic homonuclear targets. We choose to represent the initial nondistorted wave function in the fundamental state as a linear combination of products of one-center one-electron orbitals, given by

$$\Phi_i = N_M[\varphi_i^1(1)\varphi_i^2(2)+\varphi_i^1(2)\varphi_i^2(1)]\exp\{i\mathbf{K}_i\cdot\mathbf{R}_i\}\ , \tag{23}$$

where $\varphi_i^j(1)$ and $\varphi_i^j(2)$ $(j=1,2)$ are the initial orbitals corresponding to electrons 1 and 2 in the effective center j, respectively, and N_M is the molecular normalization factor of Φ_i. We assume that electron 1 is captured and only distortions corresponding to this electron will be introduced. Hence, the initial distorted wave function ξ_i is chosen as

$$\xi_i = N_M[\varphi_i^1(1)\varphi_i^2(2)L_i^1+\varphi_i^1(2)\varphi_i^2(1)L_i^2]\exp\{i\mathbf{K}_i\cdot\mathbf{R}_i\}\ . \tag{24}$$

In the exit channel, the final distorted wave function $\xi_f^\pm$ is chosen as

$$\xi_f^\pm = \varphi_f N_i^\pm[\tau_1(2)\pm\tau_2(2)]\exp\{i\mathbf{K}_f\cdot\mathbf{R}_f\}L_f^1L_f^2\ , \tag{25}$$

where $N_i^\pm[\tau_1(2)\pm\tau_2(2)]$ represents the final stationary molecular state of electron 2, with $\tau_j(2)$ the orbital corresponding to electron 2 and effective center j and the signs $+$ and $-$ correspond to gerade and ungerade states of the residual molecular ion, respectively. $N_i^\pm$ is the normalization factor corresponding to such states. In Eqs. (24) and (25) the distortion factors L_i^j and L_f^j correspond to the OBK, B1B, and Ba1 approximations as given by Eqs. (7), (8), and (9), respectively.

If, as it has been done before for the OBK model [3], we assume that during the collision process electron 2 does not influence the capture of electron 1, the molecular T-matrix results in

$$T_{if}^{M,\pm} \cong N_i^\pm N_M \sum_{j=1}^{2} N_{iM}^{j,\pm}\langle\varphi_f\exp\{i\mathbf{K}_f\cdot\mathbf{R}_f\}L_f^1L_f^2|W_i^j \times|\varphi_i^j(1)\exp\{i\mathbf{K}_i\cdot\mathbf{R}_i\}L_i^j\rangle\ , \tag{26}$$

where $N_{iM}^{j,\pm}$ is an overlap integral between ionic and molecular wave functions given by

$$N_{iM}^{1,\pm} = \langle\tau_1(2)\pm\tau_2(2)|\varphi_i^2(2)\rangle\ , \tag{27a}$$

$$N_{iM}^{2,\pm} = \langle\tau_1(2)\pm\tau_2(2)|\varphi_i^1(2)\rangle\ . \tag{27b}$$

In expressions (27a) and (27b), the brackets indicate integration over coordinates of electron 2. As we have done in the monoelectronic case, we neglect the influence of one molecular center on the other one, so that one has

$$T_{if}^{M,\pm} \cong N_i^\pm N_M \sum_{j=1}^{2} N_{iM}^{j,\pm}\langle\varphi_f\exp\{i\mathbf{K}_f\cdot\mathbf{R}_f\}L_f^j|W_i^j \times|\varphi_i^j(1)\exp\{i\mathbf{K}_i\cdot\mathbf{R}_i\}L_i^j\rangle\ . \tag{28}$$

Expression (2) is again recovered for the dielectronic case, now with the normalization factors corresponding to the dielectronic target.

For simplicity we have considered a purely covalent initial molecular wave function, but the present formulation can be easily extended to the case of a Weinbaum wave function [3], where *ionic* terms are included. In such a case, expression (23) takes the form

$$\Phi_i = N_M\{\varphi_i^1(1)\varphi_i^2(2)+\varphi_i^1(2)\varphi_i^2(1) +c[\varphi_i^1(1)\varphi_i^1(2)+\varphi_i^2(2)\varphi_i^2(1)]\}\exp(i\mathbf{K}_i\cdot\mathbf{R}_i\}\ , \tag{29}$$

with N_M the normalization factor corresponding to the Weinbaum wave function. Now, the overlap constant in Eq. (28) results in

$$N_{iM}^{1,\pm} = \langle\tau_1(2)\pm\tau_2(2)|\varphi_i^2(2)\rangle(1\pm c)\ , \tag{30a}$$

$$N_{iM}^{2,\pm} = \langle\tau_1(2)\pm\tau_2(2)|\varphi_i^1(2)\rangle(1\pm c)\ . \tag{30b}$$

Differential and total cross sections can be obtained as indicated previously in Sec. II A, multiplying each quantity by a factor of 2 in order to take account of the two electrons of the molecule.

III. RESULTS AND DISCUSSIONS

The approximations presented in Sec. II (OBK, B1B, and Ba1) have been applied to calculate probabilities $P_M(\mathbf{B})$ and single-differential cross sections $d\sigma/d(\cos\theta_\rho)$ for the case of a monoelectronic target H_2^+. We have analyzed the reaction $H^+ + H_2{}^+(\sigma_g 1s) \rightarrow H(1s) + 2H^+$ and for the calculations we have taken $\rho=2$ a.u., $Z_1=Z_2=1$, $Z_1^*=Z_2^*=1.228$, and $\varepsilon_i=-1.083$ a.u. In Figs. 1–3 probabilities $P_M(\mathbf{B})$ are represented at a 1-MeV collision energy for fixed orientation of the molecular axis vector $\boldsymbol{\rho}$. In Fig. 1 we have set $\theta_\rho=\phi_\rho=0°$ and it may be observed, as in the case of atomic targets [10], that the B1B model does not give an adequate representation of the transition amplitude at small impact parameters where a divergence occurs at $B=0$ a.u. When $\theta_\rho=90°$ and $\phi_\rho=0°$ (Fig. 2), a similar behavior is seen at $B=1$ a.u. Let us note that this value of B corresponds to an impact param-

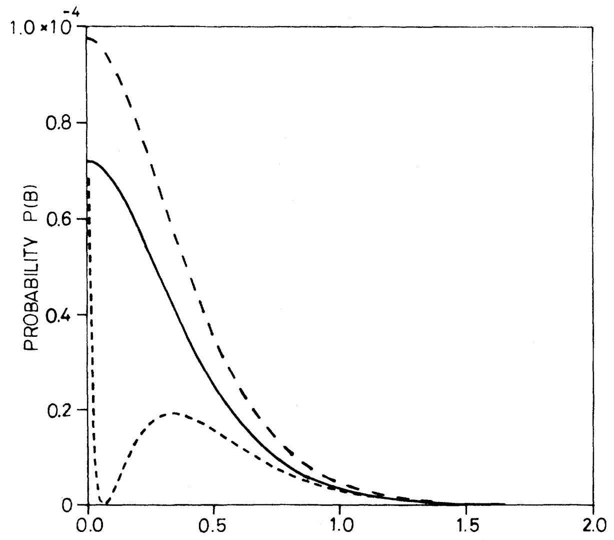

FIG. 1. Impact-parameter probabilities for electron capture in $H^+ + H_2{}^+$ collisions at 1 MeV for fixed orientation of the molecular axis $\theta_\rho=\phi_\rho=0°$. Theoretical calculations: ———, OBK; ——, Ba1; - - -, B1B.

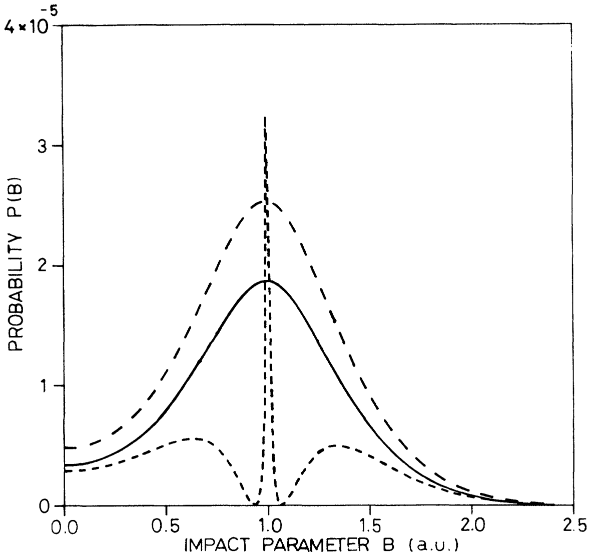

FIG. 2. Impact-parameter probabilities for electron capture in $H^+ + H_2{}^+$ collisions at 1 MeV for fixed orientation of the molecular axis: $\theta_p = 90°$ and $\phi_p = 0°$. Theoretical calculations: OBK, B1B, and Ba1 results, as for Fig. 1.

eter B_1, referred to the molecular center 1, equal to zero. If the molecular axis is placed out of the collision plane setting $\theta_p = 90°$ and $\phi_p = 45°$ (Fig. 3), no spurious divergences appear. In this case both B_1 and B_2 are different from zero for any value of B. In the three figures shown, the OBK and Ba1 models present similar qualitative behavior, with the OBK results larger than the Ba1 results. In Figs. 4–6 we have plotted $d\sigma/d(\cos\theta_p)$ vs θ_p for impact energies of 100 keV, 1 MeV, and 2 MeV, respectively. The molecular alignment effect can be seen from these figures where interference patterns due to scattering from the two effective molecular centers appear. For each impact energy all three approximations present similar profiles but their forms depend strongly on the incident energy. We also observe that even when the B1B model has spurious contributions in the impact-parameter probability, the singularities are avoided when we integrate these probabilities over the impact parame-

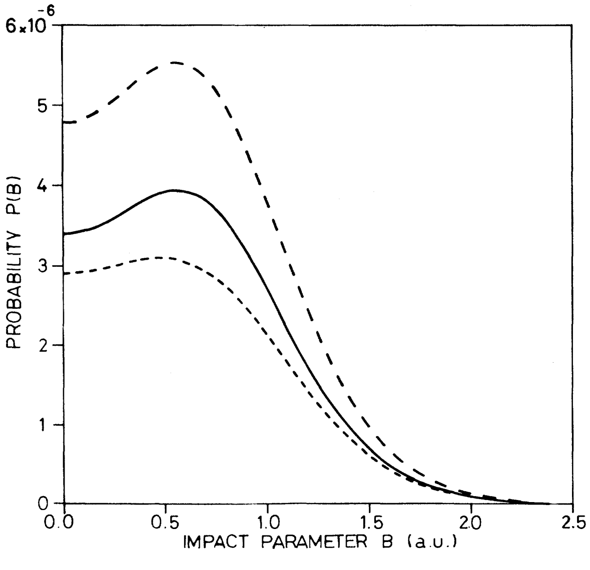

FIG. 3. Impact-parameter probabilities for electron capture in $H^+ + H_2{}^+$ collisions at 1 MeV for fixed orientation of the molecular axis: $\theta_p = 90°$ and $\phi_p = 45°$. Theoretical calculations: OBK, B1B, and Ba1 results, as for Fig. 1.

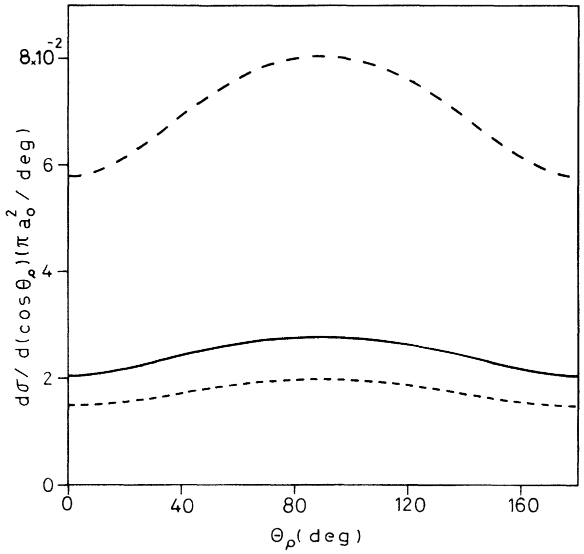

FIG. 4. Single-differential cross section as a function of θ_p for $H^+ + H_2{}^+$ collisions at 100-keV impact energy. Theoretical calculations: OBK, B1B, and Ba1 results, as for Fig. 1.

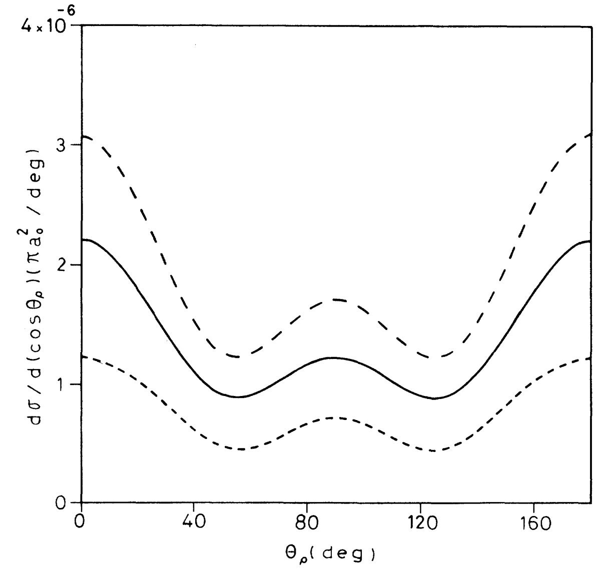

FIG. 5. Single-differential cross section as a function of θ_p for $H^+ + H_2{}^+$ collisions at 1-MeV impact energy. Theoretical calculations: OBK, B1B, and Ba1 results, as for Fig. 1.

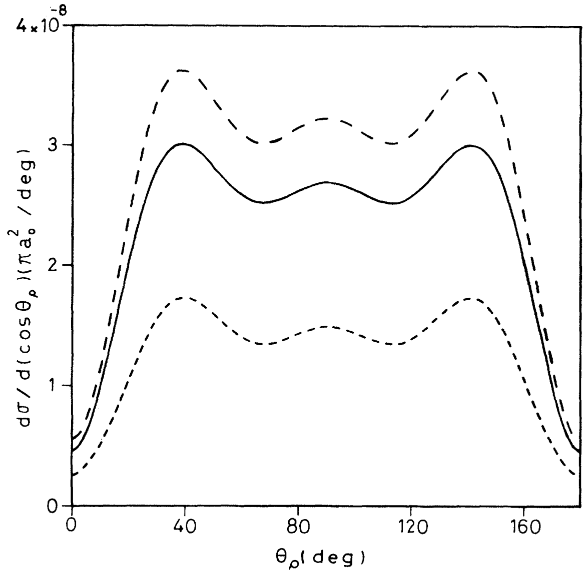

FIG. 6. Single-differential cross section as a function of θ_ρ for $H^+ + H_2^+$ collisions at 2-MeV impact energy. Theoretical calculations: OBK, B1B, and Ba1 results, as for Fig. 1.

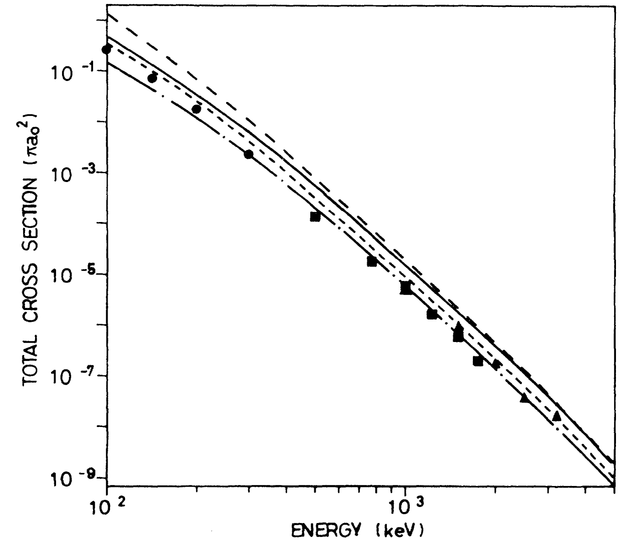

FIG. 7. Total cross section for ground-state capture in $H^+ + H_2$ collisions. Theoretical results: — — —, OBK; ——, Ba1; - - - - -, B1B; —·—·— twice atomic B1B. Experimental data: ●, Barnett and Reynolds (1958); ■, Toburen, Nakai, and Langley (1968); ▲, Schryber (1966).

ter **B** and over the azimuthal angle ϕ_ρ to obtain $d\sigma/d(\cos\theta_\rho)$. At asymptotic high velocities Rivarola, Maidagan, and Hanssen [7] have shown that the Ba1 transition amplitude in the atomic case converges to the OBK amplitude. In the figures presented here, even when the impact energies are not very high, the Ba1 results approach the OBK results as the the energy increases.

Because the experimental data available in $H^+ + H_2$ collisions do not give information about the alignment of the molecular axis, we have calculated total cross sections within the OBK, B1B, and Ba1 models, averaged over all orientations of ρ as previously done by Tuan and Gerjuoy [2] and by Ray and Saha [11,12]. The calculations, shown in Fig. 7, correspond to the capture process $H^+ + H_2(^1\Sigma_g^+) \rightarrow H(1s) + H_2^+(\sigma_g 1s)$. A purely covalent wave function is used to represent the initial stationary molecular state. Cross sections for the ungerade state $\sigma_u^* 1s$ of the residual H_2^+ ion are expected to be only a few percent of the gerade cross sections [11], and are not plotted in Fig. 7. The parameters used in the calculations are $\rho = 1.4$ a.u., $Z_1 = Z_2 = 1$, $Z_1^* = Z_2^* = 1.193$, and the effective charge corresponding to orbitals τ_j $(j = 1,2)$ of Eq. (25) is taken equal to 1.4. The initial electronic binding energy is taken as $\varepsilon_i = -1.07$ a.u. Figure 7 also shows twice the total cross section for the atomic reaction $H^+ + H(1s) \rightarrow H(1s) + H^+$ in B1B model and it is seen from the figure, by comparison with the molecular B1B results, that the molecular cross section is not just equal to twice the atomic cross section [2,11]. The experimental data are from Barnett and Reynolds [13], Toburen, Nakai, and Langley [14], and Schryber [15]. As the distorted functions used in the Ba1 model give a better representation of the projectile-electron and electron-residual target interactions in the entry and exit channel, respectively, at intermediate distances between the projectile and the target, we expect for this approximation the best agreement with the experiments. However, when the three molecular approximations described above are compared with experiments, we observe that within the energy range considered, the B1B calculations give the best agreement with the experimental data. Also it must be noted that a "fortuitous" coincidence between B1B and the previously developed molecular Jackson-Schiff model [2,11] would be obtained in this particular case (where $Z_P = Z_1 = Z_2 = 1$) if the same parameters characterizing the molecule were used.

IV. CONCLUSIONS

Two distorted-wave models B1B and Ba1 are developed in order to describe single-electron capture from diatomic molecular targets. Two-effective-center pictures are derived from the distorted-wave treatment for the ion-molecule collisions. The introduction of these models allows us to determine the influence of the interactions between the *active* electron and the projectile and target nuclei on the studied reaction. It is shown that for the impact of protons on H_2^+ ions, the B1B approximation yields spurious singularities when impact-parameter probabilities are studied. On the contrary, OBK and Ba1 give smooth curves with a simple maximum in the impact-parameter region for which the singularities appear in the B1B model. Even when OBK and Ba1 give similar qualitative profiles, Ba1 results are lower than the OBK ones. When single-differential cross sections $d\sigma/d(\cos\theta_\rho)$ are calculated the singularities of B1B are avoided and the three approximations give the same qualitative representation of the interference patterns characteristic of scattering from the two effective centers of the target. However, OBK overestimates the Ba1 results, while B1B underestimates them.

The distorted-wave approximations here introduced may be a good starting point to analyze experimental data for heavier projectiles [1]. In one such case it has been shown that OBK results give a large overestimation of experimental measurements [4]. In the case of an atomic H target, it has been shown [16] that the B1B approximation gives a good representation of experimental cross sections for impact of B^{5+} and C^{6+} ions at collision energies larger than 1 MeV. At present we are developing a similar study for the molecular H_2 target case.

Comparisons between theoretical total cross sections for $H^{+}+H_2$ collisions (calculated in the OBK, B1B, and Ba1 approximations) and experimental data show that the best agreement between theory and measurements is obtained for the B1B model. Differences between molecular and atomic pictures are observed for total cross sections.

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*Also at Departamento de Física, Escuela de Ciencias Exactas y Naturales, Facultad de Ciencias Exactas, Ingeniería y Agrimensura, Universidad Nacional de Rosario, 2000 Rosario, Argentina.

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