Ionization and electron capture to the continuum in the H^+–hydrogen-atom collision

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The equivalence of the two-body interactions between the final particles of the ion-atom ionization process is considered in the T-matrix formalism. This defines a final wave function which is product of Coulomb waves and describes simultaneously the capture to the continuum and the direct ionization. The relation of that approach with the wave equation for the three-particle system and the asymptotic behavior are discussed. The doubly differential cross section for the ionization of hydrogen atoms by proton impact is calculated, in first order, and compared with experimental values.

I. INTRODUCTION

Considerable theoretical progress has been made for the calculation of the doubly differential cross section (DDCS), in energy and angle, for electrons ejected by atoms under light-ion impact. The major theoretical methods used have been first-order approximations[1] and binary-encounter theories.[2] Early first-order calculations considered that the final state of the electron was described by a Coulomb plane wave centered at the residual ion, neglecting distortion due to the projectile. These methods dealt with direct ionization (DI) and were not able to explain the forward peaking in the DDCS. This enhanced yield of electrons has been interpreted as arising from charge exchange to continuum states centered around the projectile (CTC).[3-6] However, the symmetry of the final system strongly suggests that the ejected electron should be described by a two-center wave function. Furthermore, as has been pointed out by Macek,[3] there is no physical distinction between DI and CTC. Then, the cross sections for DI and for CTC should not be added. Macek proposed a linear combination of Coulomb plane waves centered at the residual target and at the projectile for the final-state wave function of the electron.[3,5] With this description the amplitudes for both processes are added. This approach allows for the possible occurence of an interference pattern between both amplitudes. Recently, this interference structure has been searched for experimentally.[7]

From the exact final wave function, Dettman *et al.* factor out the Coulomb wave centered at the projectile, and give an analytic expression for the forward cusp. As in charge exchange theories, the second Born term is very important.[8] In this work we factor out a two-center wave function for the electron in the scattering amplitude. In Sec. III we recognize the equivalent status of the three final Coulomb interactions, and we propose a final state which is the product of functions centered at the projectile and at the target. We have also studied the influence of the interaction between the protons in the final state. In Sec. IV we discuss the meaning of the model starting from the Schrödinger equation for the three-particle system. We find that the approach used here is an improvement of the Vainshtein, Presnyakov, and Sobelman method.[9] Numerical results for proton–hydrogen-atom collisions are discussed in Sec. VI.

II. KINEMATICS

We consider a system composed by an incoming ion of mass M_2 and charge Z_2, colliding with a hydrogenlike atom. The electron mass is called m and the target nucleus has mass M_1 and charge Z_1. In the center of mass system, the problem can be described by any one of the pairs of relative coordinates $(\vec{r}_1, \vec{R}_2)$, $(\vec{r}_2, \vec{R}_1)$, or $(\vec{r}, \vec{R})$, as shown in Fig. 1. The coordinates $\vec{R}_1, \vec{R}_2, \vec{R}$ refer each particle to the center of mass of the other two. They are related by the following equations (atomic units):

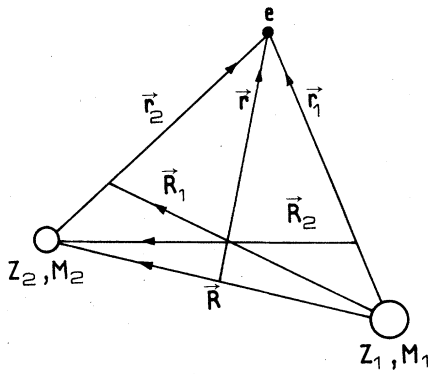

FIG. 1. Coordinate system.

$$\vec{r}_2=\mu_1\vec{r}_1-\vec{R}_2,\quad \vec{r}=(\nu/\nu_2)\vec{r}_1-(\nu/\mu_2)(1-\mu_2)\vec{R}_2,$$
$$\vec{R}_1=\mu_2\vec{R}_2+(1-\mu_1\mu_2)\vec{r}_1,\quad \vec{R}=\vec{R}_2+(1-\mu_1)\vec{r}_1, \tag{2.1}$$

where

$$\mu_1=\frac{M_1}{M_1+1},\quad M_2=\frac{M_2}{M_2+1},\quad \mu=\frac{M_1+M_2}{M_1+M_2+1},$$
$$\nu_1=\frac{(M_2+1)M_1}{M_1+M_2+1},\quad \nu_2=\frac{(M_1+1)M_2}{M_1+M_2+1},\quad \nu=\frac{M_1+M_2}{M_1+M_2}, \tag{2.2}$$

are the associated reduced masses. According to the choice of the spatial coordinates, the system is described in the momentum space by one pair $(\vec{k}_1,\vec{K}_2)$, $(\vec{k}_2,\vec{K}_1)$, or $(\vec{k},\vec{K})$, where $\vec{k}_1$, $\vec{k}_2$, and $\vec{k}$ are the momentum of the electron relative to M_1, M_2, or to the center of mass of M_1,M_2, respectively. These pairs are related by

$$\vec{k}_2=\mu_2\vec{k}_1-(1-\mu_1\mu_2)\vec{K}_2,\quad \vec{k}=\vec{k}_1-(1-\mu_1)\vec{K}_2,$$
$$\vec{K}_1=\mu_1\vec{K}_2+\vec{k}_1,\quad \vec{K}=(\nu/\nu_2)\vec{K}_2+(1-\mu_2)(\nu/\mu_2)\vec{k}_1, \tag{2.3}$$

and the kinematical relation

$$\vec{k}_1\cdot\vec{r}_1+\vec{K}_2\cdot\vec{R}_2=\vec{k}_2\cdot\vec{r}_2+\vec{K}_1\cdot\vec{R}_1=\vec{k}\cdot\vec{r}+\vec{K}\cdot\vec{R} \tag{2.4}$$

follows from the equations above.

The mutual interactions between the particles are Coulomb potentials:

$$V_1=-Z_1/r_1,\quad V_2=-Z_2/r_2,\quad V=Z_1Z_2/R, \tag{2.5}$$

and we define $V_i=V_2+V$ as the initial interaction, $V_f=V_1+V$ as the final one, and $W=V_1+V_2+V$ as the total potential. Then the Hamiltonian operator reads

$$H=H_0+W=H_i+V_i=H_f+V_f, \tag{2.6}$$

where

$$\begin{aligned}H_0&=-(1/2\mu_2)\nabla^2_{r_2}-(1/2\nu_1)\nabla^2_{R_1}\\&=-(1/2\mu_1)\nabla^2_{r_1}-(1/2\nu_2)\nabla^2_{R_2}\\&=-(1/2\mu)\nabla^2_r-(1/2\nu)\nabla^2_R,\end{aligned} \tag{2.7}$$

depending upon which set of independent variables we choose. In the ionization process that we are considering the Schrödinger equation

$$H\Psi=E\Psi \tag{2.8}$$

has eigenvalue

$$\begin{aligned}E&=K^2_{2i}/2\nu_2+\epsilon_i=K_2^2/2\nu_2+k_1^2/2\mu_1\\&=K_1^2/2\nu_1+k_2^2/2\mu_2=K^2/2\nu+k^2/2\mu;\end{aligned} \tag{2.9}$$

$\vec{K}_{2i}$ is the momentum of the projectile relative to the atom, ϵ_i is the ionization energy of the atom, and the other quantities refer to the final state with three particles in continuum states.

The initial-state wave function, in which particles m and M_1 are bound together and M_2 is free, is

$$|i,\vec{K}_{2i}\rangle=e^{i\vec{K}_{2i}\cdot\vec{R}_2}\varphi_i(\vec{r}_1), \tag{2.10}$$

where

$$(H_0+V_1)|i,\vec{K}_{2i}\rangle=E|i,\vec{K}_{2i}\rangle. \tag{2.11}$$

Defining the Green's functions

$$G_0^{\pm}=1/(E-H_0\pm i\epsilon),\quad G_1^{\pm}=1/(E-H_0-V_1\pm i\epsilon),$$
$$G^{\pm}=1/(E-H\pm i\epsilon),\quad G_i^{\pm}=1/(E-H_0-V_i\pm i\epsilon), \tag{2.12}$$

we can write the equation (2.8), for the solution which evolves into a three-particle free state, as a Lippmann-Schwigner equation[10]:

$$\Psi^-_{\vec{k},\vec{K}}=(1-G_0^-W)^{-1}|\vec{k},\vec{K}\rangle=|\vec{k},\vec{K}\rangle+G_0^-W\Psi^-_{\vec{k},\vec{K}}, \tag{2.13}$$

with

$$|\vec{k},\vec{K}\rangle=[1/(2\pi)^3]e^{i(\vec{k}\cdot\vec{r}+\vec{K}\cdot\vec{R})}.$$

In this equation we have explicitly used the pair of momentum coordinates $(\vec{k},\vec{K})$, but anyone of the pairs defined below Eq. (2.2) could be used to write the integral equation.

III. THEORY

Now we define two wave functions $|\vec{k}^-,\vec{K}\rangle$ and $|\vec{k}^-,\vec{K}^-\rangle$ by means of the equations:

$$\begin{aligned}|k_1^-,\vec{K}_2\rangle&=(1+G_1^-V_1)|\vec{k}_1,\vec{K}_2\rangle\\&=|\vec{k}_1,\vec{K}_2\rangle+G_0^-V_1|k_1^-,\vec{K}_2\rangle,\end{aligned} \tag{3.1}$$

and

$$\begin{aligned}|\vec{k}_2^-,\vec{K}_1^-\rangle&=(1+G_i^-V_i)|\vec{k}_2,\vec{K}_1\rangle\\&=|\vec{k}_2,\vec{K}_1\rangle+G_0^-V_i|\vec{k}_2^-,\vec{K}_1^-\rangle.\end{aligned} \tag{3.2}$$

The first equation corresponds to a free wave for the projectile and, in the unscreened limit, to a Coulombian continuum state, with ingoing conditions, for the e-M_1 systems, i.e.,

$$\langle\vec{r}_1,\vec{R}_2|\vec{k}_1^-,\vec{K}_2\rangle=[1/(2\pi)^{3/2}]e^{i\vec{K}_2\cdot\vec{R}_2}\psi^-_{\vec{k}_1}(\vec{r}_1), \tag{3.3}$$

and Eq. (3.2) contains the interactions e-M_2 and M_1-M_2. Because $\vec{R}\sim\vec{R}_1+\mathcal{O}(1/M_2)$, we can assume $\vec{R}_1=\vec{R}_2=\vec{R}$ for a heavy projectile. Then, Eq. (3.2) is the wave equation with both particles, M_1 and m, in continuum states centered around the incoming ion (in Sec. IV this point will deserve further study using the Schrödinger equation), i.e.,

$$\langle\vec{r}_2,\vec{R}_1|\vec{k}_2^-,\vec{K}_1^-\rangle=\Psi^-_{\vec{k}_2}(\vec{r}_2)\,\Psi^-_{\vec{K}_1}(\vec{R}_1). \tag{3.4}$$

We write the continuum wave function for a Coulomb interaction between two particles A and B,

with reduced mass μ and relative momentum $\vec{k}$, in the following way[10]:

$$\psi_{\vec{k}}^{-}(\vec{r}) = [1/(2\pi)^{3/2}] f(\alpha)\, {}_1F_1(-i\alpha, 1, -ikr - i\vec{k}\cdot\vec{r}) e^{i\vec{k}\cdot\vec{r}}$$
$$= f(\alpha)\langle \vec{r}\,|F(\alpha)|\vec{k}\rangle\,, \tag{3.5}$$

where

$$\alpha = -Z_A Z_B \mu/k, \quad f(\alpha) = e^{\pi\alpha/2}\,\Gamma(1+i\alpha)\,.$$

The $f(\alpha)$ is the Coulomb factor, and $F(\alpha)$ is an operator which defines the hypergeometric function in the $\vec{r}$ representation. Then, Eq. (3.4) can be written

$$\langle \vec{r}_2, \vec{R}_1 | \vec{k}_2^{-}, \vec{K}_1^{-}\rangle = f(a_2) f(a_1) \langle \vec{r}_2, \vec{R}_1 | F(a_2) F(a_1) | \vec{k}_2, \vec{K}_1\rangle\,, \tag{3.6}$$

where

$$a_1 = Z_1\mu_1/k_1, \quad a_2 = Z_2\mu_2/k_2, \quad a = -Z_1 Z_2 \nu_1/K_1\,. \tag{3.7}$$

Those wave functions are substituted in the matrix element[4]

$$T_{fi} = \langle \vec{K}_2, \vec{k}_1^{-} | V_i (1 + G V_i) | i, \vec{K}_{2i}\rangle\,, \tag{3.8}$$

to give the transition amplitude for the ionization process. From Eqs. (3.1), (3.3), and (2.4) we get

$$T_{fi} = f^*(a_1)\langle \vec{K}_1, \vec{k}_2 | F(a_1) V_i (1 + G V_i) | i, \vec{K}_{2i}\rangle\,,$$

and introducing the wave function defined by Eq. (3.2):

$$T_{fi} = f^*(a_1)\langle \vec{K}_1^{-}, \vec{k}_2^{-} | (1 - V_i G_0) F(a_1) (1 + V_i G) V_i | i, \vec{K}_{2i}\rangle\,. \tag{3.9}$$

With the assumption of a heavy projectile Eq. (3.4) gives an explicit form for the bracket and an approximate form for the amplitude:

$$T_{fi} = f^*(a_1) f^*(a) f^*(a_2) \times \langle \vec{K}_1, \vec{k}_2 | F(a) F(a_2) (1 - V_i G_0) \times F(a_1)(1 + V_i G) V_i | i, \vec{K}_{2i}\rangle\,. \tag{3.10}$$

The relation between the total and free Green's functions

$$G = G_0 + G_0 W G$$

allows for a perturbative expansion of Eq. (3.10). The first term in this expansion is

$$T_1 = f^*(a_1) f^*(a_2) f^*(a) \times \langle \vec{K}_1, \vec{k}_2 | F(a) F(a_2) F(a_1) V_i | i, \vec{K}_{2i}\rangle, \tag{3.11}$$

and the second one is

$$T_2 = f^*(a_1) f^*(a_2) f^*(a) \times \langle \vec{K}_1, \vec{k}_2 | F(a) F(a_2) \times [F(a_1) V_i G_0 - V_i G_0 F(a_1)] V_i | i, \vec{K}_{2i}\rangle\,. \tag{3.12}$$

Because F and V_i are diagonal operators in the $\vec{r}$ representation

$$F(a_1) V_i G_0 - V_i G_0 F(a_1) = V_i [F(a_1), G_0]\,. \tag{3.13}$$

When k_1 is very large, so that $a_1 = Z_1\mu_1/k_1 \ll 1$, then $F(a_1) \sim 1$ and the commutator bracket will be small $[\mathcal{O}(a_1)]$. Furthermore, if V_i is a small perturbation (a_2 small) the first order given by Eq. (3.11), should provide a good description of the ionization amplitude.

In complete analogy we can start from the amplitude in the rearranged coordinates[4]

$$T_{fi} = \langle \vec{K}_1, \vec{k}_2^{-} | (1 + V_f G) V_i | i, \vec{K}_{2i}\rangle, \tag{3.14}$$

to obtain

$$T_{fi} = f(a_1) f(a) f(a_2) \langle \vec{K}_2, \vec{k}_1 | F(a) F(a_1) (1 - V_f G_0) \times F(a_2)(1 + V_f G) V_i | i, \vec{K}_{2i}\rangle\,. \tag{3.15}$$

The first order of a perturbative expansion T_1 is given by Eq. (3.11). Meanwhile, for the second order we have

$$T_2' = f^*(a_1) f^*(a) f^*(a_2) \langle \vec{K}_1, \vec{k}_2 | F(a) F(a_1) V_f \times [F(a_2), G_0] V_i | i, \vec{K}_{2i}\rangle, \tag{3.16}$$

which should be small for large k_2, i.e., $a_2 = Z_2\mu_2/k_2 \ll 1$.

We can relate the formalism described here with that proposed by Dettmann *et al.*[4] We have established a complete symmetry between the three final Coulomb interactions. Then, to get the amplitude used in Ref. 4 [Eq. (4.14a)] we must switch off the interaction between the ions and between the electron and the residual target ion in the final state. This is achieved by setting $a = a_1 = 0$ and $V = 0$ in Eq. (3.15).

IV. WAVE FUNCTION

The transition amplitude for the ionization process can be written

$$T_{fi} = \langle \psi_{\vec{k},\vec{K}}^{-} | V_i | i, \vec{K}_{2i}\rangle\,, \tag{4.1}$$

where $\psi_{\vec{k},\vec{K}}^{-}$ is a solution of Eq. (2.13). Our first-order expression in Eq. (3.11) is equivalent to writing an approximate value for $\psi_{\vec{k},\vec{K}}^{-}$, that is,

$$\psi_{\vec{k}_2,\vec{K}_1}^{-} \sim \psi_A(\vec{R}_1, \vec{r}_2) = f(a_1) f(a) f(a_2) e^{i\vec{K}_2\cdot\vec{R}_2 + i\vec{k}_1\cdot\vec{r}}\, {}_1F_1[-ia_1, 1, -i(k_1 r_1 + \vec{k}_1\cdot\vec{r}_1)]$$
$$\times {}_1F_1[-ia_2, 1, -i(k_2 r_2 + \vec{k}_2\cdot\vec{r}_2)]\, {}_1F_1[-ia, 1, -i(K_1 R_1 + \vec{K}_1\cdot\vec{R}_1)]\,(2\pi)^{-3}\,. \tag{4.2}$$

A discussion of the meaning of such an approximation will be given in what follows. We consider the wave equation for the three-particle system and see which terms are neglected by using the approximate function. To perform this task we write

$$\psi^{-}_{\vec{k}_2,\vec{K}_1} = \phi(\vec{R}_1,\vec{r}_2)\cdot\psi^{-}_{\vec{k}_1}(\vec{r}_1). \tag{4.3}$$

Now we substitute this wave function into the Schrödinger equation [Eq. (2.8)] to obtain an equation for the $\phi(\vec{R}_1,\vec{r}_2)$.[10] After some algebra we obtain

$$[-(1/2\mu_2)\nabla^2_{r_2}-(1/2\nu_1)\nabla^2_{R_1}+Z_1Z_2/R_1-Z_2/r_2-E+k_1^2/2\mu_1]\,\phi(\vec{R}_1,\vec{r}_2)$$
$$=[Z_1Z_2/R_1-Z_1Z_2/R+(1/\mu_1)\vec{\nabla}_{r_1}\ln\psi^{-}_{\vec{k}_1}(\vec{r}_1)\cdot\vec{\nabla}_{r_1}\ln\phi(\vec{R}_1,\vec{r}_2)]\,\phi(\vec{R}_1,\vec{r}_2)\ . \tag{4.4}$$

This is the starting equation for the Vainshtein, Presnyakov, and Sobelman (VPS) approximation. This approach neglects the right-hand side in Eq. (4.4) and the solution has the form shown at Eq. (3.4). Meanwhile, in our formalism the function $\phi(\vec{R}_1,\vec{r}_2)$ is already defined. From the Eqs. (4.2) and (3.5)

$$\psi_A(\vec{R}_1,\vec{r}_2) = e^{-i\vec{k}_1\cdot\vec{r}_1}\psi^{-}_{\vec{k}_2}(\vec{r}_2)\psi^{-}_{\vec{k}_1}(\vec{R}_1)\psi^{-}_{\vec{k}_1}(\vec{r}_1)(2\pi)^{3/2}\ . \tag{4.5}$$

By comparison with Eq. (4.3) we see that, in Eq. (4.2), we are assuming

$$\phi_A(\vec{R}_1,\vec{r}_2) = e^{-i\vec{k}_1\cdot\vec{r}_1}\psi^{-}_{\vec{k}_2}(\vec{r}_2)\psi^{-}_{\vec{K}_1}(\vec{R}_1)(2\pi)^{3/2}\ . \tag{4.6}$$

Recalling that by definition

$$[-\nabla^2_r-(2\alpha k/r)-k^2]\psi^{-}_{\vec{k}}(\vec{r})=0\ , \tag{4.7}$$

we applied the Hamiltonian operator to $\psi_A(\vec{R}_1,\vec{r}_2)$ and, after some algebraic work, we conclude that

$$[-(1/2\mu_2)\nabla^2_{r_2}-(1/2\nu_1)\nabla^2_{R_1}+Z_1Z_2/R_1-Z_2/r_2-E+k_1^2/2\mu_1]\,\phi_A(\vec{R}_1,\vec{r}_2)$$
$$=[(1/\mu_1)\vec{\nabla}_{r_1}\ln(e^{i\vec{k}_1\cdot\vec{r}_1})\cdot\vec{\nabla}_{r_1}\ln\phi_A]\,\phi_A(\vec{R}_1,\vec{r}_2), \tag{4.8}$$

showing that the approximate wave function, given by Eq. (4.2), is an improvement of the VPS approximation. In fact, the right-hand side of Eq. (4.4) is partially considered. For large k_1, the plane wave appearing in Eq. (4.8) gives a good approximation for the $\psi^{-}_{\vec{k}}(\vec{r}_1)$ and our function, $\Phi_A(\vec{R}_1,\vec{r}_2)$, will be an appropriate description of the exact $\phi(\vec{R}_1,\vec{r}_2)$, defined by the Eq. (4.3). This is related with the Lippmann-Schwinger approach described in Sec. II. In fact, from Eq. (3.13) we see that the second perturbative corrections would be small for large k_1, justifying the Born approximation used in our calculations.

Now we must regard the behavior of $\psi_A(\vec{R}_1,\vec{r}_2)$ for large separation between the particles. Using the asymptotic expression for the hypergeometric function,[11] we find, for large $\vec{R}_1$, $\vec{r}_2$, and $\vec{r}_1$,

$$\psi_A \to \text{Cte.}\, e^{i(\vec{k}_2\cdot\vec{r}_2+\vec{K}_1\cdot\vec{R}_1)}e^{iD} + O(1/r_1,1/R_1,1/r_2)\ , \tag{4.9}$$

where

$$D=a_1\ln(k_1r_1+\vec{k}_1\cdot\vec{r}_1)+a_2\ln(k_2r_2+\vec{k}_2\cdot\vec{r}_2) + a\ln(K_1R_1+\vec{K}_1\cdot\vec{R}_1) \tag{4.10}$$

is the divergent phase of the Coulomb potentials.

Some cases have particular interest. First, let us consider

$$k_1\sim k_2\gg K_1/\nu_1\ ,$$

meaning that the electron moves faster than the two heavy particles and travels far away from both. We could assume $r_1\sim r_2$; then

$$D\sim(a_1+a_2)\ln(k_1r_1+\vec{k}_1\cdot\vec{r}_1) + a\ln(K_1R_1+\vec{K}_1\cdot\vec{R}_1)\ . \tag{4.11}$$

So, the logaritmic divergent phase is defined by the sum of the projectile plus target, i.e., $a_1+a_2\sim(Z_1+Z_2)\nu_1/k_1$. Second, we assume $k_2\sim 0$, which corresponds to the capture into the continuum state of the projectile. Then,

$$\vec{k}_1\sim\vec{K}_1/\nu_1,\quad \vec{r}_1\sim\vec{R}_1\ ,$$

and we get

$$D=(a_1+a)\ln(k_1r_1+\vec{k}_1\cdot\vec{r}_1)+a_2\ln(k_2r_2+\vec{k}_2\cdot\vec{r}_2)\ . \tag{4.12}$$

The phase is defined by

$$a_1+a\sim -Z_1(Z_2-1)\nu_1/K_1\ . \tag{4.13}$$

The charge of the projectile is screened by the electron. Analogous results are attained when

$k_1 \sim 0$, in which case the electron screens the charge of the target.

V. CALCULATION FOR PROTON-HYDROGEN-ATOM COLLISIONS

To evaluate the first-order scattering amplitude as given by Eq. (4.1) we must perform some approximations. In this paper we will accept the Wick argument and neglect the matrix element of the interaction potential V, between the cores.[12] However, the contribution of the V is considered in the initial- and final-state wave function in order to keep the correct asymptotic behaviors. Then,

$$T_1 = \int d\vec{r}_1 \int d\vec{R}_2\, \phi_A^*(\vec{R}_1, \vec{r}_2)\psi_{\vec{k}_1}^*(\vec{r}_1)\left(-\frac{Z_2}{r_2}\right) \times e^{i\vec{K}_2\cdot\vec{R}_2}\varphi_i(\vec{r}_1)(2\pi)^{-3/2}. \quad (5.1)$$

Introducing the function

$$g(\vec{s}, \vec{k}_1) = \int d\vec{r}_1\, \psi_{\vec{k}_1}^*(\vec{r}_1)\varphi_i(\vec{r}_1)e^{i\vec{s}\cdot\vec{r}_1}, \quad (5.2)$$

we obtain

$$T_1 = -\frac{Z_2}{(2\pi)^6} f^*(a)f^*(a_2) \int d\vec{s}\, g(\vec{s}, \vec{k}_1) \int d\vec{r}_1 \times \int d\vec{R}_2\, e^{-i\vec{s}\cdot\vec{r}_1 + i\vec{P}\cdot\vec{R}_2}\, {}_1F_1^*(ia_2, 1, ik_2r_2 + i\vec{k}_2\cdot\vec{r}_2) \times {}_1F_1^*(ia, 1, iK_1R_1 + i\vec{K}_1\cdot\vec{R}_1)\cdot r_2^{-1}, \quad (5.3)$$

where

$$\vec{P} = \vec{K}_{2i} - \vec{K}_2. \quad (5.4)$$

We will evaluate this integral by using a peaking approximation. Since we have two hypergeometric functions, it is not a simple matter to find which range of values of $\vec{s}$ will dominate the integral. To get some hint, we first discuss the case $a \to 0$, so that ${}_1F_1(ia, 1, iK_1R_1 + i\vec{K}_1\cdot\vec{R}_1) \sim 1$ and $f(a) \sim 1$. That means, either that the velocity of the projectile is very large, or that we switch off the interactions between the ions. Then, replacing the coordinates $(\vec{r}_1, \vec{R}_2)$ by $(\vec{r}_2, \vec{R}_1)$ in Eq. (5.3), we have a simpler expression for the scattering amplitude

$$T_1(a=0) = -\frac{Z_2}{(2\pi)^6} f^*(a_2) \int d\vec{s}\, g(\vec{s}, \vec{k}_1) \int d\vec{r}_2 \times \int d\vec{R}_1 \frac{\exp\{i\vec{R}_1\cdot(\mu_1\vec{P} - \vec{s}) - i\vec{r}_2[\mu_2\vec{s} + (1-\mu_1\mu_2)\cdot\vec{P}]\}}{r_2}\, {}_1F_1^*(ia_2, 1, ik_2r_2 + i\vec{k}_2\cdot\vec{r}_2).$$

We see that only the point $\vec{s} = \mu_1\vec{P}$ contributes to the first integral; then

$$T_1(a=0) = -\frac{Z_2}{(2\pi)^3} f^*(a_2) g(\mu_1\vec{P}, \vec{k}_1) \times \int d\vec{r}_2 \frac{e^{-\vec{P}\cdot\vec{r}_2}}{r_2}\, {}_1F_1^*(ia_2, 1, ik_2r_2 + i\vec{k}_2\cdot\vec{r}_2). \quad (5.5)$$

The Nordsieck method gives an explicit form for this integral[13] [see also Eq. (A14) in the Appendix]:

$$T_1(a=0) = -\frac{Z_2}{(2\pi)^3} f^*(a_2) g(\mu_1\vec{P}, \vec{k}_1) \frac{4\pi}{P^2}\left(1 - \frac{2\vec{P}\cdot\vec{k}_2}{P^2}\right)^{-ia_2}. \quad (5.6)$$

We can recall the first Born approximation for the ionization process,[14]

$$T_B = -(Z_2/2\pi^2P^2) g(\mu_1\vec{P}, \vec{k}_1), \quad (5.7)$$

and write

$$T_1(a=0) = f^*(a_2)[1 - (2\vec{P}\cdot\vec{k}_2/P^2)]^{-ia_2} T_B. \quad (5.8)$$

As $P^2 > 2\vec{P}\cdot\vec{k}_2$, the differential cross sections calculated from T_1 $(a=0)$ and T_B will only differ by the factor $|f(a_2)|^2$. This factor gives rise to the cusp for electron capture to the continuum. In particular, a first-order approximation for $T_1(a=0)$ is obtained when we replace $\psi_{\vec{k}_1}(r_1)$ by a plane wave in Eq. (5.2).[15]

For moderate velocities for the projectile the quantity a is not small. However, from the discussion above, we will assume that the most important contribution to the integral, Eq. (5.3), comes from a neighborhood of the point $\vec{s} = \mu_1\vec{P}$. With this assumption the $\vec{s}$ integral can be carried out and the amplitude becomes

$$T_1 = \frac{Z_2}{(2\pi)^3} f^*(a) f^*(a_2) g(\mu_1\vec{P}, \vec{k}_1) \int d\vec{r}_1 \times \int d\vec{R}_2 \frac{e^{i\vec{P}\cdot\vec{R}_2}}{r_2}\, {}_1F_1^*(ia_2, 1, ik_2r_2 + i\vec{k}_2\cdot\vec{r}_2) \times {}_1F_1^*(ia, 1, iK_1R_1 + i\vec{K}_1\cdot\vec{R}_1)\cdot\delta(\vec{r}_1). \quad (5.9)$$

These integrals are uncoupled, and using Eq. (2.1) we have

$$T_1 = -\frac{Z_2}{(2\pi)^3} f^*(a) f^*(a_2) g(\mu_1\vec{P}, \vec{k}_1) \times \int d\vec{r}_2 \frac{e^{-i\vec{P}\cdot\vec{r}_2}}{r_2}\, {}_1F_1^*(ia_2, 1, ik_2r_2 + i\vec{k}_2\cdot\vec{r}_2) \times {}_1F_1^*[ia, 1, i\mu_2(K_1r_2 - \vec{K}_1\cdot\vec{r}_2)]. \quad (5.10)$$

In the Appendix we have evaluated this integral. From Eqs. (A8), (A13), and (5.7) we have

$$T_1 = f^*(a) f^*(a_2) T_1^B [1 + (2\mu_2 \vec{K}_1 \cdot \vec{P}/P^2)]^{-ia} \times [1 - (2\vec{k}_2 \cdot \vec{P}/P^2)]^{-ia_2} {}_2F_1(ia_2, ia, 1, x), \tag{5.11}$$

where

$$x = -2\mu_2 \frac{2(\vec{P}\cdot\vec{k}_2)(\vec{P}\cdot\vec{K}_1) - P^2(K_1 k_2 + \vec{K}_1 \cdot \vec{k}_2)}{(P^2 + 2\mu_2 \vec{K}_1 \cdot \vec{P})(P^2 - 2\vec{k}_2 \cdot \vec{P})} . \tag{5.12}$$

We note that, when $a \to 0$ Eq. (5.11) reduces to Eq. (5.8). Furthermore, for physical values of the momenta, we found always $|x| < 1$ and it is unnecessary to do analytical continuation of the hypergeometric function.

VI. RESULTS AND DISCUSSION

Using the first-order scattering amplitude Eq. (3.11) we have evaluated the DDCS,

$$\frac{d\sigma}{dE_e d\Omega_e} = \mu_1 k_1 \frac{d\sigma}{d\vec{k}_1} = \frac{\mu_1 k_1 v_2^2 K_2 (2\pi)^6}{4\pi^2 K_{2i}} \int d\Omega_P |T_1|^2 , \tag{6.1}$$

for proton-hydrogen ionization. The E_e and Ω_e refer to the ejected electron relative to M_1 and the integration runs over the whole angular distribution of the proton. We will call θ the angle between the initial velocity of the proton v_i and the final velocity of the electron v_1. Since the experimental data available for the comparison are for the ionization of the H_2 molecule, we assume it to be composed of two independent atoms. In this case the DDCS is twice the value calculated from Eq. (6.1) with a hydrogenic $1s$ state ($Z_1 = 1$) as the initial state. The only correction considered is in the ionization energy, by taking $\epsilon_i = 15.4$ eV in Eq. (2.9). The correlation effects between the H_2 electrons could be important and responsible for some of the deviation between theoretical and experimental results and deserve further study.

The scattering amplitude given by Eq. (3.11) contains the distortion of the electronic final state due to the interaction between the protons. We have also calculated the DDCS by dropping this distortion. That means $a = 0$ in Eq. (3.11). In Figs. 2 and 3 we compare the experimental angular distribution[16,17] with those obtained in our formalism. For large angle, the DDCS evaluated with nonzero value of a is close to the experimental values. In fact, for large angles and large velocities of the proton and electron, the Coulomb factor $f(a)$ compensates the $f(a_2)$ and our results agree with the simple Born approximation of Bates and Griffing.[1]

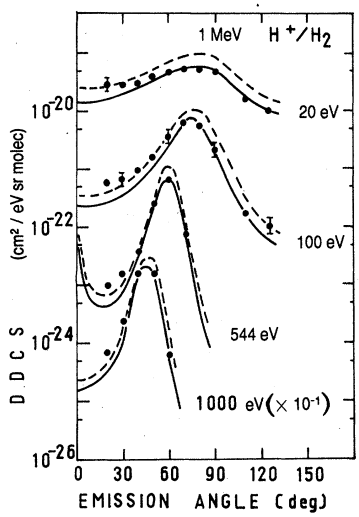

FIG. 2. Angular distributions of electrons ejected from H_2 by 1-MeV protons. Full curves: present calculations; broken curves: present calculations neglecting the proton-proton distorsion ($a = 0$); dots: experiment of Toburen and Wilson (Ref. 16). The numbers associated with the various curves indicate the energy of the ejected electron.

For small angles the DDCS obtained without the interproton distortion is better than when it is considered. The wave function given by Eq. (4.2) includes the Coulomb interaction between each pair of particles, but polarization effects are not included. We could think that, when $v_1 < v_i$ and θ is small, the electron travels between the two protons and those effects will be larger. That could account for the discrepancies but requires the

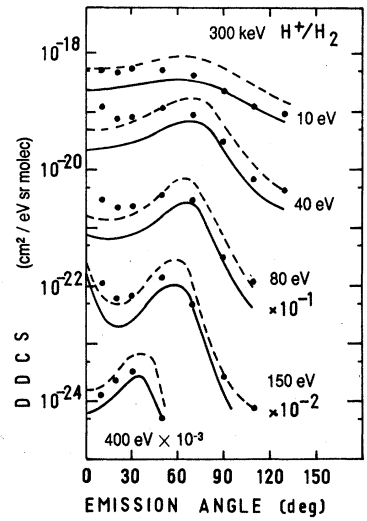

FIG. 3. Same as Fig. 2, except here the proton-energy is 300 keV and the dots are from the experiment of Rudd *et al.* (Ref. 17).

evaluation of the second-order perturbative terms. For $v_1 \gg v_i$, the electron travels away from the two protons, it is not available to set an attractive polarization, and the interactions included in the theory should be accurate enough to give a description of the process. For the largest angles the theoretical values run below the experimental points. Manson *et al.*,[18] studying H^+-He ionization, found that to explain that kind of behavior it is necessary to use an improved Hartree-Fock function for the initial and final state of the helium. We suppose that the discrepancies in H-H_2 ionization could also be overcome using a better wave function for the H_2 molecule.

In Fig. 4 we display the DDCS for $\theta = 0$, as a function of the electron energy, for 300-keV incident protons. The formalism described in this paper gives the CTC peak for any values of a (curves A and B). The cusp is given by the Coulomb factor $|f(a_2)|^2$, which does not appear in the simple Born approximation (curve C). However, second-order terms are necessary to explain asymmetries on the peak.[7]

A point which merits particular attention is the possibility of CTC effects in the ionization of atoms by negative ion impact. Curve D, at Fig. 4, shows the theoretical DDCS at 0°, for the antiproton-H_2 ionization process (with $a=0$). We note an anticapture phenomenon when $v_1 \sim v_i$. It appears as a depression in the DDCS. This behavior is also described by the $f(a_2)$ factor

$$|f(a_2)|^2 = (2\pi Z_2/k_2)(1 - e^{-2\pi Z_2/k_2})^{-1}, \xrightarrow[k_2 \to 0]{} 2\pi Z_2/k_2, \quad Z_2 > 0, \tag{6.2a}$$

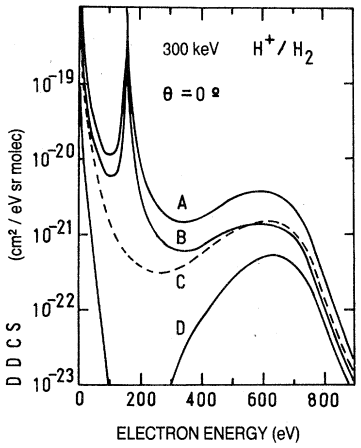

FIG. 4. Energy distribution of electrons ejected at 0° from H_2 by 300-keV protons. Curve A: present calculations, neglecting the proton-proton distortion ($a=0$); curve B: present calculations with the proton-proton distortion included; curve C: Born approximation; Curve D: energy distribution of electrons ejected at 0° from H_2 by 300-keV antiprotons.

$$\xrightarrow[k_2 \to 0]{} 2\pi |Z_2|/k_2 \, e^{-2\pi |Z_2|/k_2}, \quad Z_2 < 0. \tag{6.2b}$$

The case $Z_2 > 0$ was studied by Dettmann *et al.*,[4] and Inokuti *et al.*[19] suggested that an anticapture process could happen when massive μ and π particles are used as projectiles. From Eq. (6.2b) we see that this effect should produce a large drop in the DDCS.

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APPENDIX

In this Appendix we will be concerned with the evaluation of the integral which appears in Eq. (5.10). We introduce a screening parameter λ and write

$$I_1 = \int d\vec{r}\, \frac{e^{-\lambda r}}{r}\, e^{i\vec{q}\cdot\vec{r}}\, {}_1F_1[-ib_1, 1, i(p_1 r - \vec{p}_1 \cdot \vec{r})] \times {}_1F_1[ib_2, 1, i(p_2 r + \vec{p}_2 \cdot \vec{r})]. \tag{A1}$$

We will follow a mixed integration technique using a contour integral representation for one of the hypergeometric functions and a real representation for the other[20,21]:

$${}_1F_1(-ib_1, 1, ip_1 r - i\vec{p}_1 \cdot \vec{r}) = \frac{1}{2\pi i} \oint_C dt_1\, t_1^{-ib_1 - 1} (t_1 - 1)^{ib_1} e^{it_1 (p_1 r - \vec{p}_1 \cdot \vec{r})}, \tag{A2}$$

and

$${}_1F_1(iB_2, 1, ip_2 r + i\vec{p}_2 \cdot \vec{r}) = \frac{\Gamma(1)}{\Gamma(iB_2)\Gamma(1 - iB_2)} \times \int_0^1 dt_2\, t_1^{iB_2 - 1} (1 - t_2)^{-iB_2} e^{it_2 (p_2 r + \vec{p}_2 \cdot \vec{r})}. \tag{A3}$$

The C contour encircles the points $t=0$ and $t=1$ once in the positive direction, and we choose $iB_2 = ib_2 + \epsilon$, with ϵ a small positive number, so that

$$1 > \mathrm{Re}(iB_2) > 0. \tag{A4}$$

We now substitute (A2) and (A3) in (A1) to obtain

$$I_1 = \frac{1}{\Gamma(iB_2)\Gamma(1 - iB_2)}\, \frac{1}{2\pi i} \times \int_0^1 dt_2\, t_2^{iB_2 - 1} (1 - t_2)^{-iB_2} I_2(t_2), \tag{A5}$$

where

$$I_2(t_2) = \oint_C dt_1\, t_1^{-ib_1 - 1} (t_1 - 1)^{ib_1} I_3(t_1, t_2), \tag{A6}$$

with

$$I_3(t_1,t_2) = \int d\vec{r}\,\frac{1}{r}\exp[-\lambda r + i\vec{q}\cdot\vec{r} + it_4(p_1 r - \vec{p}_1\cdot\vec{r}) + it_2(p_2 r + \vec{p}_2\cdot\vec{r})]. \quad \text{(A7)}$$

According to Nordsieck, we introduce the following notation[20]:

$$\alpha = (q^2+\lambda^2)/2\,,\quad \beta = \vec{p}_2\cdot\vec{q} - i\lambda p_2\,, \quad \text{(A8)}$$
$$\gamma = \vec{p}_1\cdot\vec{q} + i\lambda p_1 - \alpha\,,\quad \delta = \vec{p}_1\cdot\vec{p}_2 + p_1p_2 - \beta\,.$$

The integral $I_3(t_1,t_2)$ has a simple analytic expression[21]

$$I_3(t_1,t_2) = -2\pi\{t_1[t_2(\beta+\delta)+(\alpha+\gamma)] - \alpha - \beta t_2\}^{-1}\,. \quad \text{(A9)}$$

From this equation, Nordsieck found that

$$I_2(t_2) = 4\pi^2 i[\alpha+\beta t_2]^{-ib_1-1}[-\gamma-\delta t_2]^{ib_1}\,, \quad \text{(A10)}$$

and our integral remains

$$I_1 = \frac{2\pi(-\gamma)^{ib_1}}{\alpha^{1+ib_1}\Gamma(iB_2)\Gamma(1-iB_2)} \times \int_0^1 dt_2\, t_2^{iB_2-1}(1-t_2)^{-iB_2}\left(1+\frac{\beta}{\alpha}t_2\right)^{-ib_1-1} \times\left(1+\frac{\delta}{\gamma}t_2\right)^{ib_1}. \quad \text{(A11)}$$

For B_2, so that the condition (A4) is true, Eq. (A11) is the integral representation of the hypergeometric function with two variables[22]; then

$$I = (2\pi/\alpha)(-\gamma/\delta)^{ib_1} \times {}_3F_1(iB_2, 1+ib_1, -ib_1, 1; -\beta/\alpha, -\delta/\gamma)\,. \quad \text{(A12)}$$

We can use the following relation between two and one variable hypergeometric functions[23]:

$${}_3F_1(\alpha,\beta,\beta',\beta+\beta';u,v) = (1-v)^{-\alpha}{}_2F_1[\alpha,\beta;\beta+\beta';(u-v/1-v)]\,,$$

to get a simpler expression

$$I = \frac{2\pi}{\alpha}\left(-\frac{\gamma}{\alpha}\right)^{ib_1}\left(\frac{\alpha+\beta}{\alpha}\right)^{-iB_2}{}_2F_1(iB_2,-ib_1;1;x)\,, \quad \text{(A13)}$$

where

$$x = (\beta\gamma - \alpha\delta)/\gamma(\alpha+\beta)\,.$$

The analytical continuation of Eq. (A13) when $\epsilon \to 0$ ($B_2 = b_2$), and $\lambda \to 0$, is well defined for $|x|<1$, and we obtain Eq. (5.11). Some particular limiting cases are interesting: when we consider $b_1 = 0$ we obtain[24]

$$I = (2\pi/\alpha)[(\alpha+\beta)/\alpha]^{-ib_2}\,. \quad \text{(A14)}$$

An analogous result is obtained for $b_2 = 0$.

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