PHYSICAL REVIEW A VOLUME 25, NUMBER 3 MARCH 1982

Single differential and total scattering cross sections for electrons ejected in collisions of fast bare ions with atomic hydrogen

C. R. Garibotti* and J. E. Miraglia*
Centro Atómico Bariloche,† 8400-S.C. de Bariloche, R. N., Argentina
(Received 6 April 1981)

The single differential (in electron angle or energy) and total scattering cross sections for the process $H^+ + H(1s) \rightarrow H^+ + H^+ + e$ are calculated as functions of the incident proton kinetic energy. The calculation is based on the first-order term of a multiple-scattering theory proposed in a previous paper. The results are compared with experiments and other theoretical values. The behavior of the ionization cross section is studied as a function of the projectile charge. This variation is shown for the He^{2+}-H collision.

I. INTRODUCTION

In a previous paper[1] (I) we introduce a theory for the ionization of atoms by bare ion collision. In a T-matrix formalism we considered the equivalence of the two-body interactions between the three final particles and we obtained a multiple-scattering expansion of the amplitude. The first term in that expansion describes the final state of the system as a wave function that is a product of three Coulomb waves centered on each particle and which has the correct asymptotic behavior for large distances. Then, the electron motion is symmetrically described relative to target and projectile, and we explain the capture to the continuum effect (CTC) on the ionization process. We have also shown that this approximation can be considered as a generalized VPS method for the three-particle wave equation,[2] since it includes terms that are neglected in the usual VPS formalism. The proposed amplitude gives the CTC peak on the energy distribution of the forward ejected electrons,[3] without presenting interference patterns.[4] Furthermore, that peak has an asymmetrical shape[5]; this feature, which has been observed experimentally,[6] results from the second- or higher-order terms of the perturbative expansion of the charge-exchange amplitude[7] which are partially incorporated in the first-order multiple-scattering amplitude.

In paper I we calculated the doubly differential cross section (DDCS) with respect to the energy and angle of the electron ejected in the proton-hydrogen atom collisions. We found reasonable agreement with scaled experimental data.[8] In this paper we report the calculations of the single differential (SDCS) and total scattering cross sections of the same process, and we compare the results with measurements and other theories. Most theoretical studies of the SDCS involve the Born approximation, the binary encounter theory, and the Glauber approximation.[9] However, these methods fail for the ionization DDCS because they do not incorporate CTC. Recently[10] those cross sections have been evaluated using the continuum distorted-wave method, which extends the distorted-wave Born approximation proposed by Salin.[11] In paper I a first-order perturbative term of the theory was calculated; for that reason the results should be accurate only for the relatively high energies. Nevertheless, here we extend the calculation to intermediate energies as low as 50 keV in order to study the validity range of the formalism.

Finally, we study the dependence on the charge of the projectile (Z_2) comparing the results of our theory with the Z_2^2 dependence of the Born approximation. As an explicit comparison of the behavior of the various theoretical approximations, for a multiply charged projectile, we report on the total ionization cross section for He^{2+}-H collisions.

II. MULTPLE-SCATTERING APPROACH

We consider a particle 2 colliding with an atomic system which has one active electron. The coordinates and interactions of this three-particle system are described in Fig. 1. The variables $\mu_1, \vec{r}_1, \vec{k}_1$ are the reduced mass, the position, and the momentum of the electron relative to the target nucleus; $\mu_2, \vec{r}_2, \vec{k}_2$ refer the electron to the projectile; $\nu_2, \vec{R}_2, \vec{K}_2$ refer the projectile to the center of mass of the target; and $\nu_1, \vec{R}_1, \vec{K}_1$ refer the nucleus

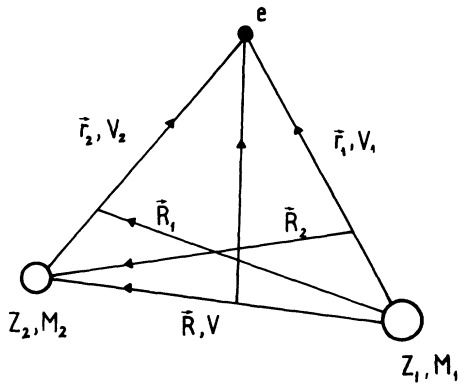

FIG. 1. Coordinate system.

to the electron-projectile system.[1]

The scattering amplitude for the direct ionization channel is given by[1]

$$T_{fi}=\langle \vec{K}_2,\vec{k}_1^- \mid V_i(1+GV_i) \mid i,\vec{K}_{2i}\rangle , \tag{2.1}$$

where

$$\langle \vec{K}_2,\vec{k}_1^- \mid \vec{R}_2,\vec{r}_1\rangle =\psi_{\vec{k}_1}^-(\vec{r}_1)e^{i\vec{K}_2\cdot\vec{R}_2}(2\pi)^{-3/2} . \tag{2.2}$$

The $\psi_{\vec{k}}^-(\vec{r})$ is an ingoing Coulomb wave, and the initial state is

$$\langle \vec{R}_2,\vec{r}_1 \mid i,\vec{K}_{2i}\rangle =e^{i\vec{K}_{2i}\cdot\vec{R}_2}\phi_i(\vec{r}_1)(2\pi)^{-3/2} , \tag{2.3}$$

where $\phi_i(\vec{r}_1)$ is the atomic state, G is the Green's function for the whole system, and V_i is the initial interaction, i.e., $V_i=V+V_2$. The amplitude given by Eq. (2.1) can be expanded in a multiple-scattering series, which may be summed allowing for the distortion of the projectile wave function.[1] The first order of that expansion is

$$T_1=\langle \chi_f^- \mid V_i \mid i,K_{2i}\rangle , \tag{2.4}$$

where

$$\chi_f^-=e^{-i\vec{k}_1\cdot\vec{r}_1}\psi_{\vec{k}_1}^-(\vec{r}_1)\psi_{\vec{k}_2}^-(\vec{r}_2)\psi_{\vec{K}_1}^-(\vec{R}_1)(2\pi)^{-3/2} . \tag{2.5}$$

This wave function approximates the final state of the three-particle system and it has the correct asymptotic behavior. Equation (2.1) gives the direct ionization scattering amplitude, but the same first order [Eq. (2.4)] is obtained by starting from the exchange amplitude.[1] T_1 has been evaluated in paper I using a peaking assumption and neglecting V. Its explicit expression is

$$T_1=f^*(a)f^*(a_2)T_B\left[1+2\mu_2\frac{\vec{K}_i\cdot\vec{P}}{P^2}\right]^{-ia}\times\left[1-2\frac{\vec{k}_2\cdot\vec{P}}{P^2}\right]^{-ia_2}{}_2F_1(ia_2,ia,1,x) , \tag{2.6}$$

where

$$a=-Z_1Z_2\nu_1/K_1,\ a_2=Z_2\mu_2/k_2,\ \vec{P}=\vec{K}_{2i}-\vec{K}_2 , \tag{2.7}$$

$$x=-2\mu_2\frac{2(\vec{P}\cdot\vec{K}_2)(\vec{P}\cdot\vec{K}_1)-P^2(K_1k_2+\vec{K}_1\cdot\vec{k}_2)}{(P^2+2\mu_2\vec{K}_1\cdot\vec{P})(P^2-2\vec{k}_2\cdot\vec{P})} .$$

T_B is the first Born approximation for the ionization process,[2] and $f(\alpha)$ is the Coulomb factor:

$$f(\alpha)=e^{\pi\alpha/2}\Gamma(1+i\alpha) . \tag{2.8}$$

From Eq. (2.6) we can evaluate the DDCS produced in proton-hydrogen atom ionization collisions:

$$\frac{d\sigma}{dE_e d\Omega_e}=\mu_1k_1\frac{d\sigma}{d\vec{k}_1}=\frac{\mu_1K_1\nu_2^2K_2(2\pi)^6}{4\pi^2K_{2i}}\int d\Omega_P \mid T_1 \mid ^2 . \tag{2.9}$$

Here, E_e and Ω_e refer to the energy and angle of the ejected electron relative to M_1 and the integration in Eq. (2.9) runs over the whole angular distribution of the proton. The SDCS are obtained by integration of the DDCS over either the electron angle or its energy:

$$\sigma(\theta_e)=2\pi\int_0^\infty\frac{d\sigma}{dE_e d\Omega_e}dE_e ,$$
$$\sigma(E_e)=2\pi\int_0^\pi\frac{d\sigma}{dE_e d\Omega_e}\sin\theta\, d\theta . \tag{2.10}$$

From these quantities we can calculate the total cross section σ_T:

$$\sigma_T=\int_0^\infty\sigma(E_e)dE_e=\int_0^\pi\sigma(\theta)\sin\theta\, d\theta . \tag{2.11}$$

III. RESULTS AND DISCUSSION

In paper I we have compared the theoretical DDCS obtained from Eq. (2.6) with experimental results for H^+-H scattering. They agree for high

collision energies. For intermediate energies the calculations describe the angular behavior of the DDCS and reproduce the CTC peak, but are somewhat low for small angles. This situation appears in the angular SDCS which are shown in Fig. 2. We have suggested[12] that the contribution of the second-order terms on the multiple-scattering expansion raises the DDCS for small angles. The experimental values correspond to H^+-H_2 scattering and they have been divided by two to compare with the present H^+-H values. This linear scaling neglects the correlation interaction with the passive electron and molecular effects of the H_2. Manson *et al.*[13] have shown that a more accurate electronic wave function for the initial atomic or molecular state is required to improve the Born approximation at large angles. We expect that this is also true in our approach and that the deviation between theoretical and experimental values observed at large angles could be corrected by avoiding the linear scaling. In Fig. 2 we have represented other theoretical calculations. The Born approximation is higher than ours, except for small angles where it does not include the CTC phenomena. For sake of comparison we include in Fig. 2 the theoretical results obtained with the continuum distorted-wave[10] and the distorted-wave modified Born approaches.[11] We have also calculated the SDCS in the energy; the results differ little from those obtained with the Glauber approximation.[14]

The present theoretical result for the total cross section are presented in Fig. 3 and compared with four sets of experimental values. The measurements'of Gilbody and Ireland[15] and Fite *et al.*[16] are absolute, while those obtained by Park *et al.*[9] were normalized to the Born approximation cross section for excitation of atomic hydrogen to the $n=2$ state. The value of Kuyatt and Jorgensen[17] were obtained by integration of the experimental SDCS for H^+-H_2 and we divided by two to obtain the H^+-H values. As we see in Fig. 3 the values ob-

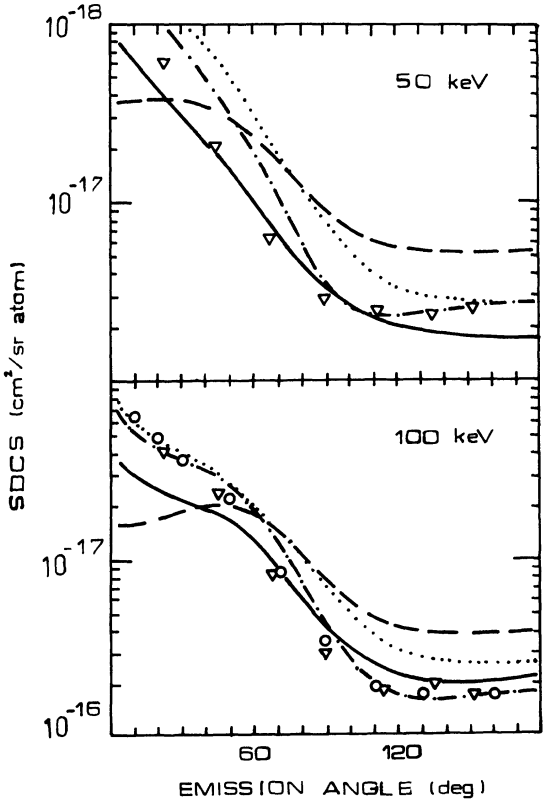

FIG. 2. Single differential scattering cross sections in scattering angle for 50- and 100-keV protons. ——, present results; — — —, first Born approximation; · · · ·, Salin (Ref. 11); —·—, Belkic (Ref. 10). Experimental values: ∇, Kuyatt and Jorgensen (Ref. 17); ○, Rudd *et al.* (Ref. 8).

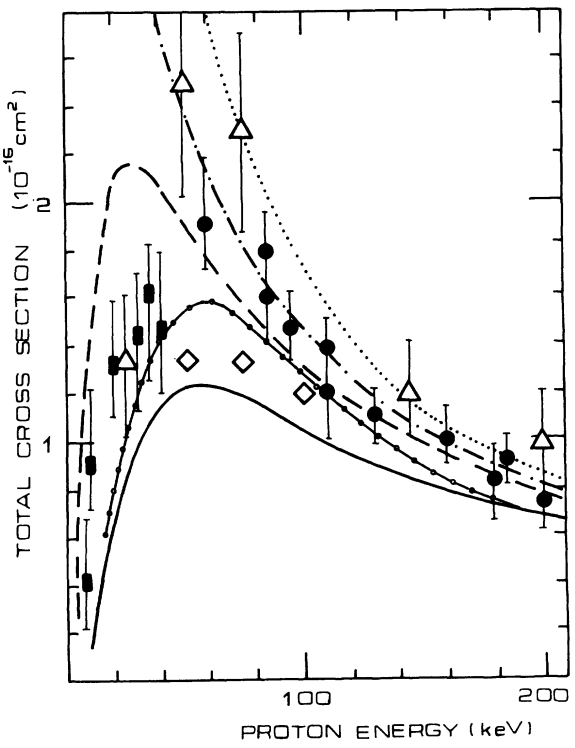

FIG. 3. Total cross sections for ionization of H atoms by protons. Captions for the curves as in Fig. 2. —○—, theoretical calculation of Shakeshaft (Ref. 18). Experimental values: △, Park *et al.* (Ref. 9); ●, Gilbody and Ireland (Ref. 15); ■, Fite *et al.* (Ref. 16); ◇, Kuyatt and Jorgensen (Ref. 17).

tained with our approach are similar to those given by the Glauber approximation.[14] It is interesting to compare our values with the most elaborate calculations at intermediate energies performed up to now; these calculations have been reported by Shakeshaft.[18] He performed a coupled-state calculation with an electron wave function which is expanded in a basis of 35 functions centered around each proton. The σ_T calculated here shows its maximum at the projectile energy suggested in Ref. 18. However, it should be noted that our approach is valid at high energies and it appears to underestimate the CTC contribution at lower energies.

In Fig. 4 we show the total cross section for ionization of H atoms by α particles. The theoretical results of the Born, Glauber, modified distorted wave, and our approach are displayed and compared with the related apparent experimental cross section.[19] As in the preceding case, our values are somewhat smaller than the measured results. The Glauber approach shows a better agreement but, like the Born approximation, it is not adequate to describe properly the CTC electrons.

Owing to the increasing availability of highly ionized beams for experimental research it is interesting to study the projectile charge dependence predicted by the present theory. Figure 5 shows the ratio between the total cross section calculated in the present work and the Born approximation results as a function of the projectile charge for two velocity values (in Bohr units). The values obtained with our method and with the distorted-wave Born approximation[11] increase less and more rapidly, respectively, than the Z_2^2 increase predicted by the Born approximation. The proposed theory gives a good description of the experimental data for energies larger than 300 keV per nucleon when only the first-order term of the multiple-scattering expansion is evaluated. At lower energies the CTC peak and the general features of the SDCS and total cross section are given by the theory but its numerical values do not agree in a absolute scale with the experimental data.

We can search for the origin of that shortcoming. In the present approach the Coulomb interac-

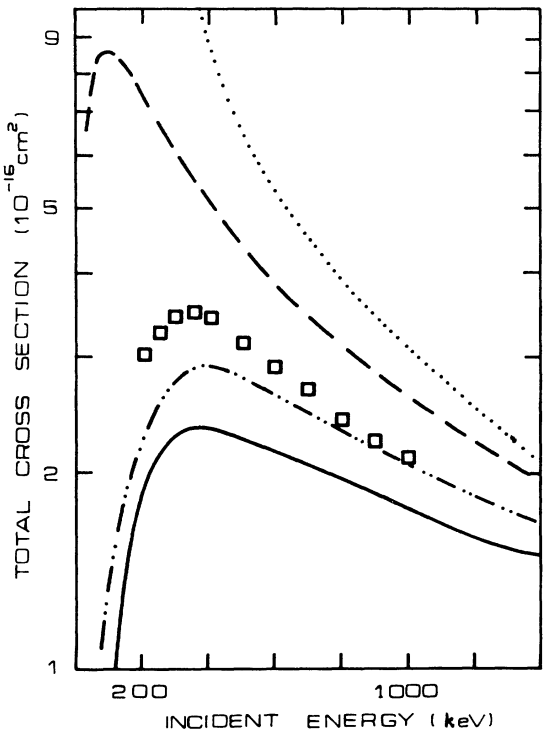

FIG. 4. Total cross section for ionization of H atoms by He^{2+}. Captions for the curves as in Fig. 2. —··— Glauber approximation (Ref. 14); □, experimental values (Ref. 19).

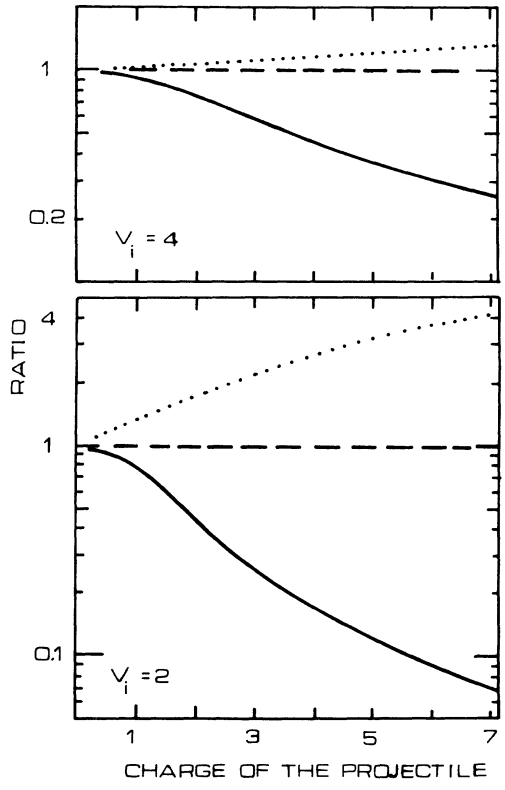

FIG. 5. Ratio between theoretical total cross sections and Born approximation as a function of the charge of the projectile and for two velocities of the incident ion: —— present theory; · · · · Salin formalism (Ref. 11).

tions between the three particles have an equivalent status in the definition of the final-state wave function. In particular, the interaction between the ion and the target nucleus introduces a Coulomb factor:

$$|f(a)|^2=2\pi Z_1 Z_2/v(1-e^{2\pi Z_1 Z_2/v}) .$$

This factor decreases rapidly as the velocity v of the ion decreases or its charge Z_2 increases. This term is a multiplicative factor in the cross sections and is responsible for the relatively low values obtained at intermediate collision energies. Furthermore, it explains the dependence as a function of Z_2 shown in Fig. 5. Several ways to improve this theory at intermediate energies are possible. These include the use of effective ion charges or momenta, second-order effect, and the contribution of the term

$$\langle \chi_f^- \mid V \mid i,K_{2i} \rangle$$

to the scattering amplitude. This additive term has been neglected in paper I by using the Wicke argument. However, it is possible that it produces a screening in the ion-target—nucleus-interaction canceling the influence of the factor $|f(a)|^2$.

ACKNOWLEDGMENTS

We would like to thank N. Stolterfoht for the critical reading of the manuscript and to I. Nemirovsky for useful discussions. One of us (J.E.M.) thanks the hospitality of the Instituto de Astronomia y Física del Espacio where part of this work was carried out.

*Consejo Nacional de Investigaciones Científicas y
† Técnicas, Argentina.
Comisión Nacional de Energía Atómica.

[1]C. R. Garibotti and J. E. Miraglia, Phys. Rev. A 21, 572 (1980).
[2]L. Vainstein, L. Presnyakov, and I. Sobelman, Zh. Eksp. Teor. Fiz. 45, 2015 (1963) [Sov. Phys.—JETP 18, 1383 (1964)]; J. P. Coleman, in *Case Studies in Atomic Collision Physics,* edited by E. W. McDaniel and M.R.C. McDowell (North-Holland, Amsterdam, 1969), Vol. 1, p. 149.
[3]G. B. Crooks and M. A. Rudd, Phys. Rev. Lett. 20, 1599 (1970).
[4]J. Macek, Phys. Rev. A 1, 235 (1970); C. R. Vane, I. A. Sellin, M. Suter, G. D. Alton, S. B. Elston, M. Griffin, and R. S. Thoe, Phys. Rev. Lett. 40, 1020 (1978); M. M. Duncan, M. G, Menéndez, F. L. Eisele, and J. Macek, Phys. Rev. A 15, 1785 (1977).
[5]C. R. Garibotti and J. E. Miraglia, J. Phys. B 14, 863 (1981).
[6]M. Breinig, S. Elston, I. Sellin, L. Liljeby, R. Thoe, C. Vane, H. Gould, R. Marrus, and R. Laubert, Phys. Rev. Lett. 45, 1689 (1980); M. Rødbro and F. D. Andersen, J. Phys. B 12, 2883 (1979); W. Meckbach, I. Nemirovsky, and C. R. Garibotti (unpublished).
[7]R. Shakeshaft and L. Spruch, Phys. Rev. Lett. 41, 1037 (1978).
[8]M. E. Rudd, C. A. Sautter, and C. L. Bailey, Phys. Rev. 151, 20 (1966).
[9]J. Park, J. Aldag, J. M. George, J. L. Peacher, and J. H. McGuire, Phys. Rev. A 15, 508 (1977); T. F. Bonsen and L. Vriens, Physica (Utrecht) 47, 307 (1970).
[10]D. Belkic, J. Phys. B 11, 3519 (1978).
[11]A. Salin, J. Phys. B 2, 631 (1969).
[12]C. R. Garibotti and J. E. Miraglia, *Abstracts of the Eleventh International Conference on the Physics of Electronic and Atomic Collisions, Kyoto, 1979,* edited by K. Takayanagi and N. Oda (The Society for Atomic Collision Research, Kyoto, 1979), p. 628.
[13]S. T. Manson, L. H. Toburen, D. H. Madison, and N. Stolterfoht, Phys. Rev. A 12, 60 (1975).
[14]J. E. Golden and J. H. McGuire, J. Phys. B 9, L11 (1976).
[15]H. B. Gilbody and J. Ireland, Proc. R. Soc. London 277, 137 (1963).
[16]W. L. Fite, R. F. Stebbings, D. G. Hummer, and R. T. Brackmann, Phys. Rev. 119, 663 (1960).
[17]C. E. Kuyatt and T. Jorgensen, Phys. Rev. 130, 1444 (1963).
[18]R. Shakeshaft, Phys. Rev. A 18, 1930 (1978).
[19]L. J. Puckett, G. O. Taylor, and D. W. Martin, Phys. Rev. 178, 271 (1969).