

Electron capture from multielectron atoms by fast ions in the continuum intermediate-state approximation

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A method has been derived for the evaluation of the Coulomb integral containing the product of a Coulomb wave function with a Slater-type orbital in a closed form. This method which is relevant to the charge transfer in second-order theories has been applied for the calculation of cross sections from the K shell of C, N, O, Ne, and Ar atoms by fast protons in the framework of the continuum intermediate-state approximation. The present calculated results are found to be in good agreement with the available experimental findings and the existing theoretical calculations in the high-energy region.

I. INTRODUCTION

Electron-capture processes from multielectron atoms by fast bare projectiles have received appreciable attention in recent years due to their various applications. In particular, the data of charge transfer cross sections from atomic oxygen or iron are essential in finding the charge equilibrium of a high-energy beam passing through different gases, or in finding the radiation of cosmic rays passing through interstellar matter. Moreover, as the interstellar medium is far from thermodynamic equilibrium, capture is an important factor in controlling the level of ionization of the constituent ions and thus the state of the system.¹

The calculation of cross sections for electron capture from inner shells of complex atoms has been one of the recent trends of theoretical activity in atomic collisions. However, exact quantal calculations present formidable difficulties due to many-electron effects. The existing theoretical calculations²⁻⁶ are based on the independent-electron approximation which treats only the electron to be transferred as active. The other electrons in these approximations are considered to be passive and provide only screening during the collision process. The use of this independent-particle model is justified⁷ due to the wide separation of binding energies for the inner subshell electrons. The theoretical calculations for asymmetric collisions have been performed in the two-state atomic expansion (TSAE) method,² the continuum distorted-wave approximation³ (CDWA), the impulse approximation⁴ (IA), the eikonal approximation⁵ (EA), and the strong-potential Born approximation⁶ (SPBA) in the intermediate- and high-energy region. The wave functions for the target atoms have been represented by unmodified hydrogenic wave functions and the experimental binding energies in conjunction with effective charges have been employed in all those calculations. Belkić *et al.*³ have also performed the CDWA calculation mak-

ing use of the Roothan-Hartree-Fock wave function⁸ of the captured electron. On comparison with the experimental findings, it has been found that in the energy region near the peak of the cross section, the SPBA cross sections are in much better agreement with the experimental data as compared to the CDWA, IA, and EA cross sections. This may be due to the fact that the SPBA takes proper account of the correct target spectrum of intermediate states. The errors in this approximation are of the order of $(z_p/v)^2$ whereas that in IA is of the order of $(z_t/v)^2$; z_p and z_t being the projectile and target charge, respectively. The SPBA requires only that z_p/v be very small and is applicable even if z_t/v is large provided that $(z_p/v)^2 \ll 1$. However, in the high-energy region, the CDWA, IA, and EA cross sections like the SPBA consistently follow the trend of the experiment. Recently, the continuum intermediate-state approximation^{3,9} (CISA) obtained by making further approximation to the IA has been applied with reasonable success¹⁰⁻¹² for electron capture from the ground state to an nlm final state and from an nlm initial state to an $n'l'm'$ final state in bare-projectile-hydrogenic-target systems.

In the SPBA or IA it is a formidable task to calculate the cross sections for electron capture from the multielectron atoms with a realistic wave function into the final hydrogenic states with arbitrary quantum numbers. Therefore, one is prone to seek other approximations that could be able to yield with moderate computational effort reasonably good results in the high-energy region. Although the CISA introduces an error of the order of $(z_t/v)^2$, one can have an estimation of the cross section with reasonable accuracy in the high-energy region.

In the present paper, we generalize the CISA method to calculate the cross sections for single electron capture from the inner shells of a multielectron atom by a fast bare projectile. We consider the active electron moving in the field of an effective nuclear charge and expand the bound-state wave function of complex atoms onto the

basis of Slater-type orbitals.

The present paper is organized as follows. In Sec. II we outline the general expression for the CISA scattering amplitude for electron capture by a bare ion from a multielectron atom into arbitrary n' , l' , and m' states and then show the reduction of the scattering amplitude to a closed analytical form. In Sec. III our calculations are compared with the experimental data and existing theoretical calculations for capture by H^+ from C, N, O, Ne, and Ar in the intermediate- and high-energy region. Finally, conclusions are given in Sec. IV. Atomic units are used throughout the paper unless otherwise stated.

II. THEORY

A. General expression for the scattering amplitude

The prior form of the CISA transition probability³ appropriate for systems^{13,14} $z_p < z_t$ for electron capture by fast bare projectiles from the multielectron atoms, within the framework of an independent-electron model, can be written as

$$T_{if} = N(v)IJ, \quad (1)$$

where

$$I = \int d\mathbf{x} e^{i\mathbf{p}\cdot\mathbf{x}} \Phi_i(\mathbf{x}) {}_1F_1(iv_t, 1; i\mathbf{v}\mathbf{x} + i\mathbf{v}\cdot\mathbf{x}),$$

$$J = \int d\mathbf{s} \frac{e^{i\mathbf{q}\cdot\mathbf{s}}}{s} \Phi_f^*(\mathbf{s}),$$

$$\mathbf{p} = -\boldsymbol{\eta} - \left[\frac{E_i - E_f}{v} + v/2 \right] \hat{\mathbf{v}},$$

$$\mathbf{q} = \boldsymbol{\eta} + \left[\frac{E_i - E_f}{v} - v/2 \right] \hat{\mathbf{v}}, \quad (2)$$

$$N(v) = \exp(\pi v_t/2) \Gamma(1 - iv_t) z_p,$$

$$v_t = z_t^*/v.$$

The phase factor involved in the transition probability has been neglected because this does not contribute to the cross sections. E_i is the Roothan-Hartree-Fock (RHF) energy corresponding to the RHF orbital $\Phi_i(\mathbf{x})$ of the active electron. E_f and Φ_f correspond, respectively, to the energy and wave function in the final state of the hydrogenic ion. $\boldsymbol{\eta}$ is the transverse momentum transfer perpendicular to the incident velocity \mathbf{v} and z_t^* is the effective charge of the target atom related with the principal quantum number n_j of the active electron by the relation

$$z_t^* = (-2n_j E_i)^{1/2}. \quad (3)$$

$$I = \sum_j 4\pi C_j N_{\alpha_j} (2i)^{l_j} \frac{1}{2\pi i} \sum_{\delta=0}^{[(n_j-l_j)/2]} (-1)^{2n_j-2l_j-\delta} \frac{(n_j-l_j)!(n_j-\delta)!}{(n_j-l_j-2\delta)!(2\delta!!)} 2^{n_j-l_j-\delta}$$

$$\times \oint_{\Gamma} dt t^{iv_t-1} (t-1)^{-iv_t} Q^{l_j} Y_{l_j m_j}(\hat{\mathbf{Q}}) \mu^{n_j-l_j-2\delta} (\mu^2 + Q^2)^{-(n_j-\delta+1)}, \quad (11)$$

where $[(n_j-l_j)/2]$ represents the largest integer $\leq (n_j-l_j)/2$. We choose our axis of quantization along the direction of \mathbf{v} and using the addition theorem¹⁸ of regular solid harmonics, we get

The capture cross section Q_{if} is defined as

$$Q_{if}(a_0^2) = \int |T_{if}/2\pi v|^2 d\boldsymbol{\eta}. \quad (4)$$

B. Evaluation of the integral I

The wave function of the multielectron atom may be expanded onto the basis of Slater-type orbitals as

$$\Phi_i(\mathbf{x}) = \sum_j C_j \chi_j(\mathbf{x}), \quad (5)$$

where the basis function $\chi_j(\mathbf{x})$ represents the normalized Slater-type orbitals

$$\chi_j(\mathbf{x}) = N_{\alpha_j} x^{n_j-1} e^{-\alpha_j x} Y_{l_j m_j}(\hat{\mathbf{x}}), \quad (6)$$

with

$$N_{\alpha_j} = [(2\alpha_j)^{2n_j+1}/(2n_j!)]^{1/2}, \quad (7)$$

α_j being a variational parameter associated with the orbital quantum number n_j .

We use the integral representation¹⁵ for the confluent hypergeometric function appearing in Eq. (2) and obtain the I integral as

$$I = \sum_j C_j N_{\alpha_j} \frac{1}{2\pi i} \oint_{\Gamma} dt t^{iv_t-1} (t-1)^{-iv_t}$$

$$\times \int d\mathbf{x} x^{n_j-1} e^{-\mu x + i\mathbf{Q}\cdot\mathbf{x}} Y_{l_j m_j}(\hat{\mathbf{x}}) \quad (8)$$

with

$$\mu = \alpha_j - iv_t,$$

$$\mathbf{Q} = \mathbf{v}t - \mathbf{p}', \quad (9)$$

$$\mathbf{p}' = -\mathbf{p}.$$

The space part of the integration in Eq. (8) can be performed following a procedure similar to Datta *et al.*¹⁶ and we arrive at

$$I = \sum_j 4\pi C_j N_{\alpha_j} (2i)^{l_j} (l_j!) \frac{1}{2\pi i}$$

$$\times \oint_{\Gamma} dt t^{iv_t-1} (t-1)^{-iv_t} dt Q^{l_j} Y_{l_j m_j}(\hat{\mathbf{Q}})$$

$$\times \left[-\frac{\partial}{\partial \mu} \right]^{n_j-l_j} (\mu^2 + Q^2)^{-(l_j+1)}. \quad (10)$$

The (n_j-l_j) th-order differentiation with respect to μ in Eq. (10) is performed by using the procedure of Todd *et al.*¹⁷ and we get

$$Q^{l_j} Y_{l_j m_j}(\hat{Q}) = \sum_{l''=0}^{l_j} N_{l''} t^{l''}, \quad (12)$$

with

$$N_{l''} = (-1)^{l''} v^{l''} (p')^{l''} Y_{l'' 0}(\hat{\nu}) Y_{l'' m_j}(\hat{p}') \left[\frac{4\pi(2l_j+1)(l_j-m_j)!(l_j+m_j)!}{(2l''+1)(2l''+1)(l''-m_j)!(l'')^2(l''+m_j)!} \right]^{1/2}, \quad (13)$$

and

$$l'' = l_j - l'.$$

Since μ and $(\mu^2 + Q^2)$ are linear functions of t , we can write

$$(\mu^2 + Q^2)^{-(n_j - \delta + 1)} = a^{-(n_j - \delta + 1)} \sum_{u=0}^{\infty} \frac{(n_j - \delta + 1)_u}{u!} \left[\frac{b}{a} \right]^u t^u, \quad (14)$$

and

$$\mu^{n_j - l_j - 2\delta} = \sum_{\omega=0}^{n_j - l_j - 2\delta} \binom{n_j - l_j - 2\delta}{\omega} d^\omega c^{n_j - l_j - 2\delta - \omega} t^\omega, \quad (15)$$

with

$$\begin{aligned} a &= \alpha_j^2 + (p')^2, \\ b &= 2i\alpha_j v + 2p' \cdot v, \\ c &= \alpha_j, \\ d &= -iv, \end{aligned} \quad (16)$$

where $(n_j - \delta + 1)_u$ represents the Pochhammer symbol.¹⁹ Making use of Eqs. (12)–(16), and using the results²⁰

$$\begin{aligned} \frac{1}{2\pi i} \oint_{\Gamma} dt t^{A-1+iv} (t-1)^{B-iv} &= \frac{(-1)^B (iv)_A (1-iv)_B}{(A+B)!}, \\ (A+B)! &= A!(A+1)_B, \end{aligned} \quad (17)$$

$$(A)_{x+y} = (A)_x (A+x)_y,$$

the I integral in Eq. (11) reduces to

$$\begin{aligned} I &= 4\pi(2i)^{l_j} \sum_j \sum_{\delta=0}^{(n_j-l_j)/2} \sum_{\omega=0}^{n_j-l_j-2\delta} \sum_{l''=0}^{l_j} C_j (-1)^{2n_j-2l_j-\delta} \frac{(n_j-l_j)!(n_j-\delta)!}{(2\delta)!(n_j-l_j-2\delta-\omega)!\omega!} 2^{n_j-l_j-\delta} N_{l''} d^\omega \\ &\quad \times c^{n_j-l_j-2\delta-\omega} a^{-(n_j-\delta+1)} \frac{(iv_t)_{\omega+l'}}{(\omega+l')!} {}_2F_1(n_j-\delta+1, iv_t+l'+\omega, \omega+l'+1, b/a). \end{aligned} \quad (18)$$

Making use of the property²¹ of the hypergeometric function in a terminating series, we get

$$\begin{aligned} I &= 4\pi(2i)^{l_j} \sum_j \sum_{\delta=0}^{(n_j-l_j)/2} \sum_{\omega=0}^{n_j-l_j-2\delta} \sum_{l''=0}^{l_j} C_j (-1)^{-\delta} \frac{(n_j-l_j)!(n_j-\delta)!}{(2\delta)!(n_j-l_j-2\delta-\omega)!\omega!} 2^{n_j-l_j-\delta} N_{l''} d^\omega \\ &\quad \times c^{n_j-l_j-2\delta-\omega} a^{-(n_j-\delta+1)} \frac{(iv_t)_{\omega+l'}}{(\omega+l')!} \left[1 - \frac{b}{a} \right]^{-n_j+\delta-iv_t} \\ &\quad \times {}_2F_1(\omega+l''-n_j+\delta, 1-iv_t, \omega+l''+1, b/a). \end{aligned} \quad (19)$$

Recently, a closed-form expression of the I integral has also been derived using parabolic coordinates by Belkić²² and Crothers²³ in terms of the Appell hypergeometric function of two and three variables and also independently by Dubé¹⁴ in terms of the Gaussian hypergeometric function.

C. Evaluation of the integral J

The reduction of the integral J has already been expressed in a closed form¹⁰ in connection with electron capture by bare projectiles from atomic hydrogen as

$$\begin{aligned} J &= 2^{2l'+3} S \frac{\pi(l'!)i^{l'}}{(2l'+1)!} Y_{l'' m'}^*(\hat{q}) q^{l'} (q^2 + \gamma_n^2)^{-(l'+1)} \\ &\quad \times {}_2F_1(a, b, c, (1-\lambda)/2), \end{aligned} \quad (20)$$

with

$$\begin{aligned} S &= \gamma_n^{3/2} \left[\prod_{r=0}^{l'} (1 - \gamma_n^2 r^2) \right]^{1/2}, \\ a &= n' + l' + 1, \\ b &= -n' + l' + 1, \\ c &= l' + \frac{3}{2}, \\ \lambda &= (q^2 - \gamma_n^2) / (q^2 + \gamma_n^2), \\ \gamma_n &= z_p / n'. \end{aligned} \quad (21)$$

III. RESULTS AND DISCUSSION

The present method has been checked by calculating the I integral in Eq. (19) for a few low-lying bound states

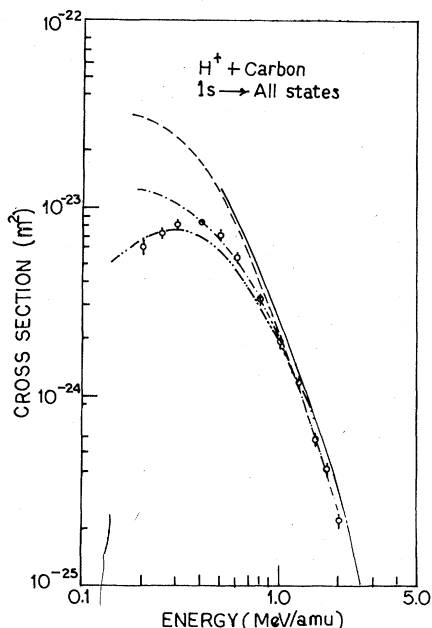


FIG. 1. Capture into all states by protons from the K shell of carbon atoms. Theory: —, present work; ---, CDWA calculation (Ref. 3); - · - ·, Lin *et al.* (Ref. 2); - - - , SPBA calculation (Ref. 6). Experiment: ○, Rødbro *et al.* (Ref. 24).

and comparing the results with those obtained with the help of the parametric differentiation technique. Identical results were found in both the methods for some particular values of the input parameter.

In Figs. 1–5, the present calculated total cross sections from the K shells of C, N, O, Ne, and Ar atoms by protons are displayed and compared with the existing theoretical results and the available experimental findings. These are the total capture cross sections per target atom, including capture to the excited states of the projectile. The theoretical values are obtained from the relation

$$Q_{\text{tot}} = Q_{1s} + 1.616(Q_{2s} + Q_{2p}),$$

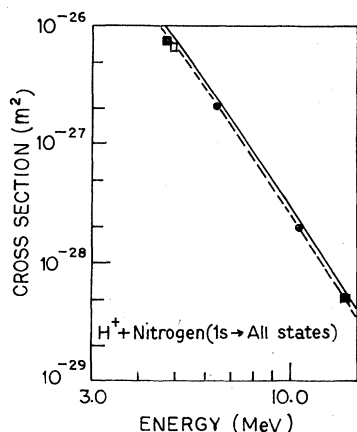


FIG. 2. Capture into all states by protons from the K shell of nitrogen atoms. Theory: —, present work; ---, CDWA calculation (Ref. 3). Experiments: atomic target; □, Cocke *et al.* (Ref. 25); ●, Berkner *et al.* (Ref. 26); ■, Welsh *et al.* (Ref. 27).

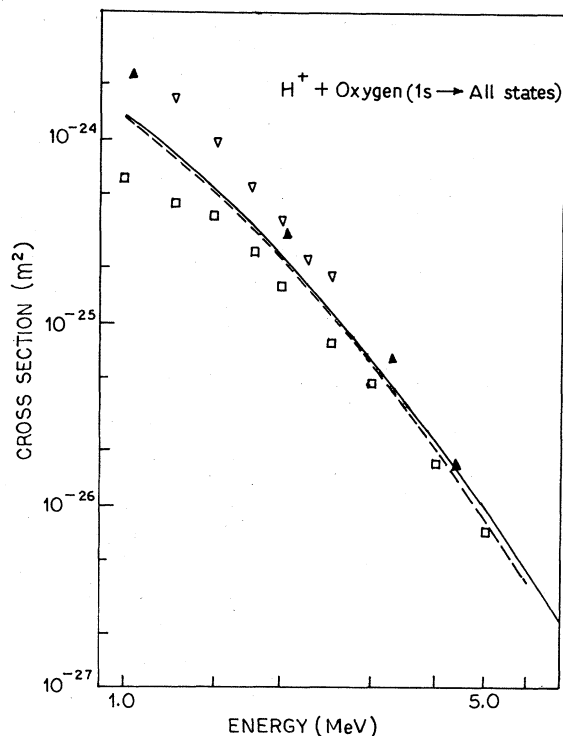


FIG. 3. Capture into all states by protons from the K shell of oxygen atoms. Theory: —, present work; ---, CDWA calculation (Ref. 3). Experiment: atomic target; □, Cocke *et al.* (Ref. 25); ▲, U. Schryder (Ref. 28); ●, Berkner *et al.* (Ref. 26); ■, Welsh *et al.* (Ref. 27); ▽, Toburen *et al.* (Ref. 29).

as the contributions from the higher excited states are found to be negligible. In all these cases it has been found that the contribution of the ground state capture is quite large as compared to any of the excited states throughout

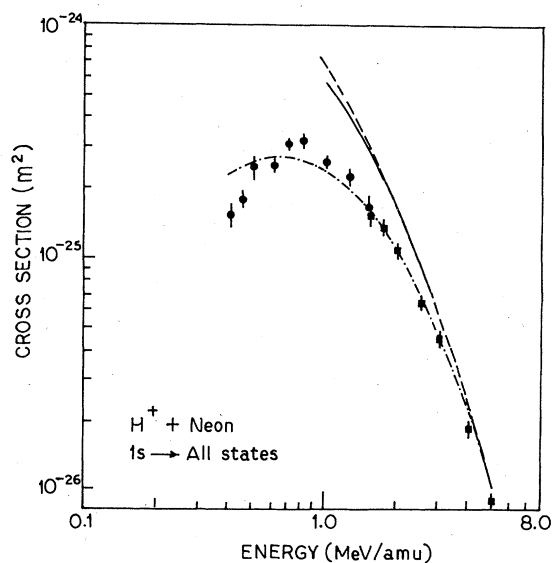


FIG. 4. Capture into all states by protons from the K shell of neon atoms. Theory: —, present work; ---, CDWA calculation (Ref. 3); - · - ·, SPBA calculation (Ref. 6). Experiment: ●, Rødbro *et al.* (Ref. 24).

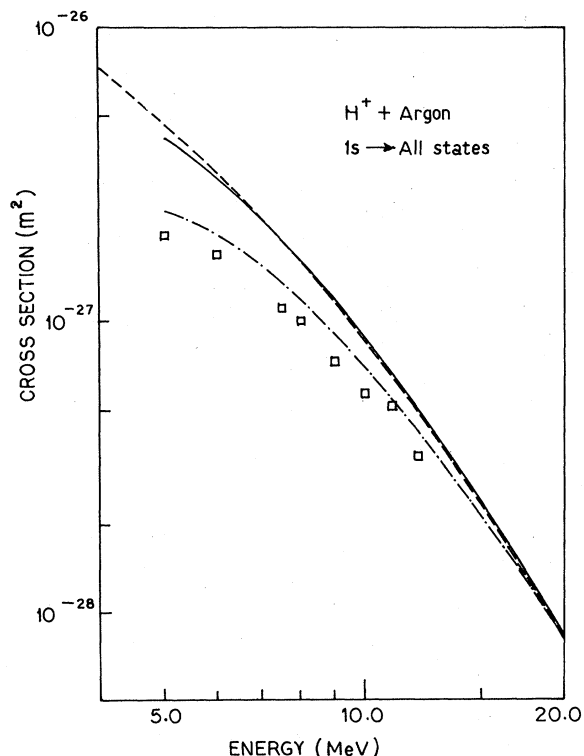


FIG. 5. Capture into all states by protons from the K shell of argon atoms. Theory: —, present work; ---, CDWA calculation (Ref. 3); - · -, SPBA calculation (Ref. 6). Experiment: \square , Macdonald *et al.* (Ref. 30).

the energy range of the projectile considered.

In the case of carbon, the present CISA results, like the CDWA results of Belkić *et al.*,³ are in good agreement with the observed data²⁴ in the high-energy region ($E > 0.9$ MeV). The calculated results of Lin *et al.*² in the two-state atomic expansion method and those of Macek and Alston⁶ in the SPBA method show a trend similar in nature to the observed curve throughout the energy region. The results of Lin *et al.*,² however, underestimate the observed results in the low- and intermediate-energy region. The calculated peak location for the SPBA theory is closer to that of the data compared to other theoretical results.

The results obtained by using the CISA method for electron capture by protons from atomic nitrogen are in excellent agreement with the CDWA calculation³ and the observed data²⁵⁻²⁷ throughout the energy range. In the case of oxygen, the present CISA results almost coincide with the CDWA results³ throughout the energy region considered. However, these theoretical results could not be properly assessed since the existing experimental values²⁵⁻²⁹ grossly diverge from one another. Further experimental investigations may be necessary to test the validity of the present theory. The present computed results for electron capture by protons from the K shell of neon and argon atoms are in excellent agreement with the CDWA calculation throughout the energy range of the projectile. In proton-neon collisions our calculated results for the K -shell capture cross sections are found to overes-

timate the observed findings²⁴ below 3 MeV. This may be due to the fact that the experimental data below 3 MeV fall below the limit of validity of the CISA method. For proton energies greater than 3 MeV, our calculated results are in excellent agreement with the observed data. On the lower-energy side the SPBA cross sections are in much better agreement with the data as compared to the CDWA and CISA calculations. For the case of argon, most of the experimental data³⁰ fall below the range of validity of a high-energy approximation. They clearly converge to the calculated results for proton impact energy close to 10 MeV. Below 10 MeV, the SPBA results are in much better agreement with the observed data as compared to the CDWA and the present CISA results calculated with the Hartree-Fock wave functions. The CDWA calculation³ with hydrogenic wave functions is found to be in excellent agreement with the data. However, this agreement below 9.5 MeV may be considered as fortuitous.³

IV. CONCLUSION

In the present paper a method has been developed for the evaluation of the Coulomb integral containing the product of a Coulomb wave function with a Slater-type orbital in a closed form in terms of the Gaussian hypergeometric function. The present method relevant for charge transfer by second-order theories has been applied for electron capture from complex atoms by fully stripped ions in the framework of the continuum intermediate-state approximation. The study of such capture processes finds practical applications in the fusion research program. The present calculated results for electron capture from the K shell of C, N, O, Ne, and Ar atoms by high-energy protons are found to be in good agreement with experimental data and are comparable to the results obtained by the use of the CDWA and SPBA calculations in the high-energy region. The cross sections calculated by using the hydrogenic and the Hartree-Fock wave functions of the complex atom are found to differ considerably with one another in H^+ -Ar collisions as observed in the CDWA calculation, especially in the intermediate-energy region. It may be interesting to have further theoretical calculations based on the TSAE, EA, IA, and SPBA methods by the use of the Hartree-Fock wave functions of the multielectron target in the intermediate- and high-energy region. In the present investigation we have used the active electron approximation ignoring the effect of passive electrons as in the case of the TSAE, EA, IA, CDWA, and SPBA methods. The imposition of restrictions on the many-electron system needs to be reviewed by using a more realistic potential for the target. Further investigation in this direction is needed.

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