PHYSICAL REVIEW A VOLUME 18, NUMBER 5 NOVEMBER 1978

# Charge transfer in collisions of atomic hydrogen with $O^{8+}$, $He^{2+}$, and $H^+$

Hiroshi Ryufuku
*Tokai Research Establishment, Japan Atomic Energy Research Institute, Tokai-mura, Naka-gun, Ibaraki 319-11, Japan*

Tsutomu Watanabe
*Department of Applied Physics, Faculty of Engineering, The University of Tokyo, Bunkyo-ku, Tokyo 113, Japan*
(Received 13 February 1978)

The charge-transfer process $O^{8+} + H(1s) \rightarrow O^{7+} + H^+$ is considered for $O^{8+}$ impact energies from 0.025 to 200 keV/amu, using the atomic base $S$ matrix formulation represented by time-dependent bases which denote moving atomic orbitals. In the evaluation of the $S$ matrix, models of two extreme types, the unitarized model and the absorption model, are introduced. The numerical results show that there is only a small difference between the cross sections obtained using the respective models for impact energies above 0.5 keV/amu, while the cross section due to the unitarized model becomes smaller than one-half of that obtained with the absorption model at an impact energy of 0.05 keV/amu. The data are also compared with other calculations of the same process. For the investigation of the validity of our formula, the unitarized formula is also applied to the processes $H^+ + H(1s) \rightarrow H + H^+$ and $He^{2+} + H(1s) \rightarrow He^+ + H^+$. The results are in good agreement with the experimental data.

## I. INTRODUCTION

In the study of the atomic processes in a controlled fusion reactor, charge-transfer processes involving impurity gas atoms are very important. Electron capture from an H atom by a highly stripped impurity ion is considered to be one of the rate-determining processes in plasma heating by neutral-hydrogen-beam injection. From this point of view and from theoretical interest itself, a plan has been formulated to evaluate the cross sections for charge transfer between hydrogen atoms and completely stripped heavy ions.

Recently, Salop and Olson[1] have calculated the cross sections for charge transfer between ground-state atomic hydrogen and completely stripped ions of C, N, O, Ne, Si, and Ar in the low-velocity range from $6 \times 10^6$ to $7 \times 10^7$ cm/sec (20–2.5 $\times 10^3$ eV/amu). Furthermore, Olson and Salop[2] have developed a formalism using the absorbing-sphere model based on the Landau-Zener method which is applicable to the class of reactions $A^{Z+} + B \rightarrow A^{(Z-1)+} + B^+$, where $4 \leq Z \leq 54$. Their method is useful for relative velocities $v \leq 1 \times 10^8$cm/sec (5 keV/amu). Bottcher[3] has also considered collisions between completely stripped ions and hydrogen atoms at low velocities using a model involving only a finite number of crossings between diabatic states, however, these results are considerably different from each other.

In the present paper, the cross sections for the charge-transfer process

$$O^{8+} + H(1s) \rightarrow O^{7+} + H^+ \quad \text{(process I)}$$

for impact energies between 0.025 and 200 keV/amu in the laboratory system are evaluated. The cross sections were calculated using an atomic-base $S$-matrix formulation represented by time-dependent bases which denote atomic orbitals moving in opposite directions. In the evaluation of the $S$ matrix, two extreme models are considered, the "unitarized-distorted-wave approximation (UDWA)" and "absorption model." For the unitarized-distorted-wave approximation, all interactions among the product channels are ignored and the matrix elements are treated as in the case of resonant charge transfer. On the contrary in the absorption model, the product channels are considered to be closely coupled and as for the absorption process, the transferred electron is assumed not to be recaptured by the hydrogen ion.

Since no experimental results are available at the present time, the present results are compared only with the theoretical results mentioned above.

The UDWA formula is also applied to the charge transfer processes

$$H^+ + H(1s) \rightarrow H + H^+ \quad \text{(process II)}$$

and

$$He^{++} + H(1s) \rightarrow He^+ + H^+ \quad \text{(process III)}.$$

In Sec. II, a formulation based on the $S$-matrix theory is described and in Sec. III, the numerical results are given and discussed. Atomic units are used throughout the paper, unless otherwise stated.

## II. FORMULATION

We will consider the rearrangement collision

$$B + (A + e) \rightarrow (B + e) + A, \tag{2.1}$$

that is, through the collision the projected particle $B$ (mass $M_B$, charge $Z_B e$) captures electron $e$ which is initially bound to the nucleus $A$ (mass $M_A$, charge $Z_A e$). The straight-line-trajectory ap-

 

proximation is used for the relative motion of the two nuclei, where the position vector $\vec{R}$ of $B$ relative to $A$ is described as

$$\vec{R}=\vec{v}t+\vec{e}_x\rho\,, \tag{2.2}$$

where $\vec{v}$ is the impact velocity, $\rho$ the impact parameter, and $\vec{e}_x$ the unit vector perpendicular to $\vec{v}$ in the collision plane. If we can obtain the probability $P(\rho)$ for process (2.1) for a given impact parameter $\rho$, then the cross section can be calculated using

$$\sigma=2\pi\int_0^\infty P(\rho)\rho\,d\rho\,. \tag{2.3}$$

The electronic wave function $\chi(\vec{r},t)$ satisfies the Schrödinger equation

$$i\frac{\partial\chi(\vec{r},t)}{\partial t}=\mathcal{H}\chi(\vec{r},t) \tag{2.4}$$

with

$$\mathcal{H}=-\tfrac{1}{2}\Delta-Z_A/r_A-Z_B/r_B\,, \tag{2.5}$$

where $r_A=|\vec{r}_A|$, $r_B=|\vec{r}_B|$, $r=|\vec{r}|$, $\vec{r}_A$, $\vec{r}_B$, and $\vec{r}$ are the position vectors of the electron relative to $A$, $B$ and the midpoint of $A$ and $B$, respectively, and $\Delta$ is the Laplacian with respect to $\vec{r}$.

As basis vectors to expand $\chi(\vec{r},t)$, we use the following time-dependent vectors $\{\xi_n^A\}$ and $\{\xi_n^B\}$ which denote atomic orbitals moving in opposite directions:

$$\xi_n^A(\vec{r},t)=\phi_n^A(\vec{r}_A)e^{-i\vec{v}/2\cdot\vec{r}} \tag{2.6a}$$

and

$$\xi_n^B(\vec{r},t)=\phi_n^B(\vec{r}_B)e^{i\vec{v}/2\cdot\vec{r}}\,, \tag{2.6b}$$

where $\phi_n^A(\vec{r}_A)$ and $\phi_n^B(\vec{r}_B)$ are hydrogenlike wave functions of the systems $A+e$ and $B+e$ having eigenenergies $\omega_n^A$ and $\omega_n^B$, respectively. In the present system nuclei $A$ and $B$ are moving with relative velocity $\vec{v}$ and the time dependence of $\xi_n^A$ and $\xi_n^B$ comes through the positions of nuclei $A$ and $B$. Hereafter we use implicit expressions with respect to $A$ and $B$, unless explicit notation is necessary. For example, we write $\{\xi_n\}$ for $\{\xi_n^A\}$ and $\{\xi_n^B\}$, and $\{\omega_n\}$ for $\{\omega_n^A\}$ and $\{\omega_n^B\}$.

We can express $\chi(\vec{r},t)$ in terms of $\xi_n(\vec{r},t)$ as

$$\chi(\vec{r},t)=\sum_n a_n(t)\xi_n(\vec{r},t)\,, \tag{2.7}$$

where $a_n(t)$ is the expansion coefficient. The expansion is not with an orthogonal set and is overdetermined. However, if we truncate the series, the problem of overdetermination is removed. At a finite internuclear distance, $\sum_n a_n(t)|^2=1$ is not satisfied due to being nonorthogonal. Considering that the charge transfer occurs mostly at an internuclear distance larger than $3a_0$ as we will see later, the charge state may approximately be expressed by either basis $\{\xi_n^A\}$ or $\{\xi_n^B\}$. The use of this expansion leads to coupled equations simpler in structure than those usually encountered and this reflects more directly the physical situation of the process. In the limit of infinite separation or $t\to\pm\infty$, $\sum_n|a_n(t)|^2$ tends to unity, and the $S$ matrix conserves the unitarity property. Here let the state vector be $|\Psi(t)\rangle$ which is composed of the components $\{a_n(t)\}$. Substituting Eq. (2.7) into Eq. (2.4), we obtain the following equation for the vector $|\Psi(t)\rangle$:

$$i\frac{d}{dt}|\Psi(t)\rangle=H|\Psi(t)\rangle \tag{2.8}$$

with

$$H=s^{-1}h\,, \tag{2.9}$$

where $s$ and $h$ are the matrices of which elements are given by

$$h_{mn}=\left(\xi_m,\left\{\mathcal{H}-i\frac{\partial}{\partial t}\right\}\xi_n\right) \tag{2.10a}$$

and

$$s_{mn}=(\xi_m,\xi_n) \tag{2.10b}$$

and $s^{-1}$ is the inverse matrix of $s$.

Using Eqs. (2.6a) and (2.6b), the elements of the matrix $H$ can be written

$$\langle m|H|n\rangle=(\omega_n+\tfrac{1}{8}v^2)\delta_{mn}+\sum_k(s^{-1})_{mk}u_{kn} \tag{2.11}$$

with

$$u_{mn}^{AB}=(\xi_m^A,[-Z_A/r_A]\xi_n^B)\,, \tag{2.12a}$$

$$u_{mn}^{BA}=(\xi_m^B,[-Z_B/r_B]\xi_n^A)\,, \tag{2.12b}$$

$$u_{nn}^{AA}=(\xi_n^A,[-Z_B/r_B]\xi_n^A)\,, \tag{2.12c}$$

$$u_{nn}^{BB}=(\xi_n^B,[-Z_A/r_A]\xi_n^B)\,. \tag{2.12d}$$

In the second term of Eq. (2.11), the factors, $(s^{-1})_{mk}$, are introduced due to the nonorthogonality of our bases, which compensates for the fact that $\sum_k|k\rangle\langle k|\neq1$.

Furthermore, we will introduce a state vector $|\Phi(t)\rangle$ which satisfies the equation

$$i\frac{d}{dt}|\Phi(t)\rangle=H^0|\Phi(t)\rangle\,, \tag{2.13}$$

where $H^0$ is the diagonal part of the matrix $H$, whose elements are given by

$$\langle m|H^0|n\rangle=\langle n|H|n\rangle\delta_{mn}\,. \tag{2.14}$$

The solution of Eq. (2.13) can be written

$$|\Phi(t)\rangle=\exp\left(-i\int_{-\infty}^{t}H^0\,dt\right)|\Phi(-\infty)\rangle\,. \tag{2.15}$$

Let the state vector $|\Psi(t)\rangle$ be expressed as

$$|\Psi(t)\rangle = \exp\left(-i\int_{-\infty}^{t} H^0\,dt\right)|\Psi^{\rm int}(t)\rangle. \tag{2.16}$$

Then upon substitution into Eq. (2.8), we get an expression of the interaction representation

$$i\frac{d}{dt}|\Psi^{\rm int}(t)\rangle = \hat{H}^{\rm int}(t)\,|\Psi^{\rm int}(t)\rangle, \tag{2.17}$$

where

$$\hat{H}^{\rm int}(t) = \exp\left(i\int_{-\infty}^{t} H^0 dt\right) H^{\rm int} \exp\left(-i\int_{-\infty}^{t} H^0 dt\right) \tag{2.18}$$

with

$$H^{\rm int} = H - H^0. \tag{2.19}$$

The solution of Eq. (2.17) is given by

$$|\Psi^{\rm int}(t)\rangle = U(t,-\infty)\,|\Psi^{\rm int}(-\infty)\rangle, \tag{2.20}$$

with

$$U(t,-\infty) = I + (-i)\int_{-\infty}^{t} dt_1\,\hat{H}^{\rm int}(t_1) + (-i)^2\int_{-\infty}^{t} dt_1\int_{-\infty}^{t_1} dt_2\,\hat{H}^{\rm int}(t_1)\hat{H}^{\rm int}(t_2)$$
$$+ (-i)^3\int_{-\infty}^{t} dt_1\int_{-\infty}^{t_1} dt_2\int_{-\infty}^{t_2} dt_3\,\hat{H}^{\rm int}(t_1)\hat{H}^{\rm int}(t_2)\hat{H}^{\rm int}(t_3) + \cdots \tag{2.21}$$

Since

$$U(-\infty,-\infty) = I,$$

we have the following relation:

$$|\Psi(-\infty)\rangle = |\Psi^{\rm int}(-\infty)\rangle. \tag{2.22}$$

The $S$ matrix defined by

$$|\Psi(\infty)\rangle = S\,|\Psi(-\infty)\rangle \tag{2.23}$$

can be written

$$S = \exp\left(-i\int_{-\infty}^{\infty} H^0\,dt\right) S^{\rm int}, \tag{2.24}$$

where

$$S^{\rm int} = U(\infty,-\infty). \tag{2.25}$$

The matrix $U(\infty,-\infty)$ can be rewritten using the $T$ exponential. Thus, we obtain

$$S^{\rm int} = T\exp\left(-i\int_{-\infty}^{\infty}\hat{H}^{\rm int}(t)dt\right)$$
$$= I + \frac{(-i)}{1!}\int_{-\infty}^{\infty} dt\,\hat{H}^{\rm int}(t) + \frac{(-i)}{2!}\int_{-\infty}^{\infty} dt_1\int_{-\infty}^{\infty} dt_2\,T\{\hat{H}^{\rm int}(t_1)\hat{H}^{\rm int}(t_2)\}$$
$$+ \frac{(-i)^3}{3!}\int_{-\infty}^{\infty} dt_1\int_{-\infty}^{\infty} dt_2\int_{-\infty}^{\infty} dt_3\;T\{\hat{H}^{\rm int}(t_1)\hat{H}^{\rm int}(t_2)\hat{H}^{\rm int}(t_3)\} + \cdots, \tag{2.26}$$

where $T$ is the chronological-ordering operator which rearranges any product of the operators $\hat{H}^{\rm int}(t)$ in chronological order with the factor $\hat{H}^{\rm int}$ containing the latest time on the left.

In the high-energy region, we can use the first-order approximation of $S^{\rm int}$ in which the terms including more than one $\hat{H}^{\rm int}(t)$ are ignored in Eq. (2.26). However, we are interested in evaluation of charge-transfer cross sections in the energy region from 10 to 100 keV/amu where the first-order approximated $S^{\rm int}$ is not always satisfied. Because of the moving factors $[\exp(\pm i\vec{v}\cdot\frac{1}{2}\vec{r})]$ in Eqs. (2.6a) and (2.6b), $\hat{H}^{\rm int}(t)$ is not a Hermitian operator. Therefore $U(t,-\infty)$ is not necessarily unitary in Eq. (2.21) whereas $S^{\rm int}$ should be unitary from its original definition. Our main objective is to obtain a proper formula which will be valid in the middle-energy region where the first few terms in (2.26) are significant. In order to obtain a unitarized $S$ matrix for this purpose we will ignore the operator $T$ and all matrix elements except $\langle m,B|\hat{H}^{\rm int}(t)|0,A\rangle$ and $\langle 0,A|\hat{H}^{\rm int}(t)|m,B\rangle$, where $|0,A\rangle$ is the initial-state vector and $|m,B\rangle$ is the state vector in the product channel. The validity of this approximation is examined later. Thus we obtain the

charge-transfer probability for a given impact parameter $\rho$ as follows:

$$P(\rho)=\sum_n |\langle n,B|S^{\rm int}|0,A\rangle|^2 \tag{2.27}$$

with

$$\langle n,B|S^{\rm int}|0,A\rangle=(-i)\int_{-\infty}^{\infty}dt\,\langle n,B|\hat{H}^{\rm int}(t)|0,A\rangle \times\left(1+\frac{(-i)^2}{3!}\sum_m\int_{-\infty}^{\infty}dt_1\int_{-\infty}^{\infty}dt_2\,\langle 0,A|\hat{H}^{\rm int}(t_1)|m,B\rangle\langle m,B|\hat{H}^{\rm int}(t_2)|0,A\rangle +\frac{(-i)^4}{5!}\sum_l\sum_m\int_{-\infty}^{\infty}dt_1\int_{-\infty}^{\infty}dt_2\int_{-\infty}^{\infty}dt_3\int_{-\infty}^{\infty}dt_4\langle 0,A|\hat{H}^{\rm int}(t_1)|l,B\rangle\langle l,B|\hat{H}^{\rm int}(t_2)|0,A\rangle \times\langle 0,A|\hat{H}^{\rm int}(t_3)|m,B\rangle\langle m,B|\hat{H}^{\rm int}(t_4)|0,A\rangle+\cdots\right) \tag{2.28}$$

$$=(-i)\int_{-\infty}^{\infty}dt\,\langle n,B|\hat{H}^{\rm int}(t)|0,A\rangle p^{-1/2}\left(p^{1/2}-\frac{1}{3!}p^{3/2}+\frac{1}{5!}p^{5/2}-\cdots\right)$$

$$=(-i)\int_{-\infty}^{\infty}dt\,\langle n,B|\hat{H}^{\rm int}(t)|0,A\rangle p^{-1/2}\sin p^{1/2} \tag{2.29}$$

with

$$p=\sum_n\left|\int_{-\infty}^{\infty}dt\,\langle n,B|\hat{H}^{\rm int}(t)|0,A\rangle\right|^2. \tag{2.30}$$

Then we have

$$P(\rho)=\sin^2 p^{1/2}. \tag{2.31}$$

In above derivation, we made use of the property that $\hat{H}^{\rm int}(t)$ has only nondiagonal nonvanishing components according to Eq. (2.19). The charge-transfer cross section can be obtained by the substitution of Eq. (2.31) into Eq. (2.3).

Using Eqs. (2.11), (2.14), (2.18), and (2.19), we can rewrite Eq. (2.30) as follows:

$$p=\sum_n\left|\int_{-\infty}^{\infty}dt\ \sum_k(s^{-1})^{BA}_{nk}u^{AA}_{k0}+\sum_k(s^{-1})^{BB}_{nk}u^{BA}_{k0}\ \exp\left[i\int_{-\infty}^{t}\left(\omega^B_n-\omega^A_0+\sum_k(s^{-1})^{BA}_{nk}u^{AB}_{kn}+\sum_k(s^{-1})^{BB}_{nk}u^{BB}_{kn} -\sum_k(s^{-1})^{AA}_{0k}u^{AA}_{k0}-\sum_k(s^{-1})^{AB}_{0k}u^{BA}_{k0}\right)dt\right]\right|^2 \tag{2.32}$$

Ignoring the states $\{|k,A\rangle,\ k\neq 0\}$ and the off-diagonal elements $\{u^{BB}_{mn},\ m\neq n\}$, we get

$$p=\sum_n\left|\int_{-\infty}^{\infty}dt\left(u^{BA}_{n0}-s^{BA}_{n0}\frac{u^{AA}_{00}-\sum_k s^{AB}_{0k}u^{BA}_{k0}}{1-\sum_k|s^{AB}_{0k}|^2}\right)\exp\ i\int_{-\infty}^{t}\left[\left(\omega^B_n+u^{BB}_{nn}-\frac{s^{BA}_{n0}u^{AB}_{0n}-s^{BA}_{n0}s^{AB}_{0n}u^{BB}_{nn}}{1-\sum_k|s^{AB}_{0k}|^2}\right) -\left(\omega^A_0+\frac{u^{AA}_{00}-\sum_k s^{AB}_{0k}u^{BA}_{k0}}{1-\sum_k|s^{AB}_{0k}|^2}\right)\right]dt\ \right|^2. \tag{2.33}$$

Detailed derivation for Eq. (2.33) is shown in the Appendix. If $\sum_k|s^{AB}_{0k}|^2\ll 1$ is satisfied, Eq. (2.33) can be approximated as

$$p\approx\sum_n|\langle n,B|T^{\rm DWBA}|0,A\rangle|^2, \tag{2.34}$$

where

$$\langle n, B | T^{\mathrm{DWBA}} | 0, A \rangle = \int_{-\infty}^{\infty} dt (u_{n0}^{BA} - s_{n0}^{BA} u_{00}^{AA}) \exp\left( i \int_{-\infty}^{t} (\omega_n^B - \omega_0^A + u_{nn}^{BB} - u_{00}^{AA}) dt \right). \tag{2.35}$$

It should be noted that Eq. (2.35) is the classical DWBA formula of the probability amplitude which is equivalent to that of Bates derived using the two-state approximation.[4] Here we call Eq. (2.31) with Eq. (2.30) "unitarized-distorted-wave approximation (UDWA)."

It may be difficult to introduce $\langle m, B | \hat{H}^{\mathrm{int}}(t) | n, B \rangle$, which is ignored in this approach, in a more rigorous manner. However, as an extreme case it is possible to take these into account using the absorbing reaction model in which the electron transferred to nucleus $B$ cannot be recaptured by nucleus $A$. In classical treatment, the decay of the occupation probability $N$ of the electron on the orbital of the nucleus $A$ obeys

$$\frac{dN}{dt} = -\lambda N, \tag{2.36}$$

where $\lambda$ is a rate coefficient. The DWBA probability $p$ given by Eq. (2.34) is thought to be the time integral of $\lambda$, i.e.,

$$p = \int_{-\infty}^{\infty} \lambda \, dt. \tag{2.37}$$

Then the survival probability of the electron in an orbital in $A$ is $e^{-p}$. Therefore, for the absorption probability in a classical sense, we have

$$P(\rho) = 1 - e^{-p}. \tag{2.38}$$

With increasing velocity, both of the probabilities given by Eqs. (2.31) and (2.38) tend asymptotically to $p$, which is the sum of the probabilities obtained by the two-state approximation. Comparison of Eq. (2.38) with Eq. (2.31) is thought to be useful in the estimation of errors in cross sections due to the ignorance of $\langle m, B | \hat{H}^{\mathrm{int}}(t) | n, B \rangle$. The numerical comparison will be described in Sec. III.

The problem with connection to the ignorance of the chronological operator $T$ will also be discussed based on numerical results for typical cases.

## III. NUMERICAL RESULTS AND DISCUSSION

Using formula (2.35), the DWBA probabilities for electron transfer from the $1s$ state of an H atom to an $(nlm)$ state of a hydrogenlike $O^{7+}$ ion,

$$p_{nlm} = \langle nlm, O^{8+} | T^{\mathrm{DWBA}} | 1s, H^{+} \rangle, \tag{3.1}$$

were calculated for $O^{8+}$ impact energies from 0.025 to 200 keV/amu, where $n$ and $(l, m)$ denote the principal and angular momentum quantum numbers.

In order to evaluate the numerical precision, the Brinkman-Kramers-type cross section obtained using the matrices defined by Eq. (2.12b) was compared with the analytically calculated result from the formula[5,6]

$$\sigma_{\mathrm{BK}}(n) = \frac{2^{18} \pi n^2 (Z_A Z_B / n)^5 v^8}{5 [v^2 + (Z_A - Z_B/n)^2]^5 [v^2 + (Z_A + Z_B/n)^2]^5}. \tag{3.2}$$

The relative descrepancies between them are within $10^{-4}$.

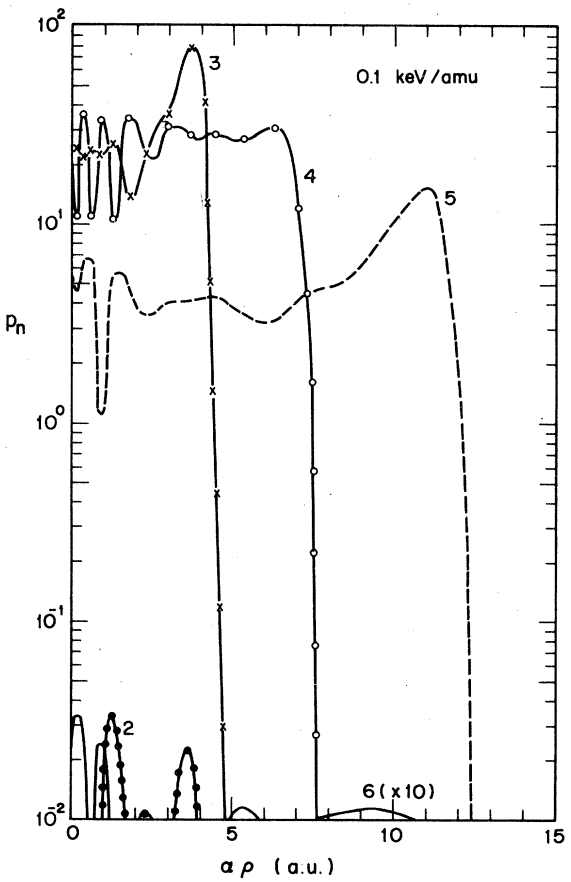


FIG. 1. Partial DWBA probabilities $p_n$ for the process $O^{8+} + H(1s) \rightarrow O^{7+} + H^{+}$ vs scaled impact parameter $\alpha\rho$ for an $O^{8+}$ impact energy of 0.1 keV/amu, where the parameter $n$ denotes the principal quantum number of the hydrogenlike ion $O^{7+}$, $\rho$ is the impact parameter, and $\alpha = \frac{1}{2}(1 + 8/n)$.

The $n$-dependent DWBA probabilities obtained using

$$p_n = \sum_{l=0}^{n-1} \sum_{m=-l}^{l} p_{nlm} \tag{3.3}$$

are shown in Figs. 1–3 versus the scaled impact parameter $\alpha\rho$, where $\alpha = \frac{1}{2}(1 + 8/n)$ and $\rho$ is the impact parameter, for impact energies of 0.1, 10, and 100 keV/amu, respectively.

The total DWBA probability was obtained using

$$p = \sum_{n=1}^{n_c} p_n , \tag{3.4}$$

where $n_c$ is the cut-off value such that the contribution of the states having principal quantum numbers greater than $n_c$ to the cross sections is negligibly small. It was sufficient to determine the cross sections having $n_c = 5$ for impact energies smaller than 0.1 keV/amu, $n_c = 6$ for 0.1 to 2.5 keV/amu, $n_c = 7$ for 5 keV/amu, and $n_c = 8$ for 10 keV/amu. However, it was necessary to set $n_c \geq 10$ for impact energies greater than 25 keV/amu. Therefore for these impact energies $p_n$ were calculated with $n = 1$–$8$ and $n = 10$, and $p_n$ with $n = 9$ were obtained by interpolation and those with $n > 10$ by extrapolation. The interpolation and the extrapolation were performed using a parabolic curve determined by the three points corresponding to $p_7$, $p_8$, and $p_{10}$ in the $\ln(n^3 p_n)$ vs $1/n^3$ plot, for a given scaled impact parameter. The probabilities for process I are obtained using

$$P(\rho) = \sin^2 p^{1/2} \tag{3.5}$$

for the UDWA and

$$P(\rho) = 1 - e^{-p} \tag{3.6}$$

for the absorption model.

The total DWBA probabilities $p$ are shown in Figs. 4 and 5, and the two types of probabilities are shown in Figs. 6–9 for impact energies of 0.05, 0.5, 10, and 100 keV/amu. In Figs. 4 and 5, for impact energies smaller than 10 keV/amu, the DWBA probability $p$ at impact parameters of 0–2, 2–5, or 5–10 a.u. results mainly from curve

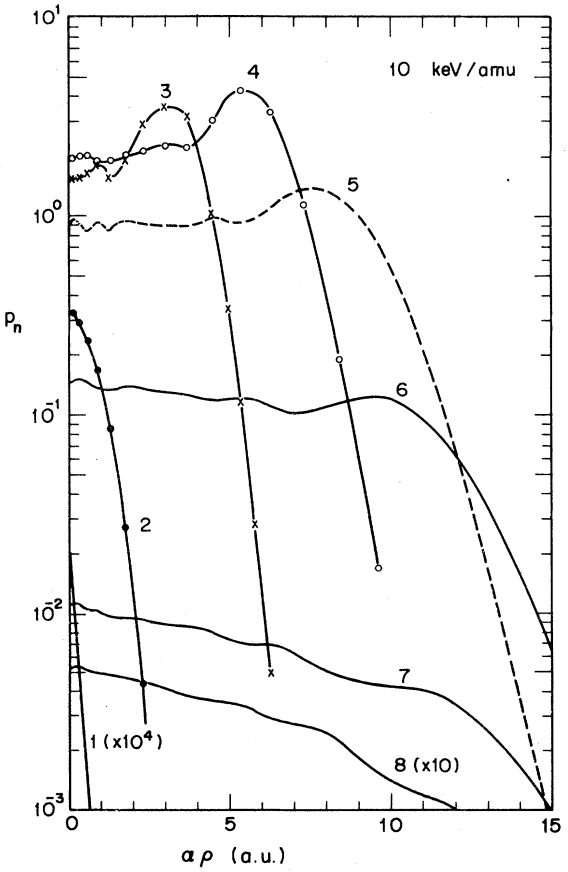


FIG. 2. Same as Fig. 1 for an $O^{8+}$ impact energy of 10 keV/amu.

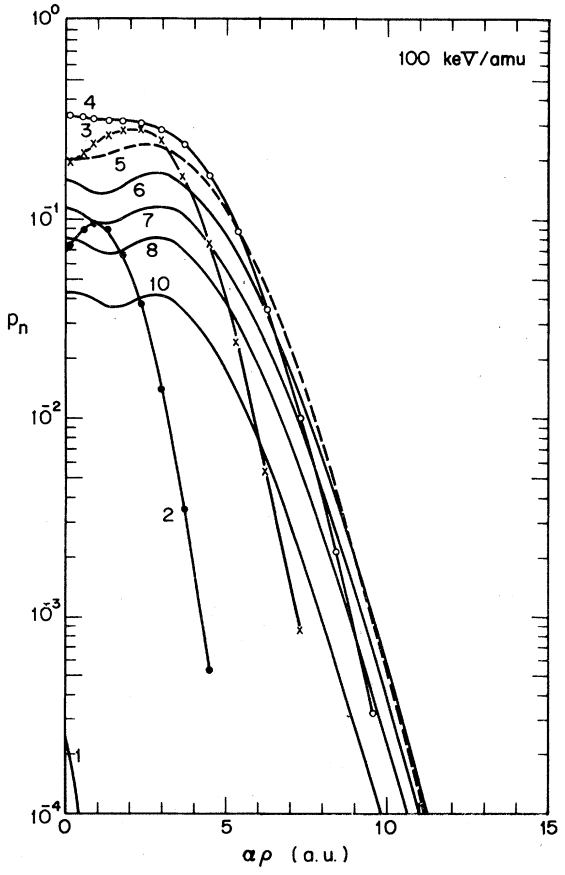


FIG. 3. Same as Fig. 1 for an $O^{8+}$ impact energy of 100 keV/amu.

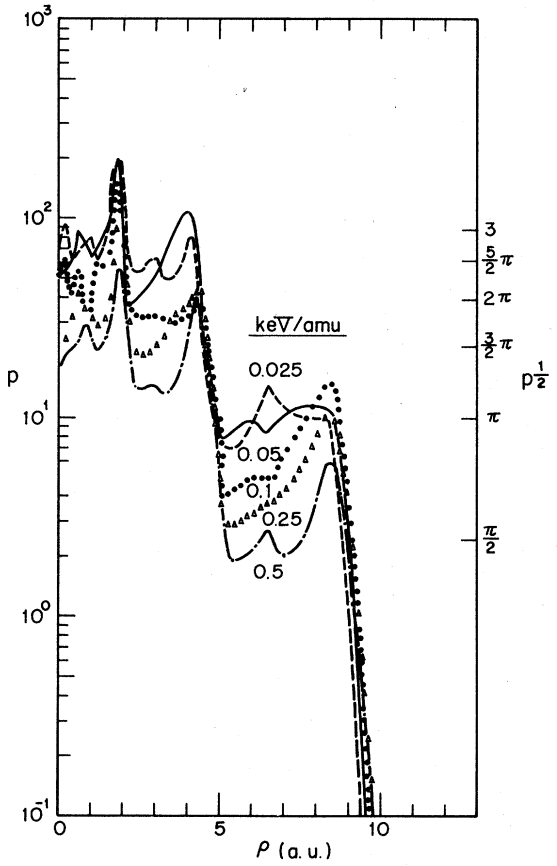


FIG. 4. Total DWBA probabilities $p$ for the process $O^{8+}+H(1s)\rightarrow O^{7+}+H^{+}$ vs impact parameter $\rho$ at $O^{8+}$ impact energies from 0.025 to 0.5 keV/amu.

TABLE I. Cross sections for the process $O^{8+}+H(1s)\rightarrow O^{7}+H^{+}$, where $\sigma_{UDWA}$, $\sigma_{abs}$, and $\sigma_{DWBA}$ denote the cross sections based on UDWA, the absorption model, and the DWBA, and $\gamma$ denotes the relative increase in the cross sections due to the extrapolation, and $Z=8$.

| $E_{O^{8+}}$ (keV/amu) | $\sigma_{UDWA}/Z^2$ (cm$^2$) | $\sigma_{abs}/Z^2$ (cm$^2$) | $\sigma_{DWBA}/Z^2$ (cm$^2$) | $\gamma$ |
|---|---|---|---|---|
| 200 | 5.67(−18) | 5.43(−18) | 6.08(−18) | <0.3 |
| 100 | 2.85(−17) | 2.63(−17) | 3.59(−17) | <0.3 |
| 75 | 4.23(−17) | 3.87(−17) | 5.87(−17) | <0.2 |
| 50 | 5.83(−17) | 5.33(−17) | 9.10(−17) | <0.1 |
| 25 | 7.31(−17) | 6.86(−17) | 1.46(−16) | <0.01 |
| 10 | 8.01(−17) | 8.41(−17) | | |
| 5 | 7.86(−17) | 9.38(−17) | | |
| 2.5 | 8.37(−17) | 1.03(−16) | | |
| 1 | 1.01(−16) | 1.12(−16) | | |
| 0.5 | 9.93(−17) | 1.16(−16) | | |
| 0.25 | 7.36(−17) | 1.21(−16) | | |
| 0.1 | 5.19(−17) | 1.21(−16) | | |
| 0.05 | 2.77(−17) | 1.18(−16) | | |
| 0.025 | 3.98(−17) | 1.14(−16) | | |

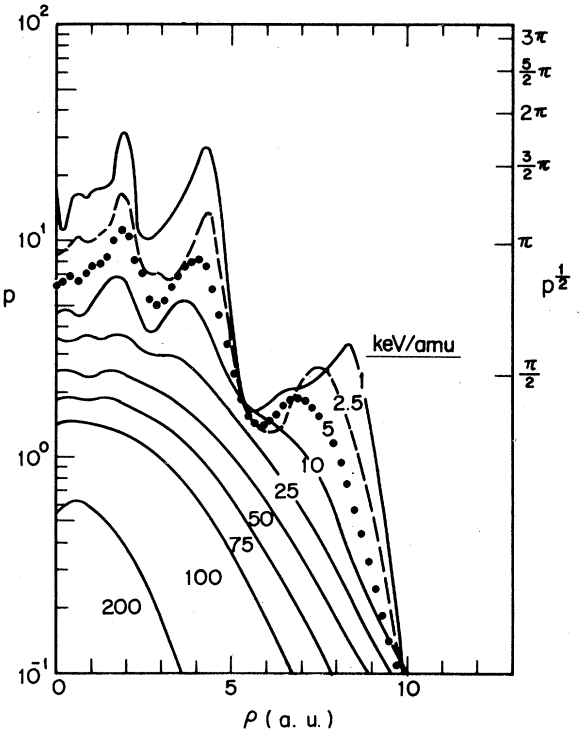


FIG. 5. Same as Fig. 4 for $O^{8+}$ impact energies from 1 to 200 keV/amu.

crossings involving the product channel states $n=3$, 4, and 5, respectively.

The charge-transfer cross sections $\sigma_{UDWA}$ and $\sigma_{abs}$ evaluated using Eqs. (3.5) and (3.6), respectively, are given in Table I, with the DWBA cross section obtained using

$$P(\rho)=p\,. \tag{3.7}$$

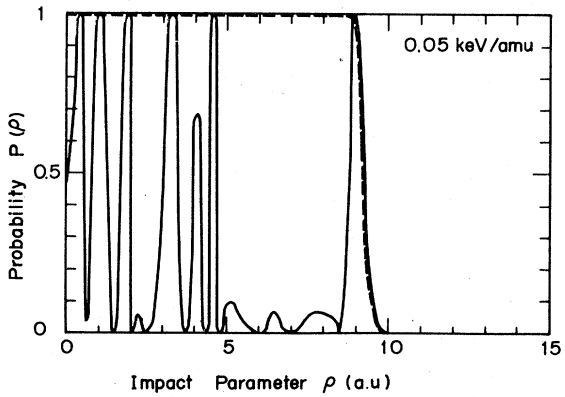


FIG. 6. Probabilities based on the two models vs impact parameter at an $O^{8+}$ impact energy of 0.05 keV/amu. The solid line (——) denotes the probability based on the UDWA and the dashed line (---) that based on the absorption model.

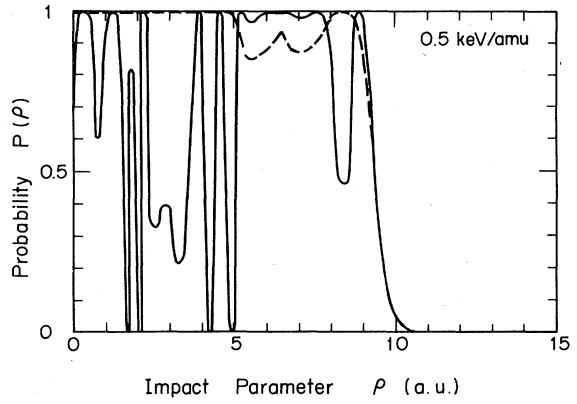


FIG. 7. Same as Fig. 6 for an $O^{8+}$-impact energy of 0.5 keV/amu.

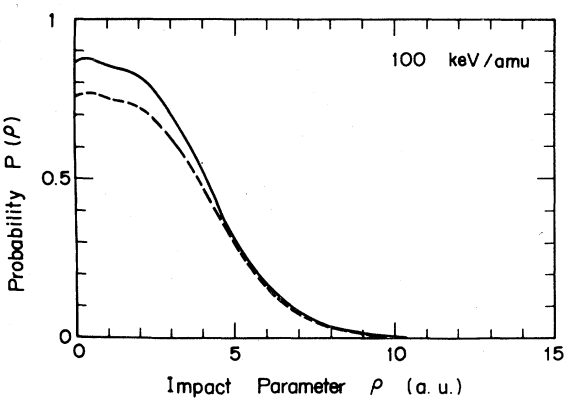


FIG. 9. Same as Fig. 6 for an $O^{8+}$-impact energy of 100 keV/amu.

In the table the relative increases, $\gamma$, in the cross sections due to the extrapolations are also shown. These are so small that the introduction of the extrapolation in the present work is acceptable.

In Fig. 10, the cross sections are shown as a function of the impact energy and are compared with the results of Salop and Olson,[1] of Olson and Salop,[2] of Bottcher[3] and of Olson and Salop.[7,8] For impact energies greater than 10 keV/amu, there is little difference between the cross sections resulting from the two models used in the present calculations. This fact shows that ignorance of matrix elements $\langle m,B|\hat{H}^{\rm int}(t)|n,B\rangle$ $(m\neq n)$ in the UDWA is reasonable. However, at impact energies smaller than 10 keV/amu they deviate with decreasing impact energy. The cross section based on the UDWA represents the minimum which results from $p^{1/2}\approx\pi$ for impact parameters from 5 to 8.5 a.u. and at an impact energy of 0.05 keV/amu (See Fig. 4). It is also seen in Fig. 10 that a considerable difference exists between the DWBA cross section and the results obtained using the two models, except at impact energies greater than 200 keV/amu.

The results of Salop and Olson[1] were derived using the Landau-Zener method. Later these authors pointed out that these results should underestimate the cross section because of disregarding quantum tunneling and transitions due to rotational coupling. They then reported a new

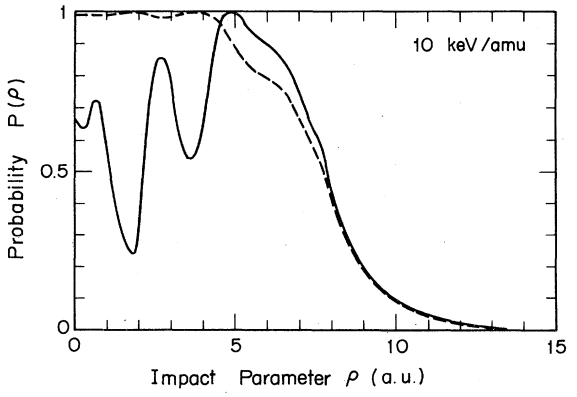


FIG. 8. Same as Fig. 6 for an $O^{8+}$ impact energy of 10 keV/amu.

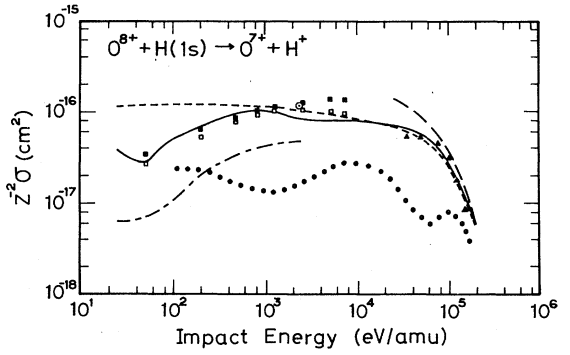


FIG. 10. Cross sections for the process $O^{8+}+H(1s)\rightarrow O^{7+}+H^{+}$ vs $O^{8+}$ impact energy with $Z=8$. —— denotes the present results (UDWA), --- the present results (absorption model), — — the present results (DWBA), — - — the results of Salop and Olson (Ref. 1) (Landau-Zener method), ⊙ the results of Olson and Salop (Ref. 2) (absorbing sphere model), ··· the results of Bottcher (Ref. 3) (unitarized approximation using stationary atomic bases and neglecting nonorthogonality of the bases), ▲ the results of Olson and Salop (Ref. 7) (Monte Carlo method), and □ and ■ the results of Salop and Olson (Ref. 8) (seven-molecular-state close-coupling method using matrix elements with the origin chosen to be on $H^{+}$ and $O^{8+}$, respectively).

value evaluated at an impact energy of 2.5 keV/amu using the absorbing-sphere model based on the Landau-Zener method.[2] This value is also shown in Fig. 10, however, it should overestimate the cross section because use was made of the perfect absorbing-sphere model. The present results based on the two models are within the range estimated from these extreme cases.

Bottcher's results based on the unitary approximation to the $S$ matrix,[3] as in the present case, present a considerably different behavior from the present results. A great difference can be found in connection with the definition of $\hat{H}^{\rm int}$ given in Eq. (2.18). Bottcher has ignored the $\{s_{mn}u_{nn}\}$ terms which are included in Eq. (2.18). These should appear due to the nonorthogonality of the atomic bases and are important in the present work. Moreover, the definition of $\omega_n - U_{mm}$ in his work is somewhat different from that used here. Furthermore, the present formula increases in validity with impact energy, while the validity of Bottcher's formula should break down for high impact energies because moving atomic bases are employed in the present work instead of the static atomic bases of Bottcher's work. He has obtained a decreasing cross section at high impact energies using a cut-off factor depending on the impact velocity.

The UDWA cross section is very close to the cross section obtained by Olson and Salop[7] using the classical trajectory Monte Carlo method and that obtained by the same authors[8] using the close-coupling method based on seven molecular states. It is now under investigation as to why the agreement is so good even below 1 keV/amu.

The validity of neglecting the chronological-ordering operator $T$ was checked by numerical calculation of the probability $P(\rho)$ for the process $O^{8+} + H(1s) \rightarrow O^{7+}(n=5) + H^+$ for impact parameters $\rho = 5.6-8.4$ a.u. where the cross section is almost determined. In Fig. 11, the results are shown against $p^{1/2}$ (square root of the DWBA probability) for impact energies of 0.25, 1, 5, 10, and 25 keV/amu. Results show that agreement of the probability obtained by the UDWA and that obtained by taking time ordering into consideration is very good for an impact energy 25 keV/amu, and that the UDWA is useful as a modified method to the DWBA for impact energies greater than 10 keV/amu.

We have also made the UDWA calculations for processes II and III, i.e., $H^+ + H(1s) \rightarrow H + H^+$ and $He^{++} + H(1s) \rightarrow He^+ + H^+$, for the purpose of investigating the validity of the UDWA method. For process II, theoretical and experimental approaches have been reported by many authors. Here, we compare our result for process II only with experimental data, because the agreement between these experiments and theories is already considered to be satisfactory for incident energies of $10-2\times10^5$ eV. In Fig. 12, the cross sections of UDWA calculation for process II are shown with the data of McClure[9] and Fite *et al.*[10] Our results (solid line) agree very well with experimental data.

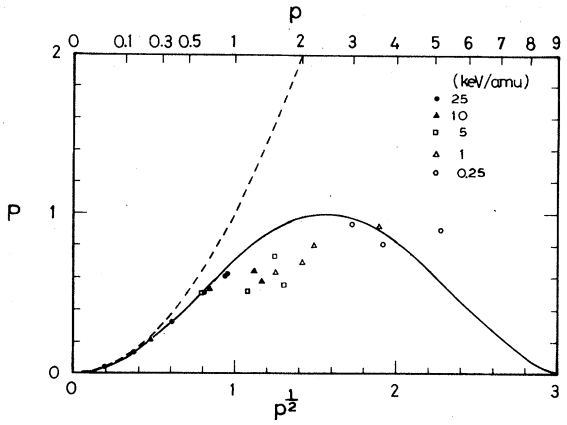


FIG. 11. Comparison of probabilities $P(\rho)$ obtained using Eq. (2.28) with and without time ordering for the process $O^{8+} + H(1s) \rightarrow O^{7+}(n=5) + H^+$, where $n$ is the principal quantum number. The abscissa represents the DWBA probability (top) or its square root (bottom). — denotes the results obtained without time ordering, O, △, □, ▲, and ● the results with time ordering for impact parameter $\rho = 5.6-8.4$ a.u. and for impact energy being 0.25, 1, 5, 10, and 25 keV/amu, respectively, and --- the DWBA probability.

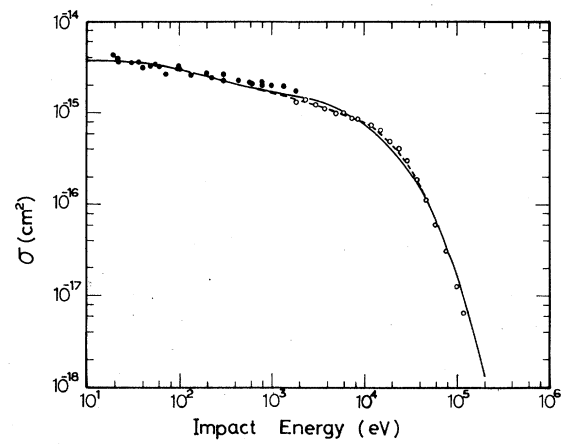


FIG. 12. Cross sections for the charge-transfer process $H^+ + H(1s) \rightarrow H + H^+$. — denotes the present results obtained using the UDWA, and --- the present results obtained by the UDWA in which Eq. (3.8) is used for the partial process $H^+ + H(1s) \rightarrow H(1s) + H^+$ instead of Eq. (2.35). Experimental data: O, McClure (Ref. 9) and ●, Fite *et al.* (Ref. 10).

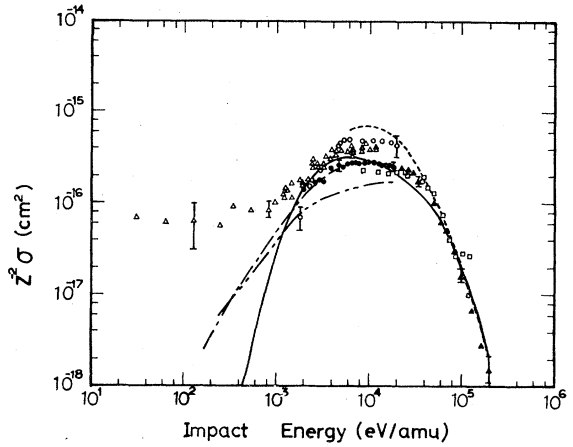


FIG. 13. Cross sections for the charge-transfer process $He^{2+} + H(1s) \rightarrow He^{+} + H^{+}$ with $Z = 2$. —— denotes the present results (UDWA), --- the results of McElroy (Ref. 11) (DWBA), — ---- the results of Piacentini and Salin (Ref. 12) (three-molecular-state close coupling method), ——— the results of Winter and Lane (Ref. 13) (20-molecular-state close-coupling method), and □ the results of Olson *et al.* (Ref. 14) (Monte Carlo method). Experimental data: △ Fite *et al.* (Ref. 10), ● Shah and Gilbody (Ref. 15), ○ Bayfield and Khayrallah (Ref. 16) and ▲ Olson *et al.* (Ref. 14).

However, for the symmetric resonance process

$$H^{+} + H(1s) \rightarrow H(1s) + H^{+} \text{ (process IV)},$$

the quantity $\sum_k |s_{0k}^{AB}|^2$ cannot be ignored compared with unity for an impact energy smaller than 40 keV. Therefore, it is reasonable for process IV that we use the following formula instead of Eq. (2.35),

$$\langle n, B | T^{\mathrm{DWBA}} | 0, A \rangle = \int_{-\infty}^{\infty} dt \frac{u_{n0}^{BA} - s_{n0}^{BA} u_{00}^{AA}}{1 - |s_{0n}^{AB}|^2}, \qquad (3.8)$$

which is obtained from Eq. (2.31) by neglecting all terms except ones for $k = n$ in the summation over $k$, where $n$ stands for the $1s$-state. Thus, we get the cross section shown by the dotted line in Fig. 12. Agreement with McClure's data[9] became considerably better.

For process III, there is also much theoretical work; i.e., those of McElroy,[11] Piancentini and Salin,[12] Winter and Lane,[13] and Olson *et al.*,[14] as well as much experimental work; i.e., those of Fite *et al.*,[10] Shah and Gilbody,[15] and Bayfield and Khayarallah.[16] The cross section versus incident energy curve is not completely established yet. The result of our UDWA calculation is shown in Fig. 13 along with the above-mentioned theoretical and experimental results. The present results agree fairly well with the experimental data except the data of Fite *et al.* below 1 keV/amu.

## ACKNOWLEDGMENTS

The authors would like to express their thanks to Professor Takeshi Ishihara and Professor Mitio Matsuzawa and to other members of the Theoretical Research Group for Atomic Processes in Heavy-Ion Science. They would like to thank Dr. Kineo Tsukada, Dr. Yohta Nakai, and other members of the Committee for Atomic and Molecular Data for Fusion, JAERI. Thanks are also due to Dr. W. Shearer-Izumi for a careful reading of the manuscript. This work was partially supported by a Grant-in-Aid for Fundamental Scientific Research from the Ministry of Education (Special Research Programme "Fundamental Research in Heavy-Ion Science" Contract No. 210103).

## APPENDIX

For the derivation of Eq. (2.33), we ignore the state $\{|k, A\rangle,\ k \neq 0\}$ and the off-diagonal elements $\{u_{mn}^{BB},\ m \neq n\}$ in Eq. (2.32), we get

$$p = \sum_n \left| \int_{-\infty}^{\infty} dt \left( (s^{-1})_{n0}^{BA} u_{00}^{AA} + \sum_k (s^{-1})_{nk}^{BB} u_{k0}^{BA} \right) \exp\left[ i \int_{\infty}^{t} \omega_n^B - \omega_0^A + (s^{-1})_{n0}^{BA} u_{0n}^{AB} + (s^{-1})_{nn}^{BB} u_{nn}^{BB} \right.\right.$$
$$\left.\left. - (s^{-1})_{00}^{AA} u_{00}^{AA} - \sum_k (s^{-1})_{0k}^{AB} u_{k0}^{BA} \right) dt \right] \Bigg|^2 . \qquad (A1)$$

The elements of the matrix $s^{-1}$ for the truncated bases, $|0, A\rangle$ and $\{|k, B\rangle\}$, are easy to evaluate since the resulting matrix $s$ should be a unit matrix except for the row and column which are the overlap matrix elements between $|0, A\rangle$ and $\{|k, B\rangle\}$. These are given by

$$(s^{-1})_{00}^{AA} = D^{-1}, \quad (s^{-1})_{kk}^{BB} = 1 + D^{-1} |s_{0k}^{AB}|^2, \qquad (A2a)$$

$$(s^{-1})_{0k}^{AB} = -D^{-1} s_{0k'}^{AB}, \quad (s^{-1})_{k0}^{BA} = -D^{-1} s_{k0}^{BA} \qquad (A2b)$$

and

$$(s^{-1})^{BB}_{kl} = D^{-1} s^{BA}_{k0} s^{AB}_{0l} \quad (k \neq l) \tag{A2c}$$

with

$$D = 1 - \sum_k |s^{AB}_{0k}|^2 , \tag{A2d}$$

$D$ being determinant of the matrix $s$. Using Eqs. (A2a)–(A2d) in Eq. (A1), we obtain Eq. (2.33).


[1]A. Salop and R. E. Olson, Phys. Rev. A 13, 1312 (1976).
[2]R. E. Olson and A. Salop, Phys. Rev. A 14, 579 (1976).
[3]C. Bottcher, J. Phys. B 10, L213 (1977).
[4]D. R. Bates, Proc. R. Soc. A 247, 294 (1958).
[5]H. C. Brinkman and H. A. Kramers, Proc. Acad. Sci. Amsterdam 33, 973 (1930).
[6]H. Schiff, Can. J. Phys. 32, 393 (1954).
[7]R. E. Olson and A. Salop, Phys. Rev. A 16, 531 (1977).
[8]A. Salop and R. E. Olson (private communication).
[9]G. W. McClure, Phys. Rev. 148, 47 (1966).
[10]W. L. Fite, A. C. H. Smith and R. F. Stebbings, Proc. R. Soc. A 268, 527 (1962).
[11]M. B. McElroy, Proc. R. Soc. A 272, 542 (1963).
[12]R. D. Piancentini and A. Salin, J. Phys. B 10, 1515 (1977).
[13]T. G. Winter and N. F. Lane, Phys. Rev. A 17, 66 (1978).
[14]R. E. Olson, A. Salop, R. A. Phaneuf, and F. W. Meyer, Phys. Rev. A 16, 1867 (1977).
[15]M. B. Shah and H. B. Gilbody, J. Phys. B 7, 637 (1974).
[16]J. E. Bayfield and G. A. Khayrallah, Phys. Rev. A 12, 869 (1975).