Ionization collisions between two excited atoms: Application of the Glauber amplitude in the framework of the impulse approximation

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(Received 16 March 1984)

The cross-section formula of Flannery [Phys. Rev. A 22, 2408 (1980)] in the semiquantal approximation for the processes referred to in the title is rewritten so as to make it more useful in practice. The formula is shown to be further simplified by taking an average over the azimuthal quantum number of a highly excited hydrogenic atom to be ionized. Numerical applications with use of the Glauber amplitude for the electron-atom inelastic scattering are made to the ionization collisions between two excited hydrogen atoms with simultaneous excitation and deexcitation of one of the atoms. The results are compared with those obtained by using the Born amplitude, and are analyzed in terms of the Glauber generalized oscillator strengths.

I. INTRODUCTION

Ionization collisions $(A+B^*\rightarrow A+B^++e)$ between highly excited atoms (B) and excited atoms or molecules (A) have been investigated quite successfully by the impulse approximation.[1] In most cases, the e-A scattering amplitude is approximated by the Born amplitude which is a function only of the momentum transfer.[1-3] In this case the cross section formula becomes very feasible for practical applications. Especially when an average is taken over the azimuthal quantum number of atom B, the formula can be reduced to just a single integral over the momentum transfer.[3] In order to take into account the higher-order corrections, however, the Born amplitude should be replaced by a more sophisticated amplitude which generally depends not only on the momentum transfer (p) but also on the relative velocity (v) in the e-A scattering. The Glauber amplitude is one of the examples. The semiquantal formula proposed by Flannery[4] can be used in this case. From the practical point of view, however, this formula is not very convenient, because the integration of the differential cross section $\sigma_{eA}(p,v)$ for the e-A scattering occupies the innermost position in a fourfold integral, and the calculation of the total cross section becomes very time consuming.

In this paper we propose an expression which differs from the semiquantal formula only in the integration order, but is more practically useful. The difference in the integration order is conceptually trivial, but in practice it is not. First, computation time is greatly reduced. Second, if we take an average with respect to the azimuthal quantum number of atom B, the formula can be easily simplified to a twofold integral over p and v. Applications of this formula to the ionization collisions between two excited hydrogen atoms,

$$\mathrm{H}(n_A,l_A)+\mathrm{H}(n_B,l_B)\rightarrow\mathrm{H}(n'_A,l'_A)+\mathrm{H}^++e,\quad n_A\leq n_B \tag{1.1}$$

are carried out with use of the Glauber approximation to the electron-atom scattering amplitude.[5] Here the quantities n and l denote the principal and azimuthal quantum numbers, respectively.

In Sec. II we derive the cross-section formula from the semiquantal T matrix which differs from the impulse T matrix in that the ejected electron is considered to be free (plane wave). This approximate description of the ejected electron is good particularly in the ionization of highly excited atoms B by the collision with neutral particles A. This is primarily because the charge neutrality of a particle A reduces the relative importance of the collisions with small momentum transfer.[6] In Sec. III the ionization process (1.1) is investigated in the collision-energy (E) region from 10^{-2} to 10^3 keV in the center-of-mass system. Cross sections for $(n_A=2,\ n'_A=3,\ n_B=3,\ 10,\ \text{and}\ 15)$ with simultaneous excitation of atom A and for $(n_A=3,\ n'_A=2,\ n_B=3,\ 10,\ \text{and}\ 15)$ with simultaneous deexcitation are calculated for all possible values of azimuthal quantum numbers.

There have been found some new interesting features in the collision energy dependence of the cross sections (σ_G) in comparison with that of the cross sections (σ_B) obtained with use of the Born amplitude for the electron-hydrogen atom inelastic scattering. First, in certain combinations of l_A and l'_A with large n_B there appears a shoulder or a second maximum in the curve σ_G versus E. Second, a prominent discrepancy in the collision energy dependence of σ_G and σ_B appears at low energies in the case of simultaneous deexcitation with high n_B. That is, while σ_B generally increases monotonically as the collision energy decreases, σ_G shows a nonmonotonic energy dependence. These new phenomena are interpreted in terms of the Glauber generalized oscillator strengths for the $n_A,l_A\rightarrow n'_A,l'_A$ transitions introduced by Chan *et al.*[7] and the electron momentum distribution of the highly excited atom B.

II. DERIVATION OF CROSS-SECTION FORMULA

A. The semiquantal cross section for $A(\alpha)+B(n)\rightarrow A(\beta)+B^+ +e$

In this section, the semiquantal cross-section formula of Flannery[4] is rederived. As was shown by Flannery,[4(b)] the semiquantal T matrix is expressed as a product of an electron-atom A transition matrix t, and a Fourier transform of the initial wave function ψ of an atom B

$$T_{fi}=t_{\beta\alpha}(\vec{k}',\vec{k})\psi_n(\vec{q}) , \tag{2.1}$$

where $\hbar\vec{k}$ and $\hbar\vec{k}'$ are the initial and final relative momenta in the e-A scattering, respectively, and $\hbar\vec{q}$ ($\hbar\vec{q}'$) is the initial (final) electron momentum of atom B. Among $\vec{k}$, $\vec{k}'$, $\vec{q}$, and $\vec{q}'$ there holds the following relations:

$$\vec{k}=\mu_{Ae}(-\vec{k}_i/\mu+\vec{q}/m_e) , \tag{2.2a}$$

$$\vec{k}'=\mu_{Ae}(-\vec{k}_f/\mu+\vec{q}'/m_e) , \tag{2.2b}$$

$$\vec{\kappa}\equiv\vec{k}'-\vec{k}=\vec{k}_i-\vec{k}_f , \tag{2.3}$$

and

$$\vec{q}'=\vec{q}-b\vec{\kappa},\quad b=(m_B-m_e)/m_B , \tag{2.4}$$

with

$$1/\mu=1/m_A+1/m_B,\quad 1/\mu_{Ae}=1/m_A+1/m_e . \tag{2.5}$$

Here m_e, m_A, and m_B are masses of the electron and the atoms A and B, respectively, and $\hbar\vec{k}_i$ and $\hbar\vec{k}_f$ are the initial and final relative momenta in the atom-A–atom-B system.

The differential cross section is given as follows with use of the T_{fi} of Eq. (2.1):

$$\sigma_{fi}(\hat{k}_f)=\frac{(2\pi)^4}{\hbar}\frac{\mu}{\hbar k_i}\int d\vec{q}\,' dk_f\, k_f^2\,|T_{fi}|^2\delta(\epsilon_i-\epsilon_f) , \tag{2.6}$$

where

$$\epsilon_i=(\hbar k_i)^2/2\mu-\epsilon_\alpha+(\hbar q)^2/2m \tag{2.7}$$

and

$$\epsilon_f=(\hbar k_f)^2/2\mu-\epsilon_\beta+(\hbar q')^2/2m \tag{2.8}$$

with

$$1/m=1/m_e+1/(m_B-m_e) , \tag{2.9}$$

where the δ function represents the energy conservation of the total system before and after collision, and ϵ_α and ϵ_β denote the ionization potentials of the initial and final states of atom A, respectively. It should be noted that the energy of the bound electron of atom B is taken to be $(\hbar q)^2/2m$, not $-\epsilon_{n'}$ in Eqs. (2.7) and (2.8). This is because in the impulse approximation the electron is treated as if it were free. The binding of this electron is properly taken into account by the wave function ψ_n. With the aid of the identity with respect to δ functions,

$$\delta(\epsilon_i-\epsilon_f)=\int_{-\infty}^{\infty}d\epsilon\,\delta(\epsilon_A-\epsilon)\delta(\epsilon-\epsilon_B) , \tag{2.10}$$

where

$$\epsilon_A=\hbar^2(k_i^2-k_f^2)/2\mu-\Delta,\ \Delta=\epsilon_\alpha-\epsilon_\beta , \tag{2.11}$$

and

$$\epsilon_B=\hbar^2(q'^2-q^2)/2m , \tag{2.12}$$

the integration over k_f in Eq. (2.6) can be carried out to give

$$\sigma_{fi}(\hat{k}_f)=\left[\frac{2\pi}{\hbar}\right]^4\mu^2\frac{k_f}{k_i}\times\int_{-\infty}^{\infty}d\epsilon\int d\vec{q}\,|T_{fi}|^2\times\delta(\epsilon-\hbar^2(2\vec{q}\cdot\vec{\kappa}+b\kappa^2)/2m_e) , \tag{2.13}$$

where

$$k_f^2=k_i^2-2\mu(\epsilon+\Delta)/\hbar^2 . \tag{2.14}$$

Here Eq. (2.4) was used. In order to proceed further we assume that $t_{\beta\alpha}(\vec{k}',\vec{k})$ depends on the momentum transfer $p(=\hbar\kappa)$ and the relative velocity v between the electron and the atom A. From Eq. (2.2) the latter is given by $v(=|\hbar\vec{k}/\mu_{Ae}|)=|-\hbar\vec{k}_i/\mu+\hbar\vec{q}/m_e|$. Introducing two polar coordinate systems as $\vec{k}_i$ $(k_i,0,0)$, $\vec{q}$ (q,χ,η), $\vec{p}$ $(p,\theta,0)$ and as $\vec{k}_i$ $(k_i,\theta,\pi/2)$, $\vec{q}$ (q,ψ,ϕ), $\vec{p}$ $(p,0,0)$, we obtain the following relations:

$$\cos\chi=\cos\psi\cos\theta+\sin\psi\sin\theta\sin\phi , \tag{2.15}$$

$$v^2=\hbar^2\left[\frac{k_i^2}{\mu^2}-2\frac{k_iq}{\mu m_e}\cos\chi+\frac{q^2}{m_e^2}\right] , \tag{2.16}$$

and

$$\frac{\hbar k_i}{\mu}\cos\theta=\frac{p}{2\mu}+\frac{\epsilon+\Delta}{p} . \tag{2.17}$$

The last equation (2.17) is obtained from Eqs. (2.3) and (2.14). Employing the latter coordinate system, we get $d\hat{q}=d(-\cos\psi)d\phi$. Then from Eqs. (2.15) and (2.16), we have

$$d\phi=d(\cos\chi)/\sqrt{D} , \tag{2.18}$$

where

$$D=(\sin\psi\sin\theta\cos\phi)^2=1-\cos^2\theta-\cos^2\psi+2\cos\theta\cos\psi\cos\chi-\cos^2\chi . \tag{2.19}$$

This can be rewritten as

$$d\phi=2[(v_+^2-v^2)(v^2-v_-^2)]^{-1/2}d(v^2) \tag{2.20}$$

with

$$\left.\begin{matrix}v_+^2\\ v_-^2\end{matrix}\right\}=\hbar^2\left[\frac{k_i^2}{\mu^2}-2\frac{k_iq}{\mu m_e}\times\left\{\begin{matrix}\cos\chi_{\min}\\ \cos\chi_{\max}\end{matrix}\right\}+\frac{q^2}{m_e^2}\right] , \tag{2.21}$$

and

$$\begin{Bmatrix}\cos\chi_{\min}\\ \cos\chi_{\max}\end{Bmatrix}=\cos\theta\cos\psi\pm[(1-\cos^2\theta)(1-\cos^2\psi)]^{1/2}\ . \tag{2.22}$$

In Eq. (2.20) the factor "2" appears, because $\cos\chi$ varies between $\cos\chi_{\max}$ and $\cos\chi_{\min}$ twice when ϕ varies from 0 to 2π at fixed θ and ψ.

If the highly excited state of atom B can be assumed to be hydrogenic, namely if

$$\psi_{nlm}(\vec{q})=f_{nl}(q)Y_{lm}(\theta,\psi)\ ,$$

we can easily take an average of the cross section with respect to the magnetic quantum number m. Using the addition theorem with respect to the spherical harmonics $Y_{lm}(\theta,\psi)$, we have

$$\frac{1}{2l+1}\sum_{m=-l}^{l}|T_{fi}|^2=\frac{1}{4\pi}|f_{nl}(q)|^2|t_{\beta\alpha}(p,v)|^2\ . \tag{2.23}$$

The differential cross section can thus be given as

$$\sigma_{fi}(\hat{k}_f)=\left[\frac{2\pi}{\hbar}\right]^4\mu^2\frac{k_f}{k_i}\frac{m_e}{4\pi\hbar p}\int_{\epsilon_{\min}}^{\epsilon_{\max}}d\epsilon\int_{q_0(p,\epsilon)}^{\infty}q\,|f_{nl}(q)|^2dq\int_{v_-^2}^{v_+^2}dv^2\,2\,|t_{\beta\alpha}(p,v)|^2[(v_+^2-v^2)(v^2-v_-^2)]^{-1/2}\ , \tag{2.24}$$

where

$$q_0(p,\epsilon)=(m_e/\hbar q)\,|\,\epsilon/p-p/2M\,|\ ,\quad M\equiv\frac{m_e}{b} \tag{2.25}$$

and

$$\cos\psi=(m_e/\hbar q)(\epsilon/p-p/2M)\ . \tag{2.26}$$

The upper and lower limits of the integration over ϵ are determined from the relation

$$\hbar\,|\,k_i-k_f\,|\le p\le\hbar(k_i+k_f)\ , \tag{2.27}$$

where

$$k_f=[k_i^2-2\mu(\epsilon+\Delta)/\hbar^2]^{1/2}\ . \tag{2.28}$$

The equations (2.27) and (2.28) yield

$$\epsilon_{\max}=\epsilon^+(p)=-\frac{p^2}{2\mu}+\frac{\hbar k_i}{\mu}p-\Delta \tag{2.29}$$

and

$$\epsilon_{\min}=\begin{cases}\epsilon^-(p)=-\dfrac{p^2}{2\mu}-\dfrac{\hbar k_i}{\mu}p-\Delta & \text{for } 0\le p\le|p_{\min}| \\ & \text{with } \epsilon_n\le-\Delta \\ \epsilon_n \text{ for } |p_{\min}|\le p\le|p_{\max}| & \end{cases} \tag{2.30}$$

with

$$\begin{Bmatrix}p_{\max}\\ p_{\min}\end{Bmatrix}=\hbar k_i\pm\hbar[k_i^2-2\mu(\epsilon_n+\Delta)/\hbar^2]^{1/2}\ . \tag{2.31}$$

Integrating the differential cross section (2.24) over $\hat{k}_f$, we obtain the final expression for the total cross section as

$$\sigma_{fi}=\int\sigma_{fi}(\hat{k}_f)d\hat{k}_f=2\pi\int\sigma_{fi}(\hat{k}_f)\frac{\kappa}{k_ik_f}d\kappa$$

$$=\left[\frac{\mu}{\hbar k_i}\right]^2\frac{1}{\mu_{Ae}^2}\frac{m_e}{\hbar}\int_{p_0}^{p_{\max}}dp\int_{\epsilon_{\min}}^{\epsilon_{\max}}d\epsilon\int_{q_0(p,\epsilon)}^{\infty}q\,|f_{nl}(q)|^2dq\int_{v_-^2}^{v_+^2}dv^2\sigma_{\beta\alpha}(p,v)[(v_+^2-v^2)(v^2-v_-^2)]^{-1/2}\ , \tag{2.32}$$

where

$$p_0=\begin{cases}0 \text{ for } \epsilon_n\le-\Delta\\ p_{\min} \text{ otherwise}\end{cases}$$

and $\sigma_{\beta\alpha}(p,v)$ is the differential cross section for inelastic scattering of an electron by an atom A and is defined as

$$\sigma_{\beta\alpha}(p,v)=\left[\frac{2\pi}{\hbar}\right]^4\mu_{Ae}^2\,|\,t_{\beta\alpha}(p,v)\,|^2\ . \tag{2.33}$$

Equation (2.32) is essentially equal to the semiquantal formula, Eq. (4.50) of Flannery.[4(b)]

B. Rearrangement of integration order

From the computational point of view, this formula may not be very convenient, because the integration of the differential cross section $\sigma_{\beta\alpha}(p,v)$ occupies the innermost position in the fourfold integral. If we can change the order of the integrals and put the integrals over p and v in the outermost positions, then the cross section formula will be practically more useful. To this end we introduce the variables $u\,(=\hbar q/m)$ and $v_i\,(=\hbar k_i/\mu)$. Substituting Eqs. (2.17) and (2.26) into Eq. (2.21), we obtain

$$y^{\pm}(x)=x+A\pm 2[B(x-x_0)]^{1/2}\,, \tag{2.34}$$

where

$$y^{\pm}=v_{\pm}^2,\quad x=\left[\frac{m}{m_e}u\right]^2,\quad x_0=[u_0(p,\epsilon)]^2\,,$$

$$A=v_i^2-2v(p,\epsilon)u(p,\epsilon)\,,$$

$$B=v_i^2-[v(p,\epsilon)]^2\,,$$

$$v(p,\epsilon)=p/2\mu+(\epsilon+\Delta)/p\,,$$

$$u(p,\epsilon)=\epsilon/p-p/2M\,,$$

and

$$u_0(p,\epsilon)=\frac{\hbar}{m}q_0(p,\epsilon)=\frac{m_e}{m}\,|u(p,\epsilon)|\,. \tag{2.35}$$

Since B is always positive within the integral domains of p and ϵ, $y^{-}(x)$ is shown to take a minimum value $y_m=x_0+A-B\ \ [=(p/2\mu_{Ae}+\Delta/p)^2]$ at $x_m=x_0+B$. Now in order to change the order of the integrals we have to solve Eq. (2.34) with respect to x. The inverse function of Eq. (2.34) is given by

$$x^{\pm}(y)=y+2B-A\pm 2[B(y-y_m)]^{1/2}\,. \tag{2.36}$$

Since y_m is independent of ϵ, we can easily change the order of the integrals with respect to v and ϵ. Finally, we obtain

$$\sigma_{fi}=\frac{1}{v_i^2\mu_{Ae}^2}\left[\frac{m_e}{m}\right]^3\int_{p_0}^{p_{\max}}dp\int_{v_m^2}^{\infty}dv^2\sigma_{\beta\alpha}(p,v)\int_{\epsilon_{\min}}^{\epsilon_{\max}}d\epsilon\int_{u_-}^{u_+}du\,|f_{nl}(u)|^2u[(u_+^2-u^2)(u^2-u_-^2)]^{-1/2}\,, \tag{2.37}$$

where

$$v_m=p/2\mu_{Ae}+\Delta/p \tag{2.38}$$

and

$$u_{\pm}^2=\left[\frac{m_e}{m}\right]^2\{v^2+C\pm 2[B(v^2-v_m^2)]^{1/2}\} \tag{2.39}$$

with

$$C\equiv 2B-A=v_i^2-2v(p,\epsilon)v_m\,. \tag{2.40}$$

This is the desired expression for the total cross section. Since the integrals over p and v are usually the most cumbersome, this formula gives the best feasibility. Another advantage of this formula is that this can be easily reduced to a twofold integral if we take an average over the azimuthal quantum number l. This is proved in the next section.

C. Cross section averaged over azimuthal quantum number l

If we assume a highly excited atom to be hydrogenic, the velocity distribution of atom B is given by[8]

$$|f_{nl}(u)|^2=\frac{2^{2l+1}}{\pi u_n^3}\frac{n(l!)^2(n-l-1)!}{(n+l)!}\times(1+x)^l(1-x)^{l+4}[C_{n-l-1}^{l+1}(x)]^2\,, \tag{2.41}$$

where $u_n=(2\epsilon_n/m)^{1/2}$, $x=(u^2-u_n^2)/(u^2+u_n^2)$, and $C_r^{\nu}(x)$ denotes the Gegenbauer polynomial. Using the formula derived by Fock[9] and May,[10]

$$\frac{1}{4\pi}\sum_{l=0}^{n-1}(2l+1)|f_{nl}(u)|^2=\frac{8u_n^5n^2}{\pi^2(u^2+u_n^2)^4}\,,$$

we can easily obtain

$$\frac{1}{n^2}\sum_{l=0}^{n-1}(2l+1)|f_{nl}(u)|^2=\frac{2}{\pi u_n^3}(1-x)^4\,. \tag{2.42}$$

The integral over u in Eq. (2.37) is proportional to

$$I=\int_{x_1}^{x_2}dx\,f(x)/[(x_2-x)(x-x_1)]^{1/2}\,. \tag{2.43}$$

Putting $x=\alpha+\beta y$ with $\alpha=(x_2+x_1)/2$ and $\beta=(x_2-x_1)/2$, we can rewrite I as

$$I=\int_{-1}^{1}dy\,f(\alpha+\beta y)/(1-y^2)^{1/2}=\int_0^{\pi}f(\alpha+\beta\cos y)dy\,. \tag{2.44}$$

Then the integral over u in Eq. (2.37) is expressed as

$$I_{nl}=\frac{u_n^2}{\sqrt{D}}\int_{x_1}^{x_2}dx\frac{|f_{nl}(u)|^2}{(1-x)[(x_2-x)(x-x_1)]^{1/2}} \tag{2.45}$$

with

$$D=(u_+^2+u_n^2)(u_-^2+u_n^2) \tag{2.46}$$

and

$$x_2=(u_{\pm}^2-u_n^2)/(u_{\pm}^2+u_n^2)\,. \tag{2.47}$$

If we take an average with respect to l, we obtain

$$\begin{aligned}I_n&\equiv\frac{1}{n^2}\sum_{l=0}^{n-1}(2l+1)I_{nl}\\&=\frac{2}{\pi u_n\sqrt{D}}\int_{x_1}^{x_2}dx\,(1-x)^3[(x_2-x)(x-x_1)]^{1/2}\\&=\frac{2}{\pi u_n\sqrt{D}}\int_0^{\pi}dy(1-\alpha-\beta\cos y)^3\,.\end{aligned} \tag{2.48}$$

This integral is easily evaluated to give

$$\begin{aligned}I_n&=(1-\alpha)[2(1-\alpha)^2+3\beta^2]/u_nD^{1/2}\\&=PQ/u_nD^{7/2}\,,\end{aligned} \tag{2.49}$$

where

$$P\equiv D(1-\alpha)=u_n^2(u_+^2+u_-^2+2u_n^2) \tag{2.50}$$

and

$$Q \equiv D^2[2(1-\alpha)^2+3\beta^2]=2P^2+3[u_n^2(u_+^2-u_-^2)]^2 . \tag{2.51}$$

In order to carry out the integration of I_n over ϵ we have to know the dependence of P, Q, and D on ϵ. Equation (2.39) shows that P depends linearly on ϵ via $v(p,\epsilon)$ and that Q and D are quadratic functions of ϵ. Then the integration over ϵ is expressed as

$$S_n \equiv \int_{\epsilon_1}^{\epsilon_2} d\epsilon I_n = p\int_{t_1}^{t_2} dt I_n = 2^4\left[\frac{m}{m_e}\right]^3 \tilde{u}_n^5 p \sum_{j=0}^{3}\int_{t_1}^{t_2} dt \frac{d_j t^j}{(at^2+bt+c)^{7/2}} , \tag{2.52}$$

where $\tilde{u}_n=(m/m_e)u_n$, $t_{2,1}=v(p,\epsilon_{2,1})$, and the coefficients $a\sim c$ and d_j's are determined from Eqs. (2.46), (2.50), and (2.51). This integral can be easily evaluated analytically.[11] The final expression for the averaged total cross section is as follows:

$$\sigma_{fi}(\alpha,n\to\beta)=\frac{16}{v_i^2\mu_{Ae}^2}\tilde{u}_n^5\int_{p_0}^{p_{\max}} p\,dp\int_{v_m^2}^{\infty} dv^2\sigma_{\beta\alpha}(p,v)[F_n(v,t_{\max})-F_n(v,t_{\min})] , \tag{2.53}$$

where

$$\begin{aligned}
&F_n(v,t)=\sum_{j=0}^{3} d_j J[j],\quad J[j]=\int^t dt\frac{t^j}{(at^2+bt+c)^{7/2}} ,\\
&t_{\max}=v_i\ [\epsilon_{\max}=\epsilon^+(p)] ,\\
&t_{\min}=\begin{cases}-v_i & [\epsilon_{\min}=\epsilon^-(p)]\\ v(p,\epsilon_n) & (\epsilon_{\min}=\epsilon_n)\end{cases}\\
&a=4v^2,\quad b=-4\gamma v_m,\quad c=\gamma^2-4v_i^2(v^2-v_m^2) ,\\
&d_0=\gamma[\gamma^2+6v_i^2(v^2-v_m^2)],\quad d_1=-6v_m[\gamma^2+2v_i^2(v^2-v_m^2)] ,\\
&d_2=-6\gamma(v^2-3v_m^2),\quad d_3=4v_m(3v^2-5v_m^2) ,
\end{aligned} \tag{2.54}$$

with

$$\gamma=v^2+v_i^2+\tilde{u}_n^2 .$$

III. RESULTS AND DISCUSSION

Applications of the cross-section formulas (2.37) and (2.53) to the ionization collisions (1.1) with simultaneous excitation ($n_A=2\to n_A'=3$) and with simultaneous deexcitation ($n_A=3\to n_A'=2$) have been carried out with the use of the Glauber approximation to the electron-atom scattering amplitude.

For the convenience of later discussion, it is instructive to compare the Glauber and Born generalized oscillator strengths (GOS) for all possible transitions from $n_A=2$ to $n_A'=3$. These are shown in Fig. 1. As was found by Chan *et al.*,[7] the number of extrema and their positions of the Glauber GOS vary with the energy of the incident particle, and the values at the minima are not equal to zero in contrast to the Born approximation.

A. Ionization collisions with simultaneous excitation

First, we have calculated the cross sections for the ionization processes

$$\mathrm{H}(2,l_A)+\mathrm{H}(3,l_B)\to\mathrm{H}(3,l_A')+\mathrm{H}^+ +e , \tag{3.1}$$

in order to look into the l_B dependence of the cross sections. However, the l_B dependence has not been well discerned. So we have averaged the cross sections with respect to l_B. Figure 2 shows the results as a function of the center-of-mass collision energy (E). It should be noted that the Born results σ_B are enlarged by a factor 10^2. In the high-energy region above 500 keV both cross sections (σ_G and σ_B) become identical and decrease in proportion to $1/E$. This $1/E$ dependence of the cross section at high energies was discussed in the earlier paper.[3(b)] As the collision energy decreases, σ_G becomes smaller than σ_B, and the maximal values are about one-third of those of σ_B. It is interesting to note that the shoulder appearing in the σ_B curve in the case of the $2s\to3p$ transition disappears in the corresponding σ_G curve and vice versa in the case of the $2p\to3s$ transition. In order to interpret this phenomenon, we examine the positions of extrema of the Glauber and Born GOS, and the effective integral domains of p and v in Eq. (2.37).

Atomic units will be used hereafter, unless otherwise indicated explicitly. Since the electron-velocity distribution function $f(u)$ takes a maximum at $u\simeq 1/n_B$ and rapidly decreases in the order of u^{-8} at $u>1/n_B$, σ_{fi} becomes small when $u_->1/n_B$. We find from Eq. (2.39) that $\tilde{u}_-[\equiv(m/m_e)u_-]$ takes a minimum value $|v-v_i|$ at $\epsilon_m=-p^2/2\mu+(v_m v_i/v)p-\Delta$. Therefore the integral over v becomes significant only when v_i is larger than v_m, since in this case $\tilde{u}_-$ can be zero. In order for this condition to be realized, ϵ_m at $v=v_i$ [$\epsilon_m(v=v_i)=p^2/2M$] should also lie in the integration range of $\epsilon(\epsilon_{\min},\epsilon_{\max})$. These conditions yield the following relations:

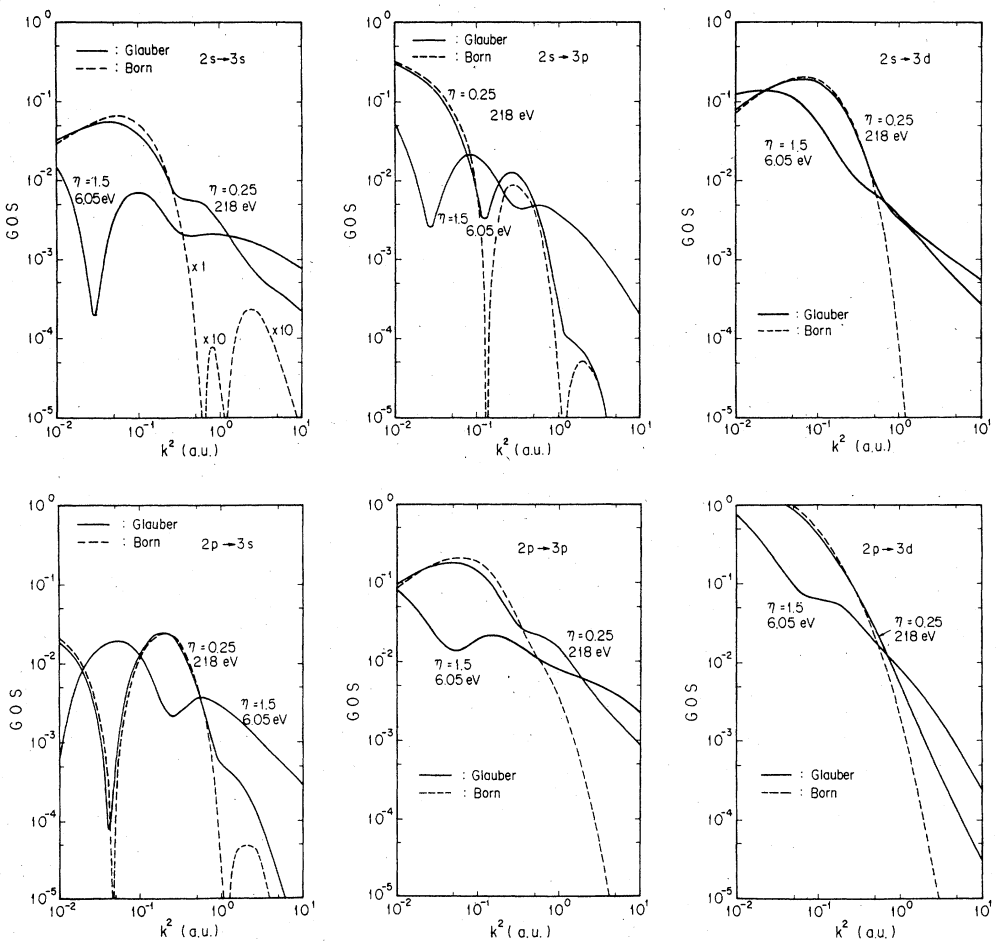

FIG. 1. Born and Glauber generalized oscillator strengths as a function of the square of momentum transfer k^2, for $e+\mathrm{H}(n_A=2,l_A)\rightarrow e+\mathrm{H}(n'_A=3,l'_A)$. The symbol η is equal to v^{-1} (a.u.), where v is the incident electron velocity.

$$p^+ \geq p \geq \max(p^-,p_B)=\begin{cases} p_B & \text{for } E>E_c \\ p^- & \text{for } E_c \geq E > E_d \end{cases} \tag{3.2}$$

where

$$p^{\pm}=\mu_{Ae}[v_i \pm (v_i^2-2\Delta/\mu_{Ae})^{1/2}],\quad p_B=(2M\epsilon_{n_B})^{1/2}, \tag{3.3}$$

$$E_c=12.5\left[\frac{M}{\mu_{Ae}}\epsilon_{n_B}+\Delta\right]^2/2M\epsilon_{n_B}\ \text{keV}, \tag{3.4}$$

and

$$E_d=12.5(2\Delta/\mu_{Ae})\ \text{keV}. \tag{3.5}$$

We see from Eq. (3.2) that the cross section decreases rapidly when the collision energy becomes smaller than E_d ($=1.74$ keV), because the minimum value of $\tilde{u}_-$ becomes greater than $1/n_B$. Since in the case of the processes (3.1) E_c is estimated to be 1.76 keV which is roughly equal to E_d, the lower limit of the p-integration range can be approximated as p_B ($=\frac{1}{3}$), which is independent of v_i. As is shown in Fig. 1, on the other hand, at $k(=p)\sim\sqrt{5}/6$ the Born GOS has a deep dip for the $2s\rightarrow 3p$ transition, while the Glauber GOS for $\eta=1.5$ ($E=5.56$ keV) has a peak there and vice versa for the $2p\rightarrow 3s$ transition. Thus we can interpret the appearance and disappearance of shoulders in the cross section curves in Fig. 2 in terms of the structures of the generalized oscillator strengths at $p\simeq p_B$.

Figure 3 shows the cross sections σ_G and σ_B for the ionization processes:

$$\mathrm{H}(2,l_A)+\mathrm{H}(15)\rightarrow\mathrm{H}(3,l'_A)+\mathrm{H}^+ +e\ . \tag{3.6}$$

In this figure we notice that there appear second maxima at $E\simeq 2\sim 10$ keV in the σ_G curves for the $2s\rightarrow 3s$, $2s\rightarrow 3p$, and $2p\rightarrow 3p$ transitions. In this case the effective integral domain of p is given as follows:

$$p^+ \geq p \geq p_B \quad \text{for } E>14.4\ \text{keV}, \tag{3.7}$$

or

$$p^+ \geq p \geq p^- \quad \text{for } 14.4\ \text{keV} \geq E > 1.74\ \text{keV}. \tag{3.8}$$

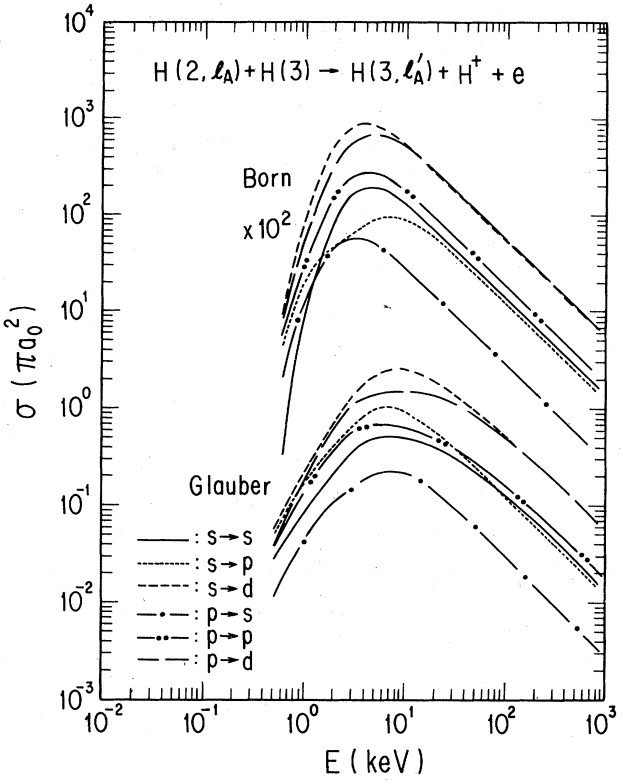

FIG. 2. Ionization cross sections for $H(n_A=2,l_A)+H(n_B=3)\rightarrow H(n'_A=3,l'_A)+H^+ +e$. E is the collision energy in the center-of-mass system. The curves marked as "Born" and "Glauber" are obtained with use of the Born and Glauber approximations to $e+H$ scattering amplitude, respectively.

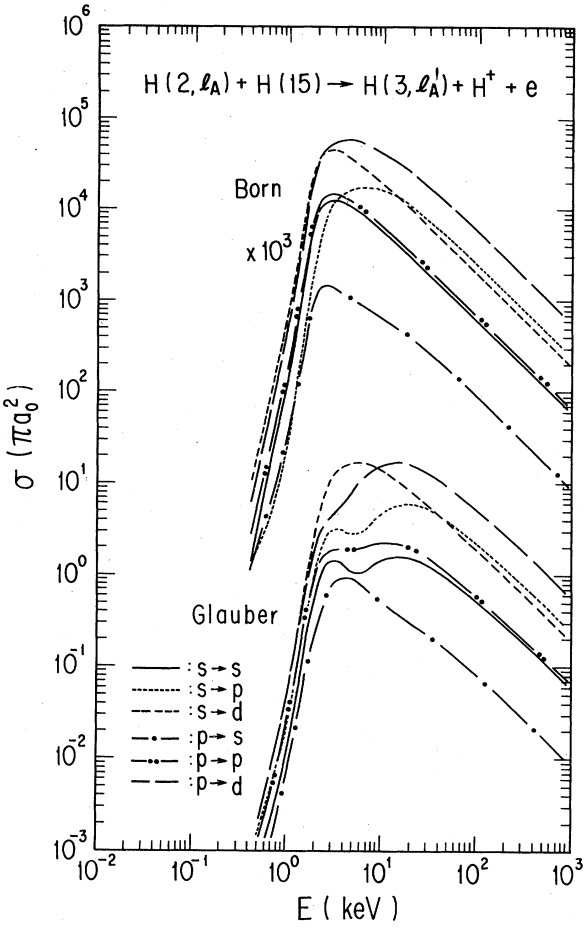

FIG. 3. The same as in Fig. 2 for $H(n_A=2,l_A)+H(n_B=15)\rightarrow H(n'_A=3,l'_A)+H^+ +e$.

At $E\simeq 5$ keV $p^{\pm}$ are estimated as ~ 1.14 and ~ 0.12, respectively. We find in Fig. 1 that the Glauber GOS for the $2s\rightarrow 3s$, $2s\rightarrow 3p$, and $2p\rightarrow 3p$ transitions have dips at $k(=p)\simeq 0.17$ in the case of $\eta=1.5$. Thus the second maxima in the σ_G curve can be explained successfully again in terms of the hollow structures of the generalized oscillator strengths at $p\simeq p^-$. Cross sections summed over final azimuthal quantum numbers and averaged over initial ones are shown in Fig. 4 for the cases of $n_B=3$, 10, and 15.

B. Ionization collisions with simultaneous deexcitation

The l_B dependence of the cross sections is again hardly discerned. Figures 5 and 6 show the calculated cross sections σ_G and σ_B for the processes

$$H(3,l_A)+H(n_B)\rightarrow H(2,l'_A)+H^+ +e \tag{3.9}$$

with $n_B=3$ and 15. These indicate the n_B and $l_A-l'_A$ dependence of the cross sections. In the high-energy region above 500 keV, σ_G becomes identical with σ_B which, as was discussed before,[3(b)] decreases in proportion to $1/E$. However, there appears a prominent discrepancy between σ_G and σ_B at lower energies $E\lesssim 10$ keV. In particular, as is seen in Fig. 6, σ_G's show nonmonotonic energy dependences with wavy structures at energies $1\sim 10$ keV. On the other hand σ_B, except for the $3p\rightarrow 2s$ transition, increases monotonically in proportion to $1/\sqrt{E}$ as the collision energy decreases.

The energy dependence of the cross section in the energy region below 500 keV can be explained in the same way as in the preceding subsection. In the case of the simultaneous deexcitation the effective integral domain of p is given as

$$p^+\geq p\geq \max(p^-,p_B)=\begin{cases} p_B & \text{for } E>E_c \\ p^- & \text{for } E\leq E_c \end{cases} \tag{3.10}$$

where

$$p^{\pm}=\mu_{Ae}[(v_i^2-2\Delta/\mu_{Ae})^{1/2}\pm v_i]\ , \tag{3.11}$$

and E_c is given by Eq. (3.4). Here the excitation energy Δ is negative. Concerning the energy dependence of the cross section in the low-energy region ($v_i\ll 1$ or $E\ll 12.5$ keV), we can give the following qualitative

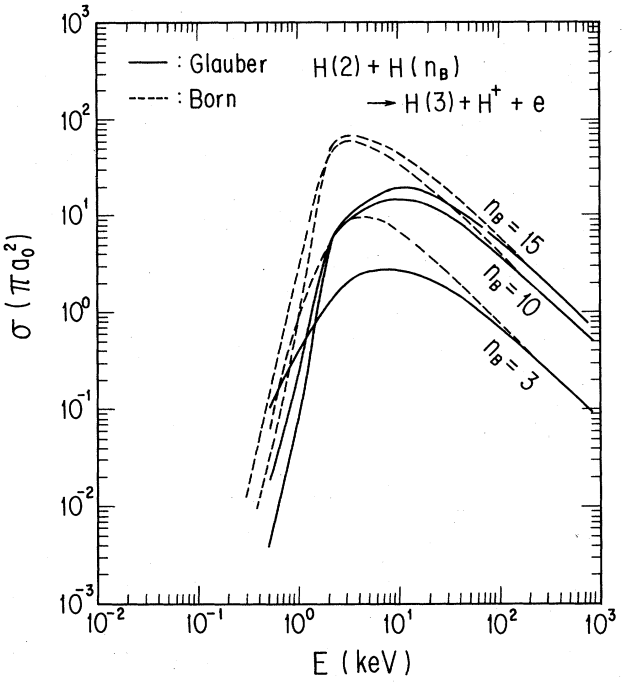

FIG. 4. Comparison between the Born and Glauber approximations for $H(n_A=2)+H(n_B)\rightarrow H(n'_A=3)+H^+ +e$ with $n_B=3$, 10, and 15. E is the collision energy in the center-of-mass system.

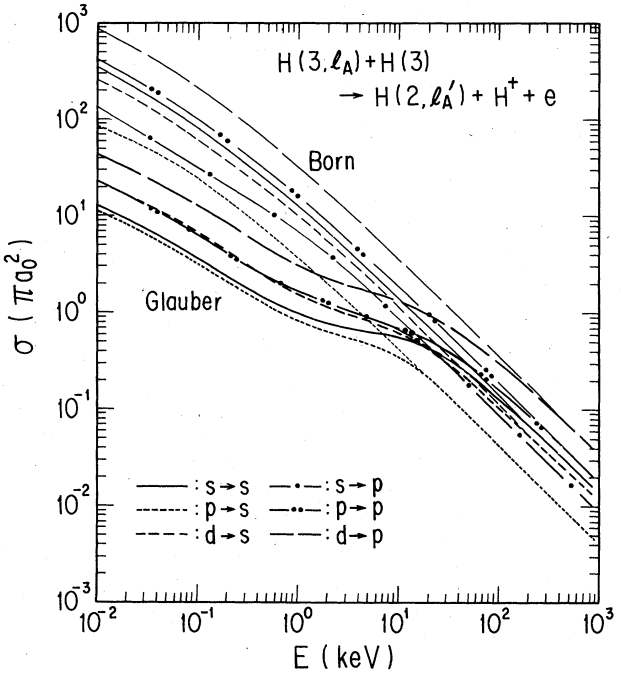

FIG. 5. Ionization cross sections for $H(n_A=3,l_A)+H(n_B=3)\rightarrow H(n'_A=2,l'_A)+H^+ +e$. E is the collision energy in the center-of-mass system. The curves marked as "Born" and "Glauber" are obtained with use of the Born and Glauber approximations to $e+H$ scattering amplitude, respectively.

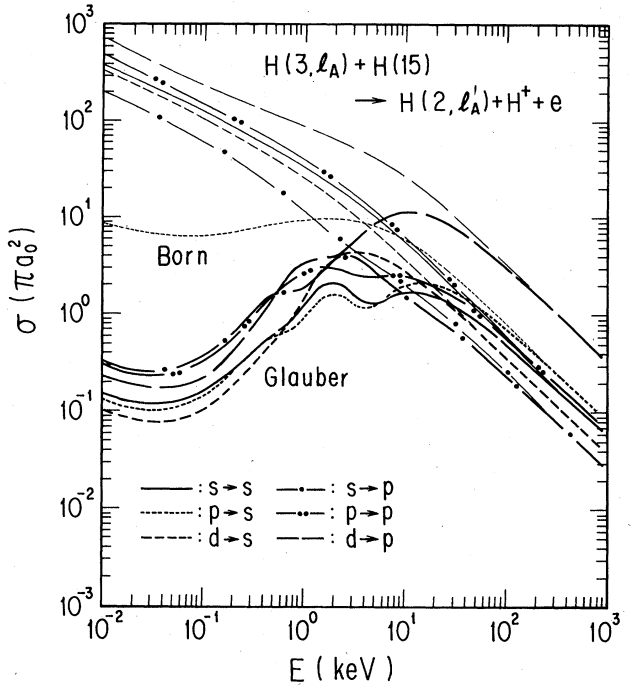

FIG. 6. The same as in Fig. 5 for $H(n_A=3,l_A)+H(n_B=15)\rightarrow H(n'_A=2,l'_A)+H^+ +e$.

description. In this limiting case Eqs. (3.10) and (3.11) are rewritten as

$$\tilde{p}^{+}\geq p\geq\tilde{p}^{-}\,, \tag{3.12}$$

where

$$\tilde{p}^{\pm}\sim p_0\pm\mu_{Ae}v_i \tag{3.13}$$

with $p_0=(-2\mu_{Ae}\Delta)^{1/2}$. Therefore the width of the integration range $[\tilde{p}^{+},\tilde{p}^{-}]$ is in proportion to v_i. Since v_m in Eq. (2.38) is always zero at $p=p_0$, we can roughly estimate the integral over v by putting $v_m=0$ in Eq. (2.37). Then the energy dependence of the cross section can again be shown to be $1/\sqrt{E}$ in the low-energy limit. There actually appears the $1/\sqrt{E}$ dependence at $E\lesssim 0.1$ keV in Fig. 5 and at $E<0.01$ keV in Fig. 6.

In the intermediate-energy region, the effective integral domain of p is given as

$$p^{+}\geq p\geq p_B \quad \text{for } E\geq 0.02 \text{ keV} \tag{3.14}$$

in the case of $n_B=3$. It should be noted that at a given v_i p^{+} given by Eq. (3.11) is large compared with p^{+} of Eq. (3.3). In other words the effective integral domain of p is wide and weakly dependent on v_i in this case. This fact explains the behavior of σ_G in Fig. 5. Namely, the differences in the structures of GOS do not show up conspicuously in the energy dependence of the cross sections. Unlike in Fig. 5, in Fig. 6 σ_G show wavy structures in the energy region from 0.5 to 5 keV. In the case of $n_B=15$, the effective integral domain of p is given as

$$p^{+}\geq p\geq p^{-} \quad \text{for } E\geq 12.7 \text{ keV}\,. \tag{3.15}$$

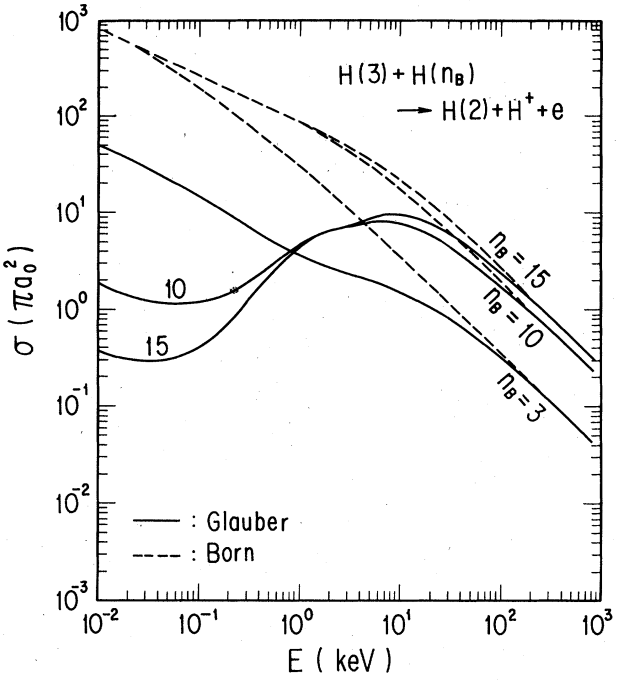

FIG. 7. Comparison between the Born and Glauber approximations for $H(n_A=3)+H(n_B)\rightarrow H(n'_A=2)+H^+ +e$ with $n_B=3$, 10, and 15. E is the collision energy in the center-of-mass system.

Since p^- increases as the collision energy decreases and the effective integral domain of p becomes narrower, the wavy behavior can be ascribed to the structures of the Glauber GOS. It is also interesting to note that σ_B for the $3p\rightarrow 2s$ transition has a minimum at $E\sim 0.04$ keV because of a deep dip of the Born GOS at $p\sim\sqrt{5}/6$.

In order to see the n_B dependence of the cross sections an average over l_A and a summation over l'_A are carried out. Figure 7 shows the results for $n_B=3$, 10, and 15. A wavy structure seen in Fig. 6 disappears. In the case of large n_B, σ_G takes a maximum at $E\simeq 10$ keV, while σ_B increases monotonically as the collision energy decreases.

Here, we describe qualitatively the energy dependence of the cross section in the low-energy limit by taking into account the spread of electron-velocity distribution. In the energy region where $v_i \ll 1/n_B$, the relative velocity (v) between the electron and the atom A is roughly equal to the velocity ($1/n_B$) of the bound electron of the atom B and is independent of v_i. Therefore, qualitatively the same discussion holds as before where the Born approximation was employed for the e-A scattering amplitude,[3(a)] and the energy dependence of the cross section is generally given as $1/\sqrt{E}$, though the absolute value of the cross section (or the proportionality constant) depends on the approximation employed for the two-body scattering amplitude. The $1/\sqrt{E}$ dependence holds from the higher collision energy in the case of small n_B than in the case of large n_B. At large n_B the cross section decreases as the collision energy decreases from 10 to 0.05 keV. Since v is nearly equal to v_i in this energy region, this energy dependence can be ascribed to the fact that the differential cross section in the Glauber approximation decreases steeply in power of v (<1) in the region of $p^+ \geq p \geq p^-$.

IV. SUMMARY AND CONCLUSION

Within the framework of the impulse approximation, we have derived the expressions (2.37) and (2.53) of practical use for calculating the cross sections for the ionization of highly excited atoms by collision with excited atoms or molecules. These formulas with use of the Glauber approximation for the electron-atom scattering were applied to the ionization collisions between two excited hydrogen atoms with simultaneous excitation and deexcitation of one of the atoms. The results were compared with those obtained by using the Born approximation. The agreement between them is very good at high collision energies $E\gtrsim\sim 100$ keV. At lower energies there appears a discrepancy. In the case of simultaneous excitation the peak values of the Glauber cross sections are roughly one-third of the corresponding Born cross sections. In the case of simultaneous deexcitation with large n_B the disagreement between the two results is unexpectedly large. This disagreement can be attributed to the difference in the structures of the Glauber and the Born generalized oscillator strengths. The Glauber cross sections show an interesting nonmonotonic energy dependence.

Unfortunately, however, it is not easy to give a quantitative validity criterion for the utilization of the Glauber approximation. The Glauber approximation is known to work well at $v\gtrsim 1(\equiv v_0^{\rm gr})$ in the case of $1s\rightarrow nl$ transition in the electron-hydrogen atom scattering.[12] If we recall the Massey's criterion, the critical velocity v_0 is considered to be proportional to the interaction range times the transition energy Δ ($\Delta\simeq\frac{1}{2}$ for the $1s\rightarrow nl$ transition). Thus in the case of the transition ($n\rightarrow n'$) between excited states we have

$$v\gtrsim v_0^{\rm ex}\simeq 2v_0^{\rm gr}n^2\Delta_{nn'}=2n^2\Delta_{nn'}$$

with $\Delta_{nn'}=(1/n^2-1/n'^2)/2$, if we simply assume that the interaction range is proportional to n^2. If we notice $v\simeq v_i$ in the case of high n_B, we obtain $E\gtrsim\mu(v_0^{\rm ex})^2/2$ as a crude criterion. This gives $E\gtrsim 3.9$ keV for the transition $n_A=2\rightarrow n'_A=3$, for instance. When n_B ($\geq n_A$) is small, this criterion would be expected to be more relaxed because of the spread of the electron-velocity distribution. Thus it would probably be all right to say that the Glauber results obtained in this paper are more accurate than the Born results at collision energies higher than several keV's. However, we cannot give any assessment conclusively at this moment about the accuracy of the Glauber results at lower energies. Further studies are required to answer this question.

The formulas (2.37) and (2.53) are also applicable to the ionization of highly excited atoms by collision with rotationally excited molecules.[1] So far calculations have been made only with use of the Born approximation for the

electron-molecule rotationally inelastic scattering. Since the analytic expression for the Glauber amplitude for the electron-polar molecule scattering is available,[13] it would be worthwhile to calculate the Glauber cross sections to investigate the validity of the Born approximation.

ACKNOWLEDGMENTS

One of the authors (T.S.) would like to express his thanks to Dr. K. Harada and Dr. S. Igarasi for their encouragement during this work.

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