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Improved impulse approximation for ionization collisions between atoms

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By taking as an example ionization collisions between atoms with simultaneous excitation of one of the atoms, a mutual relation between the impulse and the semi-quantum-mechanical approximation is made clear in the case in which the electron-atom scattering amplitude is a function only of the momentum transfer. An improved impulse approximation is proposed, which employs the smallest number of assumptions among the various formulas and has an advantage of practical usefulness. It is shown that the formula can be simplified to a single integral if an average of the cross section is taken with respect to the initial azimuthal quantum number of an atom to be ionized.

I. INTRODUCTION

Ionization collisions involving excited species have been the subject of recent interest. These processes between neutral atoms and/or molecules in high-energy collisions[1] have been quite successfully treated by the semi-quantum-mechanical theory or the impulse approximation.[2-5] These approximations have a great advantage. A better-than-simple perturbation approximation or a rigorous expression, if available, can be employed for the two-body (electron-atom) scattering amplitude so that the range of applicability of the approximations is greatly improved.

These approximations, on the other hand, have defects. First of all, they assume that the nucleus of an atom to be ionized does not change velocity relative to its electron before and after ionization. Besides, in some instances, application of the semi-quantum-mechanical theory may involve lengthy computing time because the integration of the differential cross section for the two-body scattering occupies the innermost position and is branched into many cases depending on the energy transferred to an atom to be ionized and the velocity of an electron to be ejected.[2,5] In the application of the processes involving highly excited states, this part of the integration becomes most cumbersome and time consuming. The impulse approximation, on the other hand, usually employs a mass-disparity approximation (mass ratio of electron and nucleus is completely neglected), even in the case of large-momentum transfer.[3,4] The practical usefulness of the impulse approximation owes very much to this disregard of mass ratio, since this enables the total scattering amplitude to be expressed as a product of an electron-atom inelastic scattering amplitude and a form factor of an atom to be ionized. The integration of the square of the form factor over the angle of electron ejection can further be simplified by using the binary-encounter approximation.[6]

As far as the authors know, there has been no discussion about the relation between the semi-quantum-mechanical and impulse approximations in spite of their apparent similarity. In this paper, by using an ionization collision between atoms as an example, the relation between the two approximations is made clear for the case when the electron-atom scattering amplitude is a function only of the momentum transfer. This corresponds to a special case of the semi-quantum-mechanical approximation discussed by Flannery, but presents an important class of problems in the atom-atom scattering processes.[2] A relation is also investigated to the Born approximation. In Sec. III, on the basis of these discussions, a new approximate formula is proposed for the ionization cross section. This assumes the smallest number of approximations among the various formulas. This is essentially equal to the semi-quantum-mechanical formula in the case mentioned above. The principal difference is the integration order. This simple difference, however, reduces the computer time greatly, and makes the formula more practically useful in the application to the ionization collision involving transitions between highly excited states. Especially in the case of the cross section averaged over azimuthal quantum numbers, the

formula is very much simplified to a single integral, and the numerical effort required is essentially the same as that for electron-atom scattering calculations. Flannery has discussed somewhat a modification of the integration order to derive Eq. (60) in Ref. 2(b); however not as fully as here, namely, put the integral over momentum transfer in the outermost position and thus reduce the computational effort required.

II. BORN, IMPULSE, AND SEMI-QUANTUM-MECHANICAL APPROXIMATIONS AND THEIR MUTUAL RELATIONS

In this section we will make clear the relations between the Born, impulse, and semi-quantum-mechanical approximations for the case when the electron-atom scattering amplitude is only a function of momentum transfer. We use as an example the following ionization collision process between atoms:

$$A+B(i)\rightarrow A'+B^{+}+e(f)\,. \tag{1}$$

For simplicity, each atom is considered to be composed of one electron and a structureless core.

The following is a summary of the notation used in this paper: M_A, M_B, m: mass of A^+, B^+, and electron, respectively;

$$\mu=(M_A+m)(M_B+m)/(M_A+M_B+2m)$$
$$\simeq \mu_{AB}=M_AM_B/(M_A+M_B);$$
$$\mu_{eA}=(M_A+m)m/(M_A+2m)\simeq m;$$
$$M_{eB}=M_B\,m/(M_B+m)\simeq m;$$
$$M=m(1+m/M_B)\simeq m;$$

$\vec{k}_i$, $\vec{k}_f$: initial and final wave vector of the relative motion between A and B, respectively; $\vec{K}=\vec{k}_i-\vec{k}_f$: momentum transfer;

$$K_{\max,\,\min}=|k_i\pm k_f|$$
$$=(2\,\mu/\hbar^2)^{1/2}\left|(\epsilon_m)^{1/2}\pm(\epsilon_{\max}-\epsilon)^{1/2}\right|;$$

Δ: internal energy difference between the initial and final state of atom A ($\Delta>0$ in the case of an excitation of atom A); ϵ: internal energy transferred to atom B; $\epsilon_m=\hbar^2(k_i)^2/2\mu$; $\epsilon_{\max}=\epsilon_m-\Delta$: maximum internal energy transfer; ϵ_B: kinetic energy of an ejected electron; $|E_B^i|$: ionization potential of atom B, $\epsilon=\epsilon_B+|E_B^i|$; $g_B^i(Q)$: radial part of the momentum (Q) wave function of the initial atom B; $\psi_A^{i,f}$, $\psi_B^{i,f}$: initial and final electronic wave functions of atoms A and B, respectively.

A. Born approximation

In the Born approximation the cross section for process (1) can be written

$$\sigma_{\text{Born}}(i\rightarrow f)=\frac{2\pi}{k_i^2}\left(\frac{2\mu e^2}{\hbar^2}\right)^2\int_{|E_B^i|}^{\epsilon_{\max}}d\epsilon\int_{K_{\min}}^{K_{\max}}dK\,\frac{1}{K^3}\left|\epsilon_A\left(\frac{M_A}{M_A+m}K\right)\right|^2\int d\Omega\left|\epsilon_B\left(\frac{M_B}{M_B+m}K\right)\right|^2, \tag{2}$$

where

$$\epsilon_\alpha(x)=\langle\psi_\alpha^f|e^{ix}|\psi_\alpha^i\rangle,\quad \alpha=A,B \tag{3}$$

and Ω is the solid angle of the ejected electron. Here the last integral over Ω can be replaced, with good accuracy, by using binary-encounter theory[6]:

$$\int d\Omega\,|\epsilon_B(x)|^2=\frac{M_{eB}}{2\hbar x}\int_{Q_0(K,\epsilon)}^{\infty}|g_B^i(Q)|^2Q\,dQ\,, \tag{4}$$

where

$$Q_0(K,\epsilon)=(m/\hbar K)\left|\epsilon-\hbar^2K^2/2M\right|\,. \tag{5}$$

Thus the total ionization cross section can finally be expressed as

$$\sigma_{\text{Born}}(i\rightarrow f)=\frac{1}{k_i^2}\frac{\pi m}{\hbar}\left(\frac{\mu}{\mu_{eA}}\right)^2\int_{|E_B^i|}^{\epsilon_{\max}}d\epsilon\int_{K_{\min}}^{K_{\max}}dK\,|f_{\text{Born}}^A(K)|^2\int_{Q_0(K,\epsilon)}^{\infty}|g_B^i(Q)|^2Q\,dQ\,, \tag{6}$$

where $f_{\text{Born}}^A(K)$ is the electron-atom A-scattering amplitude in the Born approximation, defined as

$$|f_{\text{Born}}^A(K)|^2=\frac{1}{K^4}\left(\frac{2\mu_{eA}e^2}{\hbar^2}\right)^2\left|\epsilon_A\left(\frac{M_A}{M_A+m}K\right)\right|^2\,. \tag{7}$$

B. Semi-quantum-mechanical approximation

In the semi-quantum-mechanical approximation proposed by Flannery[2] the total cross section for the same process can be written as follows when the general inelastic electron-atom cross section reduces

to a function of the momentum transfer only:

$$\sigma_{SQ}(i\to f)=\frac{1}{k_i^2}\frac{\pi M_{eB}}{\hbar}\left(\frac{\mu}{\mu_{eA}}\right)^2\int_{|E_B^i|}^{\epsilon_{\max}}d\epsilon\int_0^{\infty}|g_B^i(Q)|^2\,Q\,dQ\int_{p_-}^{p_+}|f^A(K)|^2\,dK\,, \tag{8}$$

where $f^A(K)$ is the electron-atom scattering amplitude (can be an exact one), and

$$p_-=\max(p_u^-,p_v^-),\quad p_+=\min(p_u^+,p_v^+)\,, \tag{9}$$

where

$$p_v^{+(-)}=K_{\max}(K_{\min}),\quad p_u^{\pm}=\frac{M}{\hbar}\left\{\left[\left(\frac{Q}{M_{eB}}\right)^2+\frac{2\epsilon}{M}\right]^{1/2}\pm\frac{Q}{M_{eB}}\right\}. \tag{10}$$

The upper (p_+) and lower (p_-) limit of the integration over K are dependent on the values of ϵ and Q. The (Q,ϵ) diagram defining these is shown in Fig. 1 of Ref. 5.[7]

C. Impulse approximation

An exact scattering amplitude for process (1) is given by

$$F(i\to f)=-\frac{\mu e^2}{2\pi\hbar^2}\int\psi_A^{f*}(\vec{r}_{1A})\,\psi_B^{f*}(\vec{r}_{2B})e^{-i\vec{k}_f\cdot\vec{\rho}}\frac{1}{r_{12}}\Psi_{\vec{k}_i}^{-}(\vec{r}_{1A},\vec{r}_{2B},\vec{\rho})\,d\vec{r}_{1A}\,d\vec{r}_{2B}\,d\vec{\rho}\,. \tag{11}$$

The coordinate system used here is defined in Fig. 1. Equation (11) can be rewritten

$$\begin{aligned}F(i\to f)=-\frac{1}{(2\pi)^4}\frac{\mu e^2}{\hbar^2}\int\psi_A^{f*}(\vec{r}_{1A})\,g_B^{f*}(\vec{q}_f)\,e^{-i\vec{q}_f\cdot\vec{r}_{2B}}\\ \times\exp\left(-i\frac{M_B}{M_B+m}\vec{k}_f\cdot\vec{r}_{2B}+i\vec{k}_f\cdot\vec{\rho}_A\right)\frac{1}{|[-M_A/(M_A+m)]\vec{r}_{1A}+\vec{\rho}_A|}\,g_B^i(\vec{q}_i)\\ \times\Phi_{\vec{k}_i}^{-}(\vec{q}_i,\vec{r}_{1A},\vec{r}_{2B},\vec{\rho}_A)\,d\vec{r}_{1A}\,d\vec{r}_{2B}\,d\vec{\rho}_A\,d\vec{q}_i\,d\vec{q}_f\,.\end{aligned} \tag{12}$$

Here we have used momentum representations of wave functions defined as

$$\psi_B^f(\vec{r}_{2B})=(2\pi)^{-3/2}\int g_B^f(\vec{q}_f)\,e^{i\vec{q}_f\cdot\vec{r}_{2B}}\,d\vec{q}_f$$

and

$$\Phi_{\vec{k}_i}^{-}(\vec{r}_{1A},\vec{r}_{2B},\vec{\rho}_A)=(2\pi)^{-3/2}\int g_B^i(\vec{q}_i)\Phi_{\vec{k}_i}^{-}(\vec{q}_i,\vec{r}_{1A},\vec{r}_{2B},\vec{\rho}_A)d\vec{q}_i\,. \tag{13}$$

Assuming a free relative motion between B^+ and the rest of the system, we can employ the following approximation for $\Phi_{\vec{k}_i}^{-}$:

$$\Phi_{\vec{k}_i}^{-}(\vec{q}_i,\vec{r}_{1A},\vec{r}_{2B},\vec{\rho}_A)=\exp\left[i\left(\vec{q}_i+\frac{M_B}{M_B+m}\vec{k}_i\right)\cdot\vec{r}_{GB}\right]\phi(\vec{k}_i,\vec{q}_i,\vec{r}_{1A},\vec{\rho}_A)\,. \tag{14}$$

This is one of the most essential approximations used in the impulse theory.[3] Substituting Eq. (14) into Eq. (12), and using a mass-disparity approximation (m/M_A and $m/M_B=0$), we obtain

$$F_{\mathrm{imp}}(i\to f)=(\mu_{AB}/m)f^A(K)\,\epsilon_B(K)\,, \tag{15}$$

where $f^A(K)$ is the electron-atom A-scattering amplitude defined as

$$f^A(K)=-\frac{\mu_{eA}e^2}{2\pi\hbar^2}\int\psi_A^{f*}(\vec{r}_{1A})\,e^{-i\vec{q}\cdot\vec{\rho}_A}\frac{1}{r_{12}}\phi(\vec{k}_i,\vec{q}_i,\vec{r}_{1A},\vec{\rho}_A)\,d\vec{r}_{1A}\,d\vec{\rho}_A\,. \tag{16}$$

The total ionization cross section can be expressed as

$$\sigma_{\mathrm{imp}}(i\to f)=\frac{2\pi}{k_i^2}\left(\frac{\mu_{AB}}{m}\right)^2\int_{|E_B^i|}^{\epsilon'_{\max}}d\epsilon\int_{K'_{\min}}^{K'_{\max}}dK\,|f^A(K)|^2K\int d\Omega\,|\epsilon_B(K)|^2\,, \tag{17}$$

where prime means that the mass-disparity approximation is used in the corresponding unprimed quantities. Using the binary-encounter theory (4), we have finally

$$\sigma_{\mathrm{imp}}(i\to f)=\frac{1}{k_i^2}\frac{\pi}{\hbar}\frac{\mu_{AB}^2}{m}\int_{|E_B^i|}^{\epsilon'_{\max}}d\epsilon\int_{K'_{\min}}^{K'_{\max}}dK\,|f^A(K)|^2\int_{Q_0^*(K,\epsilon)}^{\infty}dQ\,|g_B^i(Q)|^2Q\,. \tag{18}$$

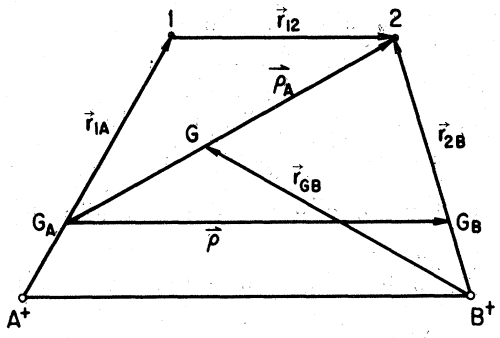


FIG. 1. Coordinate system used in the derivation of the impulse approximation. G_A, G_B, and G are the center of masses of the A^+-1, B^+-2, and A^+-1-2 system, respectively.

D. Mutual relations

Here we investigate the mutual relations of the three approximate formulas (6), (8), and (18). It is well known and obvious that Eqs. (6) and (8) coincide if we use the mass-disparity approximation in Eq. (6) and replace $f^A(K)$ by $f^A_{\text{Born}}(K)$ in Eq. (8). Except for the apparent differences in the mass factors and the approximation for $f^A(K)$, the main difference between the Born or impulse approximation and the semi-quantum-mechanical formula consists in the integration ordering. By interchanging the order of integrations, we will show here the essential equivalence of the Born approximation with the semi-quantum-mechanical formula. It is shown that the only difference between the two is the Born approximation for $f^A(K)$ used in Eq. (6) and the neglect of a certain mass factor in Eq. (8).

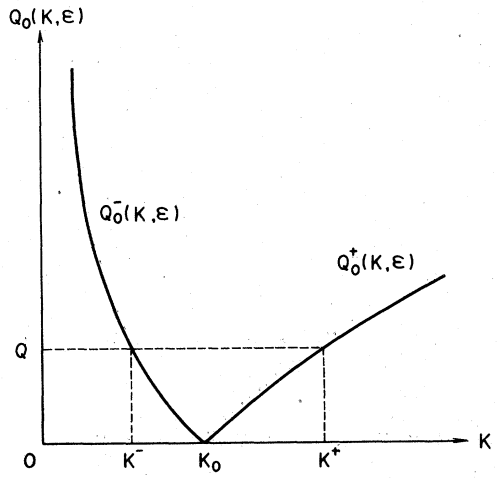


FIG. 2. Lower limit $Q_0(K,\epsilon)$ of the integral over Q in Eq. (6) as a function of K. $Q_0(K,\epsilon)=(m/\hbar)|\epsilon/K-\hbar^2K/2M|$.

The lower limit $Q_0(K,\epsilon)$ of the integral over Q is given in Fig. 2 as a function of K. It easily can be shown that

$$K_{\max}>K_0 \quad \text{for } 0<\epsilon<\epsilon_{\max}, \tag{19}$$

$$K_{\min}>K_0 \quad \text{for } 0<\epsilon<\epsilon_b \text{ or } \epsilon_d<\epsilon<\epsilon_{\max}, \tag{20}$$

and

$$K_{\min}<K_0 \quad \text{for } \epsilon_b<\epsilon<\epsilon_d,$$

where

$$(\epsilon_{b,d})^{1/2}=\frac{(\epsilon_m M/\mu)^{1/2}\mp[(1+M/\mu)\epsilon_{\max}-\epsilon_m]^{1/2}}{1+M/\mu} \tag{21}$$

and

$$K_0=(2M\epsilon/\hbar^2)^{1/2}.$$

Thus the following two cases should be considered.

(i) $0<\epsilon<\epsilon_b$ or $\epsilon_d<\epsilon<\epsilon_{\max}$. In this case we have

$$\int_{K_{\min}}^{K_{\max}}dK\int_{Q_0(K,\epsilon)}^{\infty}dQ=\int_{Q_0^{\min}}^{Q_0^{\max}}dQ\int_{K_{\min}}^{K^+(Q,\epsilon)}dK+\int_{Q_0^{\max}}^{\infty}dQ\int_{K_{\min}}^{K_{\max}}dK, \tag{22}$$

where

$$Q_0^{\min}=\frac{m}{\hbar K_{\min}}\left|\frac{\hbar^2K_{\min}^2}{2M}-\epsilon\right|, \tag{23}$$

$$Q_0^{\max}=\frac{m}{\hbar K_{\max}}\left(\frac{\hbar^2K_{\max}^2}{2M}-\epsilon\right), \tag{24}$$

and $K^+(Q,\epsilon)$ is an inverse function of $Q_0^+(K,\epsilon)$ (Fig. 2) given as

$$K^+(Q,\epsilon)=\frac{M}{\hbar}\left\{\frac{Q}{M_{eB}}+\left[\left(\frac{Q}{M_{eB}}\right)^2+\frac{2\epsilon}{M}\left(\frac{M_B+m}{M_B}\right)^2\right]^{1/2}\right\}. \tag{25}$$

(ii) $\epsilon_b<\epsilon<\epsilon_d$. In this case we have always $Q_0^{\max}>Q_0^{\min}$ and

$$\int_{K_{\min}}^{K_{\max}}dK\int_{Q_0(K,\epsilon)}^{\infty}dQ=\int_0^{Q_0^{\min}}dQ\int_{K^-(Q,\epsilon)}^{K^+(Q,\epsilon)}dK+\int_{Q_0^{\min}}^{Q_0^{\max}}dQ\int_{K_{\min}}^{K^+(Q,\epsilon)}dK+\int_{Q_0^{\max}}^{\infty}dQ\int_{K_{\min}}^{K_{\max}}dK, \tag{26}$$

where

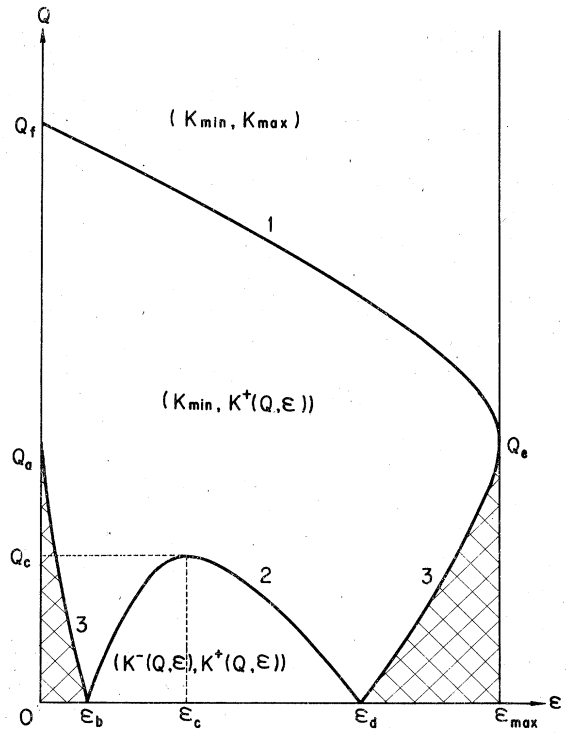


FIG. 3. (Q, ϵ) diagram defining the range of the integration over K. Shaded region is forbidden.

$$K^-(Q,\epsilon) = \frac{M}{\hbar}\left\{-\frac{Q}{M_{eB}} + \left[\left(\frac{Q}{M_{eB}}\right)^2 + \frac{2\epsilon}{M}\left(\frac{M_B+m}{M_B}\right)^2\right]^{1/2}\right\}. \tag{27}$$

From the above equations we can obtain the (Q,ϵ) diagram defining the range of the integration over K as is shown in Fig. 3. The integration range of K is shown in brackets in each region. Curves 1, 2, and 3, and the coordinates of the various points in Fig. 3 are given as follows:

curve 1:

$$Q = Q_0^{\max} \text{ [Eq. (24)]};$$

curve 2:

$$Q = Q_0^{\min} \text{ [Eq. (23)] for } \epsilon > \frac{\hbar^2}{2M} K_{\min}^2; \tag{28}$$

curve 3:

$$Q = Q_0^{\min} \text{ [Eq. (23)] for } \epsilon < \frac{\hbar^2}{2M} K_{\min}^2;$$

$$\begin{aligned} Q_a &= (\tfrac{1}{2}\mu)^{1/2}(m/M)[(\epsilon_m)^{1/2} - (\epsilon_{max})^{1/2}], \\ Q_c &= (2/\mu)^{1/2} m\{(\epsilon_m)^{1/2} - [(1+\mu/M)\Delta]^{1/2}\}, \\ Q_e &= [m/(2\mu)^{1/2}](\epsilon_m)^{-1/2}[(\mu/M)\epsilon_m - \epsilon_{max}], \\ Q_f &= (\tfrac{1}{2}\mu)^{1/2}(m/M)[(\epsilon_m)^{1/2} + (\epsilon_{max})^{1/2}], \\ \epsilon_c &= \frac{-(2+M/\mu)\Delta}{1+\mu/M} + 2\left(\frac{\epsilon_m \Delta}{1+\mu/M}\right)^{1/2}. \end{aligned} \tag{29}$$

As is seen easily from Fig. 3 and Eqs. (28) and (29), the integration range of K and Q in the Born approximation (6) coincides with that of the semi-quantum-mechanical approximation (8), which is given in Fig. 1 and Eqs. (6) of Ref. 5. The only difference is that a mass factor $(M_B+m)/M_B$ is missing in the semi-quantum-mechanical approximation. This discrepancy simply comes from the fact that the semi-quantum-mechanical theory assumes that the nucleus of an atom to be ionized does not change its velocity before and after the transition. The relation between the impulse and semi-quantum-mechanical approximations is now obvious. That is, both coincide with each other if we neglect mass ratios m/M_A and m/M_B everywhere in the derivation.

III. IMPROVED IMPULSE APPROXIMATION

From the discussions in Sec. II we propose here the following cross-section formula of practical usefulness which adopts the good parts of each approximate formula:

$$\sigma_{\text{imp imp}}(i\to f) = \frac{1}{k_i^2}\frac{\pi m}{\hbar}\left(\frac{\mu}{\mu_{eA}}\right)^2 \int_{|E_B^i|}^{\epsilon_{\max}} d\epsilon \int_{K_{\min}}^{K_{\max}} dK\, |f^A(K)|^2 \int_{Q_0(K,\epsilon)}^{\infty} dQ\, |g_B^i(Q)|^2 Q\,. \tag{30}$$

This, like the Born formula, does not use any mass-disparity approximation, and, like the semi-quantum-mechanical and impulse formulas, includes the electron-atom scattering amplitude $f^A(K)$ which can be an exact one. Finally, as in the Born and impulse formulas, the most cumbersome part (integration over K) is not in the inconvenient innermost place. It is better to change the order of the integrations over ϵ and K, considering the fact that the integration over K is the most time consuming and cumbersome. This results in

$$\sigma_{\text{imp imp}}(i\to f) = \frac{1}{k_i^2}\frac{\pi m}{\hbar}\left(\frac{\mu}{\mu_{eA}}\right)^2 \int_{K_0^{\min}}^{K_0^{\max}} dK\, |f^A(K)|^2 \int_{|E_B^i|}^{\epsilon(K)} d\epsilon \int_{Q_0(K,\epsilon)}^{\infty} dQ\, |g_B^i(Q)|^2 Q\,, \tag{31}$$

where

$$K_0^{\max,\min}=(2\mu/\hbar^2)^{1/2}[(\epsilon_m)^{1/2}\pm(\epsilon_{\max}-|E_B^i|)^{1/2}] \tag{32}$$

and

$$\epsilon(K)=-(\hbar^2/2\mu)K^2+2[(\hbar^2/2\mu)\epsilon_m]^{1/2}K-\Delta. \tag{33}$$

Equation (31) assumes the smallest number of approximations among the various formulas, besides having a great practical advantage. Hereafter we call formula (31) an improved impulse approximation. For the sake of making the formula much more practically useful, it is better to further change the order of the integrations over ϵ and Q. This reduces the expression to a double integral, since the integration over ϵ can be done analytically. For later convenience, we introduce here the following quantities:

$$\begin{aligned}
&\epsilon_0^{\pm}(Q,K)=\pm(\hbar/m)QK+(\hbar^2/2M)K^2,\\
&Q_\epsilon^+(K)=(m/\hbar)[\epsilon(K)/K-(\hbar^2/2M)K], \quad Q_\epsilon^-(K)=-Q_\epsilon^+(K),\\
&Q_B^+(K)=(m/\hbar)(|E_B^i|/K-\hbar^2K/2M), \quad Q_B^-(K)=-Q_B^+(K),\\
&K_{1,2}=\left\{\left(\frac{\hbar^2}{2\mu}\epsilon_m\right)^{1/2}\mp\left[\frac{\hbar^2}{2\mu}\epsilon_m-\frac{\hbar^2}{2}\left(\frac{1}{\mu}+\frac{1}{M}\right)\Delta\right]^{1/2}\right\}\Big/\frac{\hbar^2}{2}\left(\frac{1}{M}+\frac{1}{\mu}\right),\\
&K_{1,2}^B=\left\{\left(\frac{\hbar^2}{2\mu}\epsilon_m\right)^{1/2}\mp\left[\frac{\hbar^2}{2\mu}\epsilon_m-\frac{\hbar^2}{2}\left(\frac{1}{\mu}+\frac{2}{M}\right)(\Delta-|E_B^i|)\right]^{1/2}\right\}\Big/\frac{\hbar^2}{2}\left(\frac{1}{\mu}+\frac{2}{M}\right).
\end{aligned} \tag{34}$$

The double integral over Q and ϵ can be classified according to the following criteria:

(A) $(\hbar^2/2\mu)\epsilon_m<\frac{1}{2}\hbar^2(1/M+1/\mu)\Delta$, (A-1)

$(\hbar^2/2\mu)\epsilon_m>\frac{1}{2}\hbar^2(1/M+1/\mu)\Delta$; (A-2)

(B) $(\hbar^2/2M)K_1^2>|E_B^i|$, (B-1)

$(\hbar^2/2M)K_1^2<|E_B^i|<(\hbar^2/2M)K_2^2$, (B-2)

$(\hbar^2/2M)K_2^2<|E_B^i|$; (B-3)

(C) $K_2>k_i=[(2\mu/\hbar^2)\epsilon_m]^{1/2}=\frac{1}{2}(K_0^{\max}+K_0^{\min})$, (C-1)

$K_2<k_i$; (C-2)

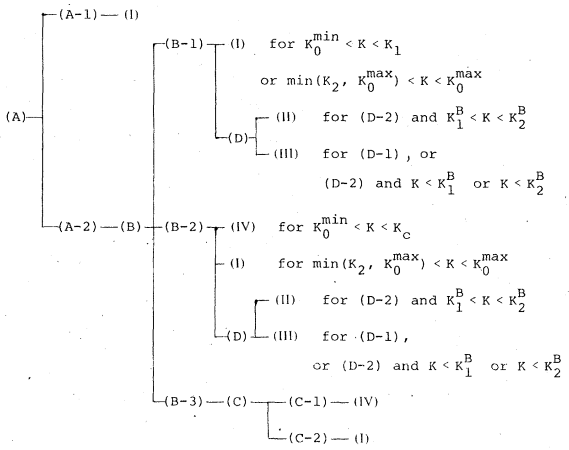
(D) $(\hbar^2/2\mu)\epsilon_m<\frac{1}{2}\hbar^2(1/\mu+2/M)(\Delta-|E_B^i|)$, (D-1)

$(\hbar^2/2\mu)\epsilon_m>\frac{1}{2}\hbar^2(1/\mu+2/M)(\Delta-|E_B^i|)$. (D-2)

The integral further branches into a few cases depending on the region of K, and then the integration over ϵ gives the following functions:

$$\begin{aligned}
&f_1(K,Q)=\epsilon(K)-\epsilon_0^-(Q,K),\\
&f_2(K)=\epsilon(K)-|E_B^i|,\\
&f_3(K,Q)=\epsilon_0^+(Q,K)-\epsilon_0^-(Q,K),\\
&f_4(K,Q)=\epsilon_0^+(Q,K)-|E_B^i|.
\end{aligned} \tag{35}$$

According to criteria (A)–(D) and the region of K, we can have the following branching diagram defining the classification of the integral over Q:



Here the Roman numerals at the end of each branching imply the following integrals, respectively:

$$\begin{aligned}
\text{(I)}\ I&\equiv\int_{|E_B^i|}^{\epsilon(K)}d\epsilon\int_{Q_0(K,\epsilon)}^{\infty}dQ\\
&=\int_{Q_\epsilon^-(K)}^{Q_B^-(K)}dQ f_1(K,Q)+\int_{Q_B^-(K)}^{\infty}dQ f_2(K),\\
\text{(II)}\ I&=\int_0^{Q_B^-(K)}dQ f_3(K,Q)+\int_{Q_B^-(K)}^{Q_\epsilon^+(K)}dQ f_4(K,Q)\\
&\quad+\int_{Q_\epsilon^+(K)}^{\infty}dQ f_2(K),
\end{aligned} \tag{36}$$

$$\text{(III)}\ I=\int_0^{Q_\epsilon^+(K)} dQ f_3(K,Q)+\int_{Q_\epsilon^+(K)}^{Q_B^-(K)} dQ f_1(K,Q) + \int_{Q_B^-(K)}^{\infty} dQ f_2(K),$$

$$\text{(IV)}\ I=\int_{Q_B^+(K)}^{Q_\epsilon^+(K)} dQ f_4(K,Q)+\int_{Q_\epsilon^+(K)}^{\infty} dQ f_2(K).$$

It may be criticized that the branching is quite complicated, and that the formula becomes unpractical. As is easily seen from criteria (A)–(D), however, we do not have to follow all the cases in the diagram for a given process (1). The number of the cases to be actually considered is at most four.

If we are interested in the ionization cross sections averaged over l_B, Eq. (31) can be simplified further to a single integral. Since we have[8]

$$\frac{1}{n_B^2}\sum_{l_B}(2l_B+1)|g_B^i(Q)|^2 = \frac{32|E_B^i|^{5/2}}{\pi(2M_{eB})^{3/2}(|E_B^i|+Q^2/2M_{eB})^4}, \quad (37)$$

we can easily obtain from Eq. (31)

$$\sigma_{\text{imp imp}}(n_Al_A\to n_A'l_A', n_B:\Delta>0)\equiv\frac{1}{n_B^2}\sum_{l_B}(2l_B+1)\sigma_{\text{imp imp}}(i\to f) = \tfrac{4}{3}|E_B^i|^{3/2}\frac{1}{k_i^2}\left(\frac{\mu}{\mu_{eA}}\right)^2\int_{K_0^{\min}}^{K_0^{\max}} dK|f^A(K)|^2K[J(y_\epsilon^+)-J(y_B)], \quad (38)$$

where

$$J(y)=\frac{y}{(y^2+|E_B^i|)^2}+\frac{3y}{2|E_B^i|(y^2+|E_B^i|)} + \frac{3}{2|E_B^i|^{3/2}}\tan^{-1}\frac{y}{|E_B^i|^{1/2}}, \quad (39)$$

$$y_\epsilon^+=\left(\frac{m^2}{2M_{eB}\hbar^2}\right)^{1/2}\left(\frac{\epsilon(K)}{K}-\frac{\hbar^2K}{2M}\right)=\frac{Q_\epsilon^+(K)}{(2M_{eB})^{1/2}},$$

and (40)

$$y_B=\left(\frac{m^2}{2M_{eB}\hbar^2}\right)^{1/2}\left(\frac{|E_B^i|}{K}-\frac{\hbar^2K}{2M}\right)=\frac{Q_B^+(K)}{(2M_{eB})^{1/2}}.$$

This is a very useful formula because the numerical effort required is essentially the same as that for the electron-atom scattering calculations. We can improve easily the cross-section estimate by employing a better-than-simple perturbation approximation for $f^A(K)$ without introducing any further complexity or numerical difficulty.

So far we have been discussing only the ionization process (1) with simultaneous excitation of atom A. Process (1) with simultaneous deexcitation of atom A ($\Delta<0$) also presents an interesting problem, since the excitation transfer is expected to enhance the process greatly. The derivation of the cross-section formula for this case is not very different from that of the excitation case. We only give here the final expression for the cross section corresponding to Eq. (38):

$$\sigma_{\text{imp imp}}(n_Al_A\to n_A'l_A', n_B:\Delta<0, |\Delta|>|E_B^i|) = \tfrac{4}{3}|E_B^i|^{3/2}\frac{1}{k_i^2}\left(\frac{\mu}{\mu_{eA}}\right)^2\left(\int_0^{K_0^{\min}} dK[J(y_\epsilon^+)-J(y_\epsilon^-)] + \int_{K_0^{\min}}^{K_0^{\max}} dK[J(y_\epsilon^+)-J(y_B)]\right)|f^A(K)|^2K, \quad (41)$$

where

$$y_\epsilon^-=\left(\frac{m^2}{2M_{eB}\hbar^2}\right)^{1/2}\left(\frac{\epsilon(-K)}{K}-\frac{\hbar^2K}{2M}\right). \quad (42)$$

In the case of $|\Delta|<|E_B^i|$ the cross-section formula coincides with Eq. (38). The detailed discussions of the process will be given in a future publication.

IV. SUMMARY

Mutual relations between the Born, impulse, and semi-quantum-mechanical approximations were made clear for the case when the electron-atom scattering amplitude depends only on the momentum transfer by taking as an example the ionization collisions between atoms with simultaneous excitation of one of the atoms. An improved impulse approximation is proposed, one which assumes the least assumptions. Except for the mass ratio factor m/M_B, this is essentially equal to the semi-quantum-mechanical formula and modifies the integration orders in that formula. This has, however, an advantage of practical usefulness in reducing the computation time. Especially formulas (38)

and (41) are very simple and useful in the applications to the processes involving highly excited states. A series of applications of the formulas derived in this paper will be made in future publications not only for the case of the simultaneous excitation, but also for the case of deexcitation of one of the atoms. Use of the Glauber approximation for the electron-atom scattering amplitude in Eq. (38) or (41) will also be interesting to test the validity of the Born approximation for the amplitude. As pointed out frequently in this paper, we have discussed only the case when the electron-atom scattering amplitude reduces to a function of the momentum transfer only. This is, of course, not the most general case, but a very important case in atom-atom scattering problems. In general, the scattering amplitude depends not only on the momentum transfer but also on the relative velocity of the two particles. A similar modification of the semi-quantum-mechanical approximation could be made together with clarification of its relation to the impulse approximation.

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[1]An energy range meant by "high" here is not a definite one, but depends on actual processes. It may be defined as the energy higher than that corresponding to the electron velocity of an excited atom to be ionized.

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