Continuum x rays produced by light-ion—atom collisions

K. Ishii
Cyclotron and Radioisotope Center, Tohoku University, Sendai 980, Japan

S. Morita
Research Center of Ion Beam Technology, Hosei University, Koganei, Tokyo 184, Japan
(Received 10 April 1984)

Radiative processes in light-ion collisions are all-inclusively formulated and discussed. Production cross sections of the radiations are calculated in terms of the second Born approximation. The cross sections of atomic bremsstrahlung production and radiative ionization have been estimated and compared with experimental results of continuum x rays from an Al target bombarded with few-MeV protons. It is found that atomic bremsstrahlung is the most predominant component in the region of x-ray energy $\hbar\omega \geq T_m$, where T_m is the maximum energy transferred from a projectile to a free electron at rest, and the disagreement between the theory and experiment, which had previously been seen in this energy region, was clearly resolved.

I. INTRODUCTION

Several kinds of processes have been studied for production of continuum x rays in ion-atom collisions; secondary-electron bremsstrahlung[1,2] (SEB) and quasi-free-electron bremsstrahlung[3] (QFEB) are characterized, respectively, by the energies T_m and T_r $(=\frac{1}{2}m_e v_p^2 = T_m/4$, where m_e is the electron mass and v_p is the projectile velocity). These radiations are remarkable for light-ion bombardments, especially SEB is a main factor for determination of the detection limit of particle-induced x-ray emission[4] (PIXE), where few-MeV protons are usually used. On the other hand, molecular-orbital x rays[5] and radiative electron capture[6] (REC) are predominant processes in cases of heavy-ion—atom collisions. However, yields and spectra of continuum x rays produced in ion-atom collisions cannot fully be understood by taking account of only these processes. Two-collision molecular-orbital x rays,[7] quasimolecular bremsstrahlung,[8] and radiative ionizations[9] have been considered to explain the continuum x-ray spectrum induced by heavy-ion impact. In a case of light-ion impact at low energies, it has been found that[2] the experimental cross sections for production of continuum x rays exceed considerably the prediction of the SEB theory, while SEB has been considered to be the most predominant process in this energy region. Recently, Amusia[10] has estimated the production cross section of bremsstrahlung coming from atomic structure of the target atom—named "atomic bremsstrahlung" (AB)—for impact with electrons, positrons, and ions. He has calculated the production cross section of AB for the x-ray energy nearly equal to the ionization potential and found that AB is a predominant process in this photon-energy region.

In this paper we discuss a system of a bare-ion projectile, a target nucleus, and target orbital electrons interacting with the radiation field and in accordance with the second Born approximation, introduce a basic formula for calculating the cross section of one-photon emission including the processes of nuclear bremsstrahlung, radiative ionization, and atomic bremsstrahlung for light-ion impact, in contrast to the former papers on ion-atom collisions, where each process has been separately treated. The cross sections calculated for AB production and radiative ionization (RI) are compared with our previous data obtained for an Al target bombarded with few-MeV protons, and good agreement is obtained. It is shown that AB is predominant even for high-energy x rays ($\hbar\omega \geq T_m$), not only for low-energy x rays as was found by Amusia.[10]

II. THEORY

We consider here a system of a bare ion and an atom, which are interacting with the radiation field. The basic formula of the Hamiltonian for such a system is given in many texts, e.g., that of Heitler.[11] In accordance with a point transformation,[12] the Hamiltonian describing the motion of the center of mass and the relative motion of the particles can be nonrelativistically expressed by

$$H_{\rm tot} = \frac{p_c^2}{2M} + H_0 + V_c + V_R + H_R \tag{1}$$

with

$$M \equiv m_T + m_p + Nm_e \;,$$

$$H_0 = \frac{(m_p+m_T)P^2}{2m_p m_T} + \frac{1}{2m_e}\sum_{i=1}^{N} P_i^2 + \frac{1}{2m_T}\left[\sum_{k=1}^{N}\vec{\mathrm{P}}_k\right]^2 + \left[\frac{1}{m_T}\sum_{k=1}^{N}\vec{\mathrm{P}}_k\right]\cdot\vec{\mathrm{P}} - \sum_{i=1}^{N}\frac{Z_T e^2}{r_i} + \sum_{i>j}^{N}\frac{e^2}{|\vec{\mathrm{r}}_i - \vec{\mathrm{r}}_j|} \;,$$

$$V_c=-\sum_{i=1}^{N}\frac{z_p e^2}{|\vec{r}_i-\vec{r}_p|}+\frac{Z_T Z_p e^2}{r_p},$$

$$V_R=-\frac{e}{c}\vec{p}\cdot\left[\frac{Z_p}{m_p}\vec{A}(\vec{r}'_p)-\frac{Z_T}{m_T}\vec{A}(\vec{r}'_T)\right]+\sum_{i=1}^{N}\frac{e}{c}\vec{p}_i\cdot\left[\vec{A}\frac{(\vec{r}'_i)}{m_e}+\frac{Z_T}{m_T}\vec{A}(\vec{r}'_T)\right]$$
$$-\frac{e}{c}\frac{\vec{P}_c}{M}\cdot\left[Z_T\vec{A}(\vec{r}'_T)+Z_p\vec{A}(\vec{r}'_p)-\sum_{i=1}^{N}\vec{A}(\vec{r}'_i)\right]+\frac{e^2Z_T^2}{2m_Tc^2}\vec{A}^2(\vec{r}'_T)$$
$$+\frac{e^2Z_p^2}{2m_pc^2}\vec{A}(\vec{r}'_p)+\sum_{i=1}^{N}\frac{e^2\vec{A}^2(\vec{r}'_i)}{2m_eC^2},$$

and H_R is the Hamiltonian of the radiation field.[11] Further,

$$\vec{A}(\vec{r}'_p)=\sqrt{4\pi c^2}\sum_{\lambda}(a_\lambda\vec{\epsilon}_\lambda e^{i\vec{K}_\lambda\cdot\vec{r}'_p}+a_\lambda^\dagger\vec{\epsilon}_\lambda e^{-i\vec{K}_\lambda\cdot\vec{r}'_p}),\tag{2}$$

where $Z_p(Z_T)$ and $m_p(m_T)$ are the atomic number and the mass of the projectile (target nucleus), respectively, N is the number of electrons, a ($a^\dagger$) is the annihilation (creation) operator of the photon with a wave vector $\vec{K}_\lambda$ and polarization $\vec{\epsilon}_\lambda$, and $\vec{P}_c$ is the momentum operator for the coordinate of the center of mass, and P and $\vec{p}_i$ are, respectively, those for $\vec{r}_p$ and $\vec{r}_i$, which are the position vectors with respect to the target nucleus. The coordinates $\vec{r}'_T$, $\vec{r}'_p$, and $\vec{r}'_i$ are position vectors of the target nucleus, the projectile, and the electrons in the frame of the center of mass, respectively, and are related to $\vec{r}_p$ and $\vec{r}_i$ by

$$\vec{r}'_T=-\frac{m_p\vec{r}_p+m_e\sum_{i=1}^{N}\vec{r}_i}{M},$$

$$\vec{r}'_p=\vec{r}_p+\vec{r}'_T \text{ and } \vec{r}'_i=\vec{r}_i+\vec{r}'_T .$$

We can easily find the eigenfunction of the Hamiltonian H_0 as expressed by

$$\Psi_i=\exp\left[i\vec{K}_i\cdot\left[\vec{r}_p-\frac{m_e}{m_T+Nm_e}\sum_{k=1}^{N}\vec{r}_k\right]\right]\psi_i(\vec{r}_1,\ldots,\vec{r}_N).\tag{3}$$

The functions Ψ_i and ψ_i satisfy the following equations:

$$H_0\Psi_i=\left[\frac{M\hbar^2}{2m_p(m_T+Nm_e)}K_i^2+\epsilon_i\right]\Psi_i$$

and

$$H_A\psi_i(\vec{r}_1,\ldots,\vec{r}_N)=\epsilon_i\psi_i(\vec{r}_1,\ldots,\vec{r}_N),$$

where H_A is the total Hamiltonian of target electrons and is expressed by

$$H_A=\frac{1}{2m_e}\sum_{i=1}^{N}\vec{P}_i^2+\frac{1}{2m_T}\left[\sum_{k=1}^{N}\vec{P}_k\right]^2+\sum_{i=1}^{N}U(\vec{r}_i)$$

with

$$U(\vec{r}_i)=-\frac{Z_Te^2}{r_i}+\tfrac{1}{2}\sum_{j(\neq i)}\frac{e^2}{|\vec{r}_i-\vec{r}_j|}.$$

If V_c and V_R are smaller than the other terms in Eq. (1), we can obtain the T-matrix element T_{fi} from the perturbation theory,[11]

$$T_{fi}=\langle\Psi_f|(V_c+V_R)|\Psi_i\rangle+\lim_{\epsilon\to 0+}\left\langle\Psi_f\left|(V_c+V_R)\frac{1}{E_i-(H_0+H_R)+i\epsilon}(V_c+V_R)\right|\Psi_i\right\rangle+\cdots,\tag{4}$$

where $|\Psi_i\rangle$ ($|\Psi_f\rangle$) and E_i (E_f) represent the initial (final) state which are the solutions for the Hamiltonian (H_0+H_R) and its energy in the center-of-mass system. Equation (4) should be valid for the case of $Z_T \gg Z_p$, that is, light-ion impact. We calculate now the matrix element T_{fi} for one-photon emission. The first term in Eq. (4) vanishes because of the conservation of energy and momentum, as we do not consider the transition of a target electron from the target frame to the projectile frame differently from the case of the REC process considered by Jakubassa and Kleber.[13] If the wavelength of the emitted photon is large enough in comparison with radii of the collision region and of the target atom, we can apply the dipole approximation[11] to the interaction V_R. From the uncertainty principle for the collision radius and for the radius of target atom, we can express the above condition for the dipole approximation by

$$1 \gg \frac{\omega}{qc}$$

and (5)

$$1 \gg \frac{\alpha\hbar\omega}{Z_T R_y} ,$$

where $\hbar\omega$ and $\hbar q$ are the energy of the emitted photon and the transfer momentum of the projectile, respectively, R_y is the Rydberg constant, and α is the fine-structure constant. From Eqs. (2)—(5), T_{fi} for one-photon emission can be calculated by

$$T_{fi}=\frac{(\vec{\epsilon}\cdot\vec{q}\,)}{\omega}\frac{4\pi}{q^2}\left[\frac{2\pi\hbar}{\omega}\right]^{1/2} Z_p e^3\left[\frac{Z_p}{m_p}-\frac{Z_T}{m_T}+\frac{N}{m_T+Nm_e}\right]\langle\psi_f\,|\,f(\vec{r}_1,\ldots,\vec{r}_N)\,|\,\psi_i\rangle+\frac{4\pi}{q^2}\left[\frac{2\pi\hbar}{\omega}\right]^{1/2}$$
$$\times Z_p e^3\left[\frac{1}{m_e}+\frac{Z_T}{m_T}\right]\lim_{\epsilon\to 0+}\left[\sum_m\frac{\langle\psi_f\,|\,f(\vec{r}_1,\ldots,\vec{r}_N)\,|\,\psi_m\rangle\left\langle\psi_m\left|\left[\vec{\epsilon}\cdot\sum_{i=1}^{N}\vec{p}_i\right]\right|\psi_i\right\rangle}{\epsilon_i-\epsilon_m-\hbar\omega+i\epsilon}\right.$$
$$\left.+\sum_m\frac{\left\langle\psi_f\left|\left[\vec{\epsilon}\cdot\sum_{i=1}^{N}\vec{p}_i\right]\right|\psi_m\right\rangle\langle\psi_m\,|\,f(\vec{r}_1,\ldots,\vec{r}_N)\,|\,\psi_i\rangle}{\epsilon_f+\hbar\omega-\epsilon_m+i\epsilon}\right] \tag{6}$$

with

$$f(\vec{r}_1,\ldots,\vec{r}_N)=\left[Z_T-\sum_{i=1}^{N}e^{i\vec{q}\cdot\vec{r}_i}\right]\exp\left[-i\frac{m_e}{m_T+Nm_e}\vec{q}\cdot\sum_{i=1}^{N}\vec{r}_i\right] . \tag{7}$$

By using the relation

$$\frac{1}{A-H_0}V=V\frac{1}{A-H_0}+\frac{1}{A-H_0}(H_0,V)\frac{1}{A-H_0} ,$$

where A is a c number and V is a function of $\vec{r}_i$, Eq. (6) can be rewritten by

$$T_{fi}=\frac{4\pi}{q^2}\left[\frac{2\pi\hbar}{\omega}\right]^{1/2}\frac{Z_p e^3}{\hbar\omega}\left\{\hbar(\vec{\epsilon}\cdot\vec{q}\,)\left[\frac{Z_p}{m_p}-\frac{Z_T}{m_T}\left[1+\frac{Nm_e}{m_T+Nm_e}\right]\right]\times\langle\psi_f\,|\,f(\vec{r}_1,\ldots,\vec{r}_N)\,|\,\psi_i\rangle\right.$$
$$-\hbar(\vec{\epsilon}\cdot\vec{q}\,)\left[\frac{1}{m_e}+\frac{Z_T}{m_T}\right]\left\langle\psi_f\left|\sum_{i=1}^{N}e^{i\vec{q}\cdot\vec{r}_i}\exp\left[-i\frac{m_e}{m_T+Nm_e}\vec{q}\cdot\sum_{i=1}^{N}\vec{r}_i\right]\right|\psi_i\right\rangle$$
$$-\left[\frac{1}{m_e}+\frac{Z_T}{m_T}\right]\lim_{\epsilon\to 0+}\left[\sum_m\frac{\langle\psi_f\,|\,f(\vec{r}_1,\ldots,\vec{r}_N)\,|\,\psi_m\rangle\left\langle\psi_m\left|\left[H_0,\left[\vec{\epsilon}\cdot\sum_{i=1}^{N}\vec{p}_i\right]\right]\right|\psi_i\right\rangle}{\epsilon_i-\epsilon_m-\hbar\omega+i\epsilon}\right.$$
$$\left.\left.+\sum_m\frac{\left\langle\psi_f\left|\left[H_0,\left[\vec{\epsilon}\cdot\sum_{i=1}^{N}\vec{p}_i\right]\right]\right|\psi_m\right\rangle\langle\psi_m\,|\,f(\vec{r}_1,\ldots,\vec{r}_N)\,|\,\psi_i\rangle}{\epsilon_f+\hbar\omega-\epsilon_m+i\epsilon}\right]\right\} . \tag{8}$$

The first term can be understood as nuclear bremsstrahlung and gives a more precise expression than that of Alder *et al.*[14] on the projectile-charge dependence, i.e., the nuclear bremsstrahlung (dipole radiation) does not completely vanish for $Z_p/m_p=Z_T/m_T$. The second and the third terms show contribution from the target electrons. When the potential $U(\vec{r}_i)$ is assumed to be constant or negligible, that is, H_0 can be approximated to a Hamiltonian of a free electron, contribution of the third term may be neglected

$$\left\{\text{because}\left[H_0,\left[\vec{\epsilon}\cdot\sum_{i=1}^{N}\vec{p}_i\right]\right]\approx 0\right\} .$$

We call this process "free electron approximation." The third term has some poles which correspond to photon emission from an excited or ionized atom and is considered to be a radiative process reflecting the atomic structure. Although the mass ratio m_e/m_T is very small, it gives a delicate effect on the energy conservation and cannot be neglected for a huge transfer momentum q [see Eq. (7)]. Under the condition

$$qa \ll \frac{m_T}{m_e}\,, \tag{9}$$

where a is the orbital radius of the target electron, Eq. (8) can be approximated by

$$T_{fi}=\frac{4\pi}{m_e q^2}\left[\frac{2\pi\hbar}{\omega}\right]^{1/2}\frac{Z_p e^3}{\omega}\left[(\vec{\epsilon}\cdot\vec{q})\left\langle\psi_f\left|\sum_{i=1}^{N}e^{i\vec{q}\cdot\vec{r}_i}\right|\psi_i\right\rangle - \lim_{\epsilon\to 0+}\left[\sum_m\frac{\left\langle\psi_f\left|\sum_{i=1}^{N}e^{i\vec{q}\cdot\vec{r}_i}\right|\psi_m\right\rangle\left\langle\psi_m\left|i\sum_{k=1}^{N}\vec{\epsilon}\cdot\vec{\nabla}_k U(\vec{r}_k)\right|\psi_i\right\rangle}{\epsilon_i-\epsilon_m-\hbar\omega+i\epsilon} + \sum_m\frac{\left\langle\psi_f\left|i\sum_{k=1}^{N}\vec{\epsilon}\cdot\vec{\nabla}_k U(\vec{r}_k)\right|\psi_m\right\rangle\left\langle\psi_m\left|\sum_{i=1}^{N}e^{i\vec{q}\cdot\vec{r}_i}\right|\psi_i\right\rangle}{\epsilon_f-\epsilon_m+\hbar\omega+i\epsilon}\right]\right]. \tag{10}$$

For the case where the final state of the target electron is the same as the initial one, Eq. (10) gives the amplitude of atomic bremsstrahlung,[10] whereas, taking an ionized state for the final state, Eq. (10) corresponds to the radiative ionization.[9] On the basis of the formula (10), we estimate the cross sections of atomic bremsstrahlung and of radiative ionizations produced by light-ion impact.

A. Atomic bremsstrahlung

Amusia[10] has calculated the cross section of the atomic-bremsstrahlung production for the case of $qa \ll 1$ and $\hbar\omega \sim I$, where I is the ionization potential. We estimate here the production cross section of the atomic bremsstrahlung on the basis of Eq. (10).

For the calculation of T_{fi}, we assume the wave function of the target electrons to be a single product of the solution[15] of H_A, where $U(\vec{r}_i)$ is replaced by the effective potential and the term

$$(1/2m_T)\left[\sum_{k=1}^{N}\vec{P}_k\right]^2$$

is neglected. Using this wave function, the matrix T_{fi} for $|\psi_i\rangle=|\psi_f\rangle$ can easily be calculated and the first term $[\equiv F_1(\vec{q})]$ in Eq. (10) is given by

$$F_1(\vec{q})=\frac{-4\pi}{m_e q^2}\left[\frac{2\pi\hbar}{\omega}\right]^{1/2}\frac{Z_p e^3}{\omega}(\vec{\epsilon}\cdot\vec{q}) \times\left[2\sum_{n,l,m}\langle\chi_{nlm}|e^{i\vec{q}\cdot\vec{r}}|\chi_{nlm}\rangle\right], \tag{11}$$

where χ_{nlm} is the hydrogenlike wave function with the principal quantum number n, azimuthal quantum number l, and magnetic quantum number m, and the factor of 2 results from the electron spin. The term $\sum_{n,l,m}\langle\chi_{nlm}|e^{i\vec{q}\cdot\vec{r}}|\chi_{nlm}\rangle$ $[\equiv S_1(q)]$ can be analytically calculated and we obtain

$$S_1(q)=\frac{16}{(Q_1+4)^2}+\frac{(2Q_2-1)(Q_2-1)}{(Q_2+1)^4}+3\frac{(1-Q_2)}{(Q_2+1)^4} +\frac{16}{27}\frac{(Q_3-\frac{4}{3})(Q_3-\frac{4}{27})(Q_3^2-8Q_3/9+\frac{16}{243})}{(Q_3+\frac{4}{9})^6} +\cdots \tag{12a}$$

with

$$Q_n+\frac{\hbar^2 q^2}{2m_e Z_n^2 R_y}\,,$$

where Z_n means the effective nuclear charge[15] for the orbital electron of the principal quantum number n which has been calculated by Slater,[16] and the summation should be taken over the number of electrons N. For a large transfer momentum, $S_1(q)$ is approximated by

$$S_1(q)\approx 16\left[\frac{2m_e R_y}{\hbar^2 q^2}\right]^2\left[Z_1^2+\frac{Z_2^2}{2^3}+\frac{Z_3^2}{3^3}+\cdots\right]. \tag{12b}$$

Since the minimum transfer momentum $q_{\min}$ (Ref. 17) is estimated to be ω/v_p, Eq. (12b) is valid for the case of $(\omega/v_p)^2(a_0/Z_1)^2[=(\hbar^2 q_{\min}^2/2m_e z_1^2 R_y)]\gg 1$.

The second term $[\equiv F_2(\vec{q})]$ in Eq. (10) for $|\psi_i\rangle=|\psi_f\rangle$ is simplified by

$$F_2(\vec{q})=\frac{4\pi}{m_e q^2}\left[\frac{2\pi\hbar}{\omega}\right]^{1/2}\frac{Z_p e^3}{\omega}$$

$$\times 2\lim_{\epsilon\to 0+}\left[\sum_{n,l,m}\sum_{n',l',m'}\frac{iZ_n e^2\langle\chi_{nlm}|e^{i\vec{q}\cdot\vec{r}}|\chi_{n'l'm'}\rangle\langle\chi_{n'l'm'}|(\vec{\epsilon}\cdot\vec{r})r^{-3}|\chi_{nlm}\rangle}{\epsilon_n-\epsilon_{n'}-\hbar\omega+i\epsilon}\right.$$

$$\left.+\sum_{n,l,m}\sum_{n',l',m'}\frac{iZ_n e^2\langle\chi_{nlm}|(\vec{\epsilon}\cdot\vec{r})r^{-3}|\chi_{n'l'm'}\rangle\langle\chi_{n'l'm'}|e^{i\vec{q}\cdot\vec{r}}|\chi_{nlm}\rangle}{\epsilon_n-\epsilon_{n'}+\hbar\omega+i\epsilon}\right], \quad (13)$$

where we assume the wave function of the intermediate state $|\chi_{n'l'm'}\rangle$ to be a solution for the same effective potential as that of $|\chi_{nlm}\rangle$. The matrix

$$\sum_m\sum_{l',m'}\langle\chi_{nlm}|e^{i\vec{q}\cdot\vec{r}}|\chi_{n'l'm'}\rangle\langle\chi_{n'l'm'}|(\vec{\epsilon}\cdot\vec{r})r^{-3}|\chi_{nlm}\rangle,$$

after some integrals over the angle, becomes

$$\sum_m\sum_{l',m'}\langle\chi_{nlm}|e^{i\vec{q}\cdot\vec{r}}|\chi_{n'l'm'}\rangle\langle\chi_{n'l'm'}|(\vec{\epsilon}\cdot\vec{r})r^{-3}|\chi_{nlm}\rangle=i\sum_{l'}\frac{(2l+1)(\vec{\epsilon}\cdot\vec{q})}{q}\left[\frac{Z_n}{a_0}\right]^2 S_{n,l;n'l'}(q) \quad (14)$$

with

$$S_{n,l;n',l'}(q)=\begin{cases}\frac{l+l'+1}{2}\left[\frac{a_0}{Z_n}\right]^2\int dr\,R_{n,l}(r)R_{n',l'}(r)\int dr\,r^2R_{n',l'}(r)j_1(qr)R_{nl}(r) & \text{for } l'=l\pm1\\ 0 \ \text{ for } l'\neq l\pm1\end{cases}$$

where $R_{n,l}(r)$ is the normalized radial wave function (see p. 15 of Ref. 15), $j_l(qr)$ is the spherical Bessel function, and a_0 is the Bohr radius. Using Eq. (14), Eq. (13) can be rewritten by

$$F_2(\vec{q})=\frac{4\pi}{m_e q^2}\left[\frac{2\pi\hbar}{\omega}\right]^{1/2}\frac{Z_p e^3}{\omega}\times 2(\vec{\epsilon}\cdot\vec{q})S_2(q), \quad (15)$$

$$S_2(q)=\sum_n\sum_l\frac{Z_n^3e^2(2l+1)}{qa_0^2}\left[\sum_{n'}\sum_{l'}\frac{2(\epsilon_{n'}-\epsilon_n)}{(\epsilon_{n'}-\epsilon_n)^2-(\hbar\omega)^2}S_{n,l;n',l'}(q)+\int dk\frac{2(k^2T_n-\epsilon_n)}{(k^2T_n-\epsilon_n)^2-(\hbar\omega)^2}S_{n,l;k,l'}(q)\right.$$

$$\left.+i\pi\frac{1}{T_n}\sum_{l'}[S_{n,l;k,l'}(q)/2k]_{k=\sqrt{(\hbar\omega+\epsilon_n)/T_n}}\right]$$

with

$$T_n=\frac{\hbar^2}{2m_e}\left[\frac{Z_n}{a_0}\right]^2. \quad (16)$$

The third term of Eq. (16) vanishes in the case of $\hbar\omega+\epsilon_n<0$. By using the integral formula[18] of hypergeometric function, we can calculate the term $S_{n,l;n'l'}(q)$ and obtain

$$S_{n,l;n'l'}(q)=f_{n,l;n',l'}(q)\frac{1}{n'^3}\left[\frac{\frac{1}{n}-\frac{1}{n'}}{\frac{1}{n}+\frac{1}{n'}}\right]^n\frac{1}{Q_n}\left[\frac{1}{n^2}-\frac{1}{n'^2}\right]^{-n+1}$$

$$\times\left[\left[\frac{1}{n}-\frac{1}{n'}\right]^2+Q_n\right]^{(n'-n)/2}\left[\left[\frac{1}{n}+\frac{1}{n'}\right]^2+Q_n\right]^{-(n'+n)/2}$$

$$\times\sin\left[n'\tan^{-1}\frac{2\sqrt{Q_n}}{n'\left[Q_n+\frac{1}{n^2}-\frac{1}{n'^2}\right]}+n\tan^{-1}\frac{2\sqrt{Q_n}}{n\left[Q_n+\frac{1}{n'^2}-\frac{1}{n^2}\right]}\right] \tag{17}$$

and

$$S_{n,l;k,l'}(q)=f_{n,l;k,l'}(q)\frac{k}{1-e^{-2\pi/k}}\left[k^2+\frac{1}{n^2}\right]^{-n+1}\frac{1}{Q_n}\exp\left[-\frac{2}{k}\tan^{-1}(nk)-\frac{1}{k}\tan^{-1}\frac{2k}{n\left[Q_n-k^2+\frac{1}{n^2}\right]}\right]$$

$$\times\left[\frac{1}{n^2}+(k-\sqrt{Q_n})^2\right]^{-n/2}\left[\frac{1}{n^2}+(k+\sqrt{Q_n})^2\right]^{-n/2}$$

$$\times\sin\left[n\tan^{-1}\frac{2\sqrt{Q_n}}{n\left[Q_n-k^2\frac{1}{n^2}\right]}+\frac{1}{2k}\ln\frac{\frac{1}{n^2}+(k+\sqrt{Q_n})^2}{\frac{1}{n^2}+(k-\sqrt{Q_n})^2}\right]. \tag{18}$$

For some values of n and l, the function $f_{n,l;n',l'}(q)$ are given by

$$\begin{aligned}
f_{1,0;n',1}(q)&=-2^4\,,\\
f_{2,0;n',1}(q)&=2\left[1-\frac{1}{n'^2}\right]\left[Q_n+\frac{1}{n'^2}-\frac{1}{4}\right],\\
f_{2,1;n',0}(q)&=\frac{1}{6}\left[3Q_n+\frac{1}{n'^2}-\frac{1}{4}\right],\\
f_{2,1;n',2}(q)&=-\frac{4}{3}\left[1-\frac{1}{n'^2}\right],\\
f_{3,0;n',1}(q)&=-\frac{16}{27}\left[1-\frac{1}{n'^2}\right]\left[\frac{7}{27}-\frac{1}{n'^2}\right]\\
&\quad\times\left[Q_n^2+2Q_n\left[\frac{1}{9}+\frac{1}{n'^2}\right]+\left[\frac{1}{9}-\frac{1}{n'^2}\right]^2-\frac{4}{27}\left[5Q_n+\frac{1}{n'^2}-\frac{1}{9}\right]\right],
\end{aligned} \tag{19}$$

and $f_{n,l;k,l'}(q)$ can be obtained by replacing $1/n'^2$ with $-k^2$ in Eq. (19).

The production cross section of atomic bremsstrahlung is expressed by

$$\frac{d\sigma^{AB}}{d\hbar\omega\, d\Omega_\omega}=\frac{1}{4\pi^2\hbar^4}\frac{(\hbar\omega)^2}{(2\pi\hbar c)^3}\frac{\hbar^2}{V_p^2}\int_{\omega/v_p}^{\infty}dq\,q\int_0^{2\pi}d\phi_q\sum_{\vec{\epsilon}}|T_{fi}|^2$$

and from Eqs. (11), (12), and (16),

$$=\frac{8a_0^2\alpha^5}{\pi\hbar\omega}Z_p^2\left[\frac{c}{v_p}\right]^2\int_{\omega/v_p}^{\infty}\frac{dq}{q}\left\{1-\left[\frac{\omega}{qv_p}\right]^2+\left[\frac{3}{2}\left[\frac{\omega}{qv_p}\right]^2-\frac{1}{2}\right]\sin^2\theta\omega\right\}|S_1(q)-S_2(q)|^2\,. \tag{20}$$

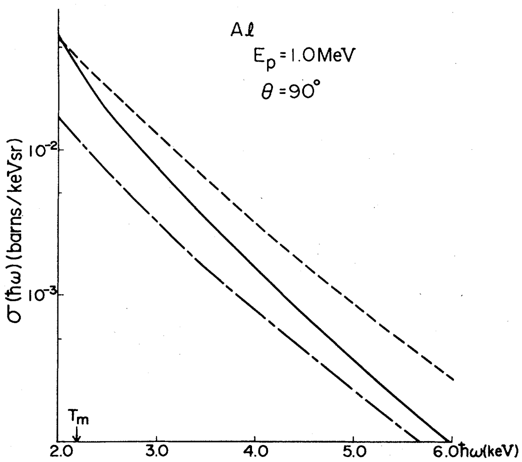

FIG. 1. Partial cross sections of atomic bremsstrahlung. The dashed, the short-dash—long-dash, and the solid curves stand for calculations of $S_1(q)$, $S_2(q)$, and both of them in Eq. (20), respectively, for the case of the Al target bombarded with 1-MeV protons.

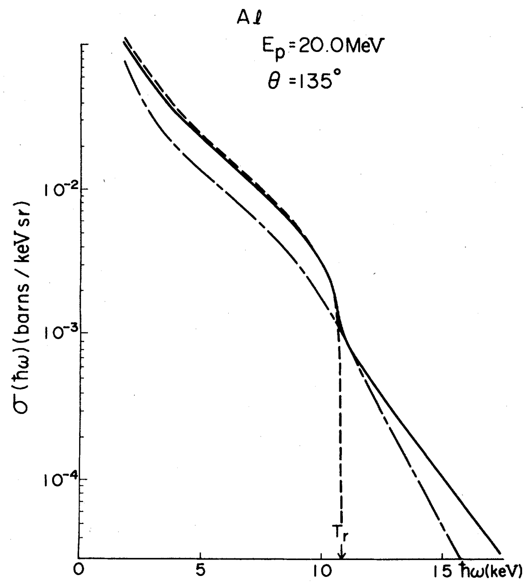

FIG. 2. Cross sections of radiative ionization for the Al target bombarded with 20-MeV protons. The solid, the dashed, and the short-dash—long-dash curves represent the calculations of, respectively, RI from Eq. (21), the simple theory[3] of QFEB, and an impulse approximation by Jakubassa and Kleber.[13]

The notation $\sum_{\vec{\epsilon}}$ means summation over the polarity of the emitted photon and θ_ω is the emission angle of the photon with respect to the direction of the incident particle. Observed values of ionization potential must be used for ϵ_n in Eq. (16).

Now we will study the contribution of $S_1(q)$ and $S_2(q)$. Figure 1 shows the production cross sections $\sigma(\hbar\omega)$ of atomic bremsstrahlung for an Al target bombarded with 1-MeV protons in the x-ray energy region $\hbar\omega=2.0$—6.0 keV. In this figure the dashed curve represents the prediction from only the term $S_1(q)$ in Eq. (20), the short-dash—long-dash curve is from $S_2(q)$, and the solid curve shows the total of Eq. (20). It is seen from Fig. 1 that $S_1(q)$ is a main component in this x-ray energy region, but the contribution of $S_2(q)$ cannot be neglected because of the interference effect between $S_1(q)$ and $S_2(q)$. For the case of atomic bremsstrahlung accompanied by a large transfer momentum such as the example shown in Fig. 1, $S_1(q)$ given by Eq. (12b) can be used for calculating the cross sections. The cross section of atomic bremsstrahlung, therefore, increases with the target atomic number Z_T under the condition of $(\omega a_0/v_p Z_T)^2 \gg 1$.

We calculate the cross section of atomic-bremsstrahlung production using the hydrogenlike wave function, which is expected to describe well the behavior of orbital electrons in a central region of the atom. As seen in Eqs. (11) and (12a), $S_1(q)$ represents the Fourier coefficient of the electron density and gives the contribution of electrons in the central region for a large q. The present calculation is therefore valid for the case of large momentum transfer $(\omega a_0/v_p Z_T)^2 \gg 1$. On the other hand, it may be necessary to calculate the cross section of atomic-bremsstrahlung production using an exact solution of H_A (e.g., Hartree-Fock wave function) for the case of small momentum transfer $(\omega Z_p/v_p Z_T)^2 \ll 1$.

B. Radiative ionization

We consider now an ionized state for the final state of the target electrons in Eq. (10). The matrix element T_{fi} for such a transition represents the ionization accompanied by radiation emission, that is, radiative ionization (RI). Jakubassa and Kleber[13] have calculated the cross section of RI for the case of radiative electron capture to a continuum state of the projectile. On the other hand, Anholt and Saylor[9] have estimated the cross section of RI for the case of $V_p \ll V_K$, where V_K is the velocity of the K electron, on the basis of binary-encounter approximation (BEA).

Calculation of the second term in Eq. (10) is very complicated for RI in comparison with the case of atomic bremsstrahlung. We calculate the cross section of RI on the basis of "the free electron approximation," in which the second term of Eq. (10) is neglected. As the calculation of $\langle \psi_f | e^{i\vec{q}\cdot\vec{r}} | \psi_i \rangle$ has been done by many workers,[17,19,20] we obtain the cross sections of RI as expressed by

$$\frac{d\sigma^{\rm RI}}{d\hbar\omega\, d\Omega_\omega} = \frac{2a_0^2\alpha^5}{\pi\hbar\omega} Z_p^2 \left[\frac{c}{v_p}\right]^2 \sum_n \int_{\theta_n/n^2}^{\infty} dW \int_{Q_{\min}}^{\infty} \frac{dQ}{Q} F_{n,W}(Q) \left[1 - \frac{Q_{\min}}{Q} + \left[\frac{3}{2}\frac{Q_{\min}}{Q} - \frac{1}{2}\right]\sin^2\theta_\omega\right] \tag{21}$$

and

$$Q_{\min}=\frac{(WZ_n^2R_y+\hbar\omega)^2}{2m_e v_p^2 Z_n^2 R_y}\ , \qquad (22)$$

where θ_n is the screening factors, and the form factors $F_{n,W}(Q)$ have been calculated in Refs. 17, 19, and 20. If the discriminant of $(WZ_n^2R_y+\hbar\omega)^2=2m_e v_p^2 Z_n^2 R_y W$ for W is positive in Eq. (22), that is, $\hbar\omega \le \frac{1}{2}m_e v_p^2$, the Bethe ridge[21] of $F_{n,W}(Q)$ is included in the integral region of W and Q, and this results in an increase of the cross section. This fact agrees with our previous result[3] of QFEB calculated from an impulse approximation. Figure 2 shows the calculations of RI cross section $\sigma(\hbar\omega)$ for the Al target bombarded with 20-MeV protons. The solid and the dashed curves represent the calculations from Eq. (21) and a simple theory[3] of QFEB, respectively. The short-dash–long-dash curve is the prediction from the impulse approximation by Jakubassa and Kleber.[13] It is seen from this figure that the present calculation for radiative ionization agrees with QFEB in the energy region of $\hbar\omega \le T_r$ and behaves like inner bremsstrahlung[9] in β decay for the $\hbar\omega \ge T_r$. Though the cross section of RI should be calculated from Eq. (10), Eq. (21) might be valid for estimation of the order of magnitude.

III. COMPARISON WITH EXPERIMENTS

Figures 3 and 4 show comparison of the present theory with our previous data[2] for the continuum x-ray production cross section $\sigma(\hbar\omega)$ from the Al target bombarded with 1- and 4-MeV protons measured at the angle of 90° with respect to the incident beam. The solid curve represents the prediction for atomic bremsstrahlung calculated from Eq. (20), the short-dash–long-dash curve is that for RI from Eq. (21), and the dashed curve is the production cross section of SEB calculated from our previous formula,[3] where the observed ionization energy is used for the binding energy of the orbital electron in contrast to the previous calculation[2] where the ideal ionization energy, which increases the cross section, has been used. The double-short-dash–long-dash curve in Fig. 4 represents the total cross section. It is seen from Figs. 3 and 4 that the experimental cross sections of continuum x-ray production agree well with the present theoretical predictions; atomic bremsstrahlung is the most predominant process in the photon-energy region of $\hbar\omega > T_m$ (see Fig. 3). On

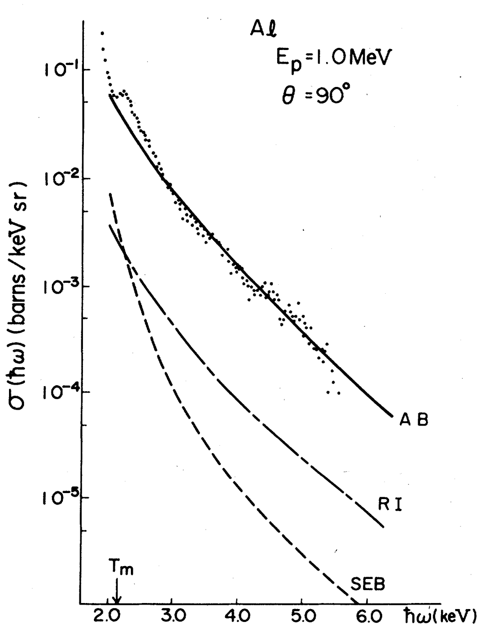

FIG. 3. Comparison between theory and experiment on the Al target bombarded with 1-MeV protons. The solid, short-dash–long-dash, and the dashed curves represent the production cross sections of AB, RI, and SEB, respectively, at the 90° emission angle. AB, RI, and SEB are estimated from Eqs. (20) and (21) and our formula previously obtained.[3] The data points are taken from Ref. 2

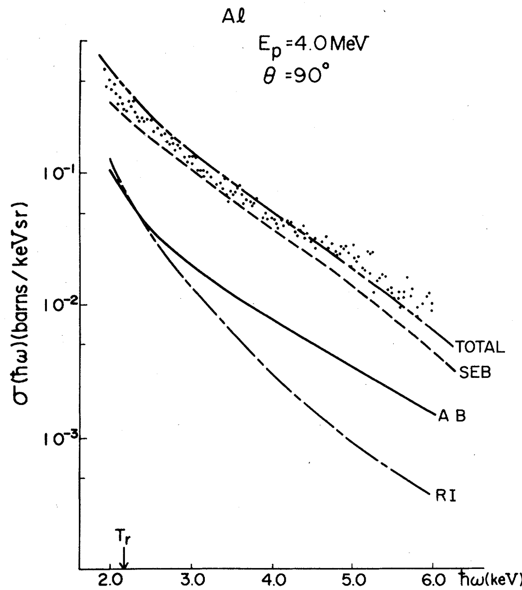

FIG. 4. Same as Fig. 3 except for 4-MeV protons.

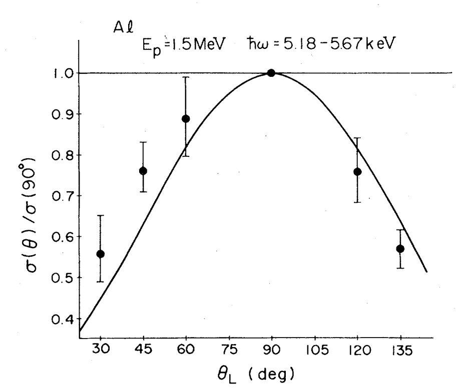

FIG. 5. Angular distribution of continuum x rays. The data points[22] are for x rays of $\hbar\omega$=5.18–5.67 keV from the Al target bombarded with 1.5-MeV protons and show the ratios of the cross section to that of the 90° emission angle. The prediction is the calculation for AB, since AB is predominant in the region of this x-ray energy.

the other hand, SEB is predominant in the region of $\hbar\omega < T_m = 4T_r$ (see Fig. 4). The angular distribution of continuum x rays, calculated from the present theory, is compared in Fig. 5 with our previous experimental result[22] obtained for x rays of $\hbar\omega = 5.18-5.69$ keV from the Al target bombarded with 1.5-MeV protons. In this figure the vertical axis represents the cross section normalized to that obtained at 90°. We find that the theory reproduces well the experimental results. The angular dependence of atomic bremsstrahlung seems to be the same as that of SEB (see Fig. 3 in Ref. 22).

IV. CONCLUSION

Starting from the total Hamiltonian for a system consisting of a bare light-ion projectile, a target nucleus, and target electrons, we obtained a formula, Eq. (8), for calculating the cross sections of radiative processes including the nuclear bremsstrahlung, atomic bremsstrahlung, and radiative ionization. It is seen easily that the nuclear bremsstrahlung can be neglected for the case of $qa \ll m_T/m_e$; this condition is satisfied in the x-ray energy region normally discussed in atomic-collision physics. By comparing the results of the calculation with our previous experiment on the Al target, it was found that atomic bremsstrahlung is the most predominant process in the x-ray energy region of $\hbar\omega > T_m$, and it was concluded that AB, SEB, and QFEB (RI) play a predominant role in the regions of $\hbar\omega > T_m$, $T_m > \hbar\omega > T_r$, and $T_r > \hbar\omega$, respectively, and these three are the main processes for continuum x-ray production in the case of light-ion—atom collisions.

ACKNOWLEDGMENTS

The authors would like to thank Dr. R. Anholt for his useful advice and discussion. They are also much indebted to Professors W. E. Meyerhof and E. Merzbacher for informative discussions in the Japan-U.S. Seminar in Hawaii in 1983.

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