PHYSICAL REVIEW A VOLUME 34, NUMBER 4 OCTOBER 1986

Continuum emission during ion-atom collisions at high projectile energies

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(Received 10 February 1986)

A general formalism to treat radiative emission of a colliding three-particle system is developed in the semiclassical approximation. The matrix element of the matter-radiation interaction is separated into three terms representing the center of mass, the intersystem bremsstrahlung, and the electron bremsstrahlung. At each step we impose the off-shell orthogonality property of the mechanical wave functions. Instead of internuclear bremsstrahlung, used so far, a more general concept of intersystem bremsstrahlung is introduced. The electron bremsstrahlung is calculated using eikonal distorted wave functions, and good agreement is found with experiment. Radiative electron excitation and deexcitation have also been calculated. The former is found to be very small, while the spectrum associated with the latter produces the continuous emission around the characteristic line, induced by the passing projectile.

I. INTRODUCTION

During ion-atom (or ion-ion) collisions continuous radiation is emitted. Several kinds of processes have been distinguished, mainly in the x-ray region. They have been generally denoted according to the model used to describe the radiative emission in a particular photon or projectile energy range. Here, we propose a simpler classification. Let us consider a single collision of a projectile P (of mass M_P and charge Z_P) with a hydrogenic atom composed of a nucleus T (M_T and Z_T), and an active electron e ($M_e=1$ and $Z_e=-1$). In accordance with the mechanical or nonradiative case, we define four radiative processes: radiative electron capture (REC), radiative ionization (RI), radiative excitation or deexcitation (REX), and radiative elastic scattering (REL). Therefore, the radiative emission process is classified in accordance with the final state of the active electron. As far as the three-particle system is concerned, any kind of radiation can be ascribed to one of these.

REC is the emission of radiation during a charge-exchange process. At high and intermediate projectile energies, REC is characterized by the presence of a peak in the x-ray region.[1–5] Its profile reflects the momentum distribution of the initial bound state. REC is quite well understood, and the theories predict photon spectra and total cross sections with an acceptable degree of agreement with experiment. REC can be seen, in the simplest form, as a binary e-P radiative recombination.

RI is a process in which the ionization of the electron is accompanied by radiative emission. Jakubassa and Kleber[6] have calculated this process with a three-particle approach, only considering the e-P continuum interaction on both the entrance and exit channels. In particular, radiative electron capture to the continuum can be considered as a part of the RI.[7] On the other hand, Anholt and Saylor[8] have estimated the RI by using the binary-encounter approximation.

This work deals mainly with REX and REL, i.e., with radiative direct processes.

In REL, the projectile transfers a part of its kinetic energy to the radiation field, while the electron ends in the same orbital. This process is here called "elastic" from the electron point of view in the sense that it ends in the same state as the initial one. But the total process is really inelastic since the projectile loses energy to the photon. This mechanism of photon emission is closely related to the so-called atomic bremsstrahlung, studied by Amusia[9] and recently developed by Ishii and Morita.[10,11]

In REX, the excitation of the electron is accompanied by the emission of light. To our knowledge, no REX cross section have ever been reported. We also calculate radiative deexcitation, which is widely known as collisional broadening, i.e., the radiative decay in the presence of a moving projectile. We show that REX can be considered as the analytical continuation to negative photon energy of the collisional broadening for the inverse process. We find that REL is orders of magnitude larger than REX at the high and intermediate projectile energies considered here.

Certainly the process is determined by the initial and final states of the electron. Such a process can be sometimes interpreted in accordance with the basis used. At low impact energy, it is convenient to use a molecular basis giving rise to a parallel classification, the so-called molecular x ray.[12] In the present work we use distorted-wave formulas to describe the mechanical wave functions, which is valid at high impact energies.

The work is organized as follows. In Sec. II we formulate a nonrelativistic semiclassical approximation for a colliding three-particle system with the continuum emission of radiation. We find that the relevant matrix element is separated into three terms with definite physical meanings, and they are calculated in Sec. III. The first term is the radiation of the center of mass and can be removed (within the dipole approximation) following the procedure of Shakeshaft and Spruch,[3] as presented in Sec. III A. In Sec. III B we find that the second matrix element represents an intersystem bremsstrahlung. In particular, when internuclear coordinates are used, it is the so-called internuclear bremsstrahlung.[13–15] The third element—by far the dominant—is due to the radiative emission of the electron in a combined field of both nuclei. This term has been calculated by using second-order Born wave functions by Amusia[9] and Ishii and Morita,[10] and it is called atomic bremsstrahlung. In Sec. III C, we calculate this matrix element using eikonal distorted-wave functions to describe the initial and final electronic states. In mechanical or nonradiative ion-atom excitations the use of these distorted-wave functions produces the so-called symmetric eikonal approximation which has proved to be a good method to deal with direct processes for high and intermediate impinging energies.[16] In Sec. IV, we present numerical results of REL and REX, and we compare them with the available experiments. Further, in the Appendix we derive from the general Eqs. (2.11)–(2.14) the expressions of REC and RI commonly found in the literature. Atomic units are used.

II. GENERAL THEORY

In the semiclassical approximation the total Hamiltonian H can be written as $H=H_m+H_r+H_{mr}$, where H_m is the mechanical Hamiltonian, i.e., the kinetic energy of the three particles plus the potentials, H_r is the radiation Hamiltonian, and H_{mr} is the matter-radiation interaction, whose expression for spontaneous emission is given by

$$\begin{aligned} H_l &= \langle 1_k \,|\, H_{mr} \,|\, 0_k \rangle \\ &= iA_0 \hat{\boldsymbol{\lambda}}_l \cdot \sum_{N=T,P,e} (Z_n/M_n)\exp(-i\mathbf{k}\cdot\mathbf{x}_n)\nabla_{\mathbf{x}_n} , \end{aligned} \tag{2.1}$$

where $A_0=(2\pi/\omega)^{1/2}$, $\hat{\boldsymbol{\lambda}}_l$ is the polarization vector versor, $\mathbf{k}$ is the photon momentum, and $\omega=kc$ is the photon energy. The coordinate $\mathbf{x}_n$ is the position of the particle n ($n=T$, P, or e) with respect to some inertial frame.

It is more convenient to introduce the relative coordinate sets which diagonalize the kinetic energy, i.e., $\{\mathbf{X},\mathbf{R}_j,\mathbf{r}_j\}$ with $j=T$, P, or N (see Fig. 1). After lengthy algebra, we find that H_l can be written as

$$H_l = iA_0\hat{\boldsymbol{\lambda}}_l \cdot \exp(-i\mathbf{k}\cdot\mathbf{X})(\beta\nabla_{\mathbf{X}}+B_j\nabla_{\mathbf{R}_j}-b_j\nabla_{\mathbf{r}_j}) , \tag{2.2}$$

where $\mathbf{X}$ is the position of the center of mass and $j=T$, P, or N represents any of the relative coordinate sets. β, which is common to any set, is given by

$$\beta=\frac{Z_T E_T + Z_P E_P - E_e}{M_T+M_P+1} , \tag{2.3}$$

where

$$E_n = \exp[-i\mathbf{k}\cdot(\mathbf{x}_n-\mathbf{X})] . \tag{2.4}$$

We find the factors of Eq. (2.2) are given by

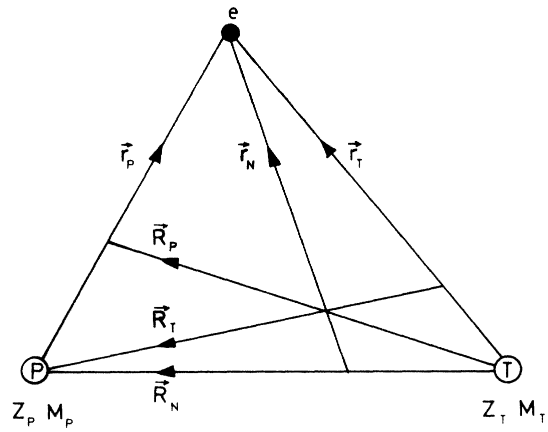

FIG. 1. Coordinate systems.

$$\begin{aligned} B_T &= \frac{Z_P E_P}{M_P} - \frac{Z_T E_T - E_e}{M_T+1} , \\ b_T &= E_e + \frac{Z_T E_T}{M_T} \end{aligned} \tag{2.5}$$

for direct coordinates, i.e., $j=T$;

$$\begin{aligned} B_P &= -\frac{Z_T E_T}{M_T} + \frac{Z_P E_P - E_e}{M_P+1} , \\ b_P &= E_e + \frac{Z_P E_P}{M_P} \end{aligned} \tag{2.6}$$

for reactive coordinates, i.e., $j=P$; and

$$\begin{aligned} B_N &= \frac{Z_P E_P}{M_P} - \frac{Z_T E_T}{M_T} , \\ b_N &= E_e + \frac{Z_P E_P + Z_T E_T}{M_P+M_T} \end{aligned} \tag{2.7}$$

for internuclear coordinates, i.e., $j=N$.

Equation (2.2) provides all the possible radiation that the three-particle system can spontaneously emit within the semiclassical approximation, *including retardation* effects contained in the factors E_n. If these effects are to be considered, then these factors must be taken into account in the corresponding integrations. In this case, it is convenient to transform the term $(\mathbf{x}_n-\mathbf{X})$ in Eq. (2.4) to the chosen coordinate system, i.e.,

$$\mathbf{x}_n - \mathbf{X} = Y_{nj}\mathbf{R}_j + y_{nj}\mathbf{r}_j , \tag{2.8}$$

where as usual $n=T$, P, or e indicates the particle and $j=T$, P, or N denotes the coordinate system. In particular we find

$$\begin{aligned} & Y_{eT} = Y_{TT} = -M_P/(M_T+M_P+1) , \\ & y_{PT}=0, \;\; y_{eT}=M_T/(M_T+1) , \\ & y_{TT} = -1/(M_T+1) , \\ & Y_{PT} = (M_T+1)/(M_T+M_P+1) , \end{aligned} \tag{2.9}$$

and the remaining ones can be calculated with the usual transformation of coordinate systems.

Note that these equations are also valid for impact of light particles such as electrons or positrons.

A. The dipole approximation

Hereafter we shall use the dipole approximation which consists of considering that $\mathbf{k}\cdot(\mathbf{x}_n-\mathbf{X})\ll 1$, i.e., the limit as $k\to 0$. In this case, the factors $\beta_j\to\beta_{j0}$, $B_j\to B_{j0}$, and $b_j\to b_{j0}$, which can be obtained from Eqs. (2.3)–(2.7) by simply replacing E_n by unity. Further, for ion-atom collisions, where $M_{T,P}\gg 1$, b_{j0} are unity.

In first perturbative order, the matrix element reads

$$\langle H_l\rangle_{fi}=(2\pi)^{-3}\langle \exp(i\mathbf{U}_f\cdot\mathbf{X})\Psi_f^- \mid H_l \mid \exp(i\mathbf{U}_i\cdot\mathbf{X})\Psi_i^+\rangle\ , \tag{2.10}$$

where the plane waves represent the movement of the center of mass, $\mathbf{U}_{i,f}$ are the initial and final *total* momenta of the three particles, and Ψ_i^+ and Ψ_f^- are the *exact* solution of the mechanical Hamiltonian H_m without the kinetic energy of the center of mass. After simple algebra we find that the matrix element can be separated into three terms with definite physical meanings:

$$\langle H_l\rangle_{fi}=\delta(\mathbf{U}_i-\mathbf{U}_f-\mathbf{k})(H_l^{\mathrm{CMB}}+H_{lj}^{\mathrm{ISB}}+H_{lj}^{\mathrm{EB}})\ , \tag{2.11}$$

where

$$H_l^{\mathrm{CMB}}=A_0\hat{\boldsymbol{\lambda}}_l\cdot\beta_0\mathbf{U}_i\langle\Psi_f^-\mid\Psi_i^+\rangle\ , \tag{2.12}$$

$$H_{lj}^{\mathrm{ISB}}=iA_0\hat{\boldsymbol{\lambda}}_l\cdot B_{j0}\langle\Psi_f^-\mid\nabla_{\mathbf{R}_j}\mid\Psi_i^+\rangle\ , \tag{2.13}$$

$$H_{lj}^{\mathrm{EB}}=iA_0\hat{\boldsymbol{\lambda}}_l\cdot b_{j0}\langle\Psi_f^-\mid\nabla_{\mathbf{r}_j}\mid\Psi_i^+\rangle\ . \tag{2.14}$$

The δ function carries on the information of the momentum conservation and can be removed in the wave-packet formulation, therefore we shall omit it. Equation (2.11) is a simple extension of Shakeshaft and Spruch's Eq. (4) (Ref. 3) to a three-particle system. As we shall see in the next section, H_l^{CMB} represents the radiation of the center of mass, H_l^{ISB} is the intersystem bremsstrahlung (ISB), and H_l^{EB} represents the electron bremsstrahlung (EB) in the field of both nuclei.

Finally, the fivefold differential cross section is given by[5]

$$\frac{d\sigma}{d\omega\, d\Omega_\omega d\Omega}=\frac{\nu_T^2\omega}{(2\pi)^4c^3}\sum_{l=1}^{2}|\langle H_l\rangle_{fi}|^2\ , \tag{2.15}$$

where ν_T is the $(T+e)-P$ reduced mass, and $d\Omega_\omega$ and $d\Omega$ are the differential solid angles of the photon and projectile, respectively.

III. CALCULATION

A. Removal of the spurious radiation of the center of mass

The exact wave functions are off-shell orthogonal, i.e., $\langle\Psi_f^-\mid\Psi_i^+\rangle=0$, and this property cancels the term H_l^{CMB}. Therefore, Galilean invariance holds, as indicated by Shakeshaft and Spruch.[3] When the proper orthogonality condition is used, there is no need to work in the center-of-mass frame. When approximate wave functions are used, the Galilean invariance may be invalidated due to spurious radiation of the center of mass. In the present work, we invoke the correct orthogonality property.

When the dipole approximation is no longer valid, retardation effects should be taken into consideration. Thus, H_l^{CMB} may account for the change-of-system emission found by Spindler *et al.*,[17] while $\delta(\mathbf{U}_i-\mathbf{U}_f-\mathbf{k})$ would produce the Doppler effect.[18]

B. Intersystem bremsstrahlung

In this section we prove that the second term H_{lj}^{ISB}, given by Eq. (2.13), is in a certain way related to the so-called internuclear bremsstrahlung. Since we shall treat direct processes, it is more convenient to work with direct coordinates.

First of all, we remove the free movement of the projectile by setting

$$\Psi_i^+=\exp(i\mathbf{K}_i\cdot\mathbf{R}_T)\phi_i^+,\quad \Psi_f^-=\exp(i\mathbf{K}_f\cdot\mathbf{R}_T)\phi_f^-\ , \tag{3.1}$$

where $\mathbf{K}_{i,f}$ are the initial and final momenta of the projectile and ϕ_i^+ and ϕ_f^- are the exact three-particle wave functions excluding the projectile kinetic. Replacing Eq. (3.1) in Eq. (2.13), we find

$$\begin{aligned}H_{lT}^{\mathrm{ISB}}&=iA_0\hat{\boldsymbol{\lambda}}_l\cdot B_{T0}[i\mathbf{K}_i\langle\Psi_f^-\mid\Psi_i^+\rangle\\&\qquad+\langle\phi_f^-\mid\exp(i\mathbf{P}\cdot\mathbf{R}_T)\nabla_{\mathbf{R}_T}\mid\phi_i^+\rangle]\\&=iA_0\hat{\boldsymbol{\lambda}}_l\cdot B_{T0}\langle\phi_f^-\mid\exp(i\mathbf{P}\cdot\mathbf{R}_T)\nabla_{\mathbf{R}_T}\mid\phi_i^+\rangle\ ,\end{aligned} \tag{3.2}$$

where, once again, we have used the off-shell orthogonality of the wave functions, and $\mathbf{P}=\mathbf{K}_i-\mathbf{K}_f$ is the momentum transfer vector. B_{T0} is of the order of $M_{T,P}^{-1}$, and the matrix element essentially involves electronic quantities and so cannot be very large. Therefore, H_{lT}^{ISB} is negligible.

The calculation of H_{lT}^{ISB} requires the exact three-particle wave functions which are unknown. In order to estimate H_{lt}^{ISB}, we resort to first-order Born wave functions with the correct Coulomb behavior at large internuclear distances (sometimes this approximation is called the Coulomb-Born approximation). The wave functions are given by

$$\begin{aligned}\Psi_i^+&\cong\exp(i\mathbf{K}_i\cdot\mathbf{R}_T)D^+(Z_N,\nu_T,\mathbf{K}_i;\mathbf{R}_T)\varphi_i(\mathbf{r}_T)\ ,\\ \Psi_f^-&\cong\exp(i\mathbf{K}_f\cdot\mathbf{R}_T)D^-(Z_N,\nu_T,\mathbf{K}_f;\mathbf{R}_T)\varphi_f(\mathbf{r}_T)\ ,\end{aligned} \tag{3.3}$$

where $\varphi_{i,f}(\mathbf{r}_T)$ are the initial and final electronic states,

$$\begin{aligned}D^\pm(Z,\nu,\mathbf{K};\mathbf{r})&=\exp(a\pi/2)\Gamma(1\mp ia)\\&\quad\times{}_1F_1(\pm ia,1,\pm iKr-i\mathbf{K}\cdot\mathbf{r})\ ,\end{aligned} \tag{3.4}$$

$a=\nu Z/K=Z/v$, where $\mathbf{v}=\mathbf{K}/\nu$ is the ion velocity, and Z_N is the product of Coulomb charges of the colliding systems, i.e., $Z_N=Z_P(Z_T-1)$.[19]

This approximation has two advantages: first, the wave functions are off-shell orthogonal—as the exact ones are—and second, the movement of the projectile is decoupled from the electron excitation. Using the wave functions given by Eq. (3.3) the matrix element H_{lT}^{ISB} reads

$$H_{IT}^{\rm ISB}=iA_0\hat{\lambda}_l\cdot B_{T0}\langle\varphi_f\,|\,\varphi_i\rangle \times\int d\mathbf{R}\exp(i\mathbf{P}\cdot\mathbf{R})D^{-*}(Z_N,\nu_T,\mathbf{K}_f;\mathbf{R}) \times\nabla_{\mathbf{R}}D^{+}(Z_N,\nu_T,\mathbf{K}_i;\mathbf{R})\ . \tag{3.5}$$

The overlap between the initial and final atomic orbitals clearly indicates that $H_{IT}^{\rm ISB}$ is different from zero in the elastic channel. So, ISB will contribute to REL but *not* to REX. In other words, the projectile radiates in the presence of the atom target as a whole, while the electron is a frozen observer.

The integral in Eq. (3.5) is a Nordsieck's integral.[20] Closed forms for this kind of integral can be obtained in terms of the hypergeometric function ${}_2F_1$. Simpler forms were developed by Bethe[21] retaining the first order in Z_N.[22] Following the Bethe's technique, and integrating on the projectile angular distribution, the triple differential cross section, given by $H_{IT}^{\rm ISB}$ alone, is found to be

$$\frac{d\sigma_T^{\rm ISB}}{d\omega\, d\Omega_\omega}=\frac{Z_N^2B_{T0}^2}{c^3v^2\omega\pi}\left[\sin^2\theta_\omega+(1+\cos^2\theta_\omega)\times\left[\ln\frac{2K_i}{\mathbf{P}\cdot\hat{\mathbf{v}}}-\frac{1}{2}\right]\right]\ , \tag{3.6}$$

where θ_ω is the angle of the emitted photon with respect to the projectile incident direction. The integration on the photon angular distribution gives the single differential cross section:

$$\frac{d\sigma_T^{\rm ISB}}{d\omega}=\frac{16Z_N^2B_{T0}^2}{3c^3v^2\omega}\ln\frac{2K_i}{\mathbf{P}\cdot\hat{\mathbf{v}}}\ . \tag{3.7}$$

Some points should be remarked upon in relation to Eq. (3.7). First, ISB cross sections are of the order $M_{T,P}^{-2}$, and so very small in comparison with EB to be calculated in the next section. As noted by Amusia[9] there is a term $M_{T,P}^{-1}$ coming from the interference between ISB and EB amplitudes. At very high photon energy, say in the very hard x-ray region, the EB cross section falls out faster than the ISB, and then the latter becomes dominant.[14,15] In this photon energy the dipole approximation is no longer valid.

Equation (3.7) is similar, but not equal, to the internuclear bremsstrahlung of Alder *et al.*,[13] later considered by Folkmann.[14,15] The difference lies in the fact that the factor B_{T0} contains (Z_T-1) instead of Z_T. This is so because we have used the set of coordinates $\{\mathbf{R}_T,\mathbf{r}_T\}$ as given by Eq. (2.5). We are of course allowed to use the reactive coordinates, i.e., $j=P$, or the internucleus ones, i.e., $j=N$, where the corresponding factors are given by Eqs. (2.6) and (2.7), respectively. In those cases, we obtain expressions similar to Eq. (3.7) with B_{P0} or B_{N0} instead of B_{T0}. The factor B_{N0} is $(Z_T/M_T-Z_P/M_P)$ which is the multiplying factor of the Alder's equation.

Then the ISB term depends on the coordinates used, but the EB term, i.e., the gradient on the electronic coordinate, must also depend on the coordinates accordingly, so that the sum is *independent* of the coordinate system used. The EB term is to be calculated with $b_{j0}\nabla_{\mathbf{r}_j}$ $(j=T,P,N)$ depending on the coordinates chosen. Since the ISB is very small, the gradient on any of the electronic coordinates should be the same (to order $M_{T,P}^{-1}$).

When approximate nonorthogonal wave functions are used, the EB does depend on the electronic coordinate chosen. To illustrate one example: Briggs and Dettmann[2] were the first to note that the REC matrix element calculated with $b_{T0}\nabla_{\mathbf{r}_T}$ is different than the one calculated with $b_{P0}\nabla_{\mathbf{r}_P}$. This is a consequence of the absence of off-shell orthogonality of the first-order Born wave functions used in that work, as later indicated by Shakeshaft and Spruch.[3]

It can be easily shown that ISB is small also for REC. Nonorthogonal—and so incorrect—wave functions allow for nonreal radiation emission. The magnitude of this spurious radiation is comparable with EB because the factor K_iB_{T0} in Eq. (3.2) is of the order of unity. Further, if this term were incorrectly kept the result would strongly depend on the target nuclear mass, giving rise to a false isotopic effect.

C. Electron bremsstrahlung

Here we calculate the third term $H_{IT}^{\rm EB}$ of Eq. (2.11) which is by far the more relevant. To begin with we shall apply, once more, the first Born approximation. Using the wave functions given by Eq. (3.3), the matrix element $H_{IT}^{\rm EB}$ reads

$$H_{IT}^{\rm EB}=(2\pi)^3\delta(\mathbf{K}_i-\mathbf{K}_f)\times\left[-iA_0\hat{\lambda}_l\cdot\int d\mathbf{r}\,\varphi_f^*(\mathbf{r})\nabla_{\mathbf{r}}\varphi_i(\mathbf{r})\right]\ . \tag{3.8}$$

This expression presents two independent features. The $\delta(\mathbf{K}_i-\mathbf{K}_f)$ means that the projectile passes through without interacting, i.e., a simple observer, while the electron interacts with the radiation field in the presence only of the target nucleus. Light is not emitted for an initial ground state, and an excited state decays, emitting the characteristic line, according to the selection rules.

Therefore, the first order is of no help to describe the continuum radiation for REL or REX. This is so because for direct processes the nondistorted wave functions have no information about the projectile potential. We have to recall that in REC, the first Born approximation describes the continuum radiation emitted, and it can be used not only to calculate total cross sections but also photon and angular distributions.[5] The difference lies in the fact that in electron capture the nondistorted wave functions implicitly contain the information of both potentials in the initial and final bound states.

From the previous discussion, it becomes clear that the electronic states should include the distortion of the electron by the projectile. Ishii and Morita,[10] following Amusia,[9] have used the second-order Born approximation. Here we shall use a distorted-wave method recently applied in atomic collision theory, the so-called symmetric eikonal method. It makes use of the following distorted-wave functions:

$$\begin{aligned}\Psi_i^+&\cong\exp(i\mathbf{K}_i\cdot\mathbf{R}_T)\varphi_i(\mathbf{r}_T)E^+(Z_P,-\mathbf{v};\mathbf{r}_P)\ ,\\ \Psi_f^-&\cong\exp(i\mathbf{K}_f\cdot\mathbf{R}_T)\varphi_f(\mathbf{r}_T)E^-(Z_P,-\mathbf{v};\mathbf{r}_P)\ ,\end{aligned} \tag{3.9}$$

where

$$E^{\pm}(Z,v;r)=\exp[\mp i(Z/v)\ln(vr\mp\mathbf{v}\cdot\mathbf{r})] \tag{3.10}$$

which can be related to the $D^{\pm}$ factor as

$$E^{\pm}(Z,v;r)=\lim_{m\to\infty}\exp[\pm i(Z/v)\ln m]D^{\pm}(Z,m,\mathbf{v};\mathbf{r}) . \tag{3.11}$$

In a recent work it has been shown that the symmetrical eikonal is one of the best methods to describe the nonradiative or mechanical excitation.[16]

Using Eq. (3.9) and neglecting terms of order $M_{T,P}^{-1}$, the EB is given by

$$H_{IT}^{\mathrm{EB}}=-iA_0\hat{\boldsymbol{\lambda}}_l\cdot(\mathbf{Q}_P+\mathbf{Q}_T) , \tag{3.12}$$

where

$$\mathbf{Q}_P=\int d\mathbf{r}_T\varphi_f^*(\mathbf{r}_T)\exp(i\mathbf{P}\cdot\mathbf{r}_T)\varphi_i(\mathbf{r}_T) \times\int d\mathbf{r}_P\exp(-i\mathbf{P}\cdot\mathbf{r}_P)E^{-*}(Z_P,-\mathbf{v};\mathbf{r}_P) \times\nabla_{\mathbf{r}_P}E^{+}(Z_P,-\mathbf{v};\mathbf{r}_P) \tag{3.13}$$

and

$$\mathbf{Q}_T=\int d\mathbf{r}_T\varphi_f^*(\mathbf{r}_T)\exp(i\mathbf{P}\cdot\mathbf{r}_T)\nabla_{\mathbf{r}_T}\varphi_i(\mathbf{r}_T) \times\int d\mathbf{r}_P\exp(-i\mathbf{P}\cdot\mathbf{r}_P)E^{-*}(Z_P,-\mathbf{v};\mathbf{r}_P) \times E^{+}(Z_P,-\mathbf{v};\mathbf{r}_P) , \tag{3.14}$$

The integrals over $\mathbf{r}_T$ are the form factor or related, while the integrals on $\mathbf{r}_P$ are of the Nordsiek type.[23]

The EB is composed of two terms, $\mathbf{Q}_T$ and $\mathbf{Q}_P$, with different physical meanings. $\mathbf{Q}_P$ represents the bremsstrahlung emission of the electron in the field of the projectile, while the nucleus target stays as an observer. Otherwise, $\mathbf{Q}_T$ indicates that the projectile passes through, provides the energy and momentum transfer, while the electron produces bremsstrahlung in the field of the target. We have found that $\mathbf{Q}_T$ tends to zero as $m\to\infty$ in Eq. (3.11).

The wave functions in Eqs. (3.9) describe collisions where both the initial and final electron states are bound to the target. Therefore Eqs. (3.12)–(3.14) represent a radiative direct process. We obtain REL by setting $\varphi_i=\varphi_f$ and REX (or deexcitation) if $\varphi_i\neq\varphi_f$.

The EB terms for REC and RI are derivated in the Appendix.

IV. CALCULATION AND COMPARISON WITH EXPERIMENTS

As we have seen in Sec. III A, there is no radiation of the center of mass in the dipole approximation, when the off-shell orthogonality property is enforced. The ISB term is very small and can be neglected in the soft x-ray region, as indicated in Sec. III B. Therefore, the remaining term, the EB, is the dominant effect in heavy-ion–atom collisions. We have calculated REL and REX cross sections using the distorted-wave functions as indicated in the last section.

The procedure can be summarized as follows: closed forms were found for form factors and related integrals for hydrogenic orbitals. A numerical code has been worked out to obtain an explicit expression of the Nordsieck's integrals using the hypergeometric function ${}_2F_1$. Afterwards, $\mathbf{Q}_P$ was projected on the photon polarization vectors to obtain the fivefold differential cross section, as indicated in Eq. (2.15).

If the magnetic numbers of the initial and (or) final bound states are nonzero, then a numerical integration on the azimuth of the projectile has to be performed. Otherwise, it has a closed form. Two integrals on $d\Omega_\omega$ can be performed in closed forms, and finally the remaining ones, on the photon energy $d\omega$ and on the projectile scattering angle $d\Omega$, have to be numerically calculated. A total cross section for REX, say $1s\to 2s$, takes about 10 min on our minicomputer (PDP 11/44) considering 100 projectile angles and 50 photon energies. The computer time is mainly spent in evaluating the hypergeometric functions ${}_2F_1$.

A. Radiative elastic scattering

Figure 2 shows the theoretical photon spectrum, emitted at 90° to the beam, produced by 1-MeV protons on aluminum. All the 13 electrons of the target may produce

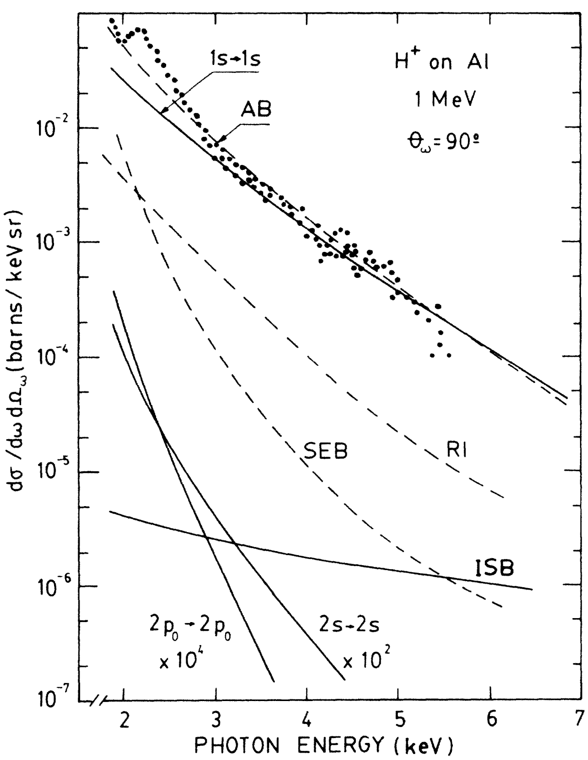

FIG. 2. X-ray continuous emission at 90° to the beam for 1-MeV protons colliding with an aluminum target as a function of the photon energy. Solid lines denote present calculations: radiative elastic scattering coming from three orbitals of the aluminum atom ($1s$, $2s$, and $2p_0$), and ISB is the intersystem bremsstrahlung as given by Eq. (3.6). Dashed lines represent theoretical results as reported by Ishii and Morita (Ref. 10): SEB, RI, and AB denote secondary electron bremsstrahlung, radiative ionization, and atomic bremsstrahlung, respectively. The points are the experimental data on an aluminum solid target (Ref. 10).

REL radiation. However, the $1s$-$1s$ transition is by far the dominant. As shown in the figure, it is about 6 orders of magnitude larger than $2s$-$2s$ and $2p_0$-$2p_0$, in the range considered here. Calculations were carried out using hydrogenic orbitals with single effective charges, given by $Z_{1s}=12.7$, $Z_{2s}=3.13$, and $Z_{2p_0}=2.51$.[24] We also plot the experiments,[10,25] which correspond to the x-ray production of an Al *solid* target. The agreement with the experiments is good. The dashed line shows the results of Ishii and Morita[10] calculated with the second Born approximation, which also gives a good description of the experiments. Since the Al target is a solid foil, another kind of process takes place: the so-called secondary electron bremsstrahlung (SEB). This process takes over the REL at higher projectile energies in the photon range considered here. RI, as reported by Ishii and Morita,[10] are also displayed. Both SEB and RI are important in the soft-photon region, and should be added to EB to account for the experiments. The ISB production calculated with Eq. (3.6) is also shown in the figure; its magnitude is very small, and can be neglected here. The REC process presents the main contribution around $\omega=v^2/2\approx 0.5$ keV, which is placed at a softer photon-energy region, not shown in the figure. As the photon energy tends to zero, the cross section diverges. This is a well-known property and is due to the long-range nature of the Coulomb potential.

Figure 3 displays the angular distribution of continuum x rays and compares it with the experiments. Our results are almost equal to those of Ishii and Morita[10] and reproduce the experiments satisfactorily. The light discrepancy at small angles may be due to the retardation effects, not considered in the present work.

A very important point is the dependence of the photon emission on the projectile charge. This subject has been first explored by Schnopper *et al.*[26] who measured continuum x rays produced by H^+ and O^{6+} on H_2 targets. These authors have suggested that the photon yield, for a fixed projectile velocity, should increase as Z_P^2. Further, the second Born approximation, used by Ishii and Morita,[10] *also* predicts a Z_P^2 dependence. We have calculated the triple differential cross section $d\sigma/d\omega\, d\Omega_\omega$ for REL produced by multiply charged bare ions on hydrogen atoms when the emitted photon energy is 1, i.e., 27.2 eV (these results can be easily scaled with Z_T if needed). Figure 4 shows the theoretical results for four different impinging velocities as a function of the projectile charge. We can observe two features: first, the larger the projectile velocity is, the larger the range where the Z_P^2 dependence holds. And second, at large projectile charge, say larger than the projectile velocity, the Z_P^2 dependence is abandoned and a sort of saturation is found. Similar effects have been found in nonradiative direct excitation.[16,27] Experiments would be welcome to study this effect, since they would provide important data for the calculation of shielding.

B. Radiative excitation and collisional broadening

Figures 5 and 6 show the photon spectrum for deexcitation and excitation of hydrogen by 100-keV protons, respectively.

Deexcitation spectra show pronounced peaks when the photon energy is equal to the difference of binding energies, and this is the so-called collisional broadening. We have to recall that our formalism, as shown in Sec. III C, includes the characteristic line of the radiative decay, when permitted. Therefore, if the projectile passed through without interacting, the electron would decay and the spectrum would be the characteristic line with a width given by the inverse of the time decay, i.e., a very sharp peak. Peaks seen in Fig. 5 are those characteristic lines now broadened by the interaction with the projectile mixing the electronic states during the collision. Note that forbidden transitions for an isolated atom, such as $2s$-$1s$, now show a well-defined enhancement with a yield as relevant as the permitted ones. Profiles diverge due to the long range of the Coulomb potential.

REX values, as shown in Fig. 6, are very small and no enhancement occurs. As $\omega \to 0$, REX (as well as collisional broadening) tends to zero as ω^1. REX is related to the absorption range of the corresponding collisional broadening. Here it is convenient to define the magnitude

$$\frac{d\sigma}{d\omega\,\omega^2\,|A_0|^2} \tag{4.1}$$

which is shown in Fig. 7 as a function of ω for excitation of hydrogen by 100-keV protons. The term $\omega^2 d\omega$ is an angular-integrated element of volume in the photon energy space, and $|A_0|^2$ is the strength of the spontaneous radiation. When the system is in the presence of an external field $|A_0|^2$ is replaced by the intensity. The magnitude defined in Eq. (4.1) represents emission for positive ω and absorption in the negative range. In other words, downward and upward transitions, respectively. REX is then restrained to the emission range, i.e., $\omega > 0$.

Results shown in Fig. 7 have another interesting interpretation. If the process is reversed, i.e., from $i \to f$ to $f \to i$, and so ω to $-\omega$, instead of nonobserved upward excitation, we have observed radiative deexcitation, and this is collisionally broadening. Therefore, in the same figure we have REX for $i \to f$ on the right, and collisional broadening for $f \to i$ on the left. With this interpretation REX contains the information of the corresponding collisional broadening in the analytical continuation, and vice versa. Then, the typical divergence at zero photon energy of the REL $1s$-$1s$, i.e., bremsstrahlung, may be seen as the half of the collisional broadening profile in the emission range, as displayed in Fig. 7.

Figure 8 displays total cross sections for excitation of hydrogen to $2s$, $2p_0$, $2p_{\pm 1}$, and $3s$ by impact of protons as a function of the projectile energy. Total cross sections are very small, that is, six orders of magnitude smaller than the nonradiative mechanism or mechanical one. The high-energy behavior is fitted to be $v^{-2}\ln(v)$, so it will never take over the mechanical or nonradiative one, which has the same behavior. By contrast, we should remember that REC becomes the dominant mechanism at very high projectile velocities when compared with the nonradiative electron capture.

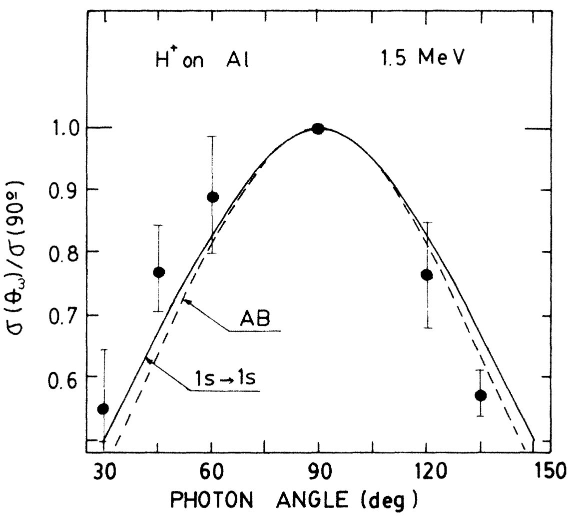

FIG. 3. X-ray angular distribution for 1-MeV protons impinging on aluminum, for photon energies in the range 5.18–5.57 keV. The solid line denotes present calculations of radiative elastic scattering $1s$-$1s$. The dashed line is the atomic bremsstrahlung result of Ishii and Morita (Ref. 10), and the points are the experiments reported by the same authors.

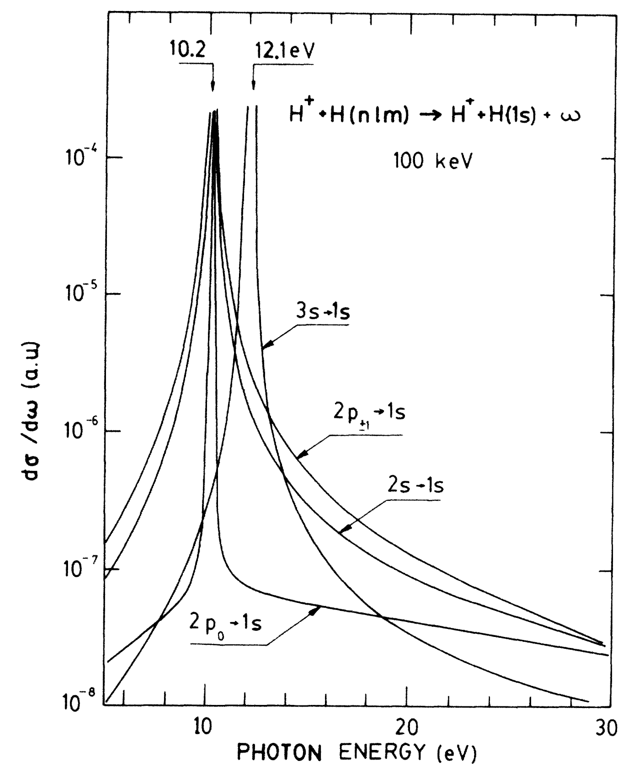

FIG. 5. Spectra for radiative deexcitation to the ground state of hydrogen atoms by impact of 100-keV protons as a function of the photon energy.

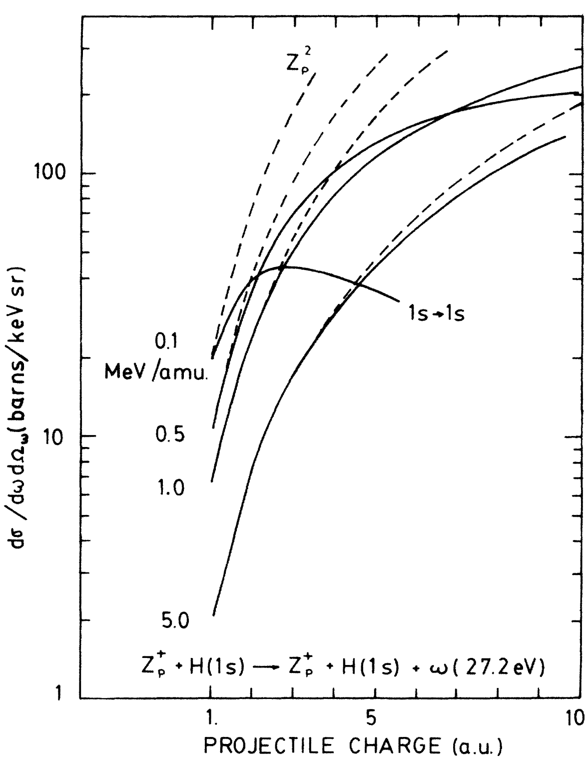

FIG. 4. Single differential cross section of continuum emission as a function of the projectile charge for four different impinging velocities on hydrogen atoms. The emitted photon energy is 1 a.u., i.e., 27.2 eV, and the angle is 90° to the beam. Solid lines denote present calculation of radiative elastic scattering $1s$-$1s$, and dashed lines, the Z_P^2 behavior.

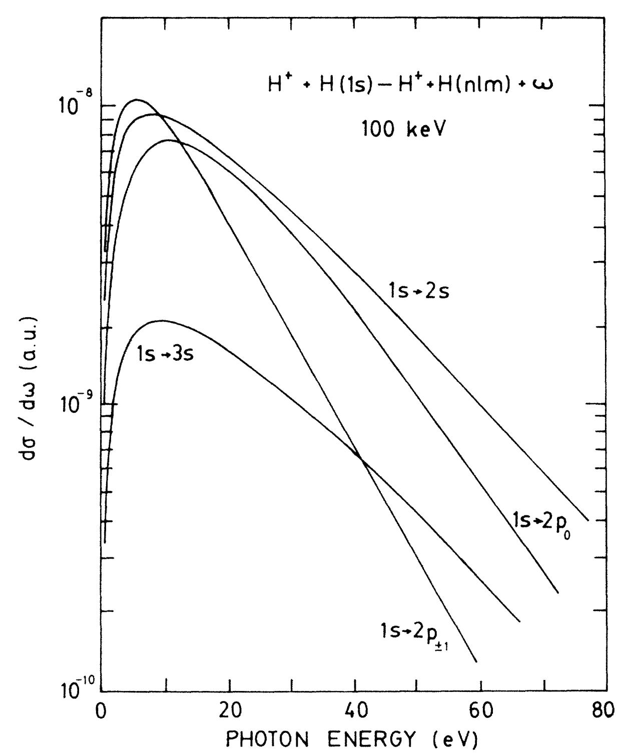

FIG. 6. Spectra for radiative excitation from the ground state of hydrogen atoms by impact of 100-keV protons as a function of the photon energy.

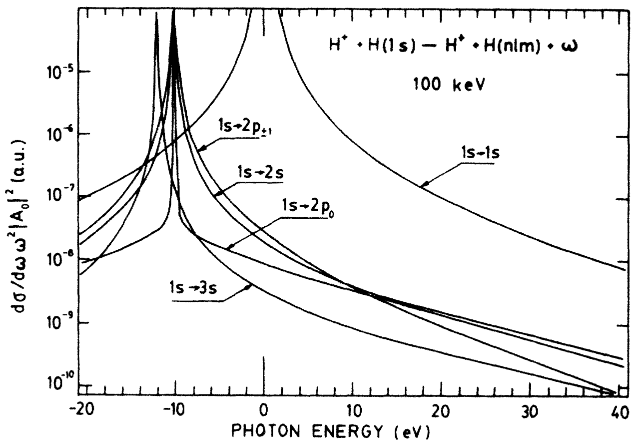

FIG. 7. Single differential cross section normalized to $\omega^2 |A_0|^2$ as a function of positive and negative photon energy for radiative excitation of hydrogen atoms by impact of 100-keV protons.

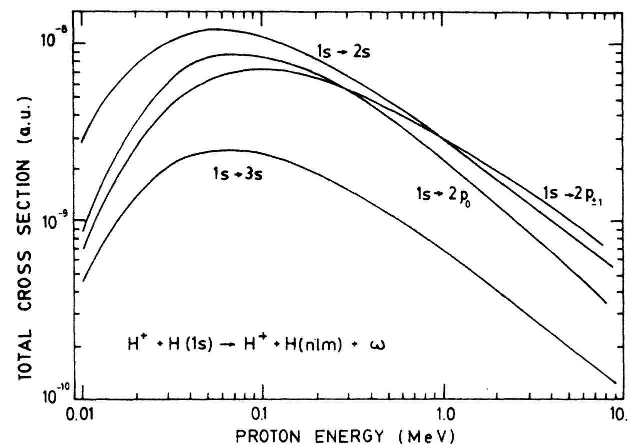

FIG. 8. Total cross section for radiative excitation of H(1s) atoms as a function of the proton incident energy.

ACKNOWLEDGMENT

The Instituto de Astronomía y Física del Espacio is affiliated with the Consejo Nacional de Investigaciones Científicas y Técnicas.

APPENDIX

Although this work mainly deals with direct radiative processes, i.e., REL and REX, we consider it illustrative to include here how the relevant matrix elements for REC and RI are derivated from Eqs. (2.11)–(2.14). Here we assume no internuclear interaction (just to simplify the problem) and the dipole approximation.

The initial state is supposed to be described by the exact impulse approximation (IA) wave function given by[28]

$$\xi_i^{\rm IA}=(2\pi)^{-3}\int d\mathbf{g}\,\tilde{\varphi}_i(\mathbf{g})\exp[i(\mu_T\mathbf{K}_i+\mathbf{g})\cdot\mathbf{R}_P]\times\Psi^+(Z_P,\mathbf{g}-\mathbf{v}_i\,|\,\mathbf{r}_P)\;, \tag{A1}$$

where $\tilde{\varphi}_i(\mathbf{g})$ is the Fourier transform of the initial electron state in the target and

$$\Psi^+(Z_P,\mathbf{g}-\mathbf{v}_i\,|\,\mathbf{r}_P)=\exp[i(\mathbf{g}-\mathbf{v}_i)\cdot\mathbf{r}_P]\times D^+(Z_P,\mathbf{g}-\mathbf{v}_i,1;\mathbf{r}_P) \tag{A2}$$

is the continuum e-P wave function.

1. Radiative electron capture

The final wave function is supposed to be—as in the nonradiative impulse approximation—given by the first-order Born wave function:

$$\xi_f^B=\exp(i\mathbf{K}_f'\cdot\mathbf{R}_P)\varphi_f(\mathbf{r}_P)\;, \tag{A3}$$

where now $\mathbf{K}_f'$ is the momentum of the final atom with respect to the residual nucleus target, and the $\varphi_f(\mathbf{r}_P)$ is the final bound state of the electron to the projectile.

Those wave functions satisfy the vital requirement of being orthogonal, i.e., $\langle \xi_f^B\,|\,\xi_i^{\rm IA}\rangle=0$, as the exact ones do. So the center of mass does not radiate, i.e., $H_l^{\rm CMB}=0$.

By using the set $\{\mathbf{R}_P,\mathbf{r}_P\}$ the ISB term reads

$$\begin{aligned}H_{lP}^{\rm ISB}&=iA_0\hat{\boldsymbol{\lambda}}_l\cdot B_{P0}\langle \xi_f^B\,|\,\nabla_{\mathbf{R}_P}\,|\,\xi_i^{\rm IA}\rangle\\&=-A_0B_{P0}\hat{\boldsymbol{\lambda}}_l\cdot\mathbf{K}_f'\tilde{\varphi}_i(\mathbf{W}_T)\\&\quad\times\int d\mathbf{r}_P\varphi_f^*(\mathbf{r}_P)\exp(-i\mathbf{W}_P\cdot\mathbf{r}_P)\\&\quad\times D^+(Z_P,-\mathbf{W}_P,1;\mathbf{r}_P)\;,\end{aligned} \tag{A4}$$

where $\mathbf{W}_T=\mathbf{K}_f'-\mu_T\mathbf{K}_i$ and $\mathbf{W}_P=\mathbf{K}_i-\mu_P\mathbf{K}_f'=\mathbf{v}_i-\mathbf{W}_T$. Equation (A4) involves the integral of the product continuum bound wave functions and so $H_{lP}^{\rm ISB}=0$.

Therefore Eq. (2.11) is finally reduced to just the EB term

$$\begin{aligned}H_{lP}^{\rm EB}&=iA_0\hat{\boldsymbol{\lambda}}_l\cdot b_{P0}\langle \xi_f^B\,|\,\nabla_{\mathbf{r}_P}\,|\,\xi_i^{\rm IA}\rangle\\&=iA_0b_{P0}\tilde{\varphi}_i(\mathbf{W}_T)\hat{\boldsymbol{\lambda}}_l\cdot\int d\mathbf{r}_P\varphi_f^*(\mathbf{r}_P)\nabla_{\mathbf{r}_P}\\&\quad\times\Psi^+(Z_P,-\mathbf{W}_P\,|\,\mathbf{r}_P)\;,\end{aligned} \tag{A5}$$

Results with this approximation for proton-hydrogen 1s-1s electron capture have been recently reported.[29]

The first Born approximation consists of replacing $\Psi^+(Z_P,-\mathbf{W}_P\,|\,\mathbf{r}_P)$ by the plane wave $\exp(-i\mathbf{W}_P\cdot\mathbf{r}_P)$, so the $H_l^{\rm EB}$ reads

$$H_{lP}^{\rm EB}\,|_{\rm Born}=A_0b_{P0}\hat{\boldsymbol{\lambda}}_l\cdot\mathbf{W}_P\tilde{\varphi}_i(\mathbf{W}_T)\tilde{\varphi}_f^*(\mathbf{W}_P)\;, \tag{A6}$$

which has been used to calculate photon spectra.[5]

2. Radiative ionization

By replacing $\varphi_f(\mathbf{r}_P)$ in Eq. (A5) by the continuum state around the projectile $\Psi^-(Z_P,\mathbf{k}_f\,|\,\mathbf{r}_P)$, where now $\mathbf{k}_f$ is the momentum of the electron with respect to the projectile, the RI expression of Jakubassa *et al.*[6] is obtained. This expression represents only radiative emission due to electron capture to the continuum. It is interesting to investigate the additional influence of the Coulomb distortion of the residual target.

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