Bremsstrahlung radiation emitted in fast-electron–H-atom collisions

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(Received 26 June 1989)

A previous calculation for free-free transitions is generalized so as to treat one-photon (spontaneous) bremsstrahlung emitted in the course of collisions of relatively fast electrons with atomic hydrogen. While the electron-atom collision is described within the first Born approximation, the role of the atomic spectrum is taken into account exactly via the use of a compact representation of the Coulomb Green's function. We discuss the main features of the cross sections and address some physically relevant issues such as the importance of the screening by the atomic electron, the role of the atomic structure, and limiting cases such as the soft-photon and the small-momentum transfer limits. We also discuss the differences observed between the cross sections for spontaneous bremsstrahlung and stimulated free-free transitions.

I. INTRODUCTION

Bremsstrahlung emission occurring during the course of an electron–H-atom collision can be symbolically represented by the following equation:

$$e(\mathbf{k}_i)+\mathrm{H}(1s)\rightarrow e(\mathbf{k}_f)+\gamma(\omega,\boldsymbol{\epsilon},\mathbf{k})+\mathrm{H}(1s)\ . \tag{1}$$

Here $\mathbf{k}_i$ ($\mathbf{k}_f$) are the wave vectors of the incoming (outgoing) electrons; $\gamma(\omega,\boldsymbol{\epsilon},\mathbf{k})$ represents a photon spontaneously emitted with frequency ω, polarization direction $\boldsymbol{\epsilon}$, and wave vector $\mathbf{k}$ and H($1s$) symbolizes a ground-state H atom. Conservation of energy imposes (atomic units will be used unless otherwise stated)

$$\frac{k_i^2}{2}=\frac{k_f^2}{2}+\omega\ . \tag{2}$$

We shall discuss here collisions of (relatively) fast electrons with kinetic energies significantly greater than typical atomic excitation energies

$$(k_i^2/2, k_f^2/2) \gg \tfrac{1}{2} \tag{3}$$

in a.u.

The theory of such radiative collisions is notably simplified in the two following limiting cases depending on the frequency of the emitted photon.

(i) One is in the high-frequency region of the spectrum, i.e., for photon frequencies relatively large with respect to characteristic atomic excitation frequencies. In such a regime it can be shown and easily verified (see below) that the projectile-nucleus interaction dominates the physics of the process and the celebrated Sommerfeld formula,[1] established for a pure Coulomb potential, provides an excellent description of the emission spectrum. For high-atomic-number elements, however, the screening effect of the atomic electrons can become important, and sophisticated theoretical methods have been developed to deal with such bremsstrahlung spectra in the x-ray range.[2]

(ii) The other is in the low-frequency (soft-photon) limit, i.e., for photon frequencies much smaller than characteristic atomic excitation frequencies. In this regime the bremsstrahlung cross section diverges as ω^{-1} and becomes proportional to the field-free elastic-scattering cross section.[3] We will illustrate this general theorem by investigating the behavior of our results in the limit $\omega\rightarrow 0$, see below.

In contrast with these limiting cases, no general theoretical analysis is available when the emitted photon frequency is comparable to characteristic atomic excitation frequencies. Indeed, as previously noted by several authors,[4–7] the coupling between the electron-atom system and empty modes of the radiation field (vacuum field) with frequencies close to atomic excitation frequencies, can create a resonant state, thus giving rise to a resonant structure in the bremsstrahlung spectrum. In such a case, one expects that the electronic structure and polarizability of the target play an important role on the dynamics of the process.

We have chosen to illustrate the main characteristics of the bremsstrahlung cross sections and spectra by considering the electron–H-atom system.[8] Though very simple, this system displays the main elements necessary to describe the dynamics of such radiative collisions. In addition, once an appropriate set of physically grounded approximations has been chosen (typically: dipole approximation for the charged-particle–field interaction and first Born approximation for the scattering stage,...), it is possible to perform an exact analytic calculation of the overall transition amplitude. This has the definite advantage of making clear the limitations of the theory and allowing one to investigate the analytic behavior of the

cross sections in interesting limiting cases.

To this end we have extended and generalized a recent calculation we had performed for the closely related process of free-free transitions (FFT) in the same system.[9] As a result of this generalization we have been able to express the bremsstrahlung transition amplitude in a very compact analytic form. In this respect our results represent an extension of previous similar works on the same process.[3]

In Sec. II, we shall outline the theoretical framework of our calculation. The numerical results of our computation will be presented and discussed in Sec. III. We will discuss, in particular, the relative magnitudes of the different terms contributing to the cross section and investigate their behavior in the soft-photon and high-frequency limits. The differences between spontaneous and stimulated bresstrahlung will be also addressed. A brief conclusion ends the paper in Sec. IV.

II. THEORY

The threefold differential cross section for detecting a spontaneously emitted photon within the frequency range ω, $\omega+d\omega$, and solid angle $d\Omega(\hat{\mathbf{k}})$, plus a scattered electron within the solid angle $d\Omega(\hat{\mathbf{k}}_f)$ is expressed as

$$\frac{d\sigma}{d\omega\, d\Omega(\hat{\mathbf{k}}) d\Omega(\hat{\mathbf{k}}_f)} = \frac{2\pi}{k_i} |T_{f/i}|^2 \rho(E_f)\rho(\omega) \ . \tag{4}$$

Here k_i is the incoming electron momentum, $\rho(E_f)=k_f/(2\pi)^3$, and $\rho(\omega)=\omega^2/(2\pi c)^3$ are the density of states for the scattered electron with energy E_f and emitted photon, respectively, and $T_{f/i}$ is the transition matrix element, the structure of which will be described below. This cross section, which has the dimensions of a surface divided by an energy, is expressed here in units of $a_0^2/(2\ \mathrm{Ry})$.

As the elementary bremsstrahlung process involves the spontaneous emission of one photon, the radiative coupling between the electrons and the vacuum field can be conveniently treated in first-order perturbation theory with respect to the interaction Hamiltonian:

$$H_r = \frac{1}{c} A_0 a^\dagger \boldsymbol{\epsilon}\cdot(\mathbf{p}_0+\mathbf{p}_1) \ , \tag{5}$$

where

$$A_0 = c(2\pi/\omega)^{1/2}$$

is the amplitude of the potential vector for a mode of the radiation field with polarization $\boldsymbol{\epsilon}$ and frequency ω, $a^\dagger$ is the creation operator for one photon in this mode, and $\mathbf{p}_0$ and $\mathbf{p}_1$ are the momentum operators for the projectile and atomic electrons, respectively.

For the relatively high projectile kinetic energies we have chosen to discuss here, a first Born approximation treatment of the electron-atom collision provides a correct description of this stage of the process. This amounts to treating the projectile-target interaction to first order in the electron-atom coupling Hamiltonian:

$$H_e^{(1)} = -\frac{1}{r_0} + \frac{1}{r_{01}} \ , \tag{6}$$

where $\mathbf{r}_0$ is the position of the projectile and $r_{01}=|\mathbf{r}_0-\mathbf{r}_1|$, $\mathbf{r}_1$ being the position of the atomic electron. Note that we will not discuss exchange effects, which are expected to be small in this collisional regime.

Within this framework the corresponding expression for the transition matrix element $T_{f/i}$ is second order in the perturbation Hamiltonians $H_e^{(1)}$ and H_r, each of them acting only once:

$$T_{f/i} = \langle f|H_r G_0(E_i) H_e^{(1)}|i\rangle + \langle f|H_e^{(1)} G_0(E_i) H_r|i\rangle \ . \tag{7}$$

Here $|i\rangle$ and $|f\rangle$ are the initial and final eigenstates of the unperturbed Hamiltonian operator

$$H_0 = H_{\mathrm{at}} + H_e + H_F \ ,$$

E_i is the energy of the state $|i\rangle$; H_{at} is the hydrogen atom Hamiltonian, H_e is the kinetic energy operator for the free-electron projectile, H_F is the radiation field Hamiltonian, and $G_0(z)=(z-H_0)^{-1}$ is the resolvent. In the initial state no photon is present (vacuum field), whereas in the final state one photon has been emitted with the frequency given by the conservation of energy relation Eq. (2). We note also that, as H_r acts on both the projectile and atomic electrons, the expression of $T_{f/i}$ contains, in fact, four amplitudes.[9]

Aside from an overall multiplicative factor, $T_{f/i}$ has the same formal structure as the corresponding second-order transition amplitude for free-free transitions. The required sum over states for the radiation field and the free-electron projectile, as well as the integration over the projectile coordinates, can be carried out exactly, and after some algebra one obtains[9,10]

$$\begin{aligned}\frac{d\sigma}{d\omega\, d\Omega(\hat{\mathbf{k}}) d\Omega(\hat{\mathbf{k}}_f)} &= \frac{\alpha^3}{\pi^2}\frac{k_f}{k_i}\frac{\omega}{\Delta^4}\left|\frac{\boldsymbol{\Delta}\cdot\boldsymbol{\epsilon}}{\omega}\langle 1s|(e^{i\boldsymbol{\Delta}\cdot\mathbf{r}}-1)|1s\rangle\right. \\ &\quad \left. + i\omega[M_{1s}(\boldsymbol{\Delta},\boldsymbol{\epsilon};E_{1s}-\omega) + M_{1s}(\boldsymbol{\Delta},\boldsymbol{\epsilon};E_{1s}+\omega)]\right|^2 \ ,\end{aligned} \tag{8}$$

where $\alpha \simeq \frac{1}{137}$ is the fine-structure constant, $\boldsymbol{\Delta}=\mathbf{k}_i-\mathbf{k}_f$ is the momentum transfer, and $M_{1s}(\boldsymbol{\Delta},\boldsymbol{\epsilon};\Omega)$ is a second-order atomic matrix element of the form

$$M_{1s}(\boldsymbol{\Delta},\boldsymbol{\epsilon};\Omega) = \langle 1s|e^{i\boldsymbol{\Delta}\cdot\mathbf{r}} G_c(\Omega)\mathbf{r}\cdot\boldsymbol{\epsilon}|1s\rangle \ , \tag{9}$$

where $G_c(\Omega)$ is the Coulomb Green's function. For computational convenience we have used the electric-dipole form of the interaction Hamiltonian.

The first term in Eq. (8) can be associated with processes in which the projectile itself emits one photon while scattered by the atom. Apart from a factor of -1 it is proportional to the atomic form factor. More precisely, this term splits into two contributions which reduce to

(i) the ground-state atomic form factor, which stems from the interaction between the projectile and the atomic electron:

$$\langle 1s|e^{i\boldsymbol{\Delta}\cdot\mathbf{r}}|1s\rangle = \frac{16}{(\Delta^2+4)^2} \ ; \tag{10a}$$

and (ii) a pure Coulomb contribution associated to the projectile-nucleus interaction:

$$-\langle 1s|1s\rangle=-1 \ . \tag{10b}$$

Note that if the nucleus charge were Z, this term would be $-Z$.

The two other terms contained in Eq. (8) account for contributions in which the target itself emits one photon while experiencing the collision with the projectile, this latter supplying the needed energy for ensuring the global conservation of energy. The magnitude of this contribution depends critically on the polarizability of the target and is strongly dependent on the frequency of the emitted photon. We note that these contributions were omitted in most earlier treatments of atomic bremsstrahlung processes and we will discuss below (Sec. III) the range of validity of such approximate treatments.

The computation of the matrix elements $M_{1s}(\Delta,\epsilon;\Omega)$ represents the main difficulty of the calculation. On using an integral representation of $G_c(\Omega)$,[11,12] we had previously obtained a fairly compact representation of these matrix elements, in terms of Appell's hypergeometric functions of two variables.[9]

In the present application, however, we needed to compute these matrix elements for values of $\Omega>0$, i.e., located on the cut of $G_c(\Omega)$, which required us to analytically continue the expressions obtained. To this end we have found it convenient to express them in terms of Gauss ${}_2F_1$ hypergeometric functions whose analytic continuation properties are easier to handle, and we have been able to derive the following very compact expression (see the Appendix for an outline of the derivation of these formulas):

$$M_{1s}(\Delta,\epsilon;\Omega)=-i\Delta\cdot\epsilon[\,A+B(+\Delta)+B(-\Delta)] \ , \tag{11}$$

with

$$A=\frac{48(4-3\Delta^2)}{\Delta^2(1-x^2)(4+\Delta^2)^3} \ , \tag{12a}$$

$$B(+\Delta)=i\frac{24(1-x+i\Delta)}{\Delta^3(1-x)(1+x)^2(2+i\Delta)^3}\frac{1}{2-1/x} \times {}_2F_1\left[1,-1-\frac{1}{x};3-\frac{1}{x};\tilde{u}^+\right] , \tag{12b}$$

where

$$\tilde{u}^+=\frac{(1-x)(1-x+i\Delta)}{(1+x)(1+x+i\Delta)}, \quad x=\sqrt{-2\Omega} \ ,$$

and $B(-\Delta)$ is obtained by changing $\Delta\rightarrow-\Delta$. Note that if x is real ($\Omega<0$), the quantities $B(+\Delta)$ and $B(-\Delta)$ are complex conjugates and their sum is real.

An interesting property of these matrix elements, resulting from the rotational invariance of the atomic system in its ground state, is the factorization of the scalar product $\Delta\cdot\epsilon$ which governs the angular dependence of the cross section with respect to the photon polarization.

This allows us to rewrite the differential cross section as follows:

$$\frac{d\sigma}{d\omega\, d\Omega(\hat{\mathbf{k}})d\Omega(\hat{\mathbf{k}}_f)}=\frac{\alpha^3}{\pi^2}\frac{k_f}{k_i}\frac{\omega}{\Delta^4}(\Delta\cdot\epsilon)^2|\tilde{T}_{1s}(\Delta;\omega)|^2 \ , \tag{13}$$

where $\tilde{T}_{1s}(\Delta;\omega)$ is a reduced matrix element that reads

$$\tilde{T}_{1s}(\Delta;\omega)=\frac{1}{\omega}\left[\frac{16}{(\Delta^2+4)^2}-1\right] +\omega[\tilde{M}_{1s}(\Delta;E_{1s}-\omega)+\tilde{M}_{1s}(\Delta;E_{1s}+\omega)] \ , \tag{14a}$$

with

$$\tilde{M}_{1s}(\Delta;\Omega)=A+B(+\Delta)+B(-\Delta) \tag{14b}$$

[see Eqs. (12)].

If, as in most bremsstrahlung experiments, the photon polarization is not detected, one has to sum over the polarization states of the spontaneously emitted photon and the triple differential cross section for the emission of an unpolarized photon is

$$\frac{d\sigma_{\text{unpol}}}{d\omega\, d\Omega(\hat{\mathbf{k}})d\Omega(\hat{\mathbf{k}}_f)} =\frac{\alpha^3}{\pi^2}\frac{k_f}{k_i}\frac{\omega}{\Delta^4}[(\Delta\cdot\epsilon_1)^2+(\Delta\cdot\epsilon_2)^2]|\tilde{T}_{1s}(\Delta;\omega)|^2 \ , \tag{15}$$

where ϵ_1 and ϵ_2 are two mutually orthogonal polarization vectors. A convenient choice of coordinate axis, adapted to the geometry of such radiative processes, is shown in Fig. 1. The scalar products then read

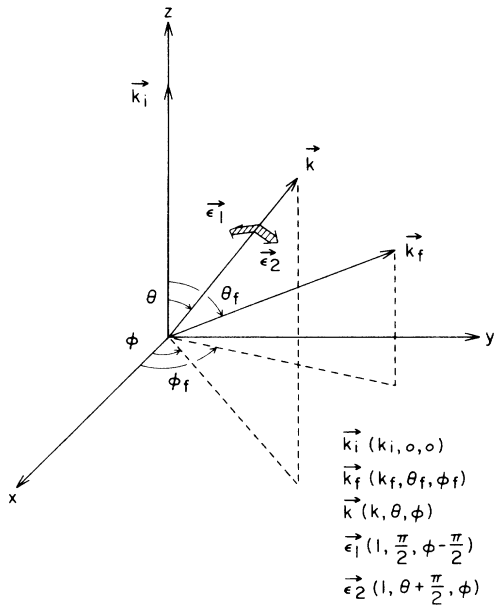

FIG. 1. Coordinate axis chosen to describe radiative collisions resulting in the emission of one bremsstrahlung photon. $\mathbf{k}_i$, incoming electron wave vector; $\mathbf{k}_f$, scattered electron wave vector; $\mathbf{k}$, wave vector of the emitted photon with polarization ϵ_1 or ϵ_2.

$$\Delta\cdot\epsilon_1 = k_f \sin\theta_f \sin(\phi_f - \phi) \ , \tag{16a}$$

$$\Delta\cdot\epsilon_2 = -k_i \sin\theta - k_f[\cos\theta \sin\theta_f \cos(\phi_f - \phi) - \sin\theta \cos\theta_f] \ , \tag{16b}$$

and

$$\Delta^2 = k_f^2 + k_i^2 - 2k_i k_f \cos\theta_f \ . \tag{16c}$$

If, in addition, one does not record the angular distribution of the outgoing electron, it is possible to partially perform the corresponding integration and one gets the following expression for the double differential cross section:

$$\frac{d\sigma_{\text{unpol}}}{d\omega\, d\Omega(\hat{\mathbf{k}})} = \frac{\alpha^3}{\pi}\frac{k_f}{k_i}\omega \int_0^{\pi} d\theta_f \sin\theta_f \frac{|\tilde{T}_{1s}(\Delta;\omega)|^2}{\Delta^4} \times [2\Delta^2 \sin^2\theta + k_f^2 \sin^2\theta_f (3\cos^2\theta - 1)] \ . \tag{17}$$

The last integration over θ_f cannot be performed analytically since $\tilde{T}_{1s}(\Delta;\omega)$ depends in a complicated fashion on θ_f, through the momentum transfer Δ; see Eqs. (12), (14), and (16c). This general expression of the twofold differential cross section will serve as a basis for discussing the properties of the bremsstrahlung spectra, as deduced from a standard numerical integration of the expression Eq. (17); see the discussion in Sec. III.

We note that a single differential cross section, associated with the overall probability for emission of one photon within the frequency range $(\omega, \omega + d\omega)$ can be deduced from Eq. (17) by integrating over the solid angle $d\Omega(\hat{\mathbf{k}})$. One then gets [$\tilde{T}_{1s}(\Delta;\omega)$ is independent from the propagation direction of the emitted photon]

$$\frac{d\sigma_{\text{unpol}}}{d\omega} = \frac{16}{3}\alpha^3 \frac{k_f}{k_i}\omega \int_0^{\pi} d\theta_f \sin\theta_f \frac{|\tilde{T}_{1s}(\Delta;\omega)|^2}{\Delta^2} \ . \tag{18}$$

Again, in most cases, the θ_f integration has to be performed numerically.

Coming back to the basic expression of the twofold differential cross section, Eq. (17), it is difficult to discuss its analytical properties in general terms, given the complicated structure of the matrix element $\tilde{T}_{1s}(\Delta;\omega)$, Eqs. (14). However, as we will show in Sec. III, some physical insight into its behavior in some limiting cases can be gained by comparing the relative contributions of the terms entering its expression.

III. RESULTS AND DISCUSSION

In the expression, Eq. (14a), of the reduced atomic transition amplitude $\tilde{T}_{1s}(\Delta;\omega)$, one can distinguish between the first term, broadly speaking associated to the generalized atomic form factor and arising from the projectile-field coupling, and the second term, more closely linked to the atom-field coupling. Accordingly, in the following, these contributions will be referred to as "electronic" and "atomic", respectively. Depending on the magnitudes of the physical parameters governing the dynamics of the radiative collision, namely, the momentum transfer Δ and the photon frequency ω, one term or the other can be dominant, thus imposing its behavior to the general cross section. This allows us to deduce some interesting features of the bremsstrahlung cross section, even before performing any numerical calculation. This can be achieved in the following particular cases.

(i) *Soft-photon limit:* $\omega \to 0$. In this limit the electronic term, preceded by the factor ω^{-1} is dominant, and the atomic term, which is proportional to ω, becomes vanishingly small. The reduced atomic matrix element $\tilde{T}_{1s}(\Delta;\omega)$ is then proportional to the field-free elastic-scattering amplitude[13]

$$\tilde{T}_{1s}(\Delta;\omega) \sim -\frac{1}{\omega}\frac{\Delta^2(\Delta^2+8)}{(\Delta^2+4)^2} \ , \tag{19}$$

and the differential cross section for bremsstrahlung, Eq. (17), reduces to

$$\frac{d\sigma_{\text{unpol}}}{d\omega\, d\Omega(\hat{\mathbf{k}})} \sim \frac{\alpha^3}{\pi}\frac{k_f}{k_i}\frac{1}{\omega}\int_0^{\pi} d\theta_f \sin\theta_f \frac{(\Delta^2+8)^2}{(\Delta^2+4)^4} \times [k_f^2(3\cos^2\theta - 1)\sin^2\theta_f + 2\sin^2\theta \Delta^2] \ . \tag{20}$$

The angular integration over θ_f can be performed exactly after some cumbersome algebra, and leads to an expression, which although of closed form, is too complicated to be reproduced here.[14] The above result clearly displays the infrared divergence of the bremsstrahlung cross section and allows us to recover a particular version of the Low theorem,[3] when applied to the case of e-H atom collisions. Here the integral is proportional to the first Born approximation for the field-free total cross section for elastic scattering of a fast electron by a ground-state H atom.

A relatively compact expression of a single differential cross section, integrated over the propagation direction of the emitted photon, can be easily obtained by substituting the approximate form, Eq. (19), in the general expression, Eq. (18),

$$\frac{d\sigma_{\text{unpol}}}{d\omega} \sim \frac{16}{3}\alpha^3 \frac{k_f}{k_i}\frac{1}{\omega}\int_0^{\pi} d\theta_f \sin\theta_f \frac{(\Delta^2+8)^2}{(\Delta^2+4)^4}\Delta^2 \ . \tag{21}$$

This analysis, based on the dominance of the electronic term in the transition amplitude, is quite general and provides an excellent description of the behavior of the cross section in the soft-photon regime. Within this context soft photon means frequencies such that $\omega \ll \omega_e$, where ω_e is the smallest atomic excitation frequency. Here, for ground-state hydrogen, ω_e corresponds to the $1s$-$2p$ transition i.e., $\omega_e = \omega_{12} = \frac{3}{8}$ a.u. So, as soon as ω does not fulfill the above condition, the soft-photon approximation is no longer valid and one has to perform the complete calculation of the expression, Eqs. (14).

Another apparent limitation of the validity of the expressions, Eqs. (20) and (21), is that they are deduced from the approximate expression, Eq. (19), for $\tilde{T}_{1s}(\Delta;\omega)$,

which is not completely correct at small scattering angles $\theta_f \to 0$, i.e., at the lower integration limit. In this angular range one has $\Delta \to 0$ as $\omega \to 0$ and the electronic contribution vanishes, being no longer dominant with respect to the atomic terms. It can be checked, however, by comparing with the exact calculation, that as this angular domain only contributes for a small amount to the integral, this does not significantly affect the validity of our general analysis concerning the soft-photon limit.

(ii) *Resonant bremsstrahlung emission.* At higher frequencies the dominance of the electronic term becomes less marked and the situation can be completely reversed, namely, the atomic contribution becomes dominant. This is particularly so if the emitted photon frequency ω matches, or nearly matches, an atomic excitation frequency $\omega \sim \omega_{1n}$, where $\omega_{1n} = \frac{1}{2}(1-n^{-2})$, $n=2,3,\ldots$. In such a case the second-order matrix element $M_{1s}(\Delta,\epsilon;E_{1s}+\omega)$, Eq. (9), or its reduced form $\tilde{M}_{1s}(\Delta;E_{1s}+\omega)$ becomes very large and dominates the total transition amplitude. This comes from the fact that these matrix elements contain the Coulomb Green's function, which has poles when its argument is equal to the energy of the bound states. To each of these poles is associated a resonance in the bremsstrahlung emission spectrum, see Fig. 2, below.

Exactly on resonance $\omega=\omega_{1n}$, our expression of the cross section becomes infinite. These unphysical infinities arise from the fact that we have neglected the radiative shifts and widths of the atomic levels. This is consistent with our lowest-order perturbative approach, which, understandably, is not valid at resonance. Note that in such particular cases, a two-level model of the atom would be relevant.

(iii) *First-Born Coulomb bremsstrahlung.* Still at higher frequencies, i.e., if $\omega \gg \omega_{1n}$, where atomic hydrogen excitation energies obey the following inequalities: $\frac{3}{8} \le \omega_{1n} < \frac{1}{2}$, the projectile-nucleus interaction dominates the dynamics of the collision.[15] This feature of the bremsstrahlung process, well known in the context of the production of x-ray spectra by electron impact, can be understood here as follows: At relatively large photon frequencies both the electronic and atomic contributions are notably modified. These modifications arise primarily from the fact that the greater ω, the greater Δ, since $k_i - k_f \le \Delta \le k_i + k_f$ and $k_i^2 - k_f^2 = 2\omega$. Accordingly, in the limit $\Delta^2 \gg 1$, the electronic term, see Eq. (8), reduces to $-1/\omega$ (or $-Z/\omega$ in case of hydrogenic ions). Parallel to this, the atomic contribution strongly decreases and becomes negligible, as the matrix elements $M_{1s}(\Delta,\epsilon;\Omega)$ are then very small because of the oscillatory nature of the operator $\exp(i\Delta\cdot\mathbf{r})$, which enters their expression, Eq. (9). This trend, concerning the atomic contribution, is even reinforced by the fact that the matrix elements M_{1s} become approximately proportional to ω^{-1} with opposed signs and that they partially cancel each other.[16] This approximate ω^{-1} dependence compensates the multiplicative factor ω, which further accentuates the decrease of the atomic contribution. As a result of these multiple cancellations the matrix element $\tilde{T}_{1s}(\Delta;\omega)$, in the limit of large ω (and Δ), becomes

$$\tilde{T}_{1s}(\Delta;\omega) \sim -\frac{1}{\omega} , \tag{22}$$

and the corresponding approximate expression for the twofold differential cross section reads

$$\frac{d\sigma_{\text{unpol}}}{d\omega\, d\Omega(\hat{\mathbf{k}})} \sim \frac{\alpha^3}{\pi}\frac{k_f}{k_i}\frac{1}{\omega} \times \int_0^{\pi} d\theta_f \sin\theta_f \Delta^{-4} \times [2\Delta^2 \sin^2\theta + k_f^2(3\cos^2\theta - 1)\sin^2\theta_f] . \tag{23a}$$

The angular integration can be easily performed and one recovers the following closed-form result:[17]

$$\frac{d\sigma_{\text{unpol}}}{d\omega\, d\Omega(\hat{\mathbf{k}})} \sim \frac{\alpha^3}{\pi}\frac{k_f}{k_i^3}\frac{1}{\omega}\left[3\sin^2\theta - 2 + \frac{\sin^2\theta(k_i^2-3k_f^2)+2(k_i^2+k_f^2)}{2k_i k_f}\ln\left[\frac{k_i+k_f}{k_i-k_f}\right]\right] . \tag{23b}$$

Again, the angular integration over the propagation direction of the emitted photon can be easily performed, and one obtains the well-known first Born approximation formula for the bremsstrahlung emission in a Coulomb field[17]

$$\frac{d\sigma_{B1}}{d\omega} = \frac{16}{3}\alpha^3\frac{1}{k_i^2}\frac{1}{\omega}\ln\left[\frac{k_i+k_f}{k_i-k_f}\right] . \tag{24}$$

These formulas, which will be referred to as the

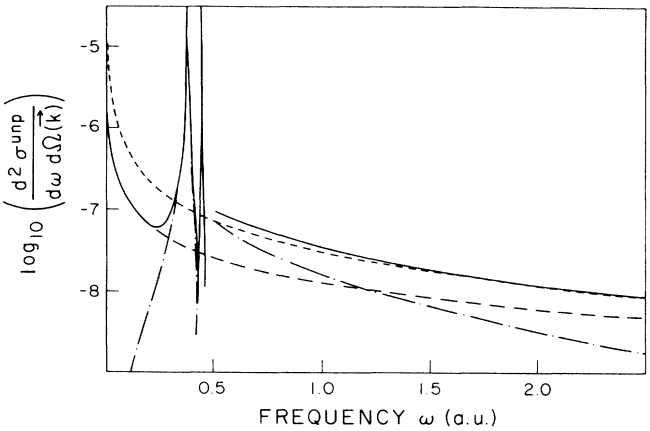

FIG. 2. Variations of $\log_{10}[d\sigma_{\text{unpol}}/(d\omega\, d\Omega)]$ in terms of the emitted photon frequency ω; $\theta=45°$, $k_i^2/2=10$ a.u. Short-dashed line, contribution of the Coulomb-Born term, Eq. (23b); long-dashed line, contribution of the electronic term, Eq. (20); dot-dashed line, atomic contribution; solid line, overall cross section Eq. (17). The cross section is expressed in units of $a_0^2/(2\ \text{Ry})$.

Coulomb-Born approximation in the following, provide a correct description of the bremsstrahlung spectra at photon frequencies well above the ionization threshold, see the discussion below.

(iv) *Small momentum transfer, Bethe-Born approximation:* $\Delta \to 0$. The calculation is notably simplified if one restricts oneself to the study of collisions resulting in a small momentum transfer. It is then convenient to expand the exponential $e^{i\Delta\cdot r}$ in powers of Δ and, if one retains only the first-order term $e^{i\Delta\cdot r}\sim 1+i\Delta\cdot\mathbf{r}$, one obtains the so-called Bethe-Born approximation for the transition amplitude. It immediately appears then that the electronic term vanishes since the dipolelike operator is not diagonal in the atomic basis. The remaining atomic terms also simplify and become

$$i\omega[M_{1s}(\Delta,\epsilon;E_{1s}-\omega)+M_{1s}(\Delta,\epsilon;E_{1s}+\omega)] \sim -\omega[\langle 1s|\epsilon\cdot\mathbf{r}G_c(E_{1s}-\omega)\Delta\cdot\mathbf{r}|1s\rangle + \langle 1s|\Delta\cdot\mathbf{r}G_c(E_{1s}+\omega)\epsilon\cdot\mathbf{r}|1s\rangle] . \quad (25)$$

The sum of the second-order matrix elements is proportional to the dipole dynamic polarizability $\alpha(\omega)$ of the ground state and one has

$$i\omega[M_{1s}(\Delta,\epsilon;E_{1s}-\omega)+M_{1s}(\Delta,\epsilon;E_{1s}+\omega)] \sim -\omega(\Delta\cdot\epsilon)\alpha(\omega) . \quad (26)$$

An explicit expression for $\alpha(\omega)$ can be obtained from our general formula for the matrix element, Eqs. (11) and (12), by taking the limit $\Delta\to 0$. After some algebra one recovers the known analytic formula which has been previously derived in several instances from a direct calculation, see Ref. 9, Eq. (21), and references therein.

This interesting result clearly shows the importance of the target dynamic polarizability on the physics of radiative collisions. It has served as a basis for general discussions on dynamic aspects of bremsstrahlung spectra.[4–7] It should be kept in mind, however, that it is valid only at small momentum transfer, i.e., for small-angle scattering and relatively low frequencies such that $k_i^2\sim k_f^2$. A detailed study of similar processes including free-free transitions,[9] and laser-assisted atomic excitation,[18] shows in fact that the Bethe-Born approximation has a very limited range of applicability and should be used with great caution.

Let us turn now to the discussion of our numerical results, obtained for the twofold differential cross section, Eq. (17), by using the analytical formula, Eqs. (14), for the atomic matrix elements. The computation of these latter quantities did not present special difficulties and was performed on a Macintosh-Plus microcomputer. In the high-frequency range $\omega > |E_{1s}|$, the hypergeometric functions ${}_2F_1$ contained in Eqs. (12) are very slowly convergent and we had to use standard analytic continuation formulas. The final angular integration over the propagation direction of the scattered electron was performed numerically, using an adapted form of a Gauss-Legendre quadrature.[14,19]

In Fig. 2 is presented the frequency dependence of the cross section at fixed incoming electron energy ($k_i^2/2=10$ a.u.) and emitted photon direction ($\theta=45°$). In addition to the exact cross section itself, we have also reported the variations of partial cross sections obtained by retaining only the contribution of either one of the electronic, or atomic or Coulomb-Born terms. Figure 2 illustrates several of the characteristic features of the dependences of the bremsstrahlung spectra on the photon frequency. In the low-frequency domain, the infrared divergence of the cross section is clearly shown. We observe also that, as expected, the electronic contribution, as given by Eq. (20), is by far dominant in this range and that the Coulomb-Born cross section, Eq. (23b), significantly overestimates the exact result.

The situation is completely reversed in the optical-vuv range (where vuv is vacuum ultraviolet) ($0.2\lesssim\omega\lesssim 0.5$), where the cross section is dominated by the atomic term, which exhibits a typical resonant behavior, see Fig. 2. In this range of frequencies the electronic contribution notably underestimates the cross section and, interestingly enough, the Coulomb-Born cross section seems to provide a smooth average of the exact result.

At still higher frequencies, i.e., above the ionization threshold $\omega > \frac{1}{2}$ a.u., the situation is again modified and one observes a steady decrease of the atomic term which does not contribute anymore at frequencies $\omega > 2$ a.u. see Fig. 2. In a parallel fashion the Coulomb-Born cross section, as given in Eq. (23b), provides an excellent approximation to the exact one, as was anticipated in our previous discussion of the high-frequency limit.

It is interesting to compare the present dispersion curve for spontaneous bremsstrahlung cross section, with the corresponding one obtained for (stimulated) free-free transitions in the frequency range $\omega\lesssim\frac{1}{2}$ a.u., see Ref. 9, Figs. 5 and 6. Common features in these curves are the infrared divergence as $\omega\to 0$ and the presence of resonances located at frequencies $\omega=\omega_{1n}$. However, the deep minima observed in the FFT dispersion curves[9] are no

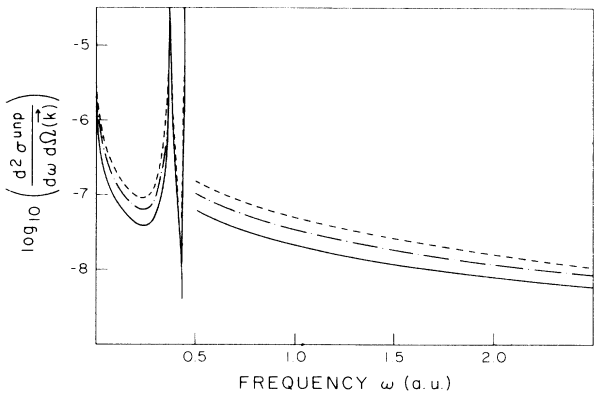

FIG. 3. Variations of $\log_{10}[d\sigma_{\text{unpol}}/(d\omega\, d\Omega)]$ in terms of the emitted photon frequency ω, at different kinetic energies $k_i^2/2$ of the incoming electron ($\theta=45°$). Dashed line, $k_i^2/2=5$ a.u.; dot-dashed line, $k_i^2/2=10$ a.u.; solid line, $k_i^2/2=20$ a.u. The cross section is expressed in units of $a_0^2/(2\text{ Ry})$.

longer present in the case of bremsstrahlung. This can be ascribed to the fact that in this latter case we have assumed that the scattered electron is not detected and that the polarization of the photon is not observed. As a consequence of the resulting integration and averaging processes, the minima are washed out. This clearly indicates that, unless the electron is detected in coincidence with the photon and the polarization state of this latter is observed, conventional bremsstrahlung cross sections are less rich in information about the dynamics of the collision than their FFT counterparts.

Figure 3 shows that the bremsstrahlung spectra depend only moderately on the kinetic energy of the incoming projectile. One observes that the cross section regularly decreases as $E_i = k_i^2/2$ increases, the dispersion curves being almost similar.

The dependence of the cross section on the incoming electron kinetic energy E_i at various photon frequencies and fixed emission angle ($\theta = 45°$) is shown in Fig. 4, which displays the variations of the different contributions to the cross section in terms of E_i within the range $5 \lesssim E_i \leq 20$ a.u.

Figure 4(a) illustrates the low-frequency regime: The electronic contribution almost coincides with the exact result while the Coulomb-Born result is significantly larger. The atomic term, which is too small to appear in the figure, does not contribute in this frequency range.

The case of ultraviolet radiation is illustrated in Fig. 4(b), corresponding to $\omega = 0.35$ a.u. The atomic term in then dominant and almost coincides with the exact results, the electronic and Coulomb-Born contributions being negligible.

In the high-frequency range ($\omega = 2$ a.u.), see Fig. 4(c), the Coulomb-Born approximation provides a fair esti-

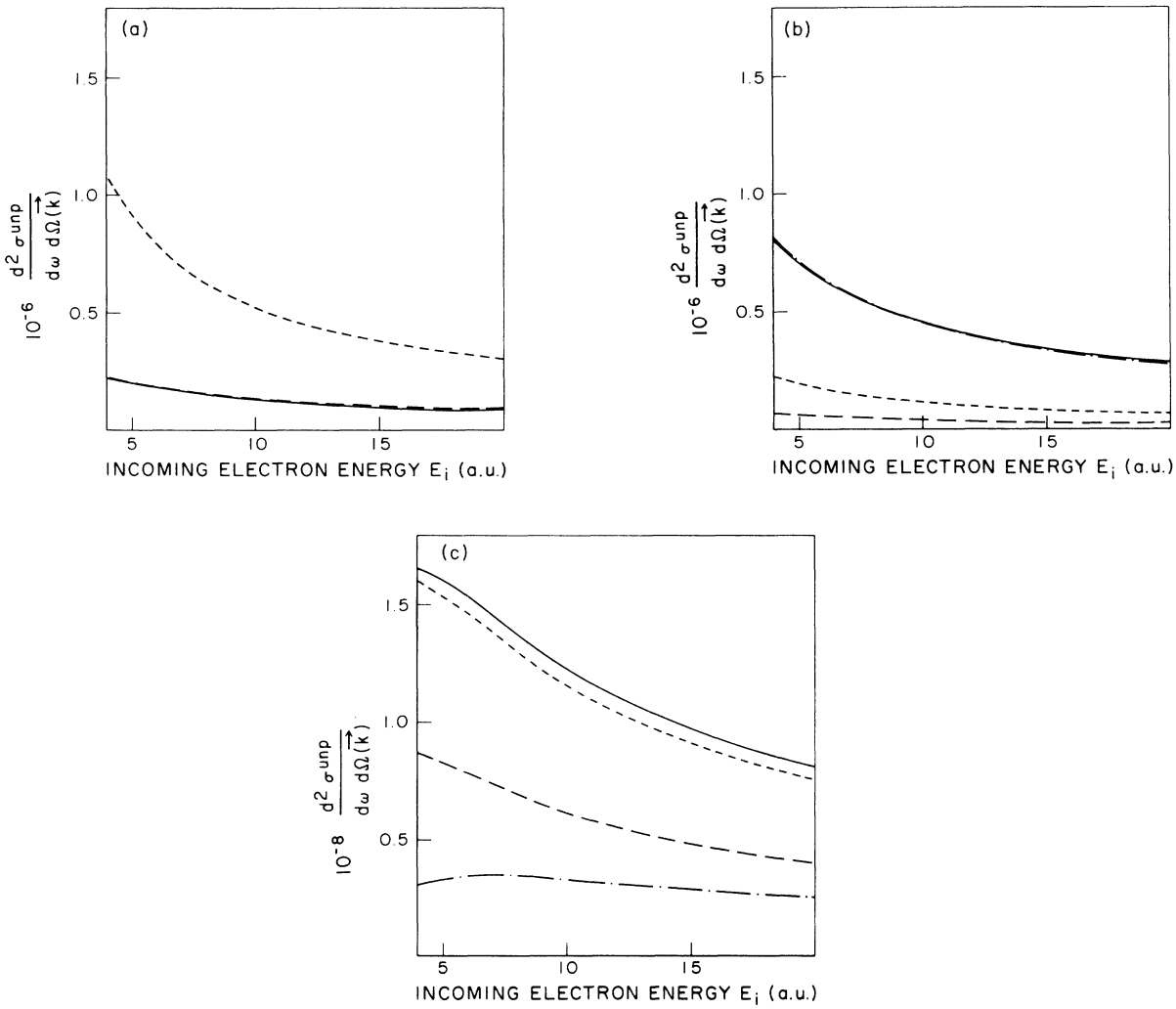

FIG. 4. Variations of the cross section $d\sigma_{\text{unpol}}/(d\omega d\Omega)$, expressed in units of $a_0^2/(2\ \text{Ry})$ as a function of the incoming electron energy $k_i^2/2$ at fixed angle of emission ($\theta = 45°$). (a) $\omega = 0.1$ a.u.; (b) $\omega = 0.35$ a.u.; (c) $\omega = 2$ a.u. Short-dashed line, Coulomb-Born approximation; long-dashed line, electronic contribution; dot-dashed line, atomic contribution; solid line, overall cross section.

mate of the exact result. Although they are not negligible, neither the atomic nor the electronic contributions can separately approximate the correct cross section. Note the change of scale for the cross section, this latter becoming much smaller in the high-frequency range.

IV. CONCLUSION

We have presented in this paper a theoretical analysis of the bremsstrahlung spectrum emitted during the course of collisions of relatively fast electrons with hydrogen atoms. We have identified different contributions to the overall cross section and compared their relative weights, depending on the frequency of the emitted photon and the magnitude of the momentum transfer.

The so-called electronic contribution, arising mainly from the projectile-field coupling, is dominant in the low-frequency (soft-photon) limit. In this case, the Low theorem[3] is applicable, and the cross section, which then varies as ω^{-1}, is proportional to the field-free elastic-scattering cross section.

The occurrence of resonances in the bremsstrahlung spectrum is recovered. In the corresponding frequency range such that $\omega \sim \omega_{1n}$, i.e., if ω is of the same order of magnitude as characteristic atomic excitation frequencies, the atom-field coupling dominates the physics of the process and the so-called atomic contribution coincides almost exactly with the overall cross section. This observation highlights the important role of the polarizability of the target in such radiative collisions.

At higher frequencies the screening of the Coulomb field of the nucleus by the atomic electron becomes negligible and the so-called Coulomb-Born approximation provides a fair description of the process. This stems from the fact that, in this frequency range, the atom-field coupling is much weaker and that accordingly, the physics of the process is dominated by the dynamics of the projectile-nucleus-field system.

The remarkably compact analytical expression, Eqs. (11)–(14), we have obtained for the transition amplitude has allowed us to perform all the numerical computations reported here on a microcomputer. The case of photon frequencies above the ionization threshold, which usually presents severe difficulties in similar calculations, was easily handled thanks to the use of standard analytic continuation formulas.

ACKNOWLEDGMENTS

One of us (A.M.) was a visiting fellow at the Joint Institute for Laboratory Astrophysics. One of us (A.D.) received support from the Institut Francais in Copenhagen.

APPENDIX: ANALYTIC CALCULATION OF THE MATRIX ELEMENTS $M_{1s}(\Delta,\epsilon;\Omega)$ EQ. (9)

The needed second-order matrix element can be obtained via the following differentiation process:[9]

$$M_{1s}(\Delta,\epsilon;\Omega)=\frac{1}{\pi}\frac{\partial}{\partial\mu}\frac{\partial}{\partial\mu'}\lim_{\Delta'\to 0}\left[i\epsilon\cdot\frac{\partial}{\partial\Delta'}\right]\times M_{\mu\mu'}(\Delta,\Delta';\Omega)\Big|_{\mu=\mu'=1}, \tag{A1}$$

where

$$M_{\mu\mu'}(\Delta,\Delta';\Omega)=\int\int d\mathbf{r}\,d\mathbf{r}'\frac{e^{-\mu' r'}}{r'}e^{-i\Delta'\cdot\mathbf{r}'}\times G_c(\mathbf{r}',\mathbf{r};\Omega)e^{i\Delta\cdot\mathbf{r}}\frac{e^{-\mu r}}{r}. \tag{A2}$$

A closed-form expression for this latter matrix element has been previously derived by Klarsfeld.[12] Its derivative with respect to Δ' is easily obtained and, after taking the limit $\Delta'\to 0$, one is left with the following expression:[9]

$$M_{1s}(\Delta,\epsilon;\Omega)=-i2^7x^3(\Delta\cdot\epsilon)\frac{\partial^2}{\partial\mu\,\partial\mu'}J(\mu,\mu')\Big|_{\mu=\mu'=1}, \tag{A3}$$

where

$$J(\mu,\mu')=[(\mu+x)^2+\Delta^2]^{-2}(\mu'+x)^{-4}\times\int_0^1 du\,u^{1-1/x}(1-u^+u)^{-2}(1-u^-u)^{-2}. \tag{A4}$$

Here $x=\sqrt{-2\Omega}$ and

$$u^{\pm}=\left[\frac{\mu'-x}{\mu'+x}\right]\left[\frac{\mu-x\pm i\Delta}{\mu+x\pm i\Delta}\right]. \tag{A5}$$

The integral entering the expression of $J(\mu,\mu')$ represents an Appell hypergeometric function F_1 of two variables,[20,21] the derivatives of which can be straightforwardly obtained.[9] We have found it convenient, however, to derive another expression of $M_{1s}(\Delta,\epsilon;\Omega)$, Eq. (A3), in terms of Gauss hypergeometric functions ${}_2F_1$ whose analytic continuation properties were more suitable here. To this end it is enough to rewrite the integrand of the integral in Eq. (A4) as follows:

$$(1-u^+u)^{-2}(1-u^-u)^{-2}=\frac{(u^+)^2}{(u^+-u^-)^2}\left[\frac{1}{(1-u^+u)^2}-\frac{2u^-}{(u^+-u^-)(1-u^+u)}\right]+\mathrm{sym}(u^+,u^-), \tag{A6}$$

which allows us to reexpress $J(\mu,\mu')$ as a sum of ${}_2F_1$ functions

$$J(\mu,\mu')=[(\mu+x)^2+\Delta^2]^{-2}(\mu'+x)^{-4}\frac{1}{2-1/x}\left\{\left[\frac{(u^+)^2}{(u^+-u^-)^2}\,{}_2F_1\left[2,2,-\frac{1}{x};3-\frac{1}{x};u^+\right]\right.\right.$$
$$\left.\left.-\frac{2(u^+)^2u^-}{(u^+-u^-)^3}\,{}_2F_1\left[1,2-\frac{1}{x};3-\frac{1}{x};u^+\right]\right]+\mathrm{sym}(u^+,u^-)\right\}. \quad \text{(A7)}$$

This expression can be notably simplified by using a contiguity relation between ${}_2F_1$ functions which, when specialized to our case, reads[21]

$${}_2F_1\left[p,2-\frac{1}{x};3-\frac{1}{x};u\right]$$
$$=\frac{(2-1/x)}{(2-1/x-p)}\frac{1}{(1-u)^p}$$
$$-\frac{p}{(2-1/x-p)}\,{}_2F_1\left[p+1,2-\frac{1}{x};3-\frac{1}{x};u\right] \quad \text{(A8)}$$

and, after some algebra, $J(\mu,\mu')$ can be expressed as

$$J(\mu,\mu')=A_1+B_1(+\Delta)+B_1(-\Delta), \quad \text{(A9)}$$

where

$$A_1=\frac{1}{1-1/x}\frac{(\mu-x)^2+\Delta}{2^5x^4\Delta^2(\mu'+x)^2[(\mu+\mu')^2+\Delta^2]},$$

$$B_1(+\Delta)=i\frac{1}{(2-1/x)(1-1/x)}\frac{(\mu^2-x^2-2i\Delta+\Delta^2)}{2^5x^3\Delta^3(\mu'^2-x^2)}$$
$$\times(u^+)^2\,{}_2F_1\left[2,2-\frac{1}{x};3-\frac{1}{x};u^+\right],$$

and $B_1(-\Delta)$ is obtained by substituting $\Delta\to-\Delta$.

The next step is to compute the derivatives with respect to the parameters μ and μ' [see Eq. (A3)]. This can be achieved by using the derivation formula[21]

$$\frac{d}{du}(u)^p\,{}_2F_1\left[p,2-\frac{1}{x};3-\frac{1}{x};u\right]$$
$$=p(u)^{p-1}\,{}_2F_1\left[p+1,2-\frac{1}{x};3-\frac{1}{x};u\right]. \quad \text{(A10)}$$

Then, by again using the contiguity relation Eq. (A8), one has

$$\frac{\delta}{\delta\mu}J(\mu,\mu')\Big|_{\mu=1}=A_2+B_2(+\Delta)+B_2(-\Delta), \quad \text{(A11)}$$

where

$$A_2=-\frac{(1+\mu')}{2^3x^3\Delta^2(\mu'+x)[(1+\mu')^2+\Delta^2]^2},$$

$$B_2(+\Delta)=-i\frac{(1+x)}{(2-1/x)4x\Delta^3(\mu'-x)^3(\mu'+x)(1-x+i\Delta)^2}$$
$$\times(u^+)^3\,{}_2F_1\left[3,2-\frac{1}{x};3-\frac{1}{x};u^+\right]\Big|_{\mu=1}.$$

The derivative with respect to the parameter μ' is computed in a similar way, and one obtains

$$\frac{\partial^2}{\partial\mu'\partial\mu}J(\mu,\mu')\Big|_{\mu'=\mu=1}=A_3+B_3(+\Delta)+B_3(-\Delta), \quad \text{(A12)}$$

where

$$A_3=\frac{3(4-3\Delta^2)}{2^3x^3\Delta^2(1-x^2)(4+\Delta^2)^3}, \quad \text{(A13a)}$$

$$B_3(+\Delta)=i\frac{3}{2(2-1/x)\Delta^3(1-x)^4(1+x)^2(1-x+i\Delta)^2}$$
$$\times(\tilde{u}^+)^3\,{}_2F_1\left[4,2-\frac{1}{x};3-\frac{1}{x};\tilde{u}^+\right], \quad \text{(A13b)}$$

with

$$\tilde{u}^+=\frac{(1-x)(1-x+i\Delta)}{(1+x)(1+x+i\Delta)}.$$

We have found it convenient to transform further the latter hypergeometric function, which leads to the following expression for $B_3(+\Delta)$:

$$B_3(+\Delta)=i\frac{3(1-x+i\Delta)}{2^4x^3(2-1/x)\Delta^3(1-x)(1+x)^2(2+i\Delta)^3}$$
$$\times{}_2F_1\left[1,-1-\frac{1}{x};3-\frac{1}{x};\tilde{u}^+\right]. \quad \text{(A13c)}$$

Replacing the expression Eq. (A12) for the derivatives in Eq. (A3) for the transition amplitude, one obtains the formulas, Eqs. (11) and (12), in the text. It should be noted that this expression is not unique and that given the numerous existing relations between contiguous ${}_2F_1$ functions, many equivalent formulas can be derived.

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[16]In the high-frequency regime discussed here, such as $\omega > |E_{1s}|$, the second-order matrix element $M_{1s}(\mathbf{\Delta}, \epsilon; E_{1s}+\omega)$ acquires also an imaginary part since the atom can be photonionized. This imaginary part, which is proportional to the photoionization amplitude times a generalized atomic form factor, remains very small for the reasons given in the text.

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