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Bremsstrahlung in collisions between electrons and atoms

B. A. Zon

Voronezh State University
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General formulas have been obtained which express the contribution of atomic electrons to the bremsstrahlung and absorption cross sections in electron-atom collisions in terms of the dynamic atomic polarisability. Application of these formulas enables experimental data on the optical breakdown threshold of alkali metal vapors to be brought into qualitative agreement with the cascade theory of breakdown.

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1. Bremsstrahlung and the absorption by electrons of photons when they are scattered by atoms play, as is well known, a determining role in the development of optical breakdown in gases.^[1] The same mechanism to a significant extent determines the heating of plasma by laser radiation, and also manifests itself in a number of other phenomena.

In theoretical calculations of the bremsstrahlung effect it is usually assumed that the electromagnetic quantum is absorbed or emitted by the scattered electron as a result of which the bremsstrahlung cross section can be related to the transport cross section for elastic (nonradiative) scattering of electrons by atoms.^[1,2] Although the question of the role played by atomic electrons in the emission and absorption of bremsstrahlung photons has been repeatedly discussed in the literature at the present time investigations of it do not exist. An exception is Ref. 3 in which the important role played by atomic electrons in bremsstrahlung was numerically demonstrated for the case of the scattering of electrons by the ground state of the hydrogen atom.

In the present paper the effect of atomic electrons on the bremsstrahlung cross section is investigated by utilizing a number of approximations of the theory of nonradiative electron-atom collisions. As a result of this we succeed in obtaining physically transparent formulas for arbitrary atoms which contain a single characteristic—the dipole dynamic polarisability of an atom at the frequency under consideration.

2. We first state some elementary considerations which enable us to understand the principal result.^[4] We consider induced bremsstrahlung which arises in the scattering of electrons by atoms in the presence of a

strong electromagnetic wave of frequency ω . Under the action of the electric field of the wave the atom becomes polarized and long range forces $\sim 1/r^2$ of the "charge-dipole" type appear which significantly alter the cross section for the process.

For an atom in an S-state the polarisability is a scalar, and the scattering potential has the form

$$V(r, t) = V_A(r) + \frac{e\alpha(\omega)}{r^3} (\mathbf{E}_0 \cdot \mathbf{r}) \cos \omega t,$$

where

$$V_A(r) = -\frac{e^2 Z}{r} + e^2 \sum_{j=1}^Z \frac{1}{|\mathbf{r} - \mathbf{r}_j|}$$

is the interaction between an electron and an atom in the absence of the wave, Z is the nuclear charge, \mathbf{r}_j are the coordinates of the atomic electrons, \mathbf{E}_0 is the amplitude of the electric field of the wave, which in the dipole approximation depends only on the time, α is the polarisability of the atom at the frequency ω .

We write the wave function for an electron in the field of the wave in the form ($c = \hbar = 1$)

$$\psi_p(\mathbf{r}, t) = \exp \left\{ i\mathbf{p} \cdot \mathbf{r} - \frac{i}{2m} \int_0^t \left(\mathbf{p} + \frac{e\mathbf{E}_0}{\omega} \sin \omega t' \right)^2 dt' \right\}.$$

The probability of scattering $\mathbf{p} \rightarrow \mathbf{p}'$ determined in the first Born approximation is by the expression

$$dw_{pp'} = \left| \int d\mathbf{r} dt \exp \left\{ i\mathbf{q} \cdot \mathbf{r} + i\mathbf{p} \cos \omega t - \frac{i}{2m} (\mathbf{p}^2 - \mathbf{p}'^2) t \right\} \times \left[V_A(\mathbf{r}) + \frac{e\alpha(\omega)}{r^3} (\mathbf{E}_0 \cdot \mathbf{r}) \cos \omega t \right] \right|^2 \frac{d^3 \mathbf{p}'}{(2\pi)^3},$$

where $\mathbf{q} = \mathbf{p} - \mathbf{p}'$ is the transferred momentum, $\rho = e\mathbf{q}\mathbf{E}_0/\omega^2$.

Expanding $\exp(i\rho \cos \omega t)$ in a Fourier series we obtain for the scattering cross section (cf., Ref. 5)

$$d\sigma^{(s)}(\mathbf{p}, \mathbf{p}') = \frac{4m^2}{q^4} \frac{p'}{p} \left| e^s J_s(\rho) [Z - F(\mathbf{q})] - \frac{1}{2} \rho m \omega^2 \alpha(\omega) [J_{s-1}(\rho) - J_{s+1}(\rho)] \right|^2 d\Omega_{\mathbf{p}'}.$$
 (1)

Here $F(\mathbf{q})$ is the atomic form factor, J are Bessel functions. The value $s=0$ corresponds to elastic ($p=p'$) scattering, $s>0$ corresponds to scattering with absorption of s quanta, $s<0$ corresponds to scattering with emission of $|s|$ quanta. But for $|s|\geq 2$ formula (1) becomes, generally speaking, inaccurate since subsequent approximations of perturbation theory in terms of the interaction between an atom and radiation lead to the dependence of the cross section on the atomic polarizability at frequencies $2\omega, 3\omega, \dots$

In the optical range of frequencies $\rho \lesssim 1$ up to fields $\sim 10^8$ V/cm. Utilizing this circumstance we expand the Bessel functions in (1) in power series

$$d\sigma^{(0)}(\mathbf{p}, \mathbf{p}') = \frac{4m^2}{q^4} \frac{p'}{p} \left| e^0 [Z - F(\mathbf{q})] + \frac{1}{2} \rho^2 m \omega^2 \alpha(\omega) \right|^2 d\Omega_{\mathbf{p}'}.$$
 (2)

$$d\sigma^{(\pm 1)}(\mathbf{p}, \mathbf{p}') = \frac{m^2}{q^4} \frac{p'}{p} \rho^2 |e^{\pm 1}[Z - F(\mathbf{q})] + m \omega^2 \alpha(\omega)|^2 d\Omega_{\mathbf{p}'}.$$
 (3)

It can be easily seen that the interaction of the atomic electrons with the field which leads to the second terms within the absolute value signs in (2), (3), almost does not change the elastic scattering ($s=0$) due to the small value of the factor ρ^2 . At the same time simple numerical estimates show the important role played by atomic electrons in transitions accompanied by absorption or emission of optical photons ($s\neq 0$) practically for all neutral atoms.

3. We now carry out more rigorous calculations which enable us to establish the limits of applicability of formulas (1)–(3) and to obtain generalizations of them.

We shall consider the interaction of an atom and a scattered electron with an electromagnetic wave in the dipole approximation which turns out to be quite satisfactory for optical frequencies. In the second quantization utilized here for a unified treatment of both forced and spontaneous transitions, and in the interaction representation, the corresponding part of the Hamiltonian is given by

$$V_1 = ie \sum_{\mathbf{k}\lambda} (2\pi\omega)^{1/2} (\mathbf{R}_{\mathbf{k}\lambda})^\mu [\mathbf{a}_{\mathbf{k}\lambda}^\dagger - \mathbf{a}_{\mathbf{k}\lambda}], \quad \mathbf{R} = \mathbf{r} + \sum_{j=1}^z \mathbf{r}_j,$$

where $\mathbf{a}_{\mathbf{k}\lambda}^\dagger, \mathbf{a}_{\mathbf{k}\lambda}$ are the operators for the creation and annihilation of photons of momentum \mathbf{k} and a unit polarization vector $\mathbf{e}_{\mathbf{k}\lambda}$. In the first order in each of the operators V_A, V_γ , the cross section for scattering with emission of a bremsstrahlung photon and transition of the atom from the state i to the state f can be represented, without taking exchange effects into account, in the following form:

$$d\sigma^{(-1)}(\mathbf{p}_i, \mathbf{p}'_f) = \frac{e^2 (N_{\mathbf{k}\lambda} + 1)}{\pi^2 q^4 \omega^3} \frac{p'}{p} |\mathbf{M}_{\mathbf{e}_{\mathbf{k}\lambda}}|^2 d\Omega_{\mathbf{p}'}, \quad (4)$$

where

$$\begin{aligned} \mathbf{M} = & e^2 \mathbf{q} [Z \delta_{fi} - F_{fi}(\mathbf{q})] + im e \omega^2 \sum_n \left[\frac{\langle f | d | n \rangle F_{ni}(\mathbf{q})}{\omega_{ni} - \omega} \right. \\ & \left. + \frac{F_{fn}(\mathbf{q}) \langle n | d | i \rangle}{\omega_{ni} + \omega} \right] \end{aligned} \quad (5)$$

$$F_{st}(\mathbf{q}) = \left\langle s \left| \sum_{j=1}^z e^{i\mathbf{q}\mathbf{r}_j} \right| t \right\rangle. \quad (6)$$

Here $N_{\mathbf{k}\lambda}$ are the occupation numbers for the photons, \mathbf{d} is the dipole moment of the atom, $E_i + p^2/2m = E_f + p'^2/2m + \omega$, the summation over n is carried out over all the states of the atom including the continuous spectrum. The first term in (5) corresponds to the emission of a photon by the incident electron, the second term corresponds to the emission of a photon by the electrons of the atom.

In discussing induced emission in the presence of a monochromatic field of frequency ω , $N_{\mathbf{k}\lambda} \gg 1$, one should integrate in (4) over $d^3\mathbf{k}$ over a small range of propagation vectors near the vector representing the external field. Denoting

$$\frac{1}{8\pi^3} \int N_{\mathbf{k}\lambda} d^3\mathbf{k} = F,$$

where F is the flux of quanta of polarization λ crossing unit area per unit time, we obtain

$$d\sigma_{\text{ind}} = \frac{8\pi e^2 F}{q^4 \omega^3} \frac{p'}{p} |\mathbf{M}_{\mathbf{e}_{\mathbf{k}\lambda}}|^2 d\Omega_{\mathbf{p}'}.$$
 (7)

In the case of spontaneous emission, $N_{\mathbf{k}\lambda} \ll 1$, we carry out in (4) summation over the polarization λ and an integration over the directions of \mathbf{k}

$$d\sigma_{\text{spont}}^{(-1)} = \frac{8\pi^2}{3\pi q^4 \omega} \frac{p'}{p} (\mathbf{M} \mathbf{M}^*) d\Omega_{\mathbf{p}'} d\omega. \quad (8)$$

In the case of inverse bremsstrahlung—absorption of a photon of the external field—the cross section differs from (4), (5) by the replacement $N_{\mathbf{k}\lambda} + 1 \rightarrow N_{\mathbf{k}\lambda}$, $\omega \rightarrow -\omega$. In this case $E_i + p^2/2m + \omega = E_f + p'^2/2m$, while the quantity $d^3\mathbf{k}$ is interpreted as the density of the incident photons. In the general case of partial polarization of incident radiation the cross section should be averaged over the polarizations. Introducing the polarization density matrix $\rho_{\mu\nu}$:

$$\frac{1}{8\pi^3} \left\langle \int N_{\mathbf{k}\lambda} (\mathbf{e}_{\mathbf{k}\lambda})_\mu (\mathbf{e}_{\mathbf{k}\lambda})_\nu d^3\mathbf{k} \right\rangle_\lambda = F \rho_{\mu\nu},$$

we obtain

$$d\sigma^{(1)} = \frac{8\pi e^2 F}{q^4 \omega^3} \frac{p'}{p} (\rho_{\mu\nu} \mathbf{M}_\mu \mathbf{M}_\nu^*) d\Omega_{\mathbf{p}'}.$$
 (9)

Here the prime on the quantity \mathbf{M} denotes the replacement $\omega \rightarrow -\omega$, a summation over the subscripts μ, ν is carried out over the values of x, y if the wave is being propagated along the z axis. In such a case

$$\rho_{\mu\nu} = \frac{1}{2} \begin{pmatrix} 1+\xi_3 & \xi_1 - i\xi_2 \\ \xi_1 + i\xi_2 & 1-\xi_3 \end{pmatrix}$$

where ξ are the Stokes parameters.

Depending on the scattering angle the value of q which determines the magnitude of the matrix element (6) varies within certain limits determined by the conservation law. If a are the atomic dimensions then $q_{\min}a \ll 1$, while for electrons of energy greater than ~ 100 eV, $q_{\max}a \gg 1$. The same matrix element F_{st} , (6) determines in the first Born approximation the amplitude for the transition of the atom between the states s and t in the case of a non-radiative scattering of the electron. From the theory of atomic collisions it is well known that the amplitude F_{st} is exponentially small for scattering at large angles for which $qa \gg 1$. In virtue of this the main contribution to the integral scattering cross section is made by such angles for which $qa \lesssim 1$.^[6] This enables us to limit ourselves in the evaluation of F_{st} to the lowest terms in the expansion of the exponential which give a nonzero result due to the selection rules in terms of angular momentum.

Thus, if we are not interested in the angular distribution of electrons accompanying bremsstrahlung, the circumstance noted above enables us to simplify significantly the formula for the amplitude (5). We consider here the case when the states i and f are of the same parity and differ in total angular momentum by 0, ± 2 . In such a case the diagonal matrix elements F_{si} do not appear in the sum (5) and in accordance with the statements made above it is possible to introduce the replacement $e^{i\mathbf{q}\cdot\mathbf{r}} - iq \cdot \mathbf{r}$, as a result of which we have:

$$M_a = e^2 [Z\delta_{fi} - F_{fi}(\mathbf{q})] q_a - m\omega^2 q_b (c_{ba}(-\omega))_{ji} \quad (10)$$

where

$$(c_{ba}(\omega))_{ji} = \sum_n \left[\frac{\langle f | d_b | n \rangle \langle n | d_a | i \rangle}{\omega_{ni} + \omega} + \frac{\langle f | d_a | n \rangle \langle n | d_b | i \rangle}{\omega_{ni} - \omega} \right]$$

is the tensor for the scattering of light by an atom which satisfies the selection rules indicated above. In the case of scattering by an atom in an S-state and for $i=f$, the tensor c_{ba} is diagonal and coincides with the dynamic polarizability of the atom at the frequency ω . In such a case the substitution of (10) into (7) leads to formula (3), if one takes into account that $F = E_0^2 / 8\pi\omega$. At the present time there is published in the literature a large number of calculation of dynamic polarizabilities of particular atoms over wide frequency ranges, reference to some of which is made in Ref. 7. In the case of a hydrogen atom one can obtain analytic formulas for the scattering tensor c_{ba} . In Ref. 8 corresponding expressions are given for the $1S - 1S$, $2S$, $3d$, $2S - 2S$ transitions. Calculations utilizing these formulas of the integral cross section for the induced bremsstrahlung in the case of scattering by the ground state of a hydrogen atom of an electron of momentum $3/a_B$ (a_B is the Bohr radius) which was investigated in Ref. 3 without the replacement $e^{i\mathbf{q}\cdot\mathbf{r}} - iq \cdot \mathbf{r}$ utilized in the present work, have demonstrated a practically identical agreement with the results of this paper.

If an electric dipole transition between the states i and f is allowed its amplitude in the approximation under

consideration can also be transformed and expressed in terms of the tensor for the scattering of light by the atom when one of the photons is a quadrupole photon.

4. The cross section for spontaneous emission (8) is of particular interest since it determines the absorption coefficient of a weakly ionized gas.^[11] We investigate this quantity in greater detail restricting ourselves to transitions not involving a change in the S-state of the atom:

$$d\sigma_{\text{spont}}^{(-1)} = \frac{8e^2}{3\pi q^2 \omega} \frac{p'}{p} |e^2 [Z - F(\mathbf{q})] - m\omega^2 \alpha(\omega)|^2 d\Omega_p d\omega. \quad (11)$$

From this formula it is easy to obtain the presently widely used connection between the total cross section for bremsstrahlung absorption and the transport cross section for the elastic scattering of an electron by an atom σ_t , if one neglects the polarizability of the atom and takes the electron energy to be considerably greater than ω ^[1, 2]:

$$\frac{d\sigma_{\text{spont}}^{(-1)}}{d\omega} = \frac{4}{3\pi} \frac{e^2 v^2}{\omega} \sigma_t, \quad v = p/m,$$

$$\sigma_t = 4m^2 e^4 \int q^{-4} (1 - \cos \theta) |Z - F(\mathbf{q})|^2 d\Omega_p,$$

As is well known, the principal contribution to the transport cross section under the conditions of applicability of the Born approximation is made by scattering angles $1 \gg \theta \gg v_0/v$, where $v_0 \approx 1/ma$ is the characteristic velocity of atomic electrons.^[6] The second term in (11) which determines the contribution of atomic polarizability to bremsstrahlung is here evaluated for scattering angles $\theta \lesssim v_0/v$ for which $qa \lesssim 1$. For larger angles it, as has already been stated, is exponentially small. Therefore in the integral cross section the two terms do not interfere, and the contribution of the polarization term can be calculated independently. Assuming, just as before, $p^2/2m\omega \gg 1$, we obtain

$$\begin{aligned} \frac{d\sigma_{\text{spont}}^{(-1)}}{d\omega} &= \frac{4}{3\pi} \frac{e^2 v^2}{\omega} \sigma_t + \frac{16}{3} e^2 m^2 \omega^3 \alpha^2(\omega) \frac{p'}{p} \int_0^{\theta_0} q^{-2} \sin \theta d\theta \\ &= \frac{4}{3\pi} \frac{e^2 v^2}{\omega} \sigma_t + \frac{8e^2 \omega^3}{3v^2} \alpha^2(\omega) \ln \left(1 + \frac{\gamma p^2}{m^2 \omega^2 a^2} \right). \end{aligned} \quad (12)$$

Here $\theta_0 = \gamma/pa$ is the limiting angle up to which the integration should be carried out, γ is a factor of the order of unity. The quantity which determines the value of the logarithm can be rewritten in the following manner $p^2/m^2 \omega^2 a^2 = (p^2/m\omega)(\Lambda\pi/a^2)$, where Λ is the Compton wavelength of the electron, π is the wavelength of the emitted radiation. It can be easily seen that this quantity is quite large and therefore the dependence of the result (12) on the value of γ is insignificant. For the same reason we can omit unity in the argument of the logarithm.

A characteristic feature of the second term in (12)—the “polarization radiation”—is its strong dependence on the frequency ω , due both to the factor ω^3 and to the frequency dependence of the dynamic polarizability which is particularly significant in the range $I^* < \omega < I_i$, where I^* , and I_i are respectively the excitation and the ionization potentials of the atom, and also its dependence on

the electron velocity which is different compared to "transport radiation."

5. In Ref. 9 the thresholds for the breakdown of Rb and Cs vapors by radiation from a ruby laser were measured. Breakdown was observed at densities approximately four orders of magnitude lower than for He, Ar, Hg. As was noted in Ref. 9, very low thresholds in cesium and rubidium are incompatible with all the theoretical explanations of the phenomenon proposed until now.

Use of formula (12) enables us in this case to reduce such a sharp divergence between theory and experiment. Indeed, the polarizabilities of Rb and Cs at the ruby laser frequency amount to approximately - 1200 and - 800 atomic units respectively.^[10] For electron velocities $\sim 10^8$ cm/sec using for the transport cross sections the theoretically calculated values of 4×10^{-15} cm²,^[11] we find that the "polarization" term in (12) is greater than the "transport" term by a factor of approximately 130. As regards He, Ar and Hg, for them the polarization term does not change the cross section as a result of the small polarizabilities of these atoms at the frequency under consideration. Utilizing for them the experimentally known transport cross sections $\sim 6 \times 10^{-16}$ cm², it can be easily seen that for Rb and Cs the probability for the scattering by an atom of an electron with a change in its momentum exceeds by approximately three orders of magnitude the corresponding values for He, Ar, Hg. In accordance with the elementary theory of optical breakdown this leads to a difference by three orders of magnitude in densities at which breakdown occurs. The remaining discrepancy by approximately an order of magnitude between experiment and the estimates given above can no longer be regarded as one involving a matter of principle. It can be connected with the difference in the ionization potentials of two groups of atoms (this was pointed out in Ref. 1) and also with

the inaccuracy of the first approximation utilized here of perturbation theory in terms of the interaction between an atom and an incident electron.

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