Bremsstrahlung cross section in scattering of an electron by a hydrogen atom

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(Submitted February 12, 1975)
Zh. Éksp. Teor. Fiz. **69**, 108–114 (July 1975)

The cross section for one-photon bremsstrahlung in scattering of an electron by a hydrogen atom is calculated in the Born approximation. The cross section is expressed in the form of a sum over the intermediate states of the atom. In contrast to the work known to us on this question, in this article the sum has been calculated over all intermediate states of the atom. Therefore the results presented here are suitable not only when the atom can be considered as the source of the external field in which the scattering of the electron occurs, but in the general case when the contribution to the cross section of the target atom is systematically taken into account. The possibility is noted of using the results in quantum electronics (in the theory of laser breakdown in a gas and in the problem of emission amplification in free-free electron transitions).

PACS numbers: 34.70., 79.2—.K

1. INTRODUCTION

Calculation of the cross section for bremsstrahlung is one of the best known problems of quantum electrodynamics, and the solutions of this problem are the subject of various monographs and reviews (see for example refs. 1 and 2). Usually one considers bremsstrahlung which arsies as the result of scattering of an electron in the specified external field of a proton or target atom. In the case of the proton this approach is quite unsatisfactory. In regard to scattering by an atom, it is evident that the atom can only be approximately considered as the source of the external field, and in actuality the target atom is an independent dynamic system with its degrees of freedom; this system must enter into the Hamiltonian of the problem on an equal basis with the incident electron.

Calculation shows that the cross section for one-photon bremsstrahlung in the Born approximation is the sum of perturbation theory over all intermediate states of the atom. To obtain results which would be suitable not just for resonance values of the radiation frequency,[3] it is necessary to calculate this sum. In the present article, as far as we know, the sum over all intermediate states of the atom in the bremsstrahlung problem is calculated for the first time. This permits calculation of the bremsstrahlung cross section as a function of the radiation frequency with a consistent account of the target atom contribution.

The importance of this type of calculation is determined particularly by the requirements of quantum electronics: Bremsstrahlung and the corresponding absorption (inverse bremsstrahlung) are being studied at the present time theoretically as an amplification mechanism[4] and as the mechanism of laser breakdown in gases.[5]

2. BREMSSTRAHLUNG CROSS SECTION

We shall calculate the cross section for induced bremsstrahlung in second-order perturbation theory: first order in the interaction (K) of the atom and incident electron with the external magnetic field and first order in the interaction (U) of the electron with the atom. Bremsstrahlung and inverse bremsstrahlung can be accompanied by a simultaneous change of the state of the atom. The cross section for induced bremsstrahlung is expressed by the following formula (in atomic units):

$$d\sigma_{n_f n_i}=\frac{p_f}{p_i(2\pi)^2}|A_{fi}|^2\,d\Omega. \tag{1}$$

Here **p** is the incident electron momentum, dΩ is the element of solid angle in **p** space, n is the set of quantum numbers characterizing the state of the atom; i and f denote the initial and final states of the system. The process which is described by the cross section $d\sigma^{\omega}_{n_f n_i}$ consists in radiation of a photon ω with simultaneous transition of the atom from the state n_i to the state n_f. The transition amplitude A_{fi} is determined by the formula

$$A_{fi}=\Sigma_i+\Sigma_f,\quad \Sigma_i=\sum_{s\neq s_f}\frac{U_{fs}L_{si}}{\varepsilon_f-\varepsilon_s},\quad \Sigma_f=\sum_{s\neq s_i}\frac{L_{fs}U_{si}}{\varepsilon_i-\varepsilon_s},$$

$$H_0=H_a+H_e,\quad H_0\Phi_s=\varepsilon_s\Phi_s,$$

$$\Phi_s=\varphi_n(\mathbf{r}_a)e^{i\mathbf{pr}},\quad H_a\varphi_n=E_n\varphi_n,\quad \varepsilon_s=E_n+p^2/2,$$

$$U=-\frac{Z}{r}+\frac{1}{|\mathbf{r}-\mathbf{r}_a|},\quad K=2\cos\omega t\cdot L(\mathbf{r},\mathbf{r}_a),$$

$$L=\alpha(\nabla_{\mathbf{r}}+\nabla_{\mathbf{r}a}),\quad \alpha=\frac{i}{2\omega}\mathbf{E}_0,\quad l^a=\alpha\nabla_{\mathbf{r}a}. \tag{2}$$

The amplitude A_{fi} is the sum over the intermediate states of the atom and incident electron. The matrix elements $U_{ss'}$ and $L_{ss'}$ are calculated in the wave functions Φ_s of the "unperturbed" Hamiltonian H_0; H_a and H_e are the Hamiltonians and $\mathbf{r}_a$ and **r** are the radius vectors of the atomic and incident electrons; s is the set of quantum numbers n; and **p**, φ_n, and E_n are the wave function and energy of the stationary state of the atom. In the Born approximation the incident electron is described by a plane wave (we use normalization to a basic region whose volume is equal to unity) and at the same time we can neglect the exchange of electrons.[6] The interaction of the electrons with the electromagnetic field is taken in the dipole approximation; $\mathbf{E}_0$ is the amplitude of the electric vector of the electromagnetic wave. It is assumed that Z is the charge of the nucleus of the atom, so that all analytical results refer also to a hydrogen-like ion.

3. CALCULATION OF SUMS OVER THE INTERMEDIATE STATES

There is a procedure which permits calculation of the sum (2) over the intermediate states. We will show that the sums Σ_i and Σ_f can be represented in the form of definite integrals over the entire configuration space:

$$\Sigma_i=\int d\tau\,\Phi_f^* U w_i,\quad \Sigma_f=\int d\tau\, w_f^* U\Phi_i,\quad d\tau=d\mathbf{r}\,d\mathbf{r}_a, \tag{3}$$

if the auxiliary functions w_i and w_f satisfy the following differential equations:

$$(H_0-\varepsilon_f)w_i=-L\Phi_i,\quad (H_0-\varepsilon_i)w_f=-L\Phi_f. \tag{4}$$

We shall be interested in what follows only in that special case in which any eigenfunction associated with an eigenvalue ϵ_f is orthogonal to the right-hand side of the equation for w_i, and any eigenfunction associated with the eigenvalue ϵ_i is orthogonal to the right-hand side of the equation for w_f. We shall discuss particular solutions of the equations (4) which can be represented in the form of an expansion in eigenfunctions of the operator H_0:

$$w_i=\sum_{s\neq s_f}\frac{L_{si}}{\varepsilon_f-\varepsilon_s}\Phi_s,\quad w_f=\sum_{s\neq s_i}\frac{L_{sf}}{\varepsilon_i-\varepsilon_s}\Phi_s. \tag{5}$$

Then expanding the right-hand sides of the equations (4) in series in eigenfunctions of the operator H_0 and substituting the formulas (5) into the equations (4), we see that the expressions (5) are actually solutions of the equations (4). Formulas (5) determine solutions orthogonal to the solutions of the homogeneous equations corresponding to the given inhomogeneous equations. It is evident that the condition of orthogonality together with the requirement that the functions w_i and w_f can be expanded in series in eigenfunctions in the operator H_0 uniquely determine the solutions of each of the equations (4). Finally, in order to convince ourselves of the validity of the expressions (3), it remains to substitute formulas (5) into formula (3) and to compare the result obtained with the expressions (2) for the sums Σ_i and Σ_f.

The method described above for the summation was derived for the nondiagonal matrix elements from the variational principle previously.[7] There we considered the more general case in which for degeneracy of the levels ϵ_i and ϵ_f the orthogonality conditions used above are not satisfied. It is interesting to note that equations (4) have a simple physical meaning. The ordinary formulation of the problem in the theory of quantum transitions consists in considering transitions under the action of a nonstationary perturbation K between stationary states of the system, which is described by a Hamiltonian $H_0 + U$. Another formulation of the problem is possible in which we consider transitions between nonstationary states of a system which is described by a Hamiltonian $H_0 + K$ under the action of a non-time-dependent perturbation U. In both cases the same transition amplitude is obtained in the form of the sum (2). However, in the second case the perturbation theory equations reduce in an obvious way to the equations (4) which contain the spatial part of the perturbation K—the operator L. These equations are simpler than the equations of stationary perturbation theory, which contain a significantly more complicated perturbation U (in the equations of stationary perturbation theory the variables are not separable, while in Eq. (4) the variables are separable).

In the problem discussed here the summation over the intermediate states of the system reduces essentially to just the summation over the intermediate states of the atom. Actually, after substitution of the function Φ_s from Eq. (2) into the initial expressions for the sums Σ_i and Σ_f and calculation of the matrix elements $L_{ss'}$ the sums over the incident electron states vanish. As a result we obtain

$$A_{fi}=\sum_n\frac{U_{n_f\mathbf{p}_f,\,n\mathbf{p}_i}l^a_{nn_i}}{E_{n_i}-\omega-E_n}+\sum_n\frac{l^a_{n_fn}U_{n\mathbf{p}_f,\,n_i\mathbf{p}_i}}{E_{n_f}+\omega-E_n}+\frac{iU_{fi}\alpha(\mathbf{p}_f-\mathbf{p}_i)}{\omega}. \tag{6}$$

It is easy to see that for definite values of the radiation frequency ω, resonances arise in the transition amplitude A_{fi}. It is also evident that we must limit the calculations to the frequency region in which the departure from the resonance in absolute value is greater than the widths of the corresponding atomic levels.

Let us now turn to the solution of equations (4). The functions w_i and w_f we will seek in the form

$$w_{i,f}=u_{i,f}^a(\mathbf{r}_a)\exp(i\mathbf{p}_{i,f}\mathbf{r})+u_{i,f}(\mathbf{r})\varphi_{n_{i,f}}(\mathbf{r}_a). \tag{7}$$

Substituting this expression into equation (4), we obtain an equation for the functions $u^a_{i,f}$ and $u_{i,f}$:

$$(H_a-E_{n_{i,f}}\pm\omega)u^a_{i,f}(\mathbf{r}_a)=-\alpha\nabla_{ra}\varphi_{n_{i,f}}(\mathbf{r}_a), \tag{8}$$

$$(H_e-{}^1/_2p_{i,f}\pm\omega)u_{i,f}(\mathbf{r})=-i\alpha\mathbf{p}_{i,f}\exp(i\mathbf{p}_{i,f}\mathbf{r}). \tag{9}$$

The solutions of Eqs. (9) are of the form

$$u_{i,f}(\mathbf{r})=\mp\frac{i\alpha\mathbf{p}_{i,f}}{\omega}\exp(i\mathbf{p}_{i,f}\mathbf{r}). \tag{10}$$

To solve Eqs. (8) it is necessary to specify the form of the initial and final atomic functions $\varphi_{n_{i,f}}$. We will consider induced bremsstrahlung without excitation of the atom ($n_i = n_f$). Then $\varphi_{n_{i,f}}$ is the wave function of the ground state of the hydrogen atom or hydrogen-like ion. We shall seek solutions of (8) in the form

$$u^a_{i,f}=\rho\cos\theta e^{-\rho/2}v(\rho),\quad \rho=2\beta_{i,f}r_a\quad \beta_{i,f}=(Z^2\pm2\omega)^{1/2}. \tag{11}$$

For the function $v(\rho)$ we obtain the equation (the subscripts i and f have been omitted)

$$\rho\frac{\partial^2v}{\partial\rho^2}+(4-\rho)\frac{\partial v}{\partial\rho}-\left(2-\frac{Z}{\beta}\right)v=-\gamma\exp\left[\pm\frac{\omega\rho}{\beta(\beta+Z)}\right],\quad \gamma=\frac{\alpha Z^{5/2}}{2\beta^2\sqrt{\pi}}. \tag{12}$$

The solution of this equation in the form of a power series has the form

$$v=\gamma\sum_{k=0}^{\infty}a_k\rho^k,\quad a_{k+1}=\frac{(k+2-Z/\beta)a_k-b_k}{(k+1)(k+4)},\quad b_k=\frac{(\pm\omega)^k}{\beta^k(\beta+Z)^kk!}. \tag{13}$$

The constant a_0 must be chosen so that the solution of the initial equation (4) can be expanded in series in eigenfunctions of the Hamiltonian H_0. This requirement reduces to definite conditions which must be satisfied by the function $v(\rho)$ for $\rho = 0$ and $\rho \to \infty$. For purely technical reasons it is convenient to go over to a new unknown function $f(\rho)$:

$$f(\rho)=e^{-\rho/2}\rho^2v(\rho),$$

$$\mathrm{F}\ \frac{\partial^2f}{\partial\rho^2}+\left(-\frac{1}{4}+\frac{Z}{\beta\rho}+\frac{{}^1/_4-({}^3/_2)^2}{\rho^2}\right)f=-\gamma\rho e^{-Z\rho/2\beta}. \tag{14}$$

The general solution of Eq. (14) can be expressed in terms of the fundamental system of solutions of the corresponding homogeneous equation (the Whittaker equation[8]) $W = W_{Z/\beta,3/2}(\rho)$, $M = M_{Z/\beta,3/2}(\rho)$:

$$f=\frac{\gamma}{\Delta}\left[M(\rho)\int_\rho^\infty W(\rho')e^{-Z\rho'/2\beta}\rho'\,d\rho'+W(\rho)\int_0^\rho M(\rho')e^{-Z\rho'/2\beta}\rho'\,d\rho'\right],$$

$$\Delta\equiv W\frac{\partial M}{\partial\rho}-M\frac{\partial W}{\partial\rho}. \tag{15}$$

In this equation the limits of integration are chosen so that the function $f(\rho)$ is finite as $\rho \to 0$ and falls off as $\rho \to \infty$. This assures the possibility of expanding the initial functions w_i and w_f in series in eigenfunctions of the operator H_0. From Eq. (15) we obtain the limit of the function f as $\rho \rightarrow 0$ and consequently the value of the coefficient a_0:

$$a_0 = \frac{16}{(2-Z/\beta)(Z/\beta+1)^4} F\left(4, 2-\frac{Z}{\beta};\ 3-\frac{Z}{\beta};\ \frac{\mp 2\omega}{(Z+\beta)^2}\right). \quad (16)$$

Having solved the equations (4) in this way, we substitute the functions w_i and w_f into the integrals (3) and obtain a final analytical expression for A_{fi} and consequently for the differential cross section $d\sigma^{\omega}_{n_e n_i}$:

$$A_{fi} = \frac{i8\pi Z^4 \alpha q}{q^2}\left[\sum_{k=0}^{\infty} C_k^i B_k^i - \sum_{k=0}^{\infty} C_k^f B_k^f + \frac{1}{\omega}\left(\frac{8}{(4Z^2+q^2)^2} - \frac{1}{2Z^3}\right)\right],$$

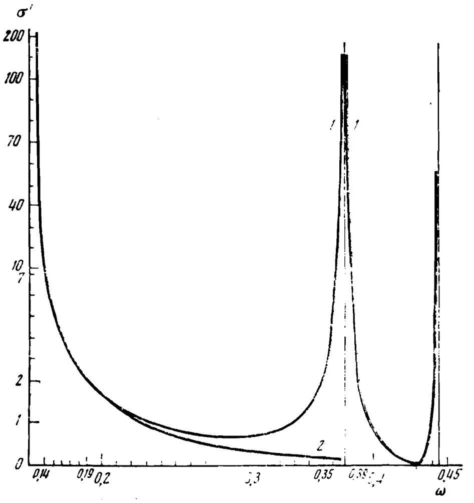
$$C_k = \frac{2^{k+1}\beta^{k-1}(k+1)!}{q^3[(Z+\beta)^2+q^2]^{(k+3)/2}} a_k, \qquad q = p_f - p_i,$$

$$B_k = (k+3) q \cos\left[(k+3)\operatorname{arctg}\frac{q}{Z+\beta}\right] - (Z+\beta)\sin\left[(k+3)\operatorname{arctg}\frac{q}{Z+\beta}\right]. \quad (17)$$

4. DISCUSSION OF RESULTS

In the figure we have shown the results of calculation (curve 1) of the integrated cross section $\sigma^{\omega}_{1s,1s} = \int_{(\Omega)} d\sigma^{\omega}_{1s,1s}$ for induced bremsstrahlung in scattering of an electron by a hydrogen atom as a function of the frequency ω (up to the frequency which corresponds to the transition between the first and third terms of the atom).

In accordance with Eq. (6) the cross section rises in a resonance manner near the points $\omega = E_n - E_{1s}$, where n refers to the discrete spectrum (the singularity at $\omega = 0$ corresponds to the infrared catastrophe). Curve 2 gives the cross section in the approximation of a specified field (the electron is scattered in the screened field of the nucleus). Such scattering is described by the last term in Eq. (6). Ordinarily only this term is taken into account in calculation of the bremsstrahlung cross section (see for example refs. 1 and 2). Comparing curves 1 and 2, we see that systematic inclusion of the contribution of the target atom to the cross section is extremely important, particularly near resonances. It is true that in the region rather close to a resonance there is no need of taking into account the entire sum over the intermediate states of the atom, and it is sufficient to take into account only the corresponding resonance term. However, already at a frequency $\omega = 0.4$ it is necessary to sum over all intermediate states and in addition at this frequency it is impossible to consider the scattering as occurring in a specified external field (in accordance with Eq. (17) for $\omega = 0.4$ the integrated cross section in relative units is $\sigma' = 0.9$; on taking into account only the resonance term in the amplitude of Eq. (6), we have $\sigma' = 1.3$, and, finally, the last term in Eq. (6) gives $\sigma' = 0.1$; $\sigma' = 10^{-2}\sigma^{\omega}_{1s,1s}/E_0^2$). This shows that there is a region of frequencies where the results obtained in the present work are important.



Bremsstrahlung cross section $\sigma^{\omega}_{1s,1s}$ in a hydrogen atom in atomic units–curve 1, $p_i = 3$, $E_0 \perp p$; curve 2 shows the bremsstrahlung cross section calculated in the approximation of a specified field. For convenience we have used a nonuniform scale as indicated in the figure (between the points marked by numbers along the axes, the scale is uniform).

Thus, accurate inclusion of the target-atom contribution to the bremsstrahlung cross section leads to new results: to appearance of resonances and also to an appreciable departure of the cross section from that which is obtained on considering scattering in the screened field of the atom, even for frequencies relatively far from a resonance.

We note that in the problem of amplification of radiation, which arises as the result of scattering of the electron with bremsstrahlung, the amplification coefficient near resonance frequencies[9] turned out to be significantly greater than the gain calculated from the formula for scattering in a specified external field.[10]

The cross section $\sigma^{\omega}_{n_i n_i}$ refers to the photon radiation process in which the state of the atom is not changed. Strictly speaking, for experimental determination of this cross section it is necessary to measure the number of electrons with an energy which is smaller than the initial electron energy by an amount ω (more accurately, the change of this number on including the momentum of the light). It is evident that simultaneously with the radiation there is also absorption of the photon (the cross sections of these processes are related by the Einstein relation). As a result, electrons appear with an energy greater than the initial energy by an amount ω. In considering laser breakdown in definite frequency intervals it is necessary to use the formulas for the absorption cross section in which the target-atom contribution is accurately taken into account. We have turned our attention to this in ref. 11.

In regard to the total cross section for radiation of a photon of a given frequency ω, it is obviously determined by the sum of the cross sections $\sum_{n_f}\sigma^{\omega}_{n_f n_i} \equiv \sigma^{\omega}_{n_i}$ over all final states of the atom n_f whose excitation is compatible with the conservation of energy. The cross section $\sigma^{\omega}_{n_i n_i}$ calculated here is the lower limit of the total cross section for radiation of a photon. Therefore the calculation of the total cross section can only aggravate the conclusion that inclusion of the resonance nature of bremsstrahlung is important.

We are grateful to S. I. Anisimov, I. B. Levinson, and É. I. Rashba for helpful discussion of this work. The questions discussed in this paper have been discussed on numerous occasions with F. V. Bunkin, and we take this occasion to express our gratitude to him.

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Translated by C. S. Robinson
12