The role of atomic electrons in bremsstrahlung

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The cross section for bremsstrahlung emitted in the scattering of a nonrelativistic electron is calculated in the approximation $\omega \gg I$ (the frequency of the radiation is much larger than the ionization energy of any of the atomic electrons). It is shown that, in contrast with the results in the low-frequency case ($\omega \ll I$) [V. M. Buĭmistrov and L. I. Trakhtenberg, Sov. Phys. JETP 42, 54 (1975)] at large frequencies a form factor cannot be used to take account of the influence of the atomic electrons, and a detailed consideration of their role in the process is required.

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Bremsstrahlung is produced when an electron collides with other atomic particles. In bremsstrahlung theory the collision of an electron with a proton is considered as the scattering of the electron in a given point-charge field, and this treatment is exact. (See, for example,[1–3].)

For radiative scattering of an electron by an atom the situation is more complicated. Although it is obvious that the atomic electrons make up an independent dynamical system with its own degrees of freedom (the Hamiltonian for the problem must contain the Hamiltonian H_a of the atom and the operator for the interaction of the atomic electrons with the electromagnetic field), this is not taken into account in most published work (see, for example, the survey in[2] and the monograph[3]). As a rule, what is considered is the radiation emitted in the scattering of the electron on the "potential of the atom"[3]: the atomic electrons are included only as a source of the external field, screening the field of the nucleus. In this way the many-particle problem is replaced with a one-particle problem, and it is assumed that the results are not changed in any important way.

In our previous papers[4–6] and in the present one it is shown that the difference turns out to be important in certain ranges of the frequency and the momentum transfer $\mathbf{q}$. Since the approximation of a fixed "potential of the atom" is equivalent to the introduction of a form factor, restrictions are thus placed on the applicability of the concept of a "form factor" in the theory of bremsstrahlung. Percival and Seaton[7] were evidently the first to point out that when the frequency of the emitted photon is close to one of the frequencies of atomic transitions the bremsstrahlung cross section increases. Obviously this result cannot be derived, even qualitatively, in the one-particle problem. The importance of treating the total scattering amplitude (including the nonresonance regions) as an amplitude for bremsstrahlung was pointed out in[4]. Thereafter the bremsstrahlung cross section for the scattering of an electron on a hydrogen atom was calculated over a wide range of frequencies (smaller than the ionization energies of the atom), and it was shown that the introduction of a form factor is justified for the emission of photons of sufficiently small frequencies (this was done for the dipole approximation of scattering theory in[5], and in the general case in[6]).

In the present paper the bremsstrahlung cross section is calculated for photons of frequencies much larger than the largest ionization energy of the atom. In this case also it is essential to use a many-particle formulation of the problem; It alone gives the correct formula for the cross section in the high-frequency limit, which can be derived by an independent argument.

The Hamiltonian for the system is

$$H=H_a+H_e+H_r+U+K,$$
$$K=\sum_{l,\sigma,j}(a_{l,\sigma}\exp\{i\varkappa_l\mathbf{r}_j\}+a^{+}_{l,\sigma}\exp\{-i\varkappa_l\mathbf{r}_j\}](\boldsymbol{\alpha}_{l\sigma}\nabla_{\mathbf{r}_j}), \qquad (1)$$
$$\boldsymbol{\alpha}_{l\sigma}=i(2\pi/\omega_l)^{1/2}\mathbf{e}_\sigma.$$

Here H_e is the Hamiltonian of the incident election, and H_r is that of the free quantized radiation field; $\mathbf{r}_j(\mathbf{r}_0, \mathbf{r}_1, \ldots, \mathbf{r}_N)$ are the radii vectors of the incident and atomic electrons; U is the energy of interaction between the incident electron and the atom; $a^{+}_{l\sigma}$ and $a_{l\sigma}$ are the creation and destruction operators of photons with frequency ω_l, wave vector $\varkappa_l$, and polarization $\sigma(\sigma=1,2)$; $\mathbf{e}_\sigma$ are the polarization unit vectors; the normalization is to unit volume of the fundamental region; and l is the set of numbers l_x, l_y, l_z ($l_{x,y,z}=0, 1, 2, \ldots$).

In second-order perturbation theory one gets the following formula, in atomic units, for the cross section for spontaneous bremsstrahlung (in the dipole approximation).

$$d\sigma^\omega=\frac{\omega^2}{(2\pi)^5c^3}\frac{p_f}{p_i}|A_{fi}|^2d\Omega_{\mathbf{p}_f}d\Omega_\varkappa d\omega,$$

where

$$A_{fi}=\frac{4\pi}{q^2}\left\{\frac{i\boldsymbol{\alpha}\mathbf{q}}{\omega}(Z\delta_{n_fn_i}-F_{n_fn_i}(q))+\sum_{n,j,j'}\frac{\langle n_f|e^{i\mathbf{q}\mathbf{r}_j}|n\rangle\langle n|\boldsymbol{\alpha}\nabla_{\mathbf{r}_{j'}}|n_i\rangle}{E_{n_i}-\omega-E_n}\right.$$
$$\left.+\sum_{n,j,j'}\frac{\langle n_f|\boldsymbol{\alpha}\nabla_{\mathbf{r}_{j'}}|n\rangle\langle n|e^{i\mathbf{q}\mathbf{r}_j}|n_i\rangle}{E_{n_f}+\omega-E_n+i\varepsilon}\right\}, \qquad (2)$$
$$F_{n_fn_i}(q)=\langle n_f|\sum_{j=1}^{N}e^{i\mathbf{q}\mathbf{r}_j}|n_i\rangle, \quad \mathbf{q}=\mathbf{p}_i-\mathbf{p}_f, \quad \varepsilon\to+0.$$

Here $\mathbf{p}$ is the momentum of the incident electron; n is a set of quantum numbers which specify a state of the at-

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om; i and f denote the initial and final states of the system; Z is the atomic number; and $F_{n_f n_i}(q)$ is the form factor of the atom. The photon is emitted in the frequency interval $d\omega$ and into the solid angle $d\Omega_\varkappa$, and the electron is scattered into the solid angle $d\Omega_{\mathbf{p}_f}$; $A_{fi} \sim U \cdot K$.[6]

Expanding the transition amplitude (2) for high frequencies in a power series in $(E_n - E_{n_{i,f}})/\omega$ and retaining only the first three terms of the expansion, we get the following expression:

$$A_{fi}=i\frac{4\pi}{\omega q^2}\left(\alpha q Z\delta_{n_f n_i}+\frac{1}{\omega^2}\langle n_f|\sum_{j,j'}e^{i\mathbf{q}\mathbf{r}_j}(\alpha\nabla_{\mathbf{r}_{j'}})(\mathbf{q}\nabla_{\mathbf{r}_j}U_a)|n_i\rangle\right). \quad (3)$$

Here U_a is the potential energy of the interaction of the atomic electrons with each other and with the nucleus.

In the derivation of Eq. (3) one makes use of the relation

$$(E_{n'}-E_n)\langle n'|\hat{B}|n\rangle=\langle n'|[H_a,\hat{B}]|n\rangle,\quad \hat{B}=\alpha\nabla\mathbf{r}_j. \quad (4)$$

For the hydrogen atom and for hydrogenlike ions, the expression (3) can be simplified when $q \ll 1$ and $n_f = n_i$. The result is the following formula for the cross section for spontaneous bremsstrahlung:

$$d\sigma^\omega=\frac{(\mathbf{e}_\sigma\mathbf{q})^2Z^2}{\pi^2c^3\omega q^4}\frac{p_f}{p_i}\left(1+\frac{4\pi}{3\omega^2}|\psi_{n_i}(0)|^2\right)^2 d\Omega_{\mathbf{p}_f}d\Omega_\varkappa d\omega. \quad (5)$$

Here Ψ_{n_i} is the wave function of the initial state of the hydrogenlike ion. It can be proved rigorously that the absolute value of the difference between the exact value of $d\sigma^\omega$ and the first term of Eq. (5) is smaller than const/ω^3.

For sufficiently large ω the cross section for bremsstrahlung in the scattering of an electron on an atom is the same as that for scattering on the nucleus. This result can be understood without any calculations. If the inequality

$$p_{i,f}^2/2 \gg I,\quad \omega \gg I, \quad (6)$$

holds, where I is the ionization energy of the atom, the atomic electron can be approximately regarded as free. Since the bremsstrahlung amplitude for electron-electron scattering is zero in the dipole approximation in both quantum theory[1] and classical theory[8] the total scattering amplitude on the atom reduces to that on the nucleus.

Let us now examine the bremsstrahlung cross section calculated with the "atomic potential"

$$d\sigma^\omega=\frac{(\mathbf{e}_\sigma\mathbf{q})^2}{\pi^2c^3\omega q^4}\frac{p_f}{p_i}\left(1-\frac{16}{(4+q^2)^2}\right)^2 d\Omega_{\mathbf{p}_f}d\Omega_\varkappa d\omega. \quad (7)$$

The scattering on the proton is described by the first term in the parentheses in Eq. (7); the effect of the atomic electron is merely to diminish the effective charge, as it must be according to the meaning of the concept of screening. For scattering through the angle $\theta = 0$ the value of q is $q = 2\omega/(p_i + p_f)$. Now for the condition $q \ll 1$, which is compatible with the inequalities (6), the bremsstrahlung cross section does not become the cross section for scattering on the nucleus; small values of q correspond to large impact parameters, and consequently to complete screening (according to Eq. (7) $d\sigma^\omega \to 0$ for $q \to 0$). The ratio of the cross sections calculated from Eqs. (5) and (7) varies from 500 down to 8 as q varies from 0.3 to 1; if $p_i \approx 10$ at.u, this means a change of θ from 0 to 5°. If we also take into account the fact that under the given conditions (which assure that the inequality $p_{i,f}^2/2 \gg \omega$ holds) the classical formula gives the correct intensity for the bremsstrahlung from scattering of electrons on the nucleus, we conclude that Eq. (7) does not approach the classical theory in the limit. This makes it obvious that the effect of the atomic electrons in bremsstrahlung does not reduce to screening. (For $q \gg 1$ Eqs. (2), (3) and (7) agree up to quantities $\approx 1/\omega^2$ and $1/q^4$, since for sufficiently small values of the impact parameter the screening is small. Along with this it must be emphasized that in this case the effect of the atomic electron on the bremsstrahlung cross section, so far as it has any importance at all, must be taken into account by using Eq. (3).)

At first glance it is tempting to suppose that only the first term in the transition amplitude (2) describes the bremsstrahlung, while the second is due to some other effect. Such an approach is unsuitable, since both terms are derived from the statement of a single physical problem. In full accordance with established tradition we define bremsstrahlung as the effect in which an electron being scattered on an atom emits in a single quantum act a photon whose energy is exactly equal to the difference of the energies of the electron before and after the scattering. Then in the many-particle case both terms necessarily appear in the transition amplitude. To make the transition amplitude receive only the first term we would have to solve the problem formulated physically in just the same way by using the less accurate one-particle approximation.

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[1]V. B. Berestetskiĭ, E. M. Lifshitz, and L. I. Pitaevskiĭ, Relyativistskaya kvantovaya teoriya (Relativistic quantum theory), Part I, "Nauka," 1968. English translation: Pergamon Press, 1974, two volumes.
[2]H. Koch and J. Motz, Revs. Mod. Phys. **31**, 920 (1959).
[3]H. A. Bethe and E. E. Salpeter, Quantum mechanics of one- and two-electron systems, Berlin, Springer Verlag, 1957.
[4]V. M. Buĭmistrov, Ukr. Fiz. Zh. **17**, 640 (1972).
[5]V. M. Buĭmistrov and L. I. Trakhtenberg, Trudy Mosk. Fiz.-Tekh. Inst., Radiotekh. Elektr., Part 2, 1971.
[6]V. M. Buĭmistrov and L. I. Trakhtenberg, Zh. Eksp. Teor. Fiz. **69**, 108 (1975) [Sov. Phys. JETP 42, 54 (1975)].
[7]I. S. Percival and M. I. Seaton, Phil. Trans. Roy. Soc. A251, 113 (1958).
[8]W. Panofsky and M. Phillips, Classical electricity and magnetism, Addison-Wesley, 1962.

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