Bremsstrahlung of electrons on atoms with allowance for polarizability

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It is shown that the cross section for the bremsstrahlung of electrons at a quantum energy on the order of the ionization potential is determined by the virtual excitations of the target atom. An actual calculation is carried out for electrons scattered by argon and xenon.

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The amplitude of bremsstrahlung of electrons on atoms breaks up naturally into two parts, one of which is expressed only in terms of the wave functions of the electron elastically scattered by the given atom, and the other in terms of the characteristics of the target atom.

The first part describes the emission of a quantum by the incident electron, where the second describes the emission of the atom itself, which is virtually excited by the electrons scattered from it. Usually[1] one considers only the contribution of the "electronic" emission, and the "atomic" emission is neglected. This approximation is valid for very low energies ω of the emitted quantum ($\omega \ll I$, where I is the ionization potential of the atom), and becomes utterly incorrect at $\omega \gtrsim I$. The present paper is devoted to a proof of this statement and to a calculation of the contributions of both the "electronic" and the "atomic" radiation. It is shown that the contribution of the "atomic" radiation, which is commensurate with the "electronic" one at low energies of the incident electron, becomes dominant at high energies of the latter.

We consider first the case of slow electrons. It is more convenient technically here to investigate not the radiation but the inverse process—inverse bremsstrahlung of a quantum. This process has been investigated, by way of an example, for argon and xenon atoms, which are a convenient object for a possible experimental study. In the language of the diagrams of many-body theory, the amplitude of the "electronic" absorption is shown in Fig. 1a,

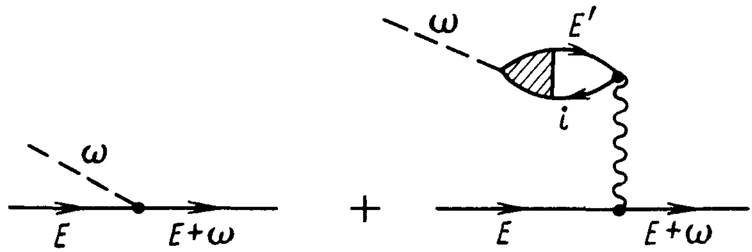

FIG. 1

whereas that of the "atomic" absorption due to the polarization of the atom by the incident electron is shown in Fig. 1b. The line with the arrow to the right represents the electron, to the left the hole i, the dashed line represents the photon, and the wavy line the Coulomb interaction U. The wave functions—electron and hole—were calculated in the Hartree—Fock approximation. The shaded triangle represents the effective dipole-moment operator D with allowance for the interaction of the electron E' and the hole I with each other, calculated in the random-phase approximation with exchange (RPAE).[2] The corresponding amplitude takes the form

$$F^{r}_{E,E+\omega} = (E|\vec{\epsilon}\mathbf{d}|E+\omega) + \sum_{\substack{i\lesssim F\\ E'>F}} (E,i|U|E+\omega,E')\,\frac{2(E'+I_i)}{\omega^2-(E'+I_i)^2}\,(E'|\vec{\epsilon}\mathbf{D}(\omega)|i), \tag{1}$$

where ϵ is the photon polarization vector, $\mathbf{d}=\mathbf{r}$,[1)] and the summation is over the occupied ($\lesssim F$) and free ($>F$) states. The amplitude D is determined in this approximation by solving an integral equation. For noble gases, the role of the interaction between the electron E' and the hole i is large, so that the matrix element D differs substantially from the matrix element d.[2]

The inverse-bremsstrahlung cross section is connected with the amplitude $F_{E,E+\omega}$ by the relation

$$\sigma_k^{l\to l_1}(\omega) = \frac{8\pi^4}{3}\,\frac{\kappa}{k^3 k_1}\,|F_{El;E+\omega,l_1}|^2, \tag{2}$$

where k, l, and $k_1 l_1$ are the initial and final angular momenta of the electron, while κ is the photon momentum. The matrix element $F_{El;E+\omega,l}$ is obtained from (1) after separating the angle variables and integrating in the cross section over all the direction of the electron momentum in the final state $-\mathbf{k}_1(l_1=l\pm 1)$. We considered slow electrons with energy $E=0.01$—0.09 Ry. At so low an energy we can confine ourselves to the contribution of the s and p waves, with $l=0$ and 1. The main contribution to the polarizability is made by virtual excitations of the outer shells, $-3p\to E'd;E's$ for Ar and $5p\to E'd;E's$ for Xe. The summation in (1) included also integration over the continuous spectrum. All the calculations were made by numerical methods. We note that in the approximation employed by us, just as in the calculation with the exact wave functions, the cross sections $\partial_k^{l\to l}$ in the form (2) and the velocities coincide.[2] The amplitude of the "electron" radiation at $\omega\sim I$ turns out to be smaller and of opposite sign than that of the "atomic" radiation. The results

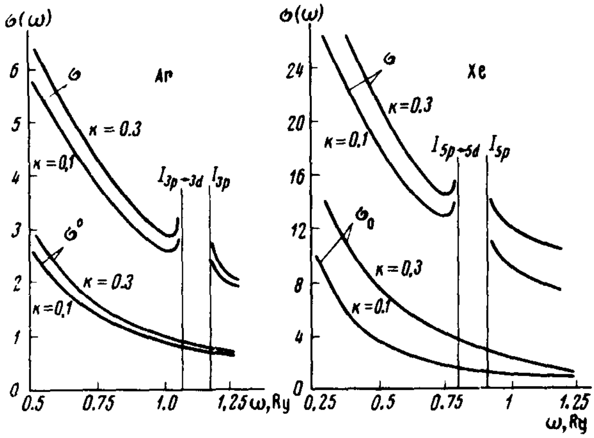

FIG. 2. Plots of $\sigma(\omega)$ and $\sigma^0(\omega)$ in Ar and Xe: $\sigma(\omega)$ includes "electronic" and "atomic" absorption, $\sigma^0(\omega)$ is the cross section for "electronic" absorption. $I_{\rm res}$ is equal to $I_{3p\to3d}$ for Ar and $I_{5p\to5d}$ for Xe.

of the calculations are shown in Fig. 2, where $\sigma(\omega) = (3k\epsilon/16\pi^4)\times\sigma_k$, and σ_k is given by (2).

The growth of σ_k at small ω is connected with the infrared divergence, and as $\omega \to I_{\rm res}$ (the excitation energy of the resonant levels) it is connected with the vanishing of the denominator in (1).

With increasing E, the relative role of the "atomic" radiation at $\omega \sim I$ becomes even larger. Choosing plane waves as the wave functions of the scattered electron, we obtain for the amplitude F

$$F_{p,|\mathbf{p}-\mathbf{q}|} = \frac{W(q)(\mathbf{q}\vec{\epsilon})}{\omega} + \frac{6\omega}{q^2}\sum_{\substack{E'>F\\ i\leqslant F}} \frac{(i|J_1(qr)\cos(\widehat{\mathbf{qr}})|E')(E'+I_i)(E'|\vec{\epsilon}\mathbf{D}(\omega)|i)}{(E'+I_i)^2-\omega^2}, \tag{3}$$

where p is the momentum of the incident electron, q is the momentum transferred to the atom, $W(q)$ is Fourier transform of the self-consistent atomic field, J_1 is a spherical Bessel function, and $\omega = p^2/2 - (\mathbf{p}-\mathbf{q})^2/2$. At small $q(q\sim\omega/p)$ we have from (3)

$$F_{p,|\mathbf{p}-\mathbf{q}|} \sim \left[\frac{W(0)q}{\omega} + \frac{\omega}{q}\alpha_1(\omega)\right], \tag{4}$$

where $\alpha_1(\omega)$ is the dipole dynamic polarizability of the atom. Approximating by way of estimate $W(r) = -Ze^{-\mu r}/r(\mu\sim\sqrt{I}$ and Z is the charge of the nucleus) and recognizing that $\alpha_1(\omega)$ exceeds $\alpha_1(0)$ up to the ionization threshold, we obtain for the ratio η of the amplitudes of the "atomic" and "electronic" radiation the relation $\eta \gtrsim p^2/I \gg 1$. It is important to note that, as shown by calculation the main contribution to the amplitude of the "atomic" radiation on atoms is made not by discrete excitations, but by the continuous spectra. According to (4), as $\omega \to 0$ and $\omega \to \infty$, the amplitude F is negative, and at $\omega \to I$ it is larger than zero. Therefore F and σ_k vanish both at $\omega < I_{res}$ and at $\omega > I$.

The results allow us to state that "atomic" radiation plays an important and sometimes the principal role in bremsstrahlung at $\omega \sim I$. This radiation must thus be taken into account in investigations of the bremsstrahlung process.

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[1)]We use a system of units with $e = \hbar = m = 1$, and with the energy in Rydbergs.

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[2]M. Ya. Amusia and N. A. Cherepkov, Case Studies in Atomic Physics **5**, 47 (1976).