Effect of resonances in elastic scattering on the bremsstrahlung of electrons in an atomic field

L. G. D'yachkov, G. A. Kobzev, and G. É. Norman

Institute of High Temperatures, USSR Academy of Sciences

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The role of resonances in elastic electron-atom scattering involving radiation emission and absorption by an electron is considered. An approach developed by Fano for describing the effect of autoionization on the photoionization and photorecombination spectra is employed. It is shown that the resonance can be approximately described as an unstable negative ion; the cross sections for the corresponding processes of photodetachment and photoattachment may exceed by an order of magnitude or more the cross sections for bremsstrahlung processes in the visible and ultraviolet spectral ranges.

Bremsstrahlung of slow electrons in the fields of atoms has been investigated theoretically and experimentally (see[1] and the references contained therein). This process can play an important role in plasma radiation. Another well investigated case is one in which the electron–atom system has a level corresponding to a stable negative ion. The contribution of photoattachment of electrons to atoms makes a much larger contribution to the plasma radiation than bremsstrahlung at frequencies higher than the threshold frequency (see, e.g.,[2]).

We consider in this paper the bremsstrahlung of an electron in the field of an atom in the case when the electron–atom system has a resonant state. It is shown that allowance for the resonance can increase the bremsstrahlung intensity by one order of magnitude and more. This increase can be interpreted as the contribution of the photo attachment with production of an unstable negative ion. This process is particularly important for plasma, where there are no stable negative ions. Expressions are obtained for the cross sections and for the absorption coefficient. The disintegration of resonant states by microfields in the plasma is discussed. The magnitude of the microfields increases with increasing charge density in the plasma, and accordingly the concentration of the resonances is decreased and the photocontinuum produced by them is suppressed. The theory developed is applied to a nitrogen plasma. The experimentally observed excess continuum is explained as a photoattachment continuum with formation of the unstable ion $N^{-3}P$.

1. The considered resonances are analogous to the autoionization states of atoms, so that we can see for their description the formalism developed by Fano[3,4] for autoionization. In the zero-order approximation, the electron–atom system has a set of states, including the continuum ψ_E and a discrete level E_φ lying in the continuum. In the presence of configuration interaction the stationary wave functions of the Hamiltonian $\hat{H}$ of the system can be expressed by a linear combination of φ and ψ_E:

$$\Psi_E = a(E)\varphi + \int dE' b_{E'}(E)\psi_{E'}. \tag{1}$$

By diagonalizing the energy matrix, Fano[3] found the coefficients in formula (1) and the shifted value of the level energy E_0:

$$|a(E)|^2 = (\Gamma/2\pi)[(E-E_0)^2+(\Gamma/2)^2]^{-1}, \tag{2}$$

$$b_{E'}(E) = a(E)\,\mathrm{P}\frac{V_{E'}}{E-E'} + \frac{(E-E_0)\delta(E-E')}{[(E-E_0)^2+(\Gamma/2)^2]^{1/2}}, \tag{3}$$

$$\Gamma = 2\pi|V_E|^2, \quad V_E = \langle\psi_E|\hat{H}|\varphi\rangle, \tag{4}$$

$$E_0 = E_\varphi + \mathrm{P}\int dE'|V_{E'}|^2(E-E')^{-1}. \tag{5}$$

The symbol P in (3) and (5) means that the integral is taken in the sense of the principal value. The quantity Ψ_E at $E \approx E_0$ is the wave function of a quasidiscrete level with width Γ, and coincides with ψ_E at $(E-E_0)/\Gamma \to \infty$.

2. We consider the case when the atom is in the state ^1S and when the electron is attached an unstable negative ion is produced with one nl_0 electron on the outer shell; later on we shall generalize the results for an arbitrary term of the atom and N equivalent nl_0 electrons. The bremsstrahlung cross section is described in the single-electron approximation by the expression (see[5])

$$\frac{d\sigma_{E,E'\omega}}{d\omega} = \frac{4\pi^2\omega^3}{3c^3E}\sum_{l=1}^{\infty} l[(R_{E,l-1}^{E'l})^2+(R_{El}^{E',l-1})^2], \tag{6}$$

$$R_{El}^{E'l'} = \int P_{El} r P_{E'l'}\,dr, \tag{7}$$

where P_{El} is the radial wave function of an electron with energy E and orbital angular momentum l.

$$\int P_{El}P_{E'l}\,dr = \delta(E-E'),$$

$\omega = E-E'$, c is the speed of light, and atomic units are used throughout.

The configuration interaction "mixes" the continuum P_{El_0} with the resonant level, so that in accordance with (1) the wave function $\tilde{P}_{El_0}$ for an electron with angular momentum l_0 is

$$\tilde{P}_{El_0} = a(E)P_{nl_0} + \int dE' b_{E'}(E)P_{El_0}.$$

If one of the numbers l or l' ($l' = l \pm 1$) in the matrix element (7) coincides with l_0, then the corresponding wave function P_{El} or $P_{E'l'}$ should be replaced by the function $\tilde{P}$. Let us assume that $l' = l_0$. Then, substituting $\tilde{P}_{E'l_0}$ in (7) in place of $P_{E'l'}$ we get

$$|\tilde{R}_{El}^{E'l_0}|^2 = (R_{El}^{E'l_0})^2 + \frac{\Gamma/2\pi}{(E'-E_0)^2+(\Gamma/2)^2}\left[\left|R_{El}^{nl_0}+\mathrm{P}\int dE''\frac{V_{E''}}{E'-E''}R_{El}^{E''l_0}\right|^2 - \frac{\pi\Gamma}{2}(R_{El}^{E'l_0})^2\right] + 2\,\mathrm{Re}\,\frac{V_{E'}^*(E'-E_0)}{(E'-E_0)^2+(\Gamma/2)^2}R_{El}^{E'l_0}\left(R_{El}^{nl_0}+\mathrm{P}\int dE''\frac{V_{E''}}{E'-E''}R_{El}^{E''l_0}\right), \tag{8}$$

where $l = l_0 \pm 1$. The right-hand side of (8) consists of three terms. The first is the usual free-free transition. We are interested in the case when the influence of the resonance on the bremsstrahlung is appreciable, i.e., $(R_{El}^{nl_0})^2 >> \Gamma\,(R_{El}^{E'l_0})^2$, and all the terms with the exception of $(R_{El}^{nl_0})^2$ in the second term can be neglected; thus, this term describes the attachment of an electron on the res-

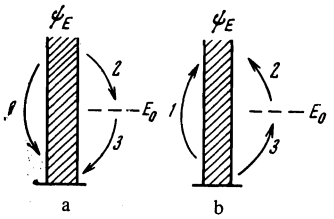

FIG. 1. Illustration of the optical transitions in emission (a) and absorption (b) in the presence of a resonant level.

onant level. The third term takes into account the interference.

We substitute $\tilde{R}^{E'l_0}_{El}$ in (6) in place of $R^{E'l_0}_{El}(l = l_0 \pm 1)$ and the analogous expression in place of $R^{E'l'}_{El_0}$ (in formula (7) we have $l = l_0$ and $l' = l_0 \pm 1$), leaving unchanged the matrix elements that are not preserved by the resonant level, and obtain an expression for the cross section. We represent this expression in the form

$$\frac{d\sigma_{E,E'\omega}}{d\omega} = \frac{d\sigma^{ff}_{E,E'\omega}}{d\omega} + \frac{d\sigma^{fb}_{E,E'\omega}}{d\omega} + \frac{d\sigma^{bf}_{E,E'\omega}}{d\omega} + \frac{d\sigma^{int}_{E,E'\omega}}{d\omega}. \quad (9)$$

The first term coincides with (6) and is the nonresonant part of the cross section (transition 1 in Fig. 1a), and the second is the cross section for the attachment on the resonant level (transition 2 on Fig. 1a):

$$\frac{d\sigma^{fb}_{E,E'\omega}}{d\omega} = \frac{\Gamma/2\pi}{(E'-E_0)^2+(\Gamma/2)^2}\sigma_{EE_0},$$

where σ_{EE_0} takes the form of the cross section for the attachment on a discrete level:

$$\sigma_{EE_0} = \frac{4\pi^2\omega^3}{3c^3E}[l_0(R^{nl_0}_{E,l_0-1})^2 + (l_0+1)(R^{nl_0}_{E,l_0+1})^2].$$

The third term in (9) is the cross section for the radiative decay of the unstable state (transition 3 on Fig. 1a):

$$\frac{d\sigma^{bf}_{E,E'\omega}}{d\omega} = \frac{(\Gamma/2\pi)\sigma_{E_0E'}}{(E-E_0)^2+(\Gamma/2)^2}, \quad \sigma_{E_0E'} = \frac{4\pi^2\omega^3}{3c^3E_0}[l_0(R^{E',l_0-1}_{nl_0})^2 + (l_0+1)(R^{E',l_0+1}_{nl_0})^2],$$

and the fourth is the interference term (this term is not interpreted with the aid of the approximate scheme of Fig. 1):

$$\frac{d\sigma^{int}_{E,E'\omega}}{d\omega} = \frac{4\pi^2\omega^3}{3c^3E}\sum_{l=l_0\pm1} l_> \cdot 2\,\mathrm{Re}\Big[\frac{V_{E'}^*(E'-E_0)}{(E'-E_0)^2+(\Gamma/2)^2}$$
$$\times R^{E'l_0}_{El}\Big(R^{nl_0}_{El} + \mathrm{P}\int dE''\,\frac{V_{E''}}{E'-E''}R^{E''l_0}_{El}\Big) + \frac{V_E^*(E-E_0)}{(E-E_0)^2+(\Gamma/2)^2}R^{E'l}_{nl_0}\Big(R^{El}_{nl_0} + \mathrm{P}\int dE''\,\frac{V_{E''}}{E'-E''}R^{E'l}_{E''l_0}\Big)\Big], \quad (10)$$

where $l_> = \max\{l, l_0\}$.

We have considered above the emission cross section. The absorption cross section $\sigma_{E'\omega,E}$ is defined, as in[5], by

$$\sigma_{E'\omega,E} = (\pi^2c^2E/\omega^2E')(d\sigma_{E,E'\omega}/d\omega). \quad (11)$$

3. The absorption coefficient K_ω can be obtained by integrating the cross section of the electron energy distribution function f(E)

$$K_\omega = N_eN_1\int_0^\infty \sigma_{E'\omega,E}(2E')^{1/2}f(E')\,dE', \quad (12)$$

where N_e and N_1 are the concentrations of the electrons and of the atoms ^1S. In the presence of equilibrium at a temperature T we have

$$f(E') = 2(E'/\pi T^3)^{1/2}e^{-E'/T}. \quad (13)$$

Like the cross section (9), the absorption coefficient breaks up into four components:

$$K_\omega = K^{ff}_\omega + K^{fb}_\omega + K^{bf}_\omega + K^{int}_\omega;$$

K^{ff}_ω is the bremsstrahlung coefficient without allowance for the resonance (transition 1 in Fig. 1b):

$$K_\omega^{ff} = N_eN_1\Big(\frac{2\pi}{T}\Big)^{3/2}\frac{4\pi^2\omega}{3c}\sum_l l\int e^{-E'/T}[(R^{E'l}_{E,l-1})^2 + (R^{E',l-1}_{El})^2]\,dE',$$

K^{fb}_ω and K^{bf}_ω are the absorption coefficients corresponding respectively to the processes of photodetachment from the resonant level (transition 2 in Fig. 1b) and attachment of an electron from the continuous spectrum lying below the level E_0 (transition 3 of Fig. 1b):

$$K_\omega^{fb} = N_eN_1\Big(\frac{2\pi}{T}\Big)^{3/2}\frac{4\pi^2\omega}{3c}\int e^{-E'/T}\Big\{\frac{\Gamma/2\pi}{(E'-E_0)^2+(\Gamma/2)^2}[l_0(R^{nl_0}_{E,l_0-1})^2 + (l_0+1)(R^{nl_0}_{E,l_0+1})^2]\Big\}dE'; \quad (14)$$

we obtain K^{bf}_ω by making the interchange $E' \longleftrightarrow E$ in the expression in the curly brackets of (14); E^{int}_ω can be easily obtained with the aid of (10)–(13).

If the configuration interaction is weak enough and the following conditions for the smallness of $\Gamma(E_0)$ are satisfied (Γ is a function of E, as can be seen from (4)):

$$\Gamma(E_0) \ll E_0,\ \Gamma(E_0) \ll T,\ \Gamma(E_0) \ll \Delta E, \quad (15)$$

where ΔE is the characteristic interval over which $R^{nl_0}_{E,l_0\pm1}$ varies significantly, then the resonant factor in (14) can be replaced by the δ-function $\delta(E'-E_0)$. Then

$$K^{fb}_\omega = N_eN_1(2\pi/T)^{3/2}(2l_0+1)e^{-E_0/T}\sigma_{E_0\omega}, \quad (16)$$

where $\sigma_{E_0\omega}$ is the photodetachment cross section

$$\sigma_{E_0\omega} = c^2E\sigma_{EE_0}/\omega^2(2l_0+1),\ E = E_0+\omega.$$

As follows from (16), the coefficient K^{fb}_ω turns out to take the form $K^{fb}_\omega = N_-\sigma_{E_0\omega}$, where N_- can be interpreted as the concentration of the unstable ion. The expression for N_- coincides with the usual formula for the concentration of stable negative ions, except that the sign of the energy E_0 is reversed.

The coefficient K^{bf}_ω corresponds to transition of type 3 in Fig. 1b. Since the configuration interaction smears out the level over an interval of width $\approx\Gamma$, the value of K_b differs from zero only in the region $\omega \lesssim E_0 + \Gamma/2$. For low-lying resonances, this region corresponds to the infrared part of the spectrum, where free-free transitions K^{ff}_ω can predominate. Thus, the contribution of K^{bf}_ω may turn out to be negligible also at $\omega \lesssim E_0 + \Gamma/2$.

To calculate K^{int}_ω it is necessary to know the function $\Gamma(E)$, but frequently one knows only the width $\Gamma(E_0)$ of the quasilevel. At a small width $\Gamma(E_0)$ it can be assumed that the contribution of the interference term to K_ω is small. The point is that the cross section (10) contains factors of the type $(E'-E_0)[(E'-E_0)^2 + (\Gamma/2)^2]^{-1}$. Thus, when the cross section is integrated in (12), the contributions from the regions $E' < E_0$ and $E' > E_0$ approximately cancel each other when the conditions (15) are satisfied ($K^{int}_\omega \to 0$ in the limit as $\to 0$). The smallness of K^{int}_ω for concrete examples must be verified with the aid of numerical calculations.

When the conditions (15) are satisfied, the resonance becomes manifest in the presence of a K_ω component in the absorption coefficient. In the case of emission, this corresponds to photoattachment on the resonant level.

4. Let us generalize the results to include the case of an arbitrary term of an atom S_1L_1 and N equivalent

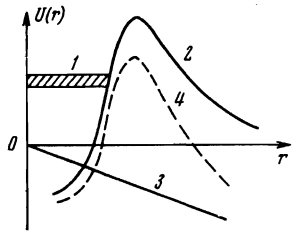

FIG. 2

nl_0 electrons on the outer shell of an unstable negative ion. Let S_0L_0 be the term of the ion and SL the term of the system comprising the atom and a free electron; $g_1 = (2S_1 + 1)(2L_1 + 1)$ and $g_- = (2S_0 + 1) \cdot (2L_0 + 1)$ are the statistical weights of the atom and of the negative ion, respectively

$$\frac{d\sigma^{ff}_{E,E'\omega}}{d\omega} = \frac{2\pi^2\omega^3}{3c^3E} \sum_{l,l'=l\pm1} \sum_{S,L,L'} \frac{(2S+1)(2L+1)}{g_1} \times (2L'+1) W^2(lLl'L'; L_1 1) l_> (R^{E'l'}_{El})^2$$

(here $l_>$ = max (l, l') and W is a Racah coefficient);

$$\frac{d\sigma^{fb}_{E,E'\omega}}{d\omega} = |a(E')|^2 \frac{2\pi^2\omega^3}{3c^3E} \frac{g_-}{g_1} N |G^{S_0L_0}_{S_1L_1}|^2 \sum_{l=l_0\pm1,L} (2L+1) W^2(lLl_0L_0; L_1 1) l_> (R^{El}_{nl_0})^2 \quad (17)$$

($l_>$ = max $\{l, l_0\}$, $G^{S_0L_0}_{S_1L_1}$ are fractional-parentage coefficients, and $|a|^2$ is defined in (2)). To obtain $d\sigma^{bf}_{E,E'\omega}/d\omega$, it is necessary to replace a(E') in (17) by a(E) and $R^{El}_{nl_0}$ by $R^{E'}_{nl_0}$;

$$\frac{d\sigma^{int}_{E,E'\omega}}{d\omega} = \frac{2\pi^2\omega^2 g_-}{3c^3 E g_1} \sqrt{N}\, G^{S_0L_0}_{S_1L_1} \sum_{l=l_0\pm1,L} (2L+1) W^2(l_0L_0lL; L_1 1) l_> \cdot 2\mathrm{Re}\left[a(E') R^{nl_0}_{El} \int dE''\, b_{E''}(E') R^{El}_{E''l_0} + a(E) R^{nl_0}_{E'l} \int dE''\, b_{E''}(E) R^{E'l}_{E''l_0} \right].$$

The generalized formulas (16) are conveniently written in the form

$$K^{fb}_\omega = N_e N_a (2\pi/T)^{3/2} [g_-/2\Sigma(T)] \exp[-(E_0+E_1)/T] \sigma_{E_0\omega},$$
$$\sigma_{E_0\omega} = \frac{2\pi^2\omega^3 g_-}{3c^2 E g_1} N |G^{S_0L_0}_{S_1L_1}|^2 \sum_{l=l_0\pm1,L} (2L+1) W^2(lLl_0L_0; L_1 1) l_> (R^{nl_0}_{El})^2, \quad (18)$$

where N_a is the total concentration of the atoms, $\Sigma(T)$ is the partition function of the atom, and E_1 is the energy of the term S_1L_1. The cross section $d\sigma^{fb}_{E,E'\omega}/d\omega$ corresponds to photodecay of the resonant state into an atom in the initial state S_1L_1 and an electron. In the general case, however, the term S_0L_0 corresponds to several parent terms, so that the decay of the unstable ion can proceed via several channels. These decays can be described by the same formula with appropriate substitution of the fraction-parentage coefficient and the Racah coefficient.

5. It was shown in[6] that a weakly-bound negative ion can disintegrate under the influence of the electric microfields of the plasma, and that the corresponding recombination continuum should decrease with increasing charge-particle concentration. The conclusions of[6] can be generalized also to include the case of the unstable state of the negative ion.

The resonant state is the level 1 (Fig. 2) in a potential well surrounded by a barrier 2. The level energy is positive, so that the level has a width. When an electric field 3 is applied, the barrier is lowered and becomes narrower (curve 4). The level width depends exponentially on the height and the width of the barrier

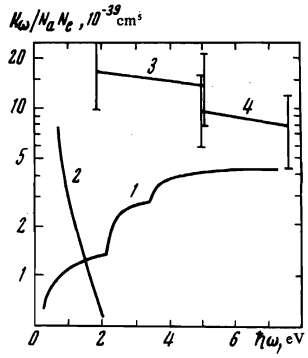

FIG. 3. Coefficient of extra absorption of nitrogen plasma per electron and per atom (T = 1100°K). Calculation: 1—attachment on resonant level, 2—bremsstrahlung without allowance for resonance. Measurement results: 3—[12], 4—by A. N. Vargin, O. A. Golubev, and O. A. Malkin.

(for a rectangular barrier see, e.g.,[7]), i.e., the level width should increase exponentially with increasing field. It is also obvious that the level vanishes at a certain critical value of the field.

At low plasma concentrations, when the average microfield intensity E in the plasma is such that $Er_0 \ll U_0$ (U_0 and r_0 are the characteristic height and radius of the potential barrier), the influence of the microfield on the resonant ions can be neglected. On the other hand, with further increase of the charge concentration in the plasma, the role of the photoattachment on the resonant level should decrease sharply. A consistent calculation of the behavior of the resonant level in an electric field and the use of these results to take into account the influence of microfields in the plasma is an independent problem.

6. By way of example of the application of the developed theory, let us consider the negative nitrogen ion N^-. Calculations performed by various methods (see[8,9] and the references contained therein) show that the ground state $2p^4\ ^3P$ of N^- is unstable and has an energy $E_0 \cong 0.1$–0.3 eV. This agrees with experiments[10] on two-electron charge exchange of N^+, O^+, and C^+ with inert gases, where no N^- ions were observed in practice, unlike O^- and C^-. At the same time, experiments have revealed in the emission of nitrogen and air plasma at a pressure 1 atm and temperatures 10 000–15 000°K an extra continuum in the visible and ultraviolet regions of the spectrum[11,12], namely, the measured intensity of the radiation is more than double the theoretical value that included the recombination, bremsstrahlung, and molecular processes.

The experimental extra absorption coefficient is compared in Fig. 3 with the result of calculation based on formula (18); it was assumed that the conditions (15) are satisfied (according to[8], $\Gamma(E_0) = 0.029$ eV[1)]). The values of $R^{nl_0}_{E,l_0\pm1}$ were taken from[12] under the assumption that these quantities can be regarded as functions of the free-electron energy E, do not change on going from $E_0 = -0.1$ to $E_0 = 0.2$ eV. The ion $N^-\ ^3P$ can be produced by attachment of an electron not only to the ground state ^4S of the N atom, but also to the excited ^2P and ^2D states of the ground-state configuration $N2p^3$; accordingly, there are two additional thresholds on curve 1 of Fig. 3. Taking into account the error in the experimental data and a certain indeterminacy of the calculations, we can consider curve 1 as agreeing with the measurement results, whereas curve 2 diverges strongly from them.

In addition to the ground state ^3P, there exist metastable states ^1D and ^1S of the ion N^-2p^4. These states, in view of their low population, make a negligible con-

tribution to the radiation, but can explain the rather weak signal that was registered in certain mass-spectrometric measurement[10].

At high pressures $\sim 10^2$ atm and at the same temperatures as in[11,12], no extra continuum was observed in a nitrogen plasma (see[13]). This can be attributed to the influence of the microfields, which was discussed in Sec. 5.

7. Calculations for a nitrogen plasma have shown that photoattachment with formation of a resonant state can increase the bremsstrahlung intensity by one order of magnitude and more. Analogous atomic and molecular resonant states can exist also for other elements, and they must be taken into account in the calculation of the radiation intensities and the absorption coefficients of the corresponding plasmas. Excited resonant states (H^-, Al^-, Si^-, C^-, etc.) can also contribute.

The possible role of resonances in bremsstrahlung was pointed out in[14], where the interaction of the configurations was not considered and where it was assumed that the resonance leads only to the appearance of a transition of type 3 in Fig. 1, it being assumed that all the radiation is emitted in a band of width Γ in the frequency region $\hbar\omega \sim E_0$. Estimates were made of the role of the molecular resonance of N_2^- in the emission of a nitrogen plasma at $T \sim 8000°K$. At a maximum oscillator strength $f \sim 1$ of the resonant transition, it was found in[14] that the resonance can increase the bremsstrahlung by not more than 30%. This agrees with our estimate of the negligible role of transitions of type 3. However, as shown above, the principal role of the resonance consists in the appearance of a transition of type 2 of Fig. 1.

In conclusion, we note that the results obtained by direct analogy with[3] are valid only if the width Γ is small, in which case they coincide with the sum of the unperturbed photoattachment for φ and the bremsstrahlung processes for ψ_E. The point is that the cross sections calculated under the assumption that Γ is independent of E no longer satisfy the sum rule for the oscillator strengths when Γ increases. When the interaction is so large ($\Gamma \cong E_0$) that a redistribution of the energy over the spectrum takes place, it is necessary to obtain and use in the radiation calculations a function $\Gamma(E)$ capable of satisfying the sum rules.

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