Spectrum of atomic radiation at sudden perturbation

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Abstract

A general expression for the spectrum of photons emitted by atom at sudden perturbation is obtained. Some concrete examples of application of the obtained result are considered. The conclusion about the coherence of radiation of the atomic electrons under the such influences is made.

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It is known many examples when the excitation or ionization of atoms occurs as result of the action of sudden perturbations. First of all these are atomic excitation or ionization in the nuclear reactions [1,2]. For example in β -decay of nucleus, when the fast β -electron's escape is perceived by atomic electrons as a sudden changing of nuclear charge or in neutron impact with nucleus, when the sudden of momentum transfer to the nucleus occurs etc. The sudden approximation [3] can be used for consideration multielectron transition in complex atoms, when transition occurring in internal shells, are perceived by relatively slow electrons of external shells as instantaneous (see [4,5]). As a result of action of sudden perturbation can be considered inelastic processes in the collisions of fast multicharged ions with atoms [6 -12 and in the collisions of charged particles with highly-excited atoms [13]. After action of sudden perturbation, the excited atom can relax with radiation of photons belonging to known spectrum of isolated atom. However, if sudden perturbation causes the change of velocities of atomic electrons, atom can radiate during the action of perturbation. Classical analogue of such a problem is the [14] radiation of a free electron under the sudden changing of velocity. In many practically important cases perturbation is not sufficiently small to use a perturbation theory. However the situations when the time of action of perturbation is considerably less than the characteristic atomic time that enables one to solve the problem without restricting the value of perturbation (see for instance [9,15-17]).

Thus, it is necessary to state a general problem on the spectrum of photons emitted by atom during the time of action of sudden perturbation, i.e. - on the spectrum of photons emitted simultaneously by all atomic electrons as a result of action of perturbation. In this paper we derive a general expression for the spectrum of photons emitted by the atom under sudden perturbation and apply this result to some concrete processes.

Consider "collision" type sudden perturbation [3], when the perturbation $V(t) \equiv V(\mathbf{r}_a, t)$ (where \mathbf{r}_a are the coordinates of atomic electrons) acts only during the time τ , which is much smaller than the characteristic period of unperturbed atom, describing by Hamiltonian H_0 . To be definite we will assume that V(t) is not equal zero near t = 0 only. Then in the exact solution of Schrödinger equation (atomic units are used throughout in this paper)

$$i\frac{\partial \psi}{\partial t} = (H_0 + V(t))\psi$$

one can neglect by evolution of ψ (during the time τ) caused by unperturbed Hamiltonian H_0 . Therefore the transition amplitude of atom from the initial state φ_0 to a

final state φ_n , as a result of actions of sudden perturbation V(t), has the form [3,6]:

$$a_{0n} = \langle \varphi_n \mid exp(-i \int_{-\infty}^{+\infty} V(t)dt) \mid \varphi_0 \rangle , \qquad (1)$$

where φ_0 and φ_n belong to the full set of orthonormalized eigenfunctions of the unperturbated Hamiltonian H_0 , i.e. $H_0\varphi_n = \epsilon_n\varphi_n$.

Thus in the sudden perturbation approximation the evolution of the initial state has the form

$$\psi_0(t) = \exp(-i \int_{-\infty}^t V(t')dt')\varphi_0 , \qquad (2)$$

where $\psi_0(t)$ satisfies the equation

$$i\frac{\partial\psi_0(t)}{\partial t} = V(t)\psi_0(t) , \qquad (3)$$

and $\psi_0(t) \to \varphi_0$ under $t \to -\infty$. Let's introduce full and orthonormal set of functions

$$\Phi_n(t) = \exp\left(i \int_{t}^{+\infty} V(t')dt'\right) \varphi_n , \qquad (4)$$

obeying eq. (3), and $\Phi_n(t) \to \varphi_n$ at $t \to +\infty$. Obviously the amplitude (1) can be rewritten as

$$a_{0n} = \langle \Phi_n(t) \mid \psi_0(t) \rangle.$$

Therefore the one photon radiation amplitude can be calculated in the first order of perturbation theory (as a corrections to the states (2) and (4)) over the interaction of atomic electrons with electromagnetic field [18,19]

$$W = -\sum_{a,\mathbf{k},\sigma} \left(\frac{2\pi}{\omega}\right)^{\frac{1}{2}} \mathbf{u}_{\mathbf{k}\sigma} (a_{\mathbf{k}\sigma}^{\dagger} e^{-i\mathbf{k}\mathbf{r}_a} + a_{\mathbf{k}\sigma} e^{-i\mathbf{k}\mathbf{r}_a}) \hat{\mathbf{p}}_a ,$$

where $a_{\mathbf{k}\sigma}^+$ and $a_{\mathbf{k}\sigma}$ are the creation and annihilation operators of the photon with a frequency ω , momentum \mathbf{k} and polarization σ , $(\sigma=1,2)$, $\mathbf{u}_{\mathbf{k}\sigma}$ are the unit vectors of polarization, \mathbf{r}_a are the coordinates of atomic electrons $(a=1,..,Z_a)$, here Z_a is the number of atomic electrons, $\hat{\mathbf{p}}_a$ are the momentum operators of atomic electrons. Then in the dipole approximation the amplitude of emission of photon with simultaneous transition of atom from the state φ_0 to a state φ_n has the form

$$b_{0n}(\omega) = i \left(\frac{2\pi}{\omega}\right)^{\frac{1}{2}} \mathbf{u}_{\mathbf{k}\sigma} \int_{-\infty}^{+\infty} dt e^{i\omega t} \langle \Phi_n(t) \mid \sum_a \hat{\mathbf{p}}_a \mid \psi_0(t) \rangle.$$

Integrating this expression by parts over the time and omitting the terms vanishing (at $t \to \pm \infty$) in turning off the interaction with electromagnetic field we have

$$b_{0n}(\omega) = i \left(\frac{2\pi}{\omega}\right)^{\frac{1}{2}} \mathbf{u}_{\mathbf{k}\sigma} \int_{-\infty}^{+\infty} dt \frac{e^{i\omega t}}{\omega} \times \left(\varphi_n \mid \sum_{a} \frac{\partial V(t)}{\partial \mathbf{r}_a} exp(-i \int_{-\infty}^{+\infty} V(t') dt') \mid \varphi_0 \right).$$
 (5)

Summing $|b_{0n}(\omega)|^2$ over polarization and integrating over the photon's emission angles and summing, after this, over all final states of the atom φ_n , we find the total radiation spectrum

$$\frac{dW}{d\omega} = \frac{2}{3\pi} \frac{1}{c^3 \omega} \langle \varphi_0 \mid \sum_a \frac{\partial \tilde{V}^*(\omega)}{\partial \mathbf{r}_a} \sum_b \frac{\partial \tilde{V}(\omega)}{\partial \mathbf{r}_b} \mid \varphi_0 \rangle, \tag{6}$$

where c = 137 a.u. is the speed of light,

$$\tilde{V}(\omega) = \int_{-\infty}^{+\infty} V(t)e^{i\omega t}dt. \tag{7}$$

Thus we have obtained the radiation spectrum of atom during the time of sudden perturbation V(t).

As an application we consider the radiation spectrum of atom in the sudden transmission of momentum \mathbf{p} to the atomic electrons when V(t) has the (widely used for collision problems) form

$$V(t) = \mathbf{f}(t) \sum_{a} \mathbf{r}_{a}, \quad \mathbf{p} = \int_{-\infty}^{+\infty} dt \mathbf{f}(t), \tag{8}$$

and $\mathbf{f}(t)$ is the perturbing force which not depends on \mathbf{r}_a and interacts during a time τ that is considerable less than the characteristic periods of the unperturbed atom. The total radiation spectrum (6) in this case has the form

$$\frac{dW}{d\omega} = \frac{2}{3\pi} \frac{1}{c^3 \omega} |\tilde{\mathbf{f}}(\omega)|^2 \cdot Z_a^2, \tag{9}$$

where $\tilde{\mathbf{f}}(\omega)$, is the Fourier transform of the functions $\mathbf{f}(t)$, defined according to (7), Z_a is the number of atomic electrons. In this case the spectrum coincides (after producting to ω) with the radiation spectrum of the classical particle with mass equal to electron's one and with charge Z_a , moving in the field of homogeneous forces $\mathbf{f}(t)$. This gives us the information about the value of the spectrum (9). Since $\mathbf{f}(t) \neq 0$ just during the time τ , and the spectrum (9) is proportional to $|\tilde{\mathbf{f}}(\omega)|^2$,

only the photons belonging to continuum with characteristic frequencies $\omega \leq 1/\tau$ can be emitted by atom.

Analogously one can consider the radiation of atom in the "switching" type sudden perturbation (we use the classification of sudden perturbations introduced in [3]).

Formula (5) allows one to obtain the spectrum of photons in the transition of atom from the state φ_0 to a state φ_n under the influence of perturbation (8):

$$\frac{dw_{0n}}{d\omega} = \frac{2}{3\pi} \frac{1}{c^3 \omega} |\tilde{\mathbf{f}}(\omega)|^2 Z_a^2 |\langle \varphi_n | exp(-i\mathbf{p} \sum_a \mathbf{r}_a) | \varphi_0 \rangle|^2.$$
 (10)

Here $dW/d\omega = \sum_n dw_{0n}/d\omega$, where \sum_n means summing over the complete set of atomic states. Formula (10) allows one to express the relative contribution of transitions with excitation to an arbitrary state φ_n to the total spectrum (9)

$$\frac{dw_{0n}/d\omega}{dW/d\omega} = |\langle \varphi_n \mid exp(-i\mathbf{p}\sum_a \mathbf{r}_a) \mid \varphi_0 \rangle|^2$$

via the well known [2] inelastic atomic formfactors $\langle \varphi_n \mid exp(-i\mathbf{p}\sum_a \mathbf{r}_a) \mid \varphi_0 \rangle$.

In the most simple case of instantaneous transferring to atomic electrons the momentum \mathbf{p} , when in (8) $\mathbf{f}(t) = \mathbf{p} \cdot \delta(t)$, where $\delta(t)$ is the Dirac δ -function, then $\tilde{\mathbf{f}}(\omega) = \mathbf{p}$ and spectrum (9) coincides, after producting to ω , with the radiation spectrum of free classical particle [14] with charge Z_a , which takes (suddenly) a velocity \mathbf{p} .

As an another example we give the radiation spectrum in the influence of pulse having the Gausian form

$$\mathbf{f}(t) = \mathbf{f}_0 exp(-\alpha^2 t^2) cos(\omega_0 t) ,$$

respectively

$$\tilde{V}(\omega) = \frac{\sqrt{\pi}}{2\alpha} \mathbf{f_0} \sum_{a} \mathbf{r}_a \left\{ exp \left[-\frac{(\omega - \omega_0)^2}{4\alpha^2} \right] + exp \left[-\frac{(\omega + \omega_0)^2}{4\alpha^2} \right] \right\} .$$

Therefore the radiation spectrum has the form

$$\frac{dW}{d\Omega} = \frac{f_0^2}{6\Omega c^3 \alpha^2} \left\{ exp \left[-(\Omega + \Omega_0)^2 \right] + exp \left[-(\Omega - \Omega_0)^2 \right] \right\} Z_a^2 ,$$

where for the sake of convenience the frequencies $\Omega = \omega/(2\alpha)$ and $\Omega_0 = \omega_0/(2\alpha)$ are introduced.

One should note an important generality of radiation at sudden perturbation, namely, the radiation intensity for the multielectron atoms is proportional to the square of the number of atomic electrons. This fact allows one to conclude on the coherence of radiation of atomic electrons under such type influences.

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