Intensity distribution shift for the resonant photon scattering on the hydrogen atom

L. Labzowsky[1,2] and D. Solovjev[1]
[1]*St. Petersburg State University, 198504, Petrodvorets, St. Petersburg, Russia*
[2]*Petersburg Nuclear Physics Institute, 188350, Gatchina, St. Petersburg, Russia*
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The role of nonresonant (NR) corrections in the resonant photon scattering process on the hydrogen atom is discussed. It is shown that the average energy of the emitted photons may not coincide with the average energy of the incident photons defined by the photon source spectral function. The discrepancy is due to the NR corrections and to the interaction with the vacuum.

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The energy balance between the absorption and emission processes in atoms is ruled by the energy conservation law. It is well known that the energy E of the excited level of an atom is ''dispersed'' and this ''dispersion'' is defined by the width Γ of this level. The origin of the width is the interaction of the atomic electron with the vacuum. One may ask whether the average energy of the incident photons $\overline{\varepsilon}_{\rm in}$ defined by the spectral distribution of the photon source $I(\omega)$ is equal to the average energy of the absorbed and emitted photons $\overline{\varepsilon}_{\rm rad}$ in the process of the resonant photon scattering. We will investigate this problem in the particular case of the Lyman-α transition in the hydrogen atom. Our conclusion will be that the equality $\overline{\varepsilon}_{\rm in}=\overline{\varepsilon}_{\rm rad}$ holds only in the resonance approximation and the inclusion of the nonresonant (NR) corrections violates this equality at the level of $(\alpha Z)^6$, where α is the fine-structure constant and Z is the charge of the nucleus. The NR corrections were first introduced in [1], where the modern QED theory of the natural spectral line profile was formulated. Recently, NR corrections for the Lyman-α transition in hydrogen were considered in [2–4]. They appear to be important in the highly precise modern experiments where the one-photon $1s$-$2p$ [5] and the two-photon $1s$-$2s$ [6] resonances in the H atom were measured.

The NR corrections distort the Lorentz line shape and make it asymmetric. The asymmetry of the line shape leads eventually to the violation of the equality $\overline{\varepsilon}_{\rm in}=\overline{\varepsilon}_{\rm rad}$. The measurement of the intensity distribution shift could be the easiest way to observe the NR corrections.

We consider the process of the elastic resonant photon scattering on the one-photon atom in its ground state A. The S-matrix element corresponding to this process is

$$S_A(\omega,\omega')=-2\pi i\,\delta(\omega-\omega')e^2\left(\sum_n \frac{(\vec{\alpha}\vec{A}_{\omega jlm})_{An}(\vec{\alpha}\vec{A}^{*}_{\omega' j' l' m'})_{nA}}{E_n-E_A-\omega}+\sum_n \frac{(\vec{\alpha}\vec{A}^{*}_{\omega' j' l' m'})_{An}(\vec{\alpha}\vec{A}_{\omega jlm})_{nA}}{E_n-E_A+\omega}\right)$$
$$=-2\pi i\,\delta(\omega-\omega')U_A(\omega,\omega'). \qquad (1)$$

In Eq. (1), the relativistic units are employed; e is the electron charge. For characterization of the incident and emitted photons, we use the set of quantum numbers ωjlm, where ω is the photon frequency, jm are the total photon moment and its projection, and l defines the parity or the type of the photon (electric or magnetic). Then $\vec{A}_{\omega jlm}$ is the electromagnetic field potential, corresponding to the absorption of the photon with quantum numbers ωjlm, and $\vec{A}^{*}_{\omega' j' l' m'}$ is the potential corresponding to the emission of the photon with quantum numbers $\omega' j' l' m'$. The notation $(\vec{\alpha}\vec{A}_{\omega jlm})_{An}$ is used for the matrix element with the electron wave functions ψ_A^* and ψ_n, $\vec{\alpha}$ is the Dirac matrix, E_n are the electron energies, and the summation in Eq. (1) is extended over all the atomic electron states. Equation (1) defines also the amplitude of the process $U_A(\omega,\omega')$. The probability of the photon scattering on the atom reads

$$W_A(\omega,\omega')=\frac{2\pi}{(2j+1)(2j_A+1)}\times\sum_{mm'}|U_A(\omega,\omega')|^2\delta(\omega-\omega'), \qquad (2)$$

where the summation over the final electron degenerate states and the averaging over the initial electron degenerate states is understood. The electron in the state A is characterized by the set of quantum numbers $n_A j_A l_A m_A$, where n_A is the principal quantum number, $j_A m_A$ are the total moment and its protection, and l_A characterizes the parity of the state A. The photon quantum numbers jl are fixed (this is evidently the case in the nonrelativistic approximation). In the total probability after the angular integration only the terms with $j'=j, l'=l$ survive. The probability W depends on the normalization volume for the incident photon, but our further

results will not depend on this volume. The delta function $\delta(\omega-\omega')$ in Eq. (2) implies the energy conservation law.

Introducing the spectral distribution function $I(\omega)$ for the incident photons which we normalize by the condition $\int_0^\infty I(\omega)d\omega=1$ and integrating over ω' in Eq. (2), we obtain the probability $dW_A(\omega)$ of the photon emission within the frequency interval $\omega,\omega+d\omega$,

$$dW_A(\omega,\omega')=\frac{2\pi}{(2j+1)(2j_A+1)}I(\omega)\sum_{mm'}|U_A(\omega)|^2 d\omega. \tag{3}$$

Equation (1) is analogous to the expression derived in [1] for the emission probability in the case in which the atom is excited by an effective thermal excitation potential. Equation (3) presents the probability of the photon emission by an atom, excited by the photon source with the spectral distribution $I(\omega)$.

In the case of resonant scattering, the frequency of the incident photon is close to some atomic transition frequency, $\omega\simeq E_{A'}-E_A$, where $E_{A'}$ is the energy of an excited atomic state. For the Lyman-α transition, $A=1s$, $A'=2p$. In the resonance approximation, we retain only one term $n=A'$ in the first sum over n in Eq. (1). The other terms of this sum as well as the total second sum represent the NR corrections. To avoid the singularity in the resonant term, one has to take into account the width of the level A'. Formally the width $\Gamma_{A'}$ arises due to the electron self-energy corrections to the S-matrix element in Eq. (1) [1]. Summation of these corrections in all orders of perturbation theory leads to geometric progression, which results in the shifted energy denominator $(E_A-E_A+\Delta E_{A'}-\omega)^{-1}$. Here $\Delta E_{A'}$ is the complex electron self-energy shift. The real part of this shift after the renormalization presents the lowest-order electron self-energy contribution to the Lamb shift $\Delta E^L_{A'}$ and the imaginary part gives the level width $\Gamma_{A'}$: $\Delta E_{A'}=\Delta E^L_{A'}-(i/2)\Gamma_{A'}$.

Another definition of the level width as the sum over all possible transition probabilities to the lower levels is

$$\Gamma_{A'}(\omega')=W_{A'A}=2\pi e^2\sum_{m'm_A}|(\vec{\alpha}\vec{A}^*_{\omega' j' l' m'})_{A'A}|^2. \tag{4}$$

We assume for simplicity that there is only one decay channel for the level A' (as in the case of the level $A'=2p_{1/2}$). In the resonance approximation, Eq. (3) reduces to

$$\begin{aligned} dW_{AA'}(\omega)&=F_{AA'}(\omega)d\omega \\ &=\frac{1}{2\pi(2j_A+1)(2j+1)} \\ &\quad\times I(\omega)\frac{\Gamma_{A'}(\omega_0)\Gamma_{A'}(\omega_0)d\omega}{(\omega_0-\omega)^2+\frac{1}{4}\Gamma^2_{A'}}, \end{aligned} \tag{5}$$

where $\omega_0=\tilde{E}_{A'}-\tilde{E}_A$, and $\tilde{E}_A$ denotes the atomic energy shifted by the radiative corrections. The function $F_{AA'}(\omega)$ describes the probability distribution for the emitted photons.

The normalization of the probability distribution (5) depends on the function $I(\omega)$. Note that we neglect the probability of inelastic scattering, i.e., the emission of several photons before the final stabilization of the atom.

Now we can define $\bar{\varepsilon}_{\rm rad}$ as

$$\bar{\varepsilon}_{\rm rad}=\frac{\int_0^\infty \omega dW_{AA'}(\omega)}{\int_0^\infty dW_{AA'}(\omega)} \tag{6}$$

and compare it with

$$\bar{\varepsilon}_{in}=\int_0^\infty \omega I(\omega)d\omega. \tag{7}$$

We choose the spectral function $I(\omega)$ as symmetrical with respect to ω_0. For example,

$$I(\omega)=\begin{cases}\dfrac{1}{\Gamma_{A'}}, & \omega\in\left[\omega_0-\dfrac{\Gamma_{A'}}{2},\omega_0+\dfrac{\Gamma_{A'}}{2}\right] \\ 0, & \omega\in\left[\omega_0-\dfrac{\Gamma_{A'}}{2},\omega_0+\dfrac{\Gamma_{A'}}{2}\right].\end{cases} \tag{8}$$

Then the equality $\bar{\varepsilon}_{\rm in}=\bar{\varepsilon}_{\rm rad}=\omega_0$ will hold in the resonance approximation, when the function $F_{AA'}(\omega)$ is also symmetrical with respect to ω_0.

This equality becomes violated if we take into account the NR corrections, i.e., the asymmetry of the line profile.

We consider as an example the Lyman-α $1s$-$2p_{1/2}$ transition in a hydrogen atom. As it was observed in [3], a large NR contribution to the Lyman-α transition frequency arises from the $2p_{3/2}$ state. In [2,3], only the dominant interference NR corrections were considered. These corrections with the $2p_{3/2}$ state vanish in the total cross section for the $1s$-$2p_{1/2}$ transition after the angular integration but remain in the differential cross section.

Still, as it was shown later in [4], the quadratic NR contribution with the $2p_{3/2}$ state appears to be of the same order as the contribution from the interference term due to the smallness of the fine-structure interval. Since in the present paper we consider the total probability, this quadratic $2p_{3/2}$ contribution will dominate. The probability distribution will look like

$$\begin{aligned} dW_{1s\text{-}2p}(\omega)=\frac{1}{12\pi}I(\omega)\Gamma^2_{2p}(\omega_0)\Bigg[&\frac{1}{(\omega_0-\omega)^2+\frac{1}{4}\Gamma^2_{2p}} \\ &+\frac{1}{(\omega_0+\Delta E_f-\omega)^2+\frac{1}{4}\Gamma^2_{2p}}\Bigg]d\omega, \end{aligned} \tag{9}$$

where $\Delta E_f = E_{2p_{3/2}} - E_{2p_{1/2}} = (\alpha Z)^2/32$ a.u. is the fine-structure interval and $\Gamma_{2p_{3/2}} \simeq \Gamma_{2p_{1/2}} = (2^{11}/3^9)\alpha^3\omega$ a.u. Inserting Eqs. (9) and (8) into Eq. (6) and evaluating the integrals over ω, we obtain

$$\bar{\varepsilon}_{\rm rad} = \omega_0 \left[1 + \frac{\Gamma^2}{\pi\omega_0^2} \left(2 - \frac{\pi}{2} \right) + \frac{\Gamma^4}{3\pi\omega_0 \Delta E_f^3} \right]. \qquad (10)$$

Comparison of the result (10) with the value $\bar{\varepsilon}_{\rm in} = \omega_0$ that follows from Eqs. (7) and (8) demonstrates the order of magnitude of the effect. This effect can be called ''intensity distribution shift'' for the emitted photons. In the case of the Lyman-α resonance, this shift is ''violet.''

Concluding, we should stress that in the case of the elastic scattering, the frequencies of the absorbed and emitted photons are exactly equal; this follows from the energy conservation law. If the incident light is monochromatic, then the scattered light will be also monochromatic. However, if the incident light has a spectral distribution, the scattered light frequencies will also be distributed and both distributions are not equal. The formula (10) shows that with NR corrections taken into account, the average photon energies are different for the initial and final distributions. The energy gain in Eq. (10) (or the possible loss in the other particular case) is due to the interaction with the vacuum.

The intensity distribution shift can be used for the observation of the NR corrections. The mean energy shift $\Delta E_{\rm NR} = \bar{\varepsilon}_{\rm rad} - \bar{\varepsilon}_{\rm in} = (\Gamma^2/\pi\omega_0)(2 - \pi/2) + (\Gamma^4/3\pi\Delta E_f^3) = 25.00$ Hz is 3.3 times larger than the NR correction $\Delta_{\rm NR} = 7.56$ Hz [1–3]. However, the intensity shift differs from the NR correction and the observation of this effect requires the direct measurement of the line-shape asymmetry.

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