Recombination process for hydrogen atom in presence of blackbody radiation

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The process of recombination for the hydrogen atom in the heat bath creating the blackbody radiation is described within the frameworks of quantum electrodynamics. For this purpose the self-energy for unbound electron in the field of the nucleus is considered. The imaginary part of this self-energy is directly connected with the recombination cross-section. The same procedure is applied to the hydrogen atom in the field of blackbody radiation. This leads to the new thermal correction to the process of recombination for the hydrogen atom in the heat bath. This correction takes into account the finite lifetimes of atomic levels and appears to be important for special astrophysical studies.

I. INTRODUCTION

The process of recombination and photo-ionization of atoms were intensively studied from the early stages of development of Quantum Mechanics (QM). A description of these processes for the hydrogen atom one can find in [1] and the same for many-electron atoms in [2], [3]. The cross-section of these processes are connected via the principle of the detailed balance which for the hydrogen atom looks like

\[ \sigma_{nl}^{\text{rec}} = 2(2l + 1) \frac{k^2}{p^2} \sigma_{nl}^{\text{ion}}, \]  

(1)

where \( k \) is the momentum of the emitted photon, \( p \) is the momentum of the incident electron and \( nl \) are the quantum numbers (principal and orbital) for the atomic electron state under consideration. In Eq. (1) we use the relativistic units \( \hbar = c = m = 1 \), \( m \) is the mass of the electron. The relativistic of Quantum Electrodynamical (QED) description of the photorecombination and photonization process is also well known (see for example [4], [5]).

In this paper we will apply the QED description of photorecombination and photoionization to the nonrelativistic hydrogen atom. Then the ionization cross-section for the atomic state \( nl \) will be expressed as

\[ d\sigma_{nl}^{\text{ion}} = 2\pi |U_{nl,\varepsilon}|^2 \delta(\omega - \varepsilon - I_{nl}) \frac{d^3p}{(2\pi)^3}. \]  

(2)

Here \( \omega \) is the incident photon frequency, \( \varepsilon \) is the energy of the electron in the continuum spectrum, \( I_{nl} \) is the ionization potential for the atomic state \( nl \) and \( U_{nl,\varepsilon} \) is the amplitude of the process connected with the S-matrix element via the relation

\[ S_{if} = -2\pi i \delta(E_i - E_f)U_{if}, \]  

(3)

where \( i, f \) denote the initial and final states of the system and \( E_i, E_f \) are initial and final energies. In the nonrelativistic limit for the hydrogen atom

\[ U_{if} = \frac{e}{\sqrt{2\pi \omega}} \left( \vec{e} \cdot \hat{p} \right)_{nl,\varepsilon}, \]  

(4)

where \( \vec{e} \) is the incident photon polarization vector, \( \hat{p} \) is the electron momentum operator, \( e \) is the electron charge. The cross-section \( \sigma_{nl}^{\text{rec}} \) can be obtained from Eq. (2) with the use of Eq. (1). The total photorecombination cross-section then is

\[ \sigma^{\text{rec}} = \sum_{nl} \sigma_{nl}^{\text{rec}}. \]  

(5)

II. QED EVALUATION OF THE PHOTOIONIZATION CROSS-SECTION

In this paper we employ a different QED approach to the evaluation of the total photorecombination cross-section. This approach is based on the well-known circumstance that the total width of atomic level \( \Gamma_{nl} \) equals to sum of transition rates to all the lower-lying atomic states \( W_{nl,n'l'} \)

\[ \Gamma_{nl} = \sum_{n'l'} W_{nl,n'l'}. \]  

(6)

In [6] it was demonstrated how this principle works within QED description of an atom. The one-loop electron self-energy correction for any atomic state \( a \) is presented by the Feynman graph depicted in Fig. [1].

FIG. 1. The Feynman graph corresponding to the one-loop electron self-energy correction \( \Delta E_a \) for the arbitrary atomic state \( a \). The double solid line denotes the electron in the field of the nucleus (the Furry picture of QED). The wavy line denotes the virtual photon. According to QED theory [4], [5] the real part of the correction \( \Delta E_a \) presented by Fig. [1] for the bound electron \( a \equiv nl \) corresponds to the lowest-order radiative shift (the Lamb shift \( L_a \)) for the level \( nl \). The imaginary part of \( \Delta E_a \) represents the total width \( \Gamma_{nl} \) of the level \( nl \). So

\[ \Delta E_{nl} = L_{nl} - \frac{i}{2} \Gamma_{nl}. \]  

(7)

The real part is divergent and should be renormalized. The imaginary part is finite and can be evaluated directly using
the Feynman correspondence rules within the Furry picture of QED.

This was done in [6], where the closed relativistic expression for $\Gamma_{\text{el}}$ was obtained and it was demonstrated how the relation (3) arises in the nonrelativistic limit. Our idia in the present paper is to obtain in a similar way the closed QED expression for $\sigma^{\text{rec}}$ and then to use it for describing the atomic level broadening in the field of blackbody radiation (BBR). For this purpose we define an expression corresponding to Fig. 1 in case when the atomic state $a$ belongs to continuous spectrum

$$\Delta E_{\varepsilon} = L_{\varepsilon} - \frac{i}{2} \Gamma_{\varepsilon}. \quad (8)$$

Here $\varepsilon$ denotes the energy of an unbound electron in the field of the nucleus. The radiative shift of the energy $L_{\varepsilon}$ for the electron in the continuous spectrum is out of the scope of the present paper. For the free electron $L_{\varepsilon} = 0$ due to the renormalization. For the free electron the imaginary part of $\Delta E_{\varepsilon}$ also vanishes, $\Gamma_{\varepsilon} = 0$. This happens because the radiation for the free electron is forbidden by the kinematics. However, for the unbound electron in the field of the nucleus the radiation is not forbidden: the electron can emit photon and transit to the one of the bound states. Consequently

$$\Gamma_{\varepsilon} = \sigma^{\text{rec}}(\varepsilon). \quad (9)$$

It is convenient to normalize the incident electron wave function in such a way, that the flux for the incident electron is equal to unity [3]. Then the recombination cross-section coincides with the electron capture probability (transition rate) and has the same dimensionality as energy in relativistic units.

According to the Feynman rules in the Furry picture of QED a general nondiagonal second order $S$-matrix element corresponding to Fig. 1 with $a \equiv \varepsilon$ looks like

$$\langle \varepsilon' | S^{(2)} | \varepsilon \rangle = e^{2} \int d^{4}x_{1}d^{4}x_{2}\bar{\psi}_{\varepsilon'}(x_{1})\gamma^{\mu} \times S(x_{1},x_{2})\gamma^{\nu}\psi_{\varepsilon}(x_{2})D_{\mu\nu}(x_{1}x_{2}), \quad (10)$$

where $\psi_{\varepsilon}(x)$ is the Dirac wave function for the unbound electron in the field of the nucleus, $\bar{\psi}$ is the Dirac conjugated wave function, $\gamma^{\mu}$ are the Dirac matrices, $S(x_{1},x_{2})$ is the electron propagator for the electron in the Furry picture, $D_{\mu\nu}(x_{1}x_{2})$ is the photon propagator. We use the standard expressions for $\psi_{\varepsilon}(x)$, $S(x_{1}x_{2})$ and $D_{\mu\nu}(x_{1}x_{2})$ [3], [6]:

$$\psi_{\varepsilon}(x) = \psi_{\varepsilon}(\vec{r})e^{-i\varepsilon t}, \quad (11)$$

the eigenmode decomposition for the electron propagator

$$S(x_{1}x_{2}) = \frac{1}{2\pi i} \int d\omega e^{i\omega(t_{1} - t_{2})} \sum_{n} \frac{\psi_{n}(\vec{r}_{1})\bar{\psi}_{n}(\vec{r}_{2})}{E_{n}(1 - i0) - \omega}, \quad (12)$$

where sum runs over the entire dirac spectrum for atomic electron, $E_{n}$ being the level energies, and the photon propagator in the Feynman gauge

$$D_{\mu\nu}(x_{1}x_{2}) = \frac{1}{2\pi i} \frac{g_{\mu\nu}}{r_{12}} \int d\omega e^{i\omega(t_{1} - t_{2}) + i\omega|r_{12}|}, \quad (13)$$

where $r_{12} = |\vec{r}_{1} - \vec{r}_{2}|$ and $g_{\mu\nu}$ is the metric tensor.

For the evaluation of the energy shift $\Delta E_{\varepsilon}$ we use Eq. (3) and

$$\Delta E_{\varepsilon} = \langle a|U|a \rangle, \quad (14)$$

which is valid for irreducible Feynman graphs like Fig. 1 [6]. Inserting Eqs. (10)-(13) into Eqs. (3), (14), and integrating over the time and frequency variables we find

$$\Delta E_{\varepsilon} = \frac{e^{2}}{2\pi i} \sum_{n} \left( \frac{1 - \bar{\alpha}_{1}\alpha_{1}}{r_{12}} I_{\varepsilon n}(r_{12}) \right) \varepsilon_{nn\varepsilon}, \quad (15)$$

$$I_{\varepsilon n}(r_{12}) = \int_{-\infty}^{\infty} \frac{e^{i\omega r_{12}} d\omega}{E_{n}(1 - i0) - \varepsilon + \omega}, \quad (16)$$

$$\left( \hat{A}(12) \right)_{abcd} \equiv \langle \bar{\psi}_{a}(1)\bar{\psi}_{b}(2) | \hat{A}(12) | \psi_{c}(1)\psi_{d}(2) \rangle. \quad (17)$$

Here $\alpha_{i}$ are the Dirac matrices acting on the functions depending on the variables $i = 1, 2$.

To evaluate the $\sigma_{\varepsilon}^{\text{rec}}$ according to Eq. (9) we need to consider the imaginary part $\Delta E_{\varepsilon}$, i.e. the real part of the integral $I_{\varepsilon n}(r_{12})$. We rewrite this integral in the form

$$I_{\varepsilon n}(r_{12}) = \int_{-\infty}^{\infty} \frac{e^{i\omega r_{12}} d\omega}{E_{n} - \varepsilon + \omega \mp i0} \quad (18)$$

In the second integral in Eq. (18) we can omit $\mp i0$ in the denominator since this denominator has no zeros within the interval $(-\infty, 0]$. Then the second term in the right-hand side of Eq. (18) is pure imaginary and we will concentrate at first term. The sign $\mp$ in the denominator of the first integral corresponds to $E_{n} < 0$, $E_{n} > 0$. Evaluating this integral in the complex plane we close the contour of integration in the upper half-plane since in this half-plane the integral vanishes along the half-circle with infinitely large radius. The existence of the pole inside this contour depends on the sign of $E_{n}$: the pole exists when $E_{n} > 0$. Evaluation of residue in this pole gives

$$\text{Re}I_{\varepsilon n}(r_{12}) = 2\pi \sin ((\varepsilon - E_{n})r_{12}) \quad (19)$$

and finally we obtain the closed expression for $\Gamma_{\varepsilon}$:

$$\Gamma_{\varepsilon} = -2\text{Im}\Delta E_{\varepsilon} = \sum_{n, E_{n} > 0} \left( \frac{1 - \bar{\alpha}_{1}\alpha_{1}}{r_{12}} \sin ((\varepsilon - E_{n})r_{12}) \right)_{\varepsilon n\varepsilon}. \quad (20)$$

This expression is an analog of the expression for the full radiative one-photon width for the one-electron atom derived in [6]:

$$\Gamma_{n} = 2e^{2} \sum_{n, E_{n} < E_{a}} \left( \frac{1 - \bar{\alpha}_{1}\alpha_{1}}{r_{12}} \sin ((E_{a} - E_{n})r_{12}) \right)_{\varepsilon n\varepsilon}. \quad (21)$$
The value $\Gamma_e$ also represents the one-photon (lowest order in $e$) contribution to the photorecombination for the one-electron atom. In a similar way an expression for the cross-section of bremsstrahlung for the electron scattered on the nucleus can be derived

$$\Gamma_{eBS} = 2e^2 \int d\varepsilon' \left( 1 - \frac{\alpha_1 \alpha_2}{\varepsilon_1} I_{e\varepsilon}(r_{12}) \right) \sum_{\varepsilon, \varepsilon'} (\varepsilon e') \delta(\varepsilon - \varepsilon') . \quad (22)$$

Expressions (20), (21), (22) are valid for one-electron ions with arbitrary high value of the nuclear charge $Z$. Evaluation of the level widths or cross-sections for the highly charged ions with use of these formulas is out of scope of the present paper.

III. QED EVALUATION FOR THE PHOTORECOMBINATION FOR AN ATOM IN A HEAT BATH

Our goal in the present paper is to evaluate the photorecombination cross-section for the hydrogen atom in the field of BBR by the method described in section II. When describing the processes of photonization and photorecombination in atoms the influence of the stimulated emission also has to be taken into account [3]. In a sense, the BBR also provides the stimulated emission with the Planck frequency distribution. The influence of the BBR on $\sigma_{\text{rec}}$ and $\sigma_{\text{ion}}$ is of interest also for astrophysics [11, 12] since the Cosmic Microwave Background (CMB) possesses the properties of BBR. A QED description of the heated electron-photon plasma was made for example in [9, 10], where the free electron and photon propagators in the field of BBR were derived. The application of QED theory to the atoms in the field of BBR was recently made in [11]. The electron propagators in [11] were assumed to be the same as in [9, 10], but the photon propagators were the same as for the bound electrons in atoms. The reason was that the BBR field can essentially destroy the atomic structure only at the very high temperatures. In the present paper we assume that the same remarks are valid for the unbound electrons in the field of the nucleus. The latter field is still considered to be much stronger than the BBR field.

In [11] the same one-loop electron self-energy as depicted in Fig. 1 was applied for the description of the radiative shift for atomic electrons in the field of the BBR. The only difference with the description in section II of this paper was that the photon propagator Eq. (13) was replaced by propagator for thermal photons with the Planck frequency distribution. An imaginary part of this radiative shift was considered as the atomic level broadening in the field of the BBR. In this section we will do the same for the unbound electron in the field of the nucleus. This will give us the correction to $\sigma_{\text{rec}}$ for atoms in the heat bath.

The photon propagator for the thermal photons derived in [9, 10] looks like

$$D_{\mu\nu} = -4\pi g_{\mu\nu} \int \frac{d^4k}{(2\pi)^4} n_{\beta}(|\vec{k}|) e^{i(k(x_1-x_2))} \delta(k^2), \quad (23)$$

where $k = (\vec{k}, \omega)$, $k^2 = \vec{k}^2 - \omega^2 = |\vec{k}|^2 - \omega^2$, $n_{\beta}(|\vec{k}|) = (e^{\beta|\vec{k}|} - 1)^{-1}$, $\beta = k_BT$, $k_B$ is the Boltzman constant and $T$ is the radiation temperature. An expression for the thermal radiative shift for the unbound electron in the field of the nucleus is similar to Eq. (15).

$$\Delta E_{\beta}^\varepsilon = \frac{e^2}{\pi} \sum_{(\varepsilon e')} \left( \frac{1 - \alpha_1 \alpha_2}{\varepsilon_1} I_{\varepsilon e'}^\beta(r_{12}) \right) \times \epsilon_{\varepsilon e'} \varepsilon_{\varepsilon e} . \quad (24)$$

where

$$I_{\varepsilon e}^\beta(r_{12}) = 2 \int d\omega \int d|\vec{k}| |\vec{k}| \sin\left(|\vec{k}|r_{12}\right) \frac{\delta(|\vec{k}|^2 - \omega^2)n_{\beta}(|\vec{k}|)}{E_n(1-i\omega) - \varepsilon + \omega} . \quad (25)$$

The limitation $|E_n| < I$ for the sum over $n$ in Eq. (24), where $I$ is the ionization potential for the ground state of an atom, means that the summation is carried out only over the discrete spectrum.

For obtaining Eq. (25) the integration over angles in Eq. (23) was performed. Presenting $\delta$-function in Eq. (25) in the form

$$\delta(|\vec{k}|^2 - \omega^2) = \frac{1}{2|\vec{k}|} \left[ \delta(\omega + |\vec{k}|) + \delta(\omega - |\vec{k}|) \right] \quad (26)$$

and integrating over $\omega$ in Eq. (25) we find

$$I_{\varepsilon e}^\beta(r_{12}) = \int_0^\infty d|\vec{k}| |\vec{k}| \sin\left(|\vec{k}|r_{12}\right) n_{\beta}(|\vec{k}|) \times \left[ \frac{1}{E_n(1-i\omega) - \varepsilon + |\vec{k}|} + \frac{1}{E_n(1-i\omega) - \varepsilon - |\vec{k}|} \right] . \quad (27)$$

For proceeding further we can use the "pole approximation" in Eq. (27). Then only the first term in square brackets in Eq. (27) contributes. Formally, this contribution can be obtained via the Sokhotski-Plemelj relation

$$\frac{1}{x - i\varepsilon} = P.V. \frac{1}{x} + i\pi \delta(x), \quad (28)$$

where $P.V.$ means that when integrating the left part of Eq. (28) with any complex (analytical) function the integral with the first term in the right-hand part of Eq. (28) should be understood as a principal value integral. Note also that considering the thermal corrections we limit ourselves only with positive values of $E_n$. Since we are interested in imaginary part of $\Delta E_{\beta}$ and hance of $I_{\varepsilon e}^\beta(r_{12})$ we obtain the following results

$$\text{Im} I_{\varepsilon e}^\beta(r_{12}) = \pi \sin \left( (\varepsilon - E_n)r_{12} \right) n_{\beta}(\varepsilon-E_n), \quad (29)$$

$$\text{Im} \Delta E_{\beta}^\varepsilon = \frac{e^2}{\pi c^2} \sum_n \left( \frac{1 - \alpha_1 \alpha_2}{\varepsilon_1} \sin \left( (\varepsilon - E_n)r_{12} \right) n_{\beta}(\varepsilon-E_n) \right) \times \epsilon_{\varepsilon e} \varepsilon_{\varepsilon e} . \quad (30)$$

In the nonrelativistic limit $(\varepsilon - E_n)r_{12} \approx \alpha$ (in r.u., $\alpha$ is the fine structure constant) and we can expand $\sin ((\varepsilon - E_n)r_{12})$ in Taylor series. For the term independent on $\beta$, the first term of Taylor expansion vanishes due to the orthogonality of the wave functions $|\varepsilon|n\rangle = 0$. The next
term, with the use of relation $r_{12}^2 = r_1^2 + r_2^2 - 2(r_1 r_2)$ reduces to the dipole matrix elements $\langle \epsilon | \tilde{p} | n \rangle \langle n | \tilde{r} | \epsilon \rangle$. For the term depending on $\tilde{\alpha}$-matrices in Eq. (19), the first term of Taylor expansion works. Remembering that in the nonrelativistic limit $\langle \epsilon | \tilde{\alpha} | n \rangle = \langle \epsilon | \tilde{p} | n \rangle$, where $\tilde{p}$ is the momentum operator and using the known quantum-mechanical relation $\langle \epsilon | \tilde{p} | n \rangle = -i(\epsilon - E_n)\langle \epsilon | \tilde{r} | b \rangle$ we again reduce the $\tilde{\alpha}$-matrix contribution to the product $\langle \epsilon | \tilde{r} | n \rangle \langle n | \tilde{r} | \epsilon \rangle$. Combining both contributions we finally arrive at the quantum-mechanical expression for the photorecombination cross-section for an atom in the BBR field [3]:

$$\sigma^\text{rec,}\beta = 4\pi^2 \sum_{|\epsilon_n|<\epsilon}^n (\epsilon - E_n)n_\beta(\epsilon - E_n) |\langle \epsilon | \tilde{p} | n \rangle|^2. \quad (31)$$

IV. QED THEORY OF THE PHOTORECOMBINATION IN THE HEAT BATH WITH ATOMIC LEVEL WIDTHS TAKEN INTO ACCOUNT

In our previous work [11] it was shown that the atomic level width within the QED approach for bound-bound transitions (i.e. for atomic level broadening) in the field of the BBR leads to the important change in the results. In [11] it was also argued that from the other point of view the influence of BBR can be considered as a mixing of atomic levels by the field of the BBR. Recently, this idea was applied to the astrophysics of cosmological recombination [12]. It was shown that the influence of the BBR (CMB) shifts the values of cosmological parameters by $\sim 1\%$, i.e. as much as the other important corrections. In this section we will apply the same approach to the photoionization process which are the unbound-bound transitions.

Now we have to return to Eq. (27) and to insert the atomic level widths within the frames of QED. For this purpose we have to consider the double loop Feynman graph Fig. 2. It is easy to check that after using again the Feynman rules, employing the expression [12] for the electron propagator, expression [13] for the ordinary photon propagator, expression (23) for the thermal photon propagator and after integrating over time and frequency variables in the pole approximation, we will get for $\Delta E_\beta$ the same expression as (24) but with the integral (27) replaced by

$$I^\beta_n(r_{12}) = \int_0^\infty d\omega_T \sin(\omega_T r_{12}) n_\beta(\omega_T) \times \quad (32)$$

$$1 - \frac{1}{E_n(1 - i\delta) - \epsilon + \omega_T + \Delta E_n} \quad (33)$$

where $\Delta E_n = L_n - \frac{i}{2}\Gamma_n$. Further we will neglect the Lamb shift $L_n$ and keep only the level width $\Gamma_n$ in the our calculations. In this way the spectral line profile was first derived within QED [13]. In [11] this way of inserting the atomic level widths was extended outside the pole approximation, for the second term in square brackets in Eq. (27) and for all the values of $\omega_T$ in the integral over $\omega_T$ in this expression. This contribution in [11], [12] was called "nonresonant" unlike the pure pole ("resonant") contribution. With this definition the "nonresonant" approximation includes also the "resonant" part. In [11] a procedure, that was originally applied for the resonant photon scattering on an atom, was used for introducing atomic level widths in the denominators in Eq. (27). This is strictly justified within QED for the first term in square brackets in Eq. (27). In the second term in square brackets the imaginary part in denominator can be omitted since there is no pole. Therefore, the second term in Eq. (27) is pure real and does not contribute to the imaginary part of the correction Eq. (24).

Our final expression for the photorecombination cross-section looks like

$$\sigma^\text{rec,}\beta = -2\text{Im}\Delta E_\beta =$$

$$2\epsilon^2 \frac{3}{\pi} \sum_n |\langle \epsilon | \tilde{p} | n \rangle|^2 \int_0^\infty d\omega_T \frac{n_\beta(\omega_T)\Gamma_n}{(E_n - \epsilon + \omega_T)^2 + \frac{1}{4}\Gamma_n^2}. \quad (34)$$
TABLE I. The recombination coefficients for spontaneous and stimulated recombination processes for $1s$, $2s$, $3s$, $5s$ and $10s$ states at different temperatures. Coefficients $\alpha_{nl}$ are calculated with the use of Eq. (32), while the coefficients $\alpha_{nl}^\beta$ and $\bar{\alpha}_{nl}^\beta$ are defined by Eqs. (31) and (34), respectively. All values are given in $m^3/s$.

| $T = 300 K$ | $T = 1000 K$ | $T = 3000 K$ | $T = 5000 K$ | $T = 10000 K$ | $T = 20000 K$ |
|-------------|--------------|--------------|--------------|--------------|--------------|
| $\alpha_{1s}$ | $9.4939 \times 10^{-19}$ | $5.1848 \times 10^{-19}$ | $2.9688 \times 10^{-19}$ | $2.2812 \times 10^{-19}$ | $1.5819 \times 10^{-19}$ | $1.0787 \times 10^{-19}$ |
| $\alpha_{1s}^\beta$ | 0.0 | 6.9968 $\times 10^{-88}$ | 2.0781 $\times 10^{-42}$ | 2.2263 $\times 10^{-33}$ | 1.1211 $\times 10^{-26}$ | 2.0858 $\times 10^{-23}$ |
| $\alpha_{2s}$ | $1.39195 \times 10^{-19}$ | $7.6117 \times 10^{-20}$ | $4.3716 \times 10^{-20}$ | $3.3664 \times 10^{-20}$ | $2.34199 \times 10^{-20}$ | $1.5998 \times 10^{-20}$ |
| $\alpha_{2s}^\beta$ | 5.02703 $\times 10^{-77}$ | $2.7449 \times 10^{-37}$ | $4.2385 \times 10^{-26}$ | $6.3229 \times 10^{-24}$ | $2.3283 \times 10^{-22}$ | $1.2711 \times 10^{-21}$ |
| $\alpha_{2s}^\beta$ | $6.5903 \times 10^{-39}$ | $3.5099 \times 10^{-37}$ | $4.2385 \times 10^{-26}$ | $6.3204 \times 10^{-24}$ | $2.3283 \times 10^{-22}$ | $1.2711 \times 10^{-21}$ |
| $\alpha_{3s}$ | $4.68487 \times 10^{-20}$ | $2.5616 \times 10^{-20}$ | $1.46942 \times 10^{-20}$ | $1.12941 \times 10^{-20}$ | $7.81646 \times 10^{-21}$ | $5.28975 \times 10^{-21}$ |
| $\alpha_{3s}^\beta$ | $9.4105 \times 10^{-46}$ | $3.0846 \times 10^{-28}$ | $2.13561 \times 10^{-23}$ | $1.74178 \times 10^{-22}$ | $7.83262 \times 10^{-22}$ | $1.62699 \times 10^{-21}$ |
| $\alpha_{3s}^\beta$ | $1.8846 \times 10^{-32}$ | $3.0855 \times 10^{-28}$ | $2.13561 \times 10^{-23}$ | $1.74178 \times 10^{-22}$ | $7.83262 \times 10^{-22}$ | $1.62699 \times 10^{-21}$ |
| $\alpha_{4s}$ | $2.2698 \times 10^{-20}$ | $6.67498 \times 10^{-21}$ | $3.77965 \times 10^{-21}$ | $2.87475 \times 10^{-21}$ | $1.95188 \times 10^{-21}$ | $1.2908 \times 10^{-21}$ |
| $\alpha_{4s}^\beta$ | $4.4237 \times 10^{-30}$ | $6.07121 \times 10^{-24}$ | $2.54593 \times 10^{-22}$ | $5.16808 \times 10^{-22}$ | $8.74335 \times 10^{-22}$ | $1.11702 \times 10^{-21}$ |
| $\alpha_{4s}^\beta$ | $4.4687 \times 10^{-30}$ | $6.07121 \times 10^{-24}$ | $2.54593 \times 10^{-22}$ | $5.16808 \times 10^{-22}$ | $8.74335 \times 10^{-22}$ | $1.11702 \times 10^{-21}$ |
| $\alpha_{5s}$ | $2.06681 \times 10^{-21}$ | $1.09008 \times 10^{-21}$ | $5.87262 \times 10^{-22}$ | $4.34211 \times 10^{-22}$ | $2.83431 \times 10^{-22}$ | $1.80743 \times 10^{-22}$ |
| $\alpha_{5s}^\beta$ | $5.42689 \times 10^{-24}$ | $1.34303 \times 10^{-22}$ | $3.19801 \times 10^{-22}$ | $3.74313 \times 10^{-22}$ | $4.04424 \times 10^{-22}$ | $3.92211 \times 10^{-22}$ |
| $\alpha_{5s}^\beta$ | $5.42689 \times 10^{-24}$ | $1.34303 \times 10^{-22}$ | $3.19801 \times 10^{-22}$ | $3.74313 \times 10^{-22}$ | $4.04424 \times 10^{-22}$ | $3.92211 \times 10^{-22}$ |

We remind that this expression is written in special units when the incident electron current is set equal to unity. Otherwise Eq. (34) should be divided by this current. The "nonresonant" expression (34) reduces to the "resonant" one Eq. (31) when $\Gamma_n = 0$. This can be seen with the use of the formula

$$\delta(x) = \frac{1}{\pi} \lim_{\epsilon \to 0} \frac{\epsilon}{x^2 + \epsilon^2}. \quad (35)$$

V. RECOMBINATION AND IONIZATION COEFFICIENTS

The effective cross-sections evaluated in previous sections allows for the definition of recombination and ionization coefficients [4]. The rate of recombination to the $n$-th level due to the spontaneous recombination processes, $\alpha_{nl}$, is given by

$$\alpha_{nl} = \int_0^\infty \sigma_{nl}^{\text{rec,}\beta} f(v) dv, \quad (36)$$

where $f(v)$ is the Maxwell-Boltzmann distribution function with the velocity of incident electrons $v$ ($v = p$ in our units):

$$f(v) dv = 4\pi \left( \frac{1}{2\pi k_B T} \right)^{3/2} v^2 e^{-\frac{v^2}{2k_B T}} dv. \quad (37)$$

The presence of the Maxwell-Boltzmann distribution function in recombination coefficient restricts the magnitude of the incident electron momentum $p$. The typical speed can be estimated as $p^2 \sim 2k_BT \ll 1$ upto $T \sim 10^5 K$ what justifies the nonrelativistic approximation used to obtain Eq. (31).

The similar equation can be written for the stimulated recombination coefficient

$$\alpha_{nl}^\beta = \int_0^\infty \sigma_{nl}^{\text{rec,}\beta} f(v) dv, \quad (38)$$

and the total recombination coefficient is

$$\alpha_{nl}^{\text{total}} = \alpha_A = \sum_{nl} \alpha_{nl}, \quad (39)$$

where index $A$ corresponds to the so called case A when the coefficient $\alpha_{nl}^{\text{total}}$ includes the direct recombination process to the ground state, while the case B in astrophysical researches excludes this process.

According to Eq. (34) the most curious result arises for the ground state of an atom. Since the natural level width of ground state is zero the cross-section of recombination process reduces to Eq. (31), i.e. there is the only resonant contribution. The spontaneous recombination coefficients defined by Eqs. (22), (36) and stimulated recombination coefficients making use of Eqs. (31), (34) and (38) are compared numerically in Table I.

It is shown that the stimulated recombination coefficient becomes important for the high temperatures and can exceed the spontaneous one for the highly excited states. The numerical values in Table I obtained with Eq. (31) are in a perfect
TABLE II. The total recombination coefficients for spontaneous, stimulated photorecombination and photoionization processes at different temperatures are listed. Coefficients $\alpha_A$ are calculated by the summation of Eqs. (22) and (36) over $nl$, while the coefficients $\alpha_A^\beta$ and $\alpha_A^{\alpha,\beta}$ are defined by Eqs. (31), (32) and (33), respectively. The total photoinization coefficient, $\beta_A$ is obtained with the use of Eqs. (1) and (23). These values were obtained by the direct summation over $nl$ up to $n = 70$, $T = 10000$ K and $n = 300$ (the first, second, third and fourth sublines in rows, respectively). In the last two rows the values of recombination coefficient corresponding to the case B can be easily come comparable with them at temperature about $(34)$ are significantly larger than the results obtained with Eq. (40), see [13]. All values are given in $m^3/s$. The three last sublines in the last row represent the relative difference, $(\alpha_A^\beta - \alpha_B)/\alpha_A^\beta$, in percents.

$$\begin{array}{cccccccc}
T & \alpha_A & \alpha_A^\beta & \alpha_A - \alpha_A^\beta & \beta_A & \beta_A^\beta & \beta_A - \beta_A^\beta & \alpha_B & \alpha_B^\beta \\
T = 300 K & 4.16281 \times 10^{-18} & 4.58123 \times 10^{-19} & 6.78681 \times 10^{-19} & 5.71538 \times 10^{-19} & 5.12927 \times 10^{-19} & 2.58022 \times 10^{-19} & 9.29960 \times 10^{-19} & 7.28372 \times 10^{-19} \\
T = 700 K & 4.23453 \times 10^{-18} & 4.68994 \times 10^{-19} & 6.87894 \times 10^{-19} & 5.71538 \times 10^{-19} & 5.12927 \times 10^{-19} & 2.58022 \times 10^{-19} & 9.29960 \times 10^{-19} & 7.28372 \times 10^{-19} \\
T = 1000 K & 4.28424 \times 10^{-18} & 4.58123 \times 10^{-19} & 6.78681 \times 10^{-19} & 5.71538 \times 10^{-19} & 5.12927 \times 10^{-19} & 2.58022 \times 10^{-19} & 9.29960 \times 10^{-19} & 7.28372 \times 10^{-19} \\
T = 3000 K & 4.32385 \times 10^{-18} & 4.68994 \times 10^{-19} & 6.87894 \times 10^{-19} & 5.71538 \times 10^{-19} & 5.12927 \times 10^{-19} & 2.58022 \times 10^{-19} & 9.29960 \times 10^{-19} & 7.28372 \times 10^{-19} \\
T = 5000 K & 4.32385 \times 10^{-18} & 4.68994 \times 10^{-19} & 6.87894 \times 10^{-19} & 5.71538 \times 10^{-19} & 5.12927 \times 10^{-19} & 2.58022 \times 10^{-19} & 9.29960 \times 10^{-19} & 7.28372 \times 10^{-19} \\
T = 10000 K & 4.32385 \times 10^{-18} & 4.68994 \times 10^{-19} & 6.87894 \times 10^{-19} & 5.71538 \times 10^{-19} & 5.12927 \times 10^{-19} & 2.58022 \times 10^{-19} & 9.29960 \times 10^{-19} & 7.28372 \times 10^{-19} \\
T = 20000 K & 4.32385 \times 10^{-18} & 4.68994 \times 10^{-19} & 6.87894 \times 10^{-19} & 5.71538 \times 10^{-19} & 5.12927 \times 10^{-19} & 2.58022 \times 10^{-19} & 9.29960 \times 10^{-19} & 7.28372 \times 10^{-19} \\
\end{array}$$

The two cases (A and B) of astrophysical investigations are noted by the corresponding indexes. The case B can be easily obtained by the subtraction of corresponding values of $\alpha_A$ from $\alpha_A^\beta$. The values of $\alpha_B$ are compared in the last rows of Table II with the results calculated via the extrapolation formula, see [14] and references therein:

$$\alpha_B^\beta = 10^{-19} \frac{a b}{1 + c t d} m^3 s^{-1}, \quad (40)$$

where $a = 4.309$, $b = -0.6166$, $c = 0.6703$ and $d = 0.5300$.

agreement with the quantum mechanical results [7], [8]. The values of stimulated recombination coefficient defined by Eq. (34) are significantly larger than the results obtained with Eq. (31) at low temperatures for low lying excited states and become comparable with them at temperature about 1000 K for any states.

Numerical results for the total recombination (spontaneous and stimulated) and ionization coefficients (summed over all $nl$ states) are collected in Table II.

Relative difference of our calculations and results obtained with Eq. (40) for $\alpha_B$ is about 5.2% at the temperature 300 K and decreases to 0.55% at the temperature 20000 K for the set of $nl$ states with $n_{\text{max}} = 70$. The deviation occurs due to the two circumstances: i) at low temperatures the larger number of states $nl$ should be taken into account in view of bad convergence of sum over $nl$ set; ii) the extrapolation formula does not work well at low temperatures. The discrepancy between $\alpha_B$ and $\alpha_B^\beta$ decreases with the account for the larger set of quantum states, the relative difference in percents is given
in the last rows of Table II and does not exceed the 0.5% at \( \eta_{\text{max}} = 300 \). Applying the same fit as Eq. (40) to our data for the set of quantum states with \( \eta_{\text{max}} = 300 \), i.e. taking into account 45000 atomic levels, one can find \( a = 4.2707, b = -0.6172, c = 0.6554 \) and \( d = 0.5307 \). It is expected that such fit modification can lead to the correction of the order of 0.25% for the ionization fraction of primordial plasma.

An accuracy of our calculations can be checked via the detailed balance relation. According to this the sum of spontaneous and stimulated recombination coefficient should be equal to the photoionization coefficient: \( \alpha_A + \alpha_\beta = \beta_A \). In our calculations the largest relative difference corresponds to the temperature 300 K and is about \( 5.4 \times 10^{-13} \), whereas for the temperature 20000 K it is about \( 4.5 \times 10^{-17} \). Such relative deviation allows us to analyse the effect of finite lifetimes on the photorecombination process. For this purpose we compare \( \alpha_A^\beta \) and \( \tilde{\alpha}_A^\beta \) defined by Eqs. (31), (34) and (38), respectively. As it follows from Table II the magnitude of \( \tilde{\alpha}_A^\beta \) is almost the same as \( \alpha_A^\beta \). The more or less significant difference arises at temperatures 10000 K and 20000 K, where the deviation in seventh and fourth digit is found, respectively.

We demonstrate the difference but not the relative to show that the deviation in seventh and fourth digit is found, respectively. As it follows from Table II the magnitude of \( \alpha_A^\beta \) is 'stable' for any set of atomic states. Thus, we do not calculate \( \tilde{\alpha}_A^\beta \) for the \( \eta_{\text{max}} \) larger than 100. Since the cross-section for the stimulated recombination process increases with the account for the larger set of \( nl \) states the relative difference \( (\alpha_A^\beta - \tilde{\alpha}_A^\beta)/\alpha_A^\beta \) becomes less. Nonetheless, we can evaluate the relative difference \( (\alpha_A^\beta - \tilde{\alpha}_A^\beta)/\alpha_A^\beta \) which is about 0.0083% at temperature 20000 K and becomes negligible at lower temperatures. Thus, we can conclude that the effect of finite lifetimes of atomic levels leads to violation of the detailed balance relation on the level of 0.01% for high temperatures and can be important at low temperatures for the investigations where only the partial unbound-bound transitions play the role, see Table II.

VI. CONCLUSIONS

In this paper the new closed expression for evaluating of photorecombination and photoionization cross-section is suggested within the rigorous Quantum Electrodynamics approach. This expression allows for the accurate (unphenomenological) introducing of the finite lifetimes of atomic levels. This leads to appearance of level widths in the expression for the stimulated photorecombination cross-section, see Eq. (34). Results of Table II show that this effect can be important in investigations where the partial photorecombination processes have a meaning.

Moreover, the total recombination and ionization coefficients as well as stimulated photorecombination coefficient are evaluated. It is shown that values of total recombination and ionization coefficients are close to the results obtain with the extrapolation formula Eq. (40). However, the difference of these two magnitudes increases with the decreasing of temperature, see Table II. This happens in view of slow convergence of total photorecombination coefficient for low temperatures and series of approximations used in derivation of Eq. (40). Therefore, we have used our data to find the new extrapolation coefficients: \( a = 4.2707, b = -0.6172, c = 0.6554 \) and \( d = 0.5307 \). The rough estimations show that such modification of \( \alpha_B \) coefficient can lead to 0.25% contribution in ionization fraction of primordial plasma.

Finally, the results listed in Table II show that the effect of finite lifetimes of atomic levels leads to violation of detailed balance principle: \( \alpha_A + \alpha_\beta = \beta_A \). In our calculations this relation is fulfilled on the level of 10^{-17} at high temperatures and 10^{-13} at the temperature 300 K within the Quantum Mechanical approach. The account for atomic level widths (QED effect) results in appearance of Lorentz profile instead of \( \delta \) function, see Eq. (35). In turn, such modification stretches the distribution function under the integral Eq. (34). The comparison of QM and QED results are given in Table II as the difference of \( \alpha_A^\beta - \tilde{\alpha}_A^\beta \). In particular, from Table II follows that values of the stimulated photorecombination coefficient are larger within QED approach at low temperatures and less than QM results at high temperatures, \( \alpha_A^\beta \approx \tilde{\alpha}_A^\beta \) at the temperature about 7500 K. The magnitude \( \alpha_A^\beta - \tilde{\alpha}_A^\beta \) is the same for the different sets of quantum states at fixed temperature. The relative difference with respect to \( \alpha_A \) is about 0.0083% at temperature 20000 K what demonstrates the violation of detailed balance principle.

VII. ACKNOWLEDGMENTS

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