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Non-Markovian study of the relativistic magnetic-dipole spontaneous emission process of hydrogen-like atoms

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Abstract

A relativistic and non-Markovian study is carried out on the magnetic-dipole emission of a hydrogen-like atom of large atomic number Z without perturbation approximation. The correlation spectra are derived analytically and the corresponding correlation functions are calculated numerically. The Markovian approximation is seen to be satisfied with more accuracy as compared with the case of electric-dipole emission while the relativistic corrections are quite larger. In transition $2S_{1/2}$ to $1S_{1/2}$, the relativistic values even become several times of the non-relativistic values. As a comparison with the magnetic-dipole emission, the electric-quadrupole emission in the case of the $2D_{3/2}$ to $1S_{1/2}$ transition is also studied.

1. Introduction

In a previous paper [1], we investigated the possible relativistic and non-Markovian corrections to the electric-dipole emission. Now we make a similar consideration of the magnetic-dipole spontaneous emissions.

For quite a long time the interest in magnetic-dipole emission has been limited in astrophysics [2], where the collision probability between the atoms is so small that the magnetic-dipole emission may have the chance to take place. Subsequently it also became of interest for solar physics, in connection with the solar corona observation. Only since 1970 has the development of experimental techniques made it possible to be studied in laboratories both for hydrogen-like and helium-like atoms, leading to a relatively high interest in their theoretical investigation.

In a low Z(atomic number) region, the two-photon electric-dipole emission will overwhelm the magnetic-dipole emission, but for large Z the situation becomes different; magnetic-dipole emission may turn out to be the dominant mode.

Usually the magnetic-dipole transitions are divided into two types. In the case where the non-relativistic atomic radial wavefunctions of the initial and final states are the same, such as in the process from $2P_{3/2}$ to $2P_{1/2}$, the corresponding transition is called unhindered [2]. In contrast, if the non-relativistic initial and final atomic radial functions are orthogonal to each other, such as in the process from $2S_{1/2}$ to $1S_{1/2}$, the corresponding transition is called hindered, since its transition rate will be zero in the non-relativistic theory provided the atom-size effect is neglected, namely the factor $e^{i\mathbf{k}\cdot\mathbf{x}}$ is taken as 1 within the range of atoms.

The earlier theories just calculate the emission rate, and mainly give the results in the lowest order of perturbation; some even just give an estimate of the order of magnitude [2–6]. Lin and Feinberg [7] calculated the radiative correction to the lowest order in the process $2S_{1/2} \to 1S_{1/2} + \gamma$ decay in hydrogen-like atoms. Barut and Salamin [8], on the other hand, derived the rates of spontaneous emission based on the calculation of electron self-energy formulation; their result for the $2S_{1/2} \to 1S_{1/2} + \gamma$ decay rate is the same as the known lowest perturbation value.

In [1] we used the multi-pole photon field formulation to study the whole process of electric-dipole emission without perturbation approximation. Now we still use the same formulation to study the magnetic-dipole emission process, which says the magnetic emission corresponds to radiating a photon with a total angular momentum $J = 1$ and with a parity $P = +1$. For comparison, the electric quadrupole emission is also studied which corresponds to radiating a photon with a total angular momentum $J = 2$ and with a parity $P = +1$. The general multipole photon field formulation has been described in [1], in which the multipole vector potential $\mathbf{A}_{kJMP}$ is expressed by the spherical Bessel function $g_L(kr)$ and vector spherical function $\mathbf{Y}_{JLM}(\theta, \varphi)$. If only the two atomic levels concerned need to be considered, the interaction Hamiltonian in rotating-wave approximation is given by

$$\hat{H}_{\text{int}} = i\hbar \sum_{kJMP} \left[g_{kJMP}\hat{\sigma}_+ \hat{a}_{kJMP}\, e^{-i(\omega-\omega_0^{(R)})t} - g^*_{kJMP}\hat{\sigma}_- \hat{a}^\dagger_{kJMP}\, e^{i(\omega-\omega_0^{(R)})t} \right], \tag{1}$$

where $\hat{\sigma}_+$ and $\hat{\sigma}_-$ are the atom level upward and downward change operators, $\omega_0^{(R)}$ is the relativistic value of $\frac{1}{\hbar}(E_2 - E_1)$, $\omega = kc$, g_{kJMP} is the corresponding coupling constant given by

$$g_{kJMP} = \frac{e}{\hbar} \int d^3x\, \overline{\psi}_2(\mathbf{x}) \gamma \psi_1(\mathbf{x}) \cdot \mathbf{A}_{kJMP}(\mathbf{x}), \tag{2}$$

in which $\psi_2(\mathbf{x})$ and $\psi_1(\mathbf{x})$ are the upper level and lower level atomic wavefunctions, respectively; they are now Dirac spinors.

The state of our system is expressed by

$$|t\rangle = C_2(t)|\psi_2; 0\rangle + \sum_{kJMP} C_{1,kJMP}(t)|\psi_1; kJMP\rangle \tag{3}$$

with $|\psi_2; 0\rangle$ denoting the state in which the atom is in its upper level and no photon exists, $|\psi_1; kJMP\rangle$ denoting the state in which the atom is in its lower level with one photon in the mode $(kJMP)$.

After eliminating $C_{1,kJMP}(t)$ from the coupled equation as we did in [1], one easily gets the integro-differential equation for $C_2(t)$ as

$$\frac{d}{dt} C_2(t) = -\int_0^t U(t - t') C_2(t')\, dt'. \tag{4}$$

The function $U(t - t')$, the so-called correlation function, is given by

$$U(t - t') = \int_0^\infty R(\omega)\, e^{-i(\omega-\omega_0^{(R)})(t-t')}\, d\omega \tag{5}$$

with

$$R(\omega) = \sum_{JMP} \frac{R_0}{c\pi} |g_{kJMP}|^2, \qquad \omega = kc, \tag{6}$$

in which R_0 is the radius of the normalized sphere of the photon field. The function $R(\omega)$ is called the correlation spectrum, and can be calculated by the relevant Dirac wavefunctions and corresponding multipole vector potential of the photon.

Having got $U(t - t')$, equation (4) may be solved numerically by a simple recurrence formula [9],

$$C_2(t_{n+1}) = C_2(t_n) - \sum_{m=1}^{n} U(t_m) C_2(t_{n-m}) (\Delta t)^2. \tag{7}$$

2. The magnetic-dipole emission in atomic transition $2S_{1/2}$ to $1S_{1/2}$ and $3D_{3/2}$ to $1S_{1/2}$

First, let us consider the atomic transition $2S_{1/2}$ to $1S_{1/2}$, which is also considered in [7, 8]. The only possible one-photon emission is magnetic-dipole emission, as can be seen from the angular momentum conservation and parity conservation. By these conservation laws, the quantum number set (J, P) of the emitted photon should be $(1, +1)$. However, in the non-relativistic theory, the corresponding magnetic transition moment $\mathfrak{m}_{21}$ is zero; even the spin contribution is taken into account. The reason is that

$$\mathfrak{m}_{21} = -\frac{e\hbar}{mc} \int \varphi_2^+(\mathbf{x})(\hat{\mathbf{L}} + \sigma)\varphi_1(\mathbf{x})\, \mathrm{d}^3 x \tag{8}$$

while both integrals $\int \varphi_2^+(\mathbf{x})\hat{\mathbf{L}}\varphi_1(\mathbf{x})\, \mathrm{d}^3 x$ and $\int \varphi_2^+(\mathbf{x})\sigma\varphi_1(\mathbf{x})\, \mathrm{d}^3 x$ are zero. It is evident that the first integral is equal to zero, because the orbital angular momenta of both initial and final states are zero. The second integral is also equal to zero by the reason that the radial wavefunctions of 2S and 1S are orthogonal. Thus, only when the finite size correction (of higher order of ka) and relativistic correction are taken into account, the one-photon emission for this transition becomes possible. It is evident that under rotating-wave approximation this spontaneous emission is just a two-level process, and no other atomic level can be involved in this process as an intermediate state; hence the formulation of the last section can be applied.

We take, by will, the m' of the initial state $2S_{1/2}$ as $1/2$; so its wavefunction is given by

$$\psi_2(\mathbf{x}) = \begin{pmatrix} \frac{1}{r} G_2(r)\Omega_{\frac{1}{2}0\frac{1}{2}}(\theta, \varphi) \\ \frac{1}{r} F_2(r)\Omega_{\frac{1}{2}1\frac{1}{2}}(\theta, \varphi) \end{pmatrix} = B_0' \begin{pmatrix} (1 + B_1'\rho)\rho^s\, \mathrm{e}^{-\rho}\Omega_{\frac{1}{2}0\frac{1}{2}} \\ (A_0' + A_1'\rho)\rho^s\, \mathrm{e}^{-\rho}\Omega_{\frac{1}{2}1\frac{1}{2}} \end{pmatrix} \frac{1}{r}, \tag{9}$$

in which $s = \sqrt{1 - Z^2\alpha^2}$, the same as that in ψ_1 described in [1], and

$$\begin{aligned} &A_0' = -\frac{Z\alpha}{1 + s}, \qquad A_1' = -\frac{2s - \sqrt{2(1 + s)}}{Z\alpha(1 + 2s)}, \qquad B_1' = -\frac{2Z\alpha + \sqrt{2(1 - s)}}{Z\alpha(1 + 2s)}, \\ &\rho = \frac{Z}{a_B} \frac{\sqrt{\frac{1}{2}(1 - s)}}{Z\alpha} r, \qquad E_2 = m_0 c^2 \sqrt{\frac{1}{2}(1 + s)}, \\ &|B_0'|^2 = \left(\frac{Z}{a_B}\right) \frac{\sqrt{\frac{1}{2}(1 - s)}}{Z\alpha} \frac{2^{2s+1}}{\Gamma(1 + 2s)} \left[\left(1 + A_0'^2\right) + (B_1' + A_0'A_1')(1 + 2s) \right. \\ &\qquad \left. + \frac{1}{2}\left(B_1'^2 + A_1'^2\right) \cdot (1 + s)(1 + 2s) \right]^{-1}. \end{aligned} \tag{10}$$

The final atomic wavefunction $\psi_1(\mathbf{x})$ is the same as in [1]. $\omega_o^{(R)}$ is also the same as that of the $2P_{1/2}$ to $1S_{1/2}$ transition, namely $\omega_0^{(R)} = \frac{m_0 c^2}{\hbar}\left(\sqrt{\frac{1}{2}(1+s)} - s\right)$.

The third components of angular momenta of photon and final-state atom (M, m) now have two possible combinations: $\left(0, \frac{1}{2}\right)$ and $\left(1, -\frac{1}{2}\right)$. The corresponding two coupling constants g_{kJMP} are given by

$$g_{k10(+1)} = 2e\sqrt{\frac{\pi\omega}{\hbar R_0}} \int \overline{\psi}_2(\mathbf{x})\gamma\psi_1(\mathbf{x}) \cdot g_1(kr)\mathbf{Y}_{110}(\theta, \varphi)\, \mathrm{d}^3x, \tag{11a}$$

$$g_{k11(+1)} = 2e\sqrt{\frac{\pi\omega}{\hbar R_0}} \int \overline{\psi}_2(\mathbf{x})\gamma\psi_1(\mathbf{x}) \cdot g_1(kr)\mathbf{Y}_{111}(\theta, \varphi)\, \mathrm{d}^3x. \tag{11b}$$

As described above, the quantum number m of ψ_1 is taken as $1/2$ in equation (11a), and taken as $(-1/2)$ in equation (11b).

After carrying out the integration over spatial coordinates, we get the corresponding spectrum of correlation function as

$$R(\omega) = \frac{R_0}{c\pi}(|g_{k10(+1)}|^2 + |g_{k11(+1)}|^2) = |B_0 B_0'|^2 \alpha \frac{5 + 2\sqrt{2}}{3}\frac{\pi}{\omega}|S_1(\omega) + S_1'(\omega)|^2 \tag{12a}$$

in which

$$|B_0|^2 = \frac{Z}{a_B} 2^{2s} \frac{1+s}{\Gamma(1+2s)}, \tag{12b}$$

$|B_0'|^2$ is given by equation (10) and

$$\begin{aligned} S_1(\omega) = {} & \frac{1}{2k}\left(\frac{Za}{a_{\mathrm{B}}}\right)^s \left(1 - \frac{Za}{a_{\mathrm{B}}}\right)^s \left\{ \frac{A_0'}{\mathrm{i}ka} \frac{\Gamma(2s-1)}{(1-\mathrm{i}ka)^{2s-1}} \right. \\ & \left. + \left[\frac{A_1'}{\mathrm{i}ka}\left(1 - \frac{Za}{a_{\mathrm{B}}}\right) - A_0'\right] \frac{\Gamma(2s)}{(1-\mathrm{i}ka)^{2s}} - A_1'\left(1 - \frac{Za}{a_{\mathrm{B}}}\right)\frac{\Gamma(2s+1)}{(1-\mathrm{i}ka)^{2s+1}} + \mathrm{c.c.}\right\}, \end{aligned} \tag{13a}$$

$$\begin{aligned} S_1'(\omega) = {} & -\frac{1}{2k}\frac{Z\alpha}{1+s}\left(\frac{Za}{a_{\mathrm{B}}}\right)^s \left(1 - \frac{Za}{a_{\mathrm{B}}}\right)^s \left\{ \frac{1}{\mathrm{i}ka} \frac{\Gamma(2s-1)}{(1-\mathrm{i}ka)^{2s-1}} \right. \\ & \left. + \left[\frac{B_1'}{\mathrm{i}ka}\left(1 - \frac{Za}{a_{\mathrm{B}}}\right) - 1\right] \frac{\Gamma(2s)}{(1-\mathrm{i}ka)^{2s}} - B_1'\left(1 - \frac{Za}{a_{\mathrm{B}}}\right)\frac{\Gamma(2s+1)}{(1-\mathrm{i}ka)^{2s+1}} + \mathrm{c.c.}\right\}, \end{aligned} \tag{13b}$$

with

$$a = \frac{a_{\mathrm{B}}/Z}{1 + \frac{\sqrt{(1-s)/2}}{Z\alpha}}, \tag{14}$$

and a_{B} denotes Bohr's radius.

We note in passing that $S_1(\omega)$ and $S_1'(\omega)$ come from the integrals

$$\int_0^\infty g_1(kr)G_1(r)F_2(r)\,\mathrm{d}r$$

and

$$\int_0^\infty g_1(kr)F_1(r)G_2(r)\,\mathrm{d}r,$$

respectively.

If we just keep the leading order term in $Z\alpha$, we will get the corresponding non-relativistic correlation spectrum:

$$R(\omega) = \frac{2^9}{3^7}(5+2\sqrt{2})Z^2\alpha^3\frac{\omega}{\pi}\frac{\left(\frac{\omega^2a^2}{c^2}\right)^3}{\left(1+\frac{\omega^2a^2}{c^2}\right)^6}, \tag{15}$$

in which a is reduced to

$$a = \frac{2a_B}{3Z}. \tag{16}$$

We see that in equation (15) the leading term of the last factor is proportional to $\left(\frac{\omega a}{c}\right)^6$, contrasting with the electric-dipole result: $\sim \left(\frac{\omega a}{c}\right)^0$ (cf equation (42a) of [1]). The reason is that the magnetic-dipole moment has an extra factor $\frac{v}{c} \sim \frac{\omega_0 a}{c}$ as compared with the electric-dipole moment, and $R(\omega_0)$ is proportional to the square of the relevant moment (hence in the unhindered case the leading term will be $\left(\frac{\omega_0 a}{c}\right)^2$). Now in the transition $2S_{1/2}$ to $1S_{1/2}$ the magnetic-dipole moment is zero, which is reflected in the above relativistic calculation that the leading terms from $S_1(\omega)$ and $S_1'(\omega)$ cancel each other. The next terms in non-relativistic $S_1(\omega)$ and $S_1'(\omega)$ are proportional to $\left(\frac{\omega a}{c}\right)^3$. Since $R(\omega)/\omega \propto |S_1(\omega) + S_1'(\omega)|^2$, an additional factor $\left(\frac{\omega a}{c}\right)^6$ will appear in the leading term of $R(\omega)$ as compared with electric-dipole results.

In sum, the $R(\omega)$ of equation (15) has taken into account the finite size effect of magnetic-dipole, and in equation (12) further correction of relativistic effect is included.

Next we consider the single photon transition from $3D_{3/2}$ to $1S_{1/2}$. In this case both photons with ($J = 1$, $P = +1$) and ($J = 2$, $P = 1$) may be emitted. The former corresponds to magnetic-dipole emission similarly as in the above discussion; the latter corresponds to electric-quadrupole emission which will be discussed in the next section for comparison.

The magnetic-dipole transition is also a hindered one with zero non-relativistic magnetic moment, as can be seen from the factor $\delta_{l_1 l_2}$ in the following formula:

$$\begin{aligned}\int \Omega^*_{j_2 l_2 m_2}(\hat{\mathbf{L}}+\sigma)\Omega_{j_1 l_1 m_1}\,\mathrm{d}\Omega &= \delta_{l_1 l_2}(-1)^{m_1-m_2}\mathbf{n}^{(m_1-m_2)} \\ &\quad\times\sum_{s=-1/2}^{1/2} C^{j_1,m_1}_{l_1,m_1-s;\frac{1}{2},s}\Big(\sqrt{l_1(l_1+1)}C^{j_2,m_2}_{l_1,m_2-s;\frac{1}{2},s}C^{l_1,m_2-s}_{l_1,m_1-s;1,m_2-m_1} \\ &\quad+\sqrt{3}C^{j_2,m_2}_{l_1,m_1-s;\frac{1}{2},m_2-m_1+s}C^{\frac{1}{2},m_2-m_1+s}_{\frac{1}{2},s;1,m_2-m_1}\Big).\end{aligned} \tag{17}$$

This situation will make the electric-quadrupole emission dominate in the $3D_{3/2}$ to $1S_{1/2}$ transition, as shown in section 3.

In the relativistic theory, we take, by will, $m' = 3/2$ for the initial state $3D_{3/2}$; so the initial wavefunction is

$$\psi_2(\mathbf{x}) = \begin{pmatrix}\frac{1}{r}G_2(r)\Omega_{\frac{3}{2}2\frac{3}{2}}(\theta,\varphi)\\ \frac{1}{r}F_2(r)\Omega_{\frac{3}{2}1\frac{3}{2}}(\theta,\varphi)\end{pmatrix} = B_0'\begin{pmatrix}(1+B_1'\rho)\rho^{s_2}\,\mathrm{e}^{-\rho}\Omega_{\frac{3}{2}2\frac{3}{2}}\\ -(A_0'+A_1'\rho)\rho^{s_2}\,\mathrm{e}^{-\rho}\Omega_{\frac{3}{2}1\frac{3}{2}}\end{pmatrix}, \tag{18a}$$

with

$$s_2 = \sqrt{4-Z^2\alpha^2}, \qquad \rho = \frac{1}{\sqrt{5+2s_2}}\frac{Z}{a_\mathrm{B}}r, \tag{18b}$$

$$A_0' = \frac{Z\alpha}{2-s_2}, \tag{18c}$$

$$A_1' = -\frac{2Z\alpha(9+2s_2-4\sqrt{5+2s_2})}{(1+2s_2)\left(14-2s_2^2-3s_2+3(s_2-2)\sqrt{5+2s_2}\right)}, \tag{18d}$$

$$B_1' = -\frac{2}{1+2s_2}\frac{2-\sqrt{5+2s_2}}{3-\sqrt{5+2s_2}}, \qquad E_2 = m_0c^2\frac{1+s_2}{\sqrt{5+2s_2}} \tag{18e}$$

and

$$|B_0'|^2 = \left(\frac{Z}{a_B}\right)\frac{1}{\sqrt{5+2s_2}}\frac{2^{1+2s_2}}{\Gamma(1+2s_2)} \times \frac{1}{\left[\left(1+A_0'^2\right)+(B_1'+A_0'A_1')(1+2s_2)+\frac{1}{2}\left(B_1'^2+A_1'^2\right)\cdot(1+s_2)(1+2s_2)\right]}. \tag{18f}$$

The emission frequency of this transition is

$$\omega_0^{(R)} = \frac{m_0c^2}{\hbar}\left(\frac{1+s_2}{\sqrt{5+2s_2}}-s_1\right), \tag{19}$$

where $s_1 = s$. In the magnetic-dipole emission the only allowed value of the third components of angular momenta for photon and for final atomic state, namely (M, m), is just $(1, 1/2)$; hence only one coupling constant need be calculated:

$$g_{k11(+1)} = 2e\sqrt{\frac{\pi\omega}{\hbar R_0}}\int \overline{\psi}_2(\mathbf{x})\gamma\psi_1(\mathbf{x})\cdot g_1(kr)\mathbf{Y}_{111}(\theta,\varphi)\,\mathrm{d}^3x \tag{20}$$

in which the value m for ψ_1 takes $1/2$.

After carrying out the integration over spatial coordinates, we get the relevant correlation spectrum in the two-level approximation as

$$R(\omega) = \frac{R_0}{c\pi}|g_{k11(+1)}|^2 = |B_0B_0'|^2\alpha\frac{\omega}{2\pi}|S_1(\omega)+S_1'(\omega)|^2. \tag{21}$$

$|B_0|^2$ is still given by equation (12b). As before, $S_1(\omega)$ and $S_1'(\omega)$ come from the radial integrals

$$\int_0^\infty g_1(kr)G_1(r)F_2(r)\,\mathrm{d}r$$

and

$$\int_0^\infty g_1(kr)F_1(r)G_2(r)\,\mathrm{d}r$$

respectively, and are given by

$$S_1(\omega) = \frac{1}{2k}\left[1+\frac{1}{\sqrt{5+2s_2}}\right]^{-s_1}\left[1+\sqrt{5+2s_2}\right]^{-s_2}\left\{\frac{A_0'}{\mathrm{i}ka}\frac{\Gamma(s_1+s_2-1)}{(1-\mathrm{i}ka)^{s_1+s_2+1}}+\frac{A_1'}{\mathrm{i}ka}\frac{1}{1+\sqrt{5+2s_2}}\right. \times\frac{\Gamma(s_1+s_2)}{(1-\mathrm{i}ka)^{s_1+s_2}}-A_0'\frac{\Gamma(s_1+s_2)}{(1-\mathrm{i}ka)^{s_1+s_2}}-\left.\frac{A_1'}{1+\sqrt{5+2s_2}}\frac{\Gamma(s_1+s_2+1)}{(1-\mathrm{i}ka)^{s_1+s_2+1}}+\mathrm{c.c.}\right\}, \tag{22a}$$

$$S_1'(\omega) = -\frac{1}{2k}\frac{Z\alpha}{1+s_1}\left[1+\frac{1}{\sqrt{5+2s_2}}\right]^{-s_1}\left[1+\sqrt{5+2s_2}\right]^{-s_2}\left\{\frac{1}{\mathrm{i}ka}\frac{\Gamma(s_1+s_2-1)}{(1-\mathrm{i}ka)^{s_1+s_2-1}}+\frac{1}{\mathrm{i}ka}\right. \times\frac{B_1'}{1+\sqrt{5+2s_2}}\frac{\Gamma(s_1+s_2)}{(1-\mathrm{i}ka)^{s_1+s_2}}-\frac{\Gamma(s_1+s_2)}{(1-\mathrm{i}ka)^{s_1+s_2}} -\left.\frac{B_1'}{1+\sqrt{5+2s_2}}\frac{\Gamma(s_1+s_2+1)}{(1-\mathrm{i}ka)^{s_1+s_2+1}}+\mathrm{c.c.}\right\}, \tag{22b}$$

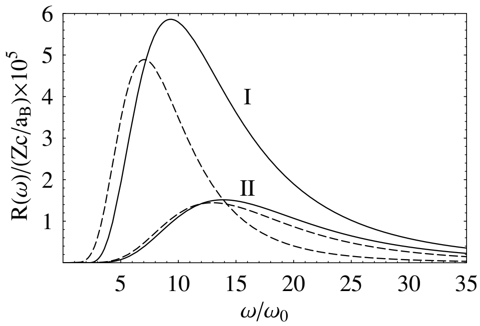

Figure 1. The relativistic correlation spectra of magnetic-dipole emission for atomic transition $2S_{1/2}$ to $1S_{1/2}$. I: $Z = 92$; II: $Z = 50$; dashed lines—the corresponding non-relativistic results.

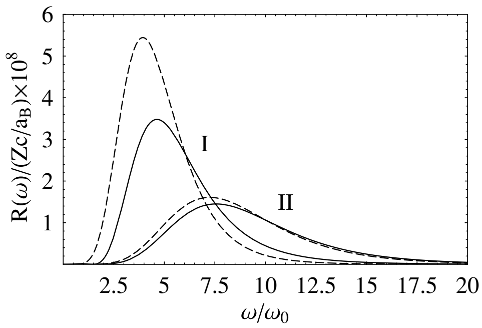

Figure 2. The relativistic correlation spectra of magnetic-dipole emission for atomic transition $3D_{3/2}$ to $1S_{1/2}$. I: $Z = 92$; II: $Z = 50$; dashed lines—the corresponding non-relativistic results.

in which case

$$a = \frac{a_B/Z}{1 + \frac{1}{\sqrt{5+2s_2}}}. \tag{23}$$

Similarly, we may just keep the term of leading order in $Z\alpha$ to get the corresponding non-relativistic spectrum, the result is

$$R(\omega) = \frac{3}{320} Z^2\alpha^3 \frac{\omega}{\pi} \frac{\left(\frac{\omega^2 a^2}{c^2}\right)^3}{\left[1 + \frac{\omega^2 a^2}{c^2}\right]^8}. \tag{24}$$

In this case, the leading term in $S_1(\omega)$ also cancels with that in $S_1'(\omega)$, hence this non-relativistic $R(\omega)$ has the same form of leading term as that in equation (15), but the numerical coefficient in equation (24) is much smaller.

Now the value of a is reduced to its non-relativistic value

$$a = \frac{3a_B}{4Z}. \tag{25}$$

We plot in figure 1 and figure 2 the correlation spectrum of magnetic-dipole emission in atomic transition $2S_{1/2}$ to $1S_{1/2}$ and $3D_{3/2}$ to $1S_{1/2}$ respectively.

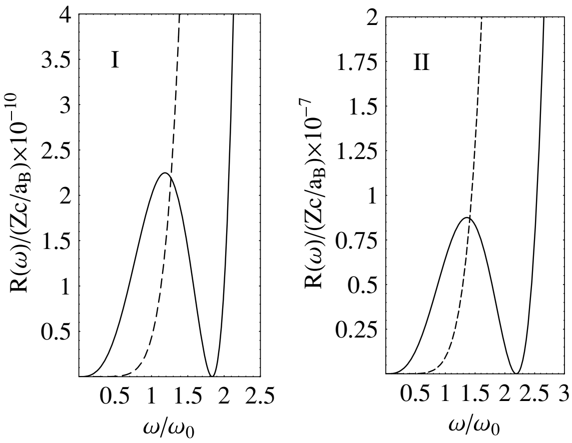

Figure 3. The small peak of relativistic correlation spectra of magnetic-dipole emission in a low frequency region for the transition $2S_{1/2}$ to $1S_{1/2}$. I: $Z = 92$; II: $Z = 50$; dashed lines are the corresponding non-relativistic $R(\omega)$.

The abscissa is taken as ω/ω_0, where the ω_0's denote the corresponding non-relativistic value. For $2S_{1/2}$ to $1S_{1/2}$, ω_0 is given by

$$\omega_0 = \frac{3}{8} Z^2 \alpha \frac{c}{a_B}, \tag{26a}$$

and for $3D_{3/2}$ to $1S_{1/2}$

$$\omega_0 = \frac{4}{9} Z^2 \alpha \frac{c}{a_B}. \tag{26b}$$

It is seen that, in the transition $2S_{1/2}$ to $1S_{1/2}$, $R(\omega)$ spread over a range somewhat larger than the range of those of electric-dipole emission. In the transition $3D_{3/2}$ to $1S_{1/2}$, the range is smaller than that of $2S_{1/2}$ to $1S_{1/2}$ for the same Z.

We note that beyond the main peak of relativistic $R(\omega)$, there is a very small peak in the low frequency region which is invisible in figures 1 and 2. We plot it separately in figures 3 and 4. These small peaks are very important, since the key values $\omega = \omega_0^{(R)}$ are located in these small peaks. The numerical values of $\omega_0^{(R)}$ calculated up to three significant digits are given by

$$\omega_0^{(R)} = \begin{cases} 1.13\omega_0, & \text{for} \quad Z = 92, \\ 1.03\omega_0, & \text{for} \quad Z = 50 \end{cases} \tag{27a}$$

for transition $2S_{1/2}$ to $1S_{1/2}$, and

$$\omega_0^{(R)} = \begin{cases} 1.16\omega_0, & \text{for} \quad Z = 92, \\ 1.04\omega_0, & \text{for} \quad Z = 50 \end{cases} \tag{27b}$$

for transition $3D_{3/2}$ to $1S_{1/2}$.

These small peaks do not appear in the non-relativistic spectrum (see the doted line of figure 3 and 4), hence their appearance is a characteristic of relativistic theory.

We also define the correspondent decay coefficient γ for magnetic-dipole emission by

$$\gamma = 2\pi R\left(\omega_0^{(R)}\right). \tag{28}$$

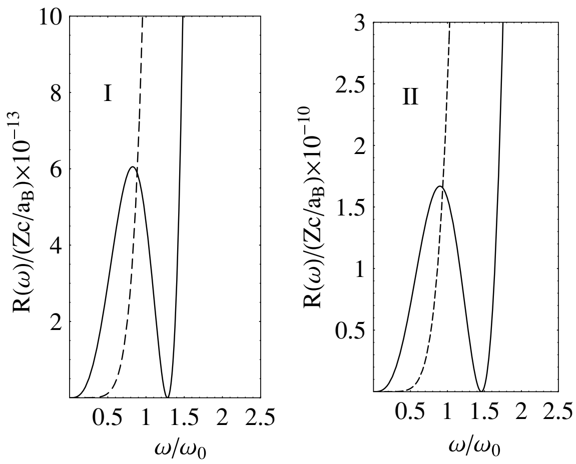

Figure 4. The small peak of relativistic correlation spectra of magnetic-dipole emission in a low frequency region for the transition $3D_{3/2}$ to $1S_{1/2}$. I: $Z = 92$; II: $Z = 50$; dashed lines are the corresponding non-relativistic $R(\omega)$.

For transition $2S_{1/2}$ to $1S_{1/2}$, calculated up to three significant digits

$$\gamma = \begin{cases} 5.66 \times 10^{-3}\gamma_A, & \text{for} \quad Z = 92, \\ 9.43 \times 10^{-5}\gamma_A, & \text{for} \quad Z = 50. \end{cases} \tag{29a}$$

γ_A is the Einstein A coefficient, characterizing the order of magnitude of the decay rate of electric-dipole emission. Equation (29a) may be compared with the non-relativistic values calculated by equation (15) for $\omega = \omega_0$:

$$\gamma = \begin{cases} 6.69 \times 10^{-4}\gamma_A, & \text{for} \quad Z = 92, \\ 1.94 \times 10^{-5}\gamma_A, & \text{for} \quad Z = 50. \end{cases} \tag{29b}$$

We see that the relativistic values are about 8.4 times and 4.9 times of non-relativistic values. The differences are quite large.

For transition $3D_{3/2}$ to $1S_{1/2}$, the relativistic results calculated by equation (28) are

$$\gamma = \begin{cases} 7.54 \times 10^{-6}\gamma_A, & \text{for} \quad Z = 92, \\ 1.78 \times 10^{-7}\gamma_A, & \text{for} \quad Z = 50, \end{cases} \tag{30a}$$

while the corresponding non-relativistic values calculated by use of equation (24) (with $\omega = \omega_0$) are given by

$$\gamma = \begin{cases} 1.81 \times 10^{-5}\gamma_A, & \text{for} \quad Z = 92, \\ 6.14 \times 10^{-7}\gamma_A, & \text{for} \quad Z = 50. \end{cases} \tag{30b}$$

We see that, in this case, the relativistic values are quite smaller than non-relativistic values, contrary to the case $2S_{1/2}$ to $1S_{1/2}$, in which the relativistic values are much larger. So one cannot generally say that magnetic-dipole emission is mainly caused by relativistic effect.

Having the correlation spectrum, the correspondent correlation function can be calculated by the numerical method as described by equation (7). The absolute value of $U(\tau)/U(0)$ are shown in figure 5 for both transitions with $Z = 50$ and $Z = 92$.

The widths τ_W at half the height of $|U(\tau)|/U(0)$ for $Z = 92$ and 50 in the transition of $2S_{1/2}$ to $1S_{1/2}$ are given by $\tau_W = 0.187/\omega_0$ and $\tau_W = 0.149/\omega_0$, respectively, while in the

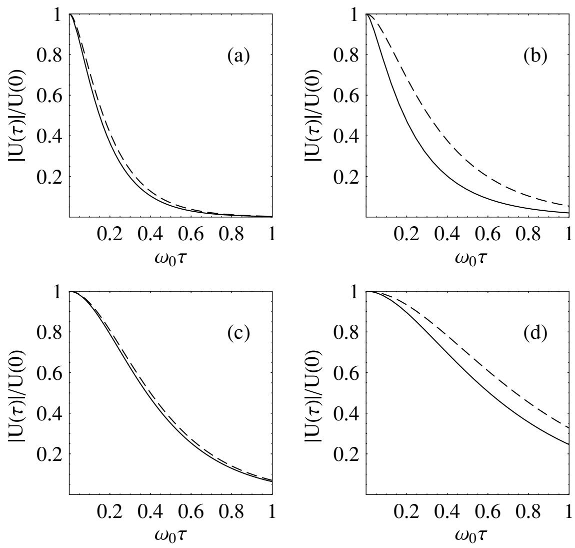

Figure 5. The relativistic correlation function $U(\tau)$ of magnetic dipole emission: the absolute value. (a) For transition $2S_{1/2}$ to $1S_{1/2}$, $Z = 50$, $U(0) = 1.98 \times 10^{-3}\omega_0^2$ for the relativistic case and $U(0) = 1.70 \times 10^{-3}\omega_0^2$ for the non-relativistic case. (b) For transition $2S_{1/2}$ to $1S_{1/2}$, $Z = 92$, $U(0) = 3.19 \times 10^{-3}\omega_0^2$ for the relativistic case and $U(0) = 1.70 \times 10^{-3}\omega_0^2$ for the non-relativistic case. (c) For transition $3D_{3/2}$ to $1S_{1/2}$, $Z = 50$, $U(0) = 6.60 \times 10^{-7}\omega_0^2$ for the relativistic case and $U(0) = 7.00 \times 10^{-7}\omega_0^2$ for the non-relativistic case. (d) For transition $3D_{3/2}$ to $1S_{1/2}$, $Z = 92$, $U(0) = 5.34\times 10^{-7}\omega_0^2$ for the relativistic case and $U(0) = 7.00\times 10^{-7}\omega_0^2$ for the non-relativistic case.

transition $3D_{3/2}$ to $1S_{1/2}$, the relevant values are $\tau_W = 0.607/\omega_0$ and $\tau_W = 0.381/\omega_0$. We see the values of τ_W for $2S_{1/2}$ to $1S_{1/2}$ transition are much smaller than $1/\omega_0$.

Figure 6 presents the correspondent arguments of $U(\tau)$ versus τ. They show a similar behaviour as those of electric-dipole emission, but they drop much deeper in the peaked region of $|U(\tau)|$, which will reduce the magnitude of γ considerably.

We have noted that the small peak of $R(\omega)$ shown in figures 3 and 4 is important for the decay behaviour, since the crucial point $\omega = \omega_0^{(R)}$ is located in this small peak. As to the large peak at higher frequency, it may greatly affect the shape of correlation function. If we just retain the small peak by removing the large peak, the curve of $|U(\tau)|$ will extend to a quite larger region than that in figure 5, as shown in figure 7. These results are according to expectation, since the small peak has a much narrower $\Delta\omega$, so its Fourier transformation will have a much wider extension $\Delta\tau$.

Now turn to the decay behaviour of the upper level population N_2. We have seen that the correlation interval τ_c in the above discussed magnetic-dipole emissions are comparable with or smaller than those in the electric-dipole emissions, and $(1/\gamma)$, which characterize the decay times, are much longer than $1/\gamma_A$ (see equations (29) and (30)); hence the Markovian approximation of $C_2(t)$ must be valid with more accuracy, resulting

$$N_2(t) \cong e^{-\gamma t} \tag{31}$$

with γ given by equation (28). This result shows that the decay coefficient γ actually represents the decay rate.

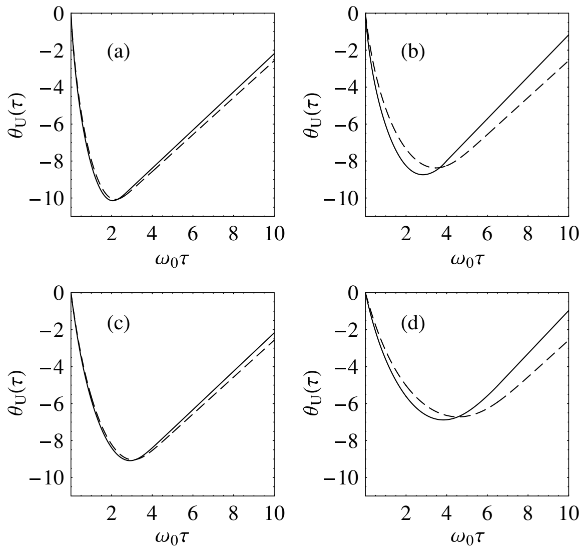

Figure 6. The relativistic correlation function $U(\tau)$ magnetic-dipole emission: θ_U (the argument of U). (a) For transition $2S_{1/2}$ to $1S_{1/2}$, $Z = 50$. (b) For transition $2S_{1/2}$ to $1S_{1/2}$, $Z = 92$. (c) For transition $3D_{3/2}$ to $1S_{1/2}$, $Z = 50$. (d) For transition $3D_{3/2}$ to $1S_{1/2}$, $Z = 92$.

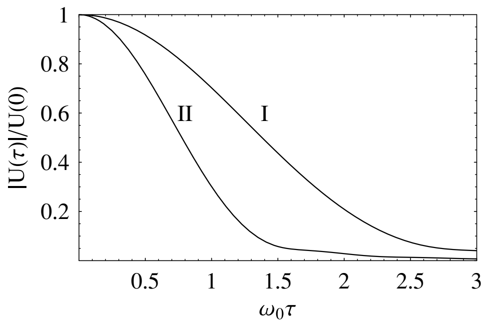

Figure 7. The absolute value of relativistic correlation function $U(\tau)$ of magnetic-dipole emission if only the small peak in the low frequency region is retained. I: for transition $3D_{3/2}$ to $1S_{1/2}$, $Z = 92$, $U(0) = 1.26 \times 10^{-9}\omega_0^2$; II: for transition $2S_{1/2}$ to $1S_{1/2}$, $Z = 92$, $U(0) = 1.39 \times 10^{-6}\omega_0^2$.

We note in passing that despite the fact that correlation function changes a lot when the large peak of spectrum is removed and hence the correlation interval τ_c is increased by several times, the decay of N_2 calculated by this modified correlation function is still almost the same as the original. The reason is that in the present case γ is extremely small, leading to the ratio of modified τ_c to $1/\gamma$ still much smaller than those for electric-dipole emission discussed in [1].

3. The electric-quadrupole emission in atomic transition $3D_{3/2}$ to $1S_{1/2}$

As a comparison we finally consider the main emission way in the transition of a hydrogen-like atom from $3D_{3/2}$ to $1S_{1/2}$—the electric-quadrupole emission.

The allowed values of (M, m), the third components of the total angular momentum of the photon and final state atom, are $\left(1, \frac{1}{2}\right)$ and $\left(2, -\frac{1}{2}\right)$. The corresponding coupling constants are given by

$$g_{k2M(+1)} = 2e\sqrt{\frac{2\pi\omega}{5\hbar R_0}} \int \overline{\psi}_2(\mathbf{x})\gamma\psi_1(\mathbf{x}) \left[\sqrt{\frac{3}{2}} g_1(kr)\mathbf{Y}_{21M}(\theta, \varphi) - g_3(kr)\mathbf{Y}_{23M}(\theta, \varphi)\right] \mathrm{d}^3x, \tag{32}$$

in which M takes the values 1 and 2, and the corresponding m for $\psi_1(\mathbf{x})$ should take $1/2$ and $-1/2$ respectively.

After carrying out the integration over space coordinates, we finally get the correlation spectrum for electric-quadrupole emission as

$$\begin{aligned} R(\omega) &= \frac{R_0}{c\pi}(|g_{k21(+1)}|^2 + |g_{k22(+1)}|^2) \\ &= |B_0 B_0'|^2 \frac{3\alpha}{25} \frac{\omega}{2\pi} |5S_1(\omega) + S_1'(\omega) - 4S_3'(\omega)|^2, \end{aligned} \tag{33}$$

in which $S_1(\omega)$ and $S_1'(\omega)$ are the same as those given by equations (22), while $S_3'(\omega)$ comes from the integral $\int g_3(kr)F_1(r)G_2(r)\,\mathrm{d}r$, with the expression

$$\begin{aligned} S_3'(\omega) = {}& \frac{1}{2k}\frac{Z\alpha}{1+s_1}\left[1 + \frac{1}{\sqrt{5+2s_2}}\right]^{-s_1} \left[1+\sqrt{5+2s_2}\right]^{-s_2} \left\{\frac{15\mathrm{i}}{k^3a^3}\frac{\Gamma(s_1+s_2-3)}{(1-\mathrm{i}ka)^{s_1+s_2-3}}\right. \\ &+ \frac{15}{k^2a^2}\left(1 + \frac{\mathrm{i}}{ka}\frac{B_1'}{1+\sqrt{5+2s_2}}\right)\frac{\Gamma(s_1+s_2-2)}{(1-\mathrm{i}ka)^{s_1+s_2-2}} - \frac{3}{ka}\left(2\mathrm{i} - \frac{5}{ka}\frac{B_1'}{1+\sqrt{5+2s_2}}\right) \\ &\times \frac{\Gamma(s_1+s_2-1)}{(1-\mathrm{i}ka)^{s_1+s_2-1}} - \left(1 + \frac{6\mathrm{i}}{ka}\frac{B_1'}{1+\sqrt{5+2s_2}}\right)\frac{\Gamma(s_1+s_2)}{(1-\mathrm{i}ka)^{s_1+s_2}} \\ &\left. + \frac{B_1'}{1+\sqrt{5+2s_2}}\frac{\Gamma(s_1+s_2+1)}{(1-\mathrm{i}ka)^{s_1+s_2+1}} + \text{c.c.}\right\}, \end{aligned} \tag{34}$$

in which a is still given by equation (23).

If we just keep the term of leading order in $Z\alpha$, the result will transit to the non-relativistic case. By this way we get the non-relativistic correlation spectrum for electric-quadrupole emission in the atomic $3D_{3/2}$ to $1S_{1/2}$ transition as

$$R(\omega) = \frac{9}{5}\left(\frac{1}{16}\right)^2 Z^2\alpha^3 \frac{\omega}{2\pi} \frac{\left(\frac{\omega a}{c}\right)^2\left(1+3\left(\frac{\omega a}{c}\right)^2\right)^2}{\left[1+\left(\frac{\omega a}{c}\right)^2\right]^8} \tag{35}$$

where a is reduced to that given by equation (25).

We see that the leading term of non-relativistic $R(\omega)/\alpha^3\omega$ is proportional to $\left(\frac{\omega a}{c}\right)^2$ compared with $\left(\frac{\omega a}{c}\right)^0$ in the electric-dipole emission. This difference reflects the fact that quadrupole moment has an additional space dimension factor a as compared with dipole moment.

On the other hand, this leading term is much larger than the leading term $\left(\frac{\omega a}{c}\right)^6$ in the non-relativistic magnetic-dipole emission of the same atomic transition, which will lead to the dominance of electric-quadrupole emission over the corresponding magnetic-dipole emission.

The correlation spectra of electric-quadrupole emission are plotted in figure 8, the abscissa being still taken as ω/ω_0 with ω_0 given by equation (26). The range of spread of $R(\omega)$ is somewhat smaller than that of electric-dipole emission.

The relevant correlation function is shown in figure 9. The widths τ_W of $|U(\tau)|/U(0)$ are $0.481/\omega_0$ for $Z = 50$, and $0.631/\omega_0$ for $Z = 92$, both of order $1/\omega_0$. The curves of

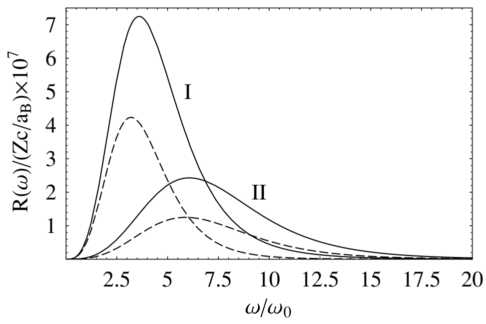

Figure 8. The relativistic correlation spectra $R(\omega)$ of electric-quadrupole emission for transition $3D_{3/2}$ to $1S_{1/2}$. I: $Z = 92$; II: $Z = 50$; dashed lines are the corresponding non-relativistic $R(\omega)$.

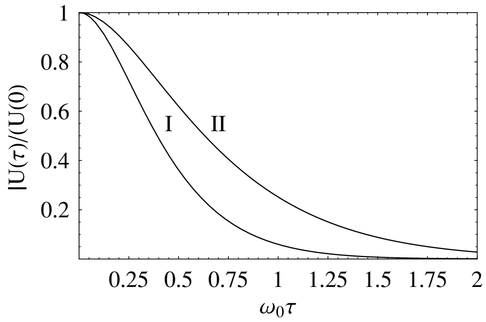

Figure 9. The relativistic correlation function $U(\tau)$ of electric-quadrupole emission for transition $3D_{3/2}$ to $1S_{1/2}$: the absolute value. I: $Z = 92, U(0) = 1.08 \times 10^{-5}\omega_0^2$; II: $Z = 50, U(0) = 1.08 \times 10^{-5}\omega_0^2$.

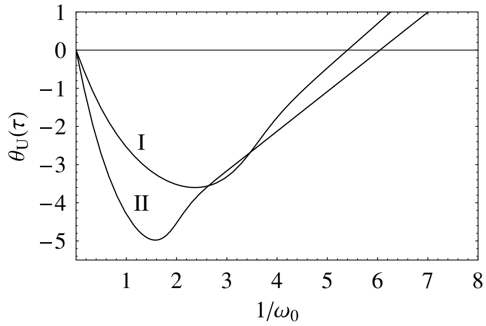

Figure 10. The relativistic correlation function $U(\tau)$ of electric-quadrupole emission for transition $3D_{3/2}$ to $1S_{1/2}$: θ_U (the argument of U). I: $Z = 92$; II: $Z = 50$.

$\theta_U(\tau)$, the argument of U(τ) versus τ are plotted in figure 10. We see $\theta_U(\tau)$ first drop down, but not so deep as those in figure 6, then rise up linearly when $\omega_0\tau$ is larger than 2.5 and 4.0.

In the present investigation, the values of γ are given by

$$\gamma = 2\pi R\big(\omega_0^{(R)}\big) = \begin{cases} 2.27 \times 10^{-3}\gamma_A, & \text{for} \quad Z = 50 \\ 6.70 \times 10^{-3}\gamma_A, & \text{for} \quad Z = 92 \end{cases} \tag{36}$$

calculated up to three significant digits, where $\omega_0^{(R)}$ is given by equation (27*b*). We see that these γ are much larger than those of corresponding magnetic-dipole emission.

As a comparison, we list the non-relativistic γ calculated by equation (35):

$$\gamma = \begin{cases} 1.15 \times 10^{-3}\gamma_A, & \text{for} \quad Z = 50, \\ 3.59 \times 10^{-3}\gamma_A, & \text{for} \quad Z = 92. \end{cases} \tag{37}$$

The difference between equations (36) and (37) gives the relativistic correction of decay coefficients. Their values are about 49% for $Z = 50$ and 46% for $Z = 92$ with positive sign.

In the present case the ratio γ/ω_0, which roughly measures the ratio of correlation internal τ_c to the decay time $1/\gamma$, is much smaller than the corresponding value for electric-dipole emission, indicating the Markovian approximation should be a good approximation. A numerical calculation confirms this assertion. Hence equation (31) holds with γ given by equation (36).

4. Brief summary

The multi-pole em field formulation is used to study the relativistic correction and non-Markovian correction of magnetic-dipole and electric-quadrupole emissions as we did in [1] for electric-dipole emission. In this formulation, the magnetic-dipole emission corresponds to the emission of a photon with $J = 1$ and $P = +1$, and the electric-quadrupole emission corresponds to the emission of a photon with $J = 2$ and $P = +1$. The electron spin current contribution is now fully included, even in the electric-quadrupole emission case.

The relativistic correlation spectra $R(\omega)$ are first analytically derived, then the corresponding correlation functions $U(\tau)$ are numerically calculated. The absolute value of $U(\tau)$ has a width smaller than $1\big/\omega_0^{(R)}$, especially in the transition of $2S_{1/2}$ to $1S_{1/2}$. Outside the peaked region $U(\tau)$ also oscillates with the frequency $\omega_0^{(R)}$. The general feature is similar to the case of electric-dipole emission.

The Markovian approximation is well satisfied over the main period of decay up to an atom of $Z = 92$, with the decay rate γ defined by the relativistic correlation spectrum $R(\omega)$ as

$$\gamma = 2\pi R\big(\omega_0^{(R)}\big).$$

But the relativistic corrections to the decay rates are quite large. For $2S_{1/2} \to 1S_{1/2}$ magnetic-dipole emission and $3D_{1/2} \to 1S_{1/2}$ electric-quadrupole emission, the relativistic corrections are positive, while for $3D_{3/2} \to 1S_{1/2}$ magnetic-dipole emission the relativistic correction on the contrary, is negative.

In our studied cases $2S_{1/2}$ to $1S_{1/2}$ and $3D_{3/2}$ to $1S_{1/2}$, the magnetic-dipole emission rates are very small. This situation reflects the fact that in the non-relativistic theory the correspondent magnetic-dipole moments are zero, namely the magnetic-dipole emission is hindered. A new feature in the relativistic correlation spectra of the investigated magnetic-dipole emission is the appearance of a small peak around $\omega_0^{(R)}$, which makes the relativistic decay rate much different from the classical value.

The electric-quadrupole emission is dominant in the atomic transition $3D_{3/2}$ to $1S_{1/2}$, as can be understood by the nonzero of non-relativistic electric-quadrupole moment. As to the relativistic correction, in this emission it is much larger than that for electric-dipole emission.

Lastly, the condition for the validity of Markovian approximation holds much better in these two kinds of emissions than in electric-dipole emission, since the corresponding γ are much smaller than that of electric-dipole emission while the correlation time τ_c's are still of order $1/\omega_0^{(R)}$ (or smaller).

Acknowledgments

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