INVESTIGATION OF FLUORESCENCE RADIATION FOLLOWING RADIATIVE RECOMBINATION OF IONS AND ELECTRONS

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Abstract

A general expression for the double differential cross section of fluorescence radiation following photorecombination (PRF) of polarized electrons and polarized ions is derived by using usual atomic theory methods and is represented in the form of multiple expansions over spherical tensors. The ways of the application of the general expression suitable for the specific experimental conditions are outlined by deriving the asymmetry parameter of angular distribution of PRF radiation in the case of nonpolarized ions and electrons. This parameter is calculated for neon-like ions and bare nuclei. A very strong dependence of the asymmetry parameter of PRF radiation angular distribution on free electron energy is obtained.

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1. Introduction

Radiative recombination (RR) is one of the dominant processes leading to the decrease of ionization degree of highly charged ions in laboratory and astrophysical plasmas. In tokamak and ion storage rings the self alignment of recombined ions arises due to the directed movement of ions that determines a strong polarization and asymmetry of the angular distribution of fluorescence radiation. The capture of an electron by an ion can take place in two ways, i.e. photorecombination (PR) and dielectronic recombination (DR). In PR, an ion $A$ with charge n+ captures a free electron, and the excess of the energy is emitted as PR radiation (PRR):

$$e^{-}(p_{m_{e}}) + A^{n+}(\alpha_{1}J_{1}M_{1}) \rightarrow A^{(n-1)+}(\alpha_{2}J_{2}M_{2}) + h\nu(\hat{\epsilon}_{1}k_{01}).$$

(1)
Here \( \mathbf{p} \) is the momentum of the electron, \( m_s \) is its spin projection onto a chosen direction, \( \hat{e}_1 \) and \( \mathbf{k}_{01} \) denote the polarization and wave vector of PRR, respectively, \( \alpha_i J_i M_i \) show other quantum numbers, total angular momentum and its projection of the ion \( i \).

If a free electron is captured into a singly excited bound state, the recombined ion can decay by emitting fluorescence radiation (PRF)

\[
A^{(n-1)+}(\alpha_2 J_2 M_2) \rightarrow A^{(n-1)+}(\alpha_3 J_3 M_3) + \hbar \nu(\hat{e}_2 \mathbf{k}_{02}).
\]  

(2)

DR is possible when the ion has one or more bound electrons. Then a free electron is captured into an ion with simultaneous excitation of a bound electron. The resulting doubly excited state of an ion can decay both radiatively and via autoionization. The DR occurs when the radiation (DRR) is emitted. The experimental investigation of PR and PRF peculiarities is possible because of fluorescence radiation emitted in the region of wavelengths much longer in comparison with those of DRR.

The aim of the present work is the derivation of a general expression for the differential cross section of PRF following PR of polarized ions and polarized electrons by using atomic theory methods [3-6] that are alternative to the density matrix formalism [7].

2. Derivation of general expression

The double differential cross section for PRF (2) following PR (1) process in two-step approximation can be written in the form of multipole expansion over non-observed states of the intermediate ion [6]:

\[
\frac{d^2\sigma(\alpha_1 J_1 M_1 m_s \rightarrow \alpha_2 J_2 \hat{e}_q \mathbf{k}_{01} \rightarrow \alpha_3 J_3 M_3 \hat{e}_q \mathbf{k}_{02})}{d\Omega_1 d\Omega_2} = \\
\sum_{K_2 N_2} \frac{d\sigma_{K_2 N_2}(\alpha_1 J_1 M_1 m_s \rightarrow \alpha_2 J_2 \hat{e}_q \mathbf{k}_{01})}{d\Omega_1} \frac{dW_{K_2 N_2}(\alpha_2 J_2 \rightarrow \alpha_3 J_3 M_3 \hat{e}_q \mathbf{k}_{02})}{d\Omega_2}.
\]  

(3)

Here \( d\sigma/d\Omega \) represents PR differential cross section that is inverse to that of photoionization. Its expression can be written by using the Milne [8] relation and its multipole expansion is [4, 6]:

\[
\frac{d\sigma_{K_2 N_2}(\alpha_1 J_1 M_1 m_s \rightarrow \alpha_2 J_2 \hat{e}_q \mathbf{k}_{01})}{d\Omega_1} = \\
\frac{\sqrt{4\pi \pi \alpha^2 E_{\text{f}}^2}}{\varepsilon^{\alpha}} \sum_{K_1 K_{\lambda}, K_{\lambda}, K_s, K_j, k_{1,1}, k_{1,1}'} B_{\text{ph}}(K_2, K_1, K_{\lambda}, K_s, K_j, K, k_{1,1}, k_{1,1}') \\
\times [2K_2 + 1]^{1/2} \sum_{N_1, N_{\lambda}, N_s, N_j, N} \left[ \begin{array}{ccc} K_{1} & K_j & K \\ N_1 & N_j & N \end{array} \right] \left[ \begin{array}{ccc} K_\lambda & K_s & K_j \\ N_\lambda & N_s & N_j \end{array} \right] \left[ \begin{array}{ccc} K_2 & K_r & K \\ N_2 & N_r & N \end{array} \right] Y_{K_\lambda N_\lambda}(\hat{p}) \\
\times T_{N_1}^{K_1}(J_1, J_1, M_1 | \hat{J}_1) T_{N_2}^{K_2}(s, s, m_s | \hat{s}) T_{N_r}^{K_r}(k_{1,1}, k_{1,1}' | \hat{k}_{01}).
\]  

(4)
Here $\varepsilon$ is the energy of the free electron in atomic units, $E_1$ is the energy of PRR in atomic units, $\alpha$ is the fine structure constant, $a_0$ is the Bohr radius, and

$$T_N^K(J, J', M|\hat{J}) = (-1)^{J' - M} \left[ \frac{4\pi}{2J + 1} \right]^{1/2} \left[ \begin{array}{ccc} J & J' & K \\ M & -M & 0 \end{array} \right] Y_{KN}(\hat{J}). \tag{5}$$

The expression for the differential probability of PRF is as follows \[5\]:

$$\frac{dW_{K_2N_2}(\alpha_2J_2 \rightarrow \alpha_3J_3M_3q_2\kappa_02)}{d\Omega_2} = \frac{\alpha^2E_2^2}{2\pi} \sum_{K'_r,K_3k_2,k'_2} \sqrt{2K_2 + 1 \over 2J_2 + 1} A^r(K_2, K'_r, K_3, k_2, k'_2) \times \sum_{N'_r,N_3} T_{N_2}^{K_2}(J_3, J_3, M_3|J_3) T_{N'_2}^{K'_2}(k_2, k'_2, q_2|\kappa_02). \tag{6}$$

Here $E_2$ is the energy of the fluorescence photon in atomic units.

The expressions for $B^{ph}(K_2, K_1, K_r, K_\lambda, K_s, K_j, K, k_1, k'_1) \tag{4}$ and $A^r(K_2, K'_r, K_3, k_2, k'_2) \tag{5}$ are:

$$B^{ph}(K_2, K_1, K_r, K_\lambda, K_s, K_j, K, k_1, k'_1) = \sum_{\lambda,j,j',J'} (2J + 1)(2J' + 1)(-1)^{\lambda'} \times \langle \alpha_1J_1\varepsilon\lambda(j)J||Q^{(k'_1)}||\alpha_0J_0 \rangle \langle \alpha_1J_1\varepsilon\lambda'(j')J'||Q^{(k_1)}||\alpha_0J_0 \rangle^* \times [(2J + 1)(2K_j + 1)((2J_2 + 1)(2k_1 + 1)(2s + 1)(2\lambda + 1)(2\lambda' + 1)(2j + 1)(2j' + 1)]^{1/2} \times \left[ \begin{array}{cccc} \lambda & \lambda' & K_\lambda & 0 \\
1 & 0 & 0 & 0 \\
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 \end{array} \right] \left[ \begin{array}{cccc} J_1 & K_1 & J_1 & 1 \\
k_1 & k_1 & k_1' & 1 \\
J' & J' & j' & J \\
K & K & K & J \end{array} \right] \left[ \begin{array}{cccc} 1 & K_2 & 2 & 1 \\
2 & J_2 & 3 & 1 \\
2 & J_2 & 3 & 1 \\
2 & J_2 & 3 & 1 \end{array} \right], \tag{7}$$

$$A^r(K_1, K'_r, K_2, k_1, k'_2) = \langle \alpha_2J_2||Q^{(k_2)}||\alpha_1J_1 \rangle \langle \alpha_2J_2||Q^{(k'_2)}||\alpha_1J_1 \rangle^* \times \left[ \frac{(2K_1 + 1)(2J_2 + 1)(2k_2 + 1)}{2K_2 + 1} \right]^{1/2} \left[ \begin{array}{cccc} J_1 & K_1 & J_1 & 1 \\
k_2 & k_2 & k_2' & 1 \\
J_2 & K_2 & J_2' & J_2' \end{array} \right]. \tag{8}$$

The reduced matrix element in (7) and (8) has the expression \[5\]:

$$\langle \alpha_2J_2||Q^{(k)}||\alpha_1J_1 \rangle = k^{k-1/2} \sum_{p=0,1} \left[ \frac{k + 1}{k} \right]^{1/2} \frac{i^k}{(2k - 1)!!} \langle \alpha_2J_2||Q^{(k)}_k||\alpha_1J_1 \rangle. \tag{9}$$

For the electrical multipole ($Ek$) transitions, $p = 0$, and the transition operator in (9) is \[5\]

$$Q_{kq}^{0} = -rk^{(k)} \tag{10}$$

and, for the magnetic multipole transition ($Mk$)($p = 1$), it is

$$Q_{kq}^{1} = \frac{iq}{c} \frac{1}{k(2k - 1)}^{1/2}r^{k-1} \left\{ \frac{1}{k + 1} \left[ C^{(k-1)} \times L^{(1)} \right]^{(k)}_q + \left[ C^{(k-1)} \times S^{(1)} \right]^{(k)}_q \right\}. \tag{11}$$

Here $L$ and $S$ are the operators of the orbital and spin angular momentum, respectively, $C^{(k)}_q$ is the operator of the spherical function normalized to $[4\pi/(2k + 1)]^{1/2}$. 


In nonrelativistic approximation, the expression (3) represents the most general case of the double differential cross section for the PRF process of polarized ions and polarized electrons. In two-step approximation, it enables us to obtain information about the polarization, asymmetry of the angular distributions of PRR and PRF as well as angular correlations between PRR and PRF. The parameters describing the polarization of the intermediate and final ions can also be derived.

3. Special cases

The cases of PRF following PR of nonpolarized and polarized or aligned ions with nonpolarized electrons are of importance for tokamak plasmas. To obtain the expression for differential cross section describing the angular distribution of PRF radiation when the PRR and final states of recombined ion and polarization of PRF radiation are not registered, one needs to perform the summation in (3) over $M_3$, polarization of radiation, $q_2 = q_1 = \pm 1$, and integration over the angles of PRR. The $\sum_M T^{K}_N(J, J, M|\hat{J}) = \delta(K, 0)\delta(N, 0)$. The integration gives $\int d\Omega Y_{KN}(\theta, \phi) = \delta(K, 0)\delta(N, 0)$. The zero ranks of the corresponding multipole expansion tensors should be inserted into (4) and (6) that leads to the simplification of (3). For the randomly oriented both ions and electrons, the expression (3) should be averaged with respect to the states of the ion and electron.

Thus, in the of PR of nonpolarized ions and electrons and the choice of the laboratory $z$ axis along the direction of electrons, the expression for the differential cross section of PRF can be written as follows:

$$\frac{d\sigma(\alpha_1 J_1 \rightarrow \alpha_2 J_2 \rightarrow \alpha_3 J_3 k_{02})}{d\Omega_2} = \frac{1}{2(2J_1 + 1)} \sum_{M_1, M_3, m_s, q_1, q_2} \int d\Omega_1 d\Omega_2 \frac{d^2\sigma(\alpha_1 J_1 M_1 p m_s \rightarrow \alpha_2 J_2 \hat{\epsilon}_{q_1} k_{01} \rightarrow \alpha_3 J_3 M_3 \hat{\epsilon}_{q_2} k_{02})}{d\Omega_1 d\Omega_2} = \sigma(\alpha_1 J_1 \rightarrow \alpha_2 J_2) \frac{W(\alpha_2 J_2 \rightarrow \alpha_3 J_3)}{4\pi} \left[ 1 + \sum_{K_r > 0} \beta_{K_r} P_{K_r}(\cos \theta) \right] . \quad (12)$$

$K_r$ acquires even values. For electrical dipole radiation $k_2 = k_2' = 1$, $K_r = 0, 2$, and

$$\beta_2 = \alpha A_2 \quad (13)$$

where

$$\alpha = \left[ \frac{5(2J_2 + 1)}{2} \right]^{1/2} \frac{A_r(2, 2, 0, 1, 1)}{A_r(0, 0, 0, 1, 1)} = (-1)^{J_2 + J_3 + 1} \left[ \frac{3(2J_2 + 1)}{2} \right]^{1/2} \left\{ \begin{array}{ccc} J_2 & J_2 & 2 \\ 1 & 1 & J_3 \end{array} \right\} \quad (14)$$

depends on only the quantum numbers of recombined ion.
The parameter $A_2$ is the alignment of recombined ion, and its expression is:

$$A_2 = \frac{5}{\sqrt{2J_2 + 1}} \frac{\mathcal{B}^{ph}(2, 0, 0, 2, 2, 1, 1)}{\mathcal{B}^{ph}(0, 0, 0, 0, 0, 0, 1, 1)}.$$  \hspace{1cm} (15)

A very strong dependence of $A_2$ on free electron energy can be expected because of the sum over $\lambda, \lambda'$ in $\mathcal{B}(2, 0, 0, 2, 2, 1, 1)$, i.e. interference of terms exists, that differs from the alignment $A_2$ of photoionization where $\lambda = \lambda'$ indicating the absence of interference terms.

In the case of PR of polarized ions and nonpolarized electrons, the expression for the differential cross section describing the angular distribution of PRF radiation is as follows:

$$\frac{d^2\sigma(\alpha_1J_1M_1 \to \alpha_2J_2 \to \alpha_3J_3k_{02})}{d\Omega_2} = \frac{1}{2} \sum_{M_3, m_s, q_1, q_2} \int d\Omega_1 \frac{d^2\sigma(\alpha_1J_1M_1p_{m_s} \to \alpha_2J_2k_{01} \to \alpha_3J_3M_3k_{02})}{d\Omega_1 d\Omega_2}
= (2J_1 + 1)\sigma(\alpha_1J_1 \to \alpha_2J_2) \frac{W(\alpha_2J_2 \to \alpha_3J_3)}{4\pi} \left[ 1 + \sum_{K_2 > 0, N_2} \beta_{K_2} Y_{K_2N_2}(\theta_2, \phi_2) A_{K_2N_2}(\theta_A, \phi_A) \right].$$ \hspace{1cm} (16)

Here the laboratory $z$ axis is aligned along the direction of free electrons. In (16),

$$\beta_{K_2} = \sum_{k_2, k'_2} (-1)^{k'_2 - q_2} \frac{4\pi}{2k_2 + 1} \left[ \begin{array}{ccc} k_2 & k'_2 & K_2 \\ q_2 & -q_2 & 0 \end{array} \right] \frac{A^r(2, 2, 0, 1, 1)}{A^r(0, 0, 0, 1, 1)},$$ \hspace{1cm} (17)

and differential alignment is defined as

$$A_{K_2N_2}(\theta_A, \phi_A) = \sum_{K_1, K_\lambda, k_1} (-1)^{K_2-N_2+J_1-M_1} \left[ \frac{4\pi(2K_2 + 1)(2K_\lambda + 1)}{2J_1 + 1} \right]^{1/2} \left[ \begin{array}{ccc} J_1 & J_1 & K_1 \\ M_1 & -M_1 & 0 \end{array} \right] \times \frac{1}{2k_2 + 1} \left[ \begin{array}{ccc} K_1 & K_\lambda & K_2 \\ N_2 & 0 & N_2 \end{array} \right] \frac{\mathcal{B}^{ph}(K_2, K_1, 0, K_\lambda, 0, K_\lambda, K_2, k_1, k_1)}{\mathcal{B}^{ph}(0, 0, 0, 0, 0, 0, 0, k_1, k_1)} Y^*_{K_1N_2}(\theta_A, \phi_A).$$ \hspace{1cm} (18)

The angles in (16) and (18) are measured from the direction of free electron.

In electrical dipole approximation, $k_1 = k'_1 = 1, K_2 = 0, 2$, and the expression for $\beta_2$ is defined by (13).

4. Calculations

The asymmetry parameters $\beta_2$ \textcolor{red}{[13]} of the angular distribution for PRF in the case of PR of bare nuclei and nonpolarized Ne-like ions Na$^+$, Mg$^{2+}$, Al$^{3+}$, Ar$^{8+}$, Fe$^{16+}$, and Zn$^{20+}$ with nonpolarized electrons were calculated. The reduced matrix elements in $\mathcal{B}^{ph}(2, 0, 0, 2, 2, 1, 1)$ \textcolor{red}{[17]} were calculated by using a computer program for the photoionization of atoms \textcolor{red}{[2]}. For the calculation of \textcolor{red}{[13]} – \textcolor{red}{[15]}, a computer program was created in the present work.
In the calculations, the energies of a free electron are chosen from 0 up to 450 eV that allows the use of dipole approximation for PRR. The energy of PRR does not exceed 1.5 keV for Al$^{18+}$ and Zn$^{20+}$, therefore, it can be expected that the contribution of higher multipoles does not exceed 2% for PR cross sections.

In the case of bare nuclei of He, F, and Ar atoms, calculated asymmetry parameters $\beta_2$ of the angular distribution of PRF for the transition $2p^2 \ P_{3/2} \rightarrow 1s \ S_{1/2}$ are shown in Fig. 1. The relativistic calculations for Xe$^{54+}$ [10] are also presented for comparison. The values of $\beta_2$ are very similar near zero energies of free electron and decrease down from 0.34 with increasing electron energy. For higher free electron energies, the values of $\beta_2$ increase if the nuclear charge increases.

For PRF of Ne-like ions via transition $2p^6 \ ^1S_0 \rightarrow 2p^63p \ ^2P_{3/2} \rightarrow 2p^63s \ ^2S_{1/2}$, the values of calculated asymmetry parameters $\beta_2$ are presented in Fig. 2. A very strong variation of $\beta_2$ on free electron energy can be noticed for ions of low ionization degree, i.e. Na$^+$ and Mg$^{2+}$ which gradually disappears with increasing nuclear charge. The minimum noticed for Na$^+$ and Mg$^{2+}$ coincides with the Cooper minimum in photoionization of Na and Mg$^+$ that is reversed to PR. The strong dependence of $\beta_2$ on free electron energy is defined by the alignment $A_2$ [15] of the recombined ion. The strong variations of $A_2$ on free electron energy occurs due to the interference of $\lambda, \lambda'$ in $\mathcal{B}(2,0,0;2,2,2,1,1)$.

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Figure captions:

Fig. 1. Asymmetry parameter $\beta_2$ of the angular distribution of fluorescence $2p^2P_{3/2} \rightarrow 1s^2S_{1/2}$ radiation following photorecombination of bare nuclei vs free electron energy. Calculations for $\text{Xe}^{54+}$ are taken from [10].

Fig. 2. Asymmetry parameter $\beta_2$ of the angular distribution of fluorescence $3p^2P_{3/2} \rightarrow 1s^2S_{1/2}$ radiation following photorecombination of neon-like ions vs free electron energy.
Figure 1

\[ A^{n+} + e^- \rightarrow A^{(n-1)+} \quad 2p^2P_{3/2} \rightarrow A^{(n-1)+} \quad 1s^2S_{1/2} + h\nu \]

Asymmetry parameter

Electron energy (eV)
Figure 2

\[
\begin{align*}
A^{(n+1)+} + e^- &\rightarrow A^{(n-1)+} + 3p^2P_{3/2} - A^{(n-1)+} + 3s^2S_{1/2} + h\nu \\
\end{align*}
\]