Linear polarization of x-rays emitted in the decay of highly-charged ions via overlapping resonances

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Abstract. The linear polarization of x-rays, emitted from highly-charged ions, has been studied within the framework of the density matrix theory and the multiconfiguration Dirac-Fock method. Emphasis was placed especially on two-photon cascades that proceed via intermediate overlapping resonances. For such two-step cascades, we here explore how the level-splitting of the resonances affects the linear polarization of the x-rays, and whether modifications in the degree of polarization may help determine small level-splittings in multiply- and highly-charged ions, if carefully analyzed along isoelectronic sequences. Detailed calculations are carried out for the 1s2p$^2$ $J_i = 3/2 \rightarrow 1s2s2p$ $J_f = 1/2$, 3/2 $\rightarrow 1s^22s$ $J_f = 1/2 + \gamma_1 + \gamma_2$ radiative cascade of lithium-like W$^{72+}$ ions. For this cascade, a quite remarkable increase of the (degree of) linear polarization is found for the second-step $\gamma_2$ photons, if the level-splitting becomes smaller than $\Delta \omega \lesssim 0.2$ a.u. $\approx 5.4$ eV. Accurate polarization measurements of x-rays may therefore be also utilized in the future to ascertain small level-splittings in multiply- and highly-charged ions.

1. Introduction

Angular distribution and polarization studies of x-rays, emitted from multiply- and highly-charged ions (HCIs), have been performed for several decades, both theoretically and experimentally. When compared to the total intensity of individual x-ray lines, angle- and polarization-resolved measurements have typically been found much more sensitive with regard to small (inner-) atomic interactions, such as the hyperfine structure [1, 2], the Breit interaction [3, 4, 5], or the mixing of different multipoles of the radiation fields [6, 7, 8]. Until the present, however, the vast majority of such angle- and polarization-resolved studies were made for sufficiently well-isolated fine-structure levels, while little attention was paid so far to photon cascades via overlapping resonances. In contrast to the decay of some isolated excited state, an overlap of two (or more) intermediate levels may lead to the depolarization of these resonances due to spin-spin, spin-orbit, and spin-other-orbit interactions. Such depolarization effects have been studied recently by us for the angular distribution and angular correlation of x-rays emitted in...
the two-step radiative cascades of lithium-like W$^{71+}$ ions [9], for which a quite strong dependence of the anisotropy of the emitted photons were found. From these investigations, we concluded that accurate measurements of the x-ray angular distributions may indeed serve as a tool for determining small level-splittings in HCl.

In this contribution, we confirm and add to our previous work [9] by analyzing the linear polarization of the emitted x-rays as function of the intermediate level-splitting. In particular, we explore how this level-splitting affects the polarization of the x-rays, and whether modifications in the degree of linear polarization may be utilized for extracting such splittings, if the selected x-ray cascades are analyzed along isoelectronic sequence. To this end, the density matrix theory was employed in order to derive general expression for the linear polarization of the emitted x-ray photons. While this formalism can be applied quite easily to any atomic (or ionic) system, independent of its particular shell structure, we here consider (again) the two-step x-ray photons. In this notation, the $A_\gamma^q$'s and $A_\gamma^p$'s denote the total angular momenta as well as all further quantum numbers that are needed for the unique specifications of the levels involved.

This paper is organized as follows. In Sec. 2, the general expression for the linear polarization of the second-step photon, emitted in a two-step radiative cascade via overlapping resonances, is derived within the density matrix theory. Moreover, this expression is further simplified for the 1$s^2p^2 \rightarrow 1s2s2p$ radiative cascade of lithium-like ions in order to obtain a proper parametrization of the (degree of) linear polarization of the second-step $\gamma_2$ photons. In Sec.3, the calculated linear polarizations of the $\gamma_2$ photons are presented and discussed as function of the level-splitting for lithium-like ions near to lithium-like W$^{71+}$. Finally, a brief summary of the present work is given in Sec. 4. Hartree atomic units ($e = m_e = \hbar = 1$) are employed throughout this work unless stated otherwise.

2. Theoretical background

Let us start from the following two-step radiative decay cascade that proceeds via two (or more) intermediate overlapping resonances

$$A_\gamma^{q+*}(\alpha_iJ_i) \rightarrow \gamma_1 + \left\{ \begin{array}{l}
A_\gamma^{q+*}(\alpha J) \\
A_\gamma^{q+*}(\alpha' J')
\end{array} \right\} \rightarrow \gamma_1 + \gamma_2 + A_\gamma^q(\alpha_fJ_f). \quad (1)$$

In this cascade, a $q$-fold charged ion $A_\gamma^{q+*}$ is assumed to be initially in the doubly excited level $\alpha_iJ_i$. In the first step, the intermediate overlapping resonances $\alpha J$ and $\alpha' J'$ are populated coherently under the emission of the first-step $\gamma_1$ photons. Thereafter, the second-step $\gamma_2$ photons are emitted, bringing the ion to its ground level $\alpha_fJ_f$, as shown schematically in Figure 1. In this notation, the $J$'s and $\alpha$'s denote the total angular momenta as well as all further quantum numbers that are needed for the unique specifications of the levels involved.

2.1. Density matrix formalism

In studying the angular distribution and polarization of x-rays, emitted in course of various “excitation-and-decay” processes of atoms (or ions), the density matrix theory [10, 11] has been found a convenient and very versatile technique, with numerous applications in the past decades; cf. [12, 13]. In particular, if well-defined (intermediate) states are formed, the excitation and subsequent decay of ions can be described separately by simply propagating the density matrix
through the various steps of the process. Since we shall here consider how the level-splitting of the overlap of the intermediate resonances affects the linear polarization of the (2nd-step) x-ray emissions, we need not discuss how the initial level $\alpha_iJ_i$ has been populated before by some excitation process. Instead, we shall just assume the statistical tensors to be known for the initial state of the ion $A^{\prime\prime\prime\prime}(\alpha_iJ_i)$.

Indeed, the second-step photon $\gamma_2$ in process (1) is a suitable candidate for investigating how the overlap of the intermediate resonances affects the linear polarization of the emitted x-rays. After the emission of the first-step photon, the two intermediate states evolve in time under the influence of the inner-atomic interactions, until they further decay into some energetically lower (or ground) state of the ions. Especially, the spin-orbit and spin-spin interactions affect the polarization states of the ions [12, 9] when the coupling of these resonances to the radiation field is comparable to their level-splitting, an effect which has been termed as lifetime-induced depolarization in literature. Of course, any change in the polarization of the intermediate ionic state(s) then also influences the polarization of the subsequently emitted $\gamma_2$ photons. In the density matrix theory, the statistical tensors of the initial- and final-state ensembles for any decay process are related to each other by [10]

$$
\rho^f_{kq}(\beta_j, \beta_j') = \frac{1}{jj'} \sum_{j_0j_0'} \langle \beta_j || T || \beta_0j_0 \rangle \langle \beta_j' || T || \beta_0'j_0' \rangle^* \rho^i_{kq}(\beta_0j_0, \beta_0'j_0') \delta_{jj_0} \delta_{jj_0'},
$$

where $jj' = \sqrt{(2j+1)(2j'+1)}$, $\langle \beta_j || T || \beta_0j_0 \rangle$ and $\langle \beta_j' || T || \beta_0'j_0' \rangle$ denote the reduced transition amplitudes for the particular process under consideration, and where $\rho^i_{kq}(\beta_0j_0, \beta_0'j_0')$ and $\rho^f_{kq}(\beta_j, \beta_j')$ refer to the statistical tensors of the initial- and final-state ensembles with total angular momenta $j_0$, $j_0'$ and $j$, $j'$, respectively. We can apply Eq. (2) twice in sequence in order to derive the density matrix of the second-step $\gamma_2$ photons, from which the (degree of) linear polarization of these photons are eventually obtained by means of Eq. (3.41) in the Ref. [10].

Following this brief outline of the theory for process (1), the statistical tensors $\rho_{kq}(\alpha J, \alpha'J')$ of the produced intermediate overlapping resonances $\alpha J$ and $\alpha'J'$ can be expressed as follows
by means of Eq. (2) above and Eq. (1.68) in the Ref. [10],
\[
\rho_{kq}(\alpha J, \alpha' J') = \sum_{p1L1} (-1)^{J'+J+L_1+k} \left\{ \begin{array}{ccc} J & J' & k \\ J_1 & J_1 & L_1 \end{array} \right\} \rho_{k_1q_1}(\alpha_i J_i) \langle \alpha J \mid \Gamma_{\gamma_1}\{p_1 L_1}\mid \alpha_i J_i \rangle \\
\times \langle \alpha' J' \mid \Gamma_{\gamma_1}\{p_1 L_1\} \mid \alpha_i J_i \rangle^* \delta_{k k_1} \delta_{q q_1},
\]
(3)

with the first-step photon supposed to be unobserved. In this expression, \(\langle \alpha J \mid \Gamma_{\gamma_1}\{p_1 L_1\} \mid \alpha_i J_i \rangle\) and \(\langle \alpha' J' \mid \Gamma_{\gamma_1}\{p_1 L_1\} \mid \alpha_i J_i \rangle\) are the reduced (radiative) transition amplitudes for the emission of the first-step \(\gamma_1\) photons with well-defined multipolarity \(p_1 L_1\), where \(p = 0\) refers to the electric multipoles and \(p = 1\) to the magnetic ones. Moreover, the standard notations have been used for the Wigner-\(6j\) symbol and the Kronecker delta function.

When compared with the radiative cascade that proceeds via well-isolated atomic (or ionic) levels, differences arise especially for the statistical tensors \(\rho_{k_2q_2}(\alpha J, \alpha' J'; t)\) of the overlapping resonances. As outlined above, these tensors evolve with time as \(\sim \exp\left\{ [i \omega_{\alpha J, \alpha' J'} - \Gamma_{\alpha J, \alpha' J'}] t \right\}\) owing to the spin-orbit interactions of the bound electrons until the second-step \(\gamma_2\) photons are emitted. However, since nothing is known about the exact time interval between the first- and second-step decays, one needs to average the statistical tensors over time. This average procedure gives rise to the depolarization factor
\[
h_{\alpha J, \alpha' J'} = \frac{\Gamma_{\alpha J, \alpha' J'} - i \omega_{\alpha J, \alpha' J'}}{\omega_{\alpha J, \alpha' J'}^2 + \Gamma_{\alpha J, \alpha' J'}^2},
\]
(4)
as well as to time-averaged statistical tensors for the intermediate overlapping resonances [11, 12].

In formula (4), \(\omega_{\alpha J, \alpha' J'} = E_{\alpha J} - E_{\alpha' J'}\) denotes the level-splitting of the intermediate resonances, and \(\Gamma_{\alpha J, \alpha' J'} = \frac{1}{2}(\Gamma_{\alpha J} + \Gamma_{\alpha' J'})\) the (averaged) total width of the two resonances.

Once the time-averaged statistical tensors are obtained for the intermediate resonances, one can use Eq. (2) again to derive the statistical tensors for the final-state assemble \(A^J_0(\alpha_J J_f) + \gamma_2\) that consists of the final ion and the second-step photon \(\gamma_2\). After this, the statistical tensors \(\rho_{k_2q_2}\{p_2 L_2, p'_2 L'_2\}\) of the second-step \(\gamma_2\) photons could be extracted from the ones of the final-state assemble by summation over the polarization states of the final ion,
\[
\rho_{k_2q_2}(\alpha J, \alpha' J'; t) = \sum_{\alpha J, \alpha' J'} (-1)^{J+J'+L_2+k} \left\{ \begin{array}{ccc} L_2 & L'_2 & k \\ J & J' \end{array} \right\} \langle \alpha J \mid \Gamma_{\gamma_2}\{p_2 L_2\} \mid \alpha J \rangle \\
\times \langle \alpha' J' \mid \Gamma_{\gamma_2}\{p_2 L_2\} \mid \alpha J \rangle^* \delta_{k_{\gamma_2} k} \delta_{q_{\gamma_2} q}.
\]
(5)

Obviously, the reduced transition amplitudes \(\langle \alpha J \mid \Gamma_{\gamma_2}\{p_2 L_2\} \mid \alpha J \rangle\) and \(\langle \alpha J \mid \Gamma_{\gamma_2}\{p'_2 L'_2\} \mid \alpha J \rangle\) here refer to the second-step decay.

To obtain the polarization of photons that are emitted in the direction \(\hat{k}_\gamma \equiv (\theta, \phi)\), one should start from the photon polarization density matrix \(\langle \hat{k}_\gamma, \lambda \mid \rho \mid \hat{k}_\gamma, \lambda' \rangle\) in the helicity representation with the helicity \(\lambda = \pm 1\). By making a transformation to the representation of total angular momentum and then applying the general relation between the density matrices and statistical tensors, the polarization density matrix can be expressed in terms of Eq. (5) as follows
\[
\langle \hat{k}_\gamma, \lambda \mid \rho \mid \hat{k}_\gamma, \lambda' \rangle = \frac{1}{8\pi} \sum_{p_2 L_2} \sum_{p'_2 L'_2} \lambda^{p_2} \lambda^{p'_2} \hat{L}_2 \hat{L}'_2 \langle -1 \rangle^{L_2+1} \langle L_2 \lambda, L'_2 - \lambda' \mid k_{\gamma 2} \lambda - \lambda' \rangle \\
\times \rho_{k_{\gamma 2} q_{\gamma 2}}(p_2 L_2, p'_2 L'_2) D_{\lambda - \lambda' q_{\gamma 2}}^{k_{\gamma 2}}(0, \theta, \phi).
\]
(6)
In this expression, the standard notations for the Clebsch-Gordan coefficients and the Wigner-D functions have been employed. In practice, however, the polarization density matrix is typically parameterized in terms of the Stokes parameters \([10, 11]\)

\[
\langle \mathbf{k}_\gamma, \lambda | \rho | \mathbf{k}_\gamma, \lambda' \rangle \equiv \frac{1}{2} \begin{pmatrix}
1 + P_3 & -P_1 + i P_2 \\
-P_1 - i P_2 & 1 - P_3
\end{pmatrix}.
\]  

(7)

These parameters can be easily used to characterize both, the linear \((P_1, 2)\) as well as the circular \((P_3)\) polarizations of the photons. By combining Eqs. (6) and (7), we then obtain the linear polarization \(P_1\) of the second-step photons as emitted in the process (1),

\[
P_1(\mathbf{k}_\gamma) = -\frac{\langle \mathbf{k}_\gamma, \lambda = +1 | \rho | \mathbf{k}_\gamma, \lambda' = -1 \rangle + \langle \mathbf{k}_\gamma, \lambda = -1 | \rho | \mathbf{k}_\gamma, \lambda' = +1 \rangle}{\langle \mathbf{k}_\gamma, \lambda = +1 | \rho | \mathbf{k}_\gamma, \lambda' = +1 \rangle + \langle \mathbf{k}_\gamma, \lambda = -1 | \rho | \mathbf{k}_\gamma, \lambda' = -1 \rangle},
\]

(8)

where the polarization density matrix elements are given by Eq. (6) together with Eqs. (3)–(5).

### 2.2. Linear polarization of second-step photons from lithiumlike ions

Equations (3)–(7) are general and applicable to any atomic (or ionic) system, independent of its (valence) shell structure. Following our previous work \([9]\), we here consider again the cascade

\[
1s2p^2 J_i = 3/2 \rightarrow \gamma_1 + \begin{cases} 
1s2s2p J = 1/2 \\
1s2s2p J' = 3/2
\end{cases} \rightarrow \gamma_1 + \gamma_2 + 1s2s2s J_f = 1/2
\]

(9)

for lithium-like ions that proceeds via two electric-dipole (E1) allowed transitions. The initial state \(1s2p^2 J_i = 3/2\) of process (9) can be produced, for instance, by the resonant electron capture or, perhaps, by the electron-impact excitations. For both processes, one can choose the direction of the incoming electron beam as the quantization \(z\) axis. Since the polarization of E1 photons is determined by just the second-rank tensors \(\rho_{20}(\alpha, J_i)\), only the single zero-component \(\rho_{20}(\alpha, J_i)\) of the statistical tensors then remains nonzero for such a particular geometry. In this scenario, therefore, the initial level population can be fully characterized by the second-rank alignment parameter \(A_2(\alpha, J_i) = \rho_{20}(\alpha, J_i)/\rho_{00}(\alpha, J_i)\).

Of course, a significant depolarization of the \(1s2s2p J = 1/2, 3/2\) intermediate states only arises if the level-splitting \(\omega_{1/2, 3/2}\) is comparable with the (averaged) natural widths \(\Gamma_{1/2, 3/2}\), as it occurs near to level crossings. Such a crossing of the \(1s2s2p J = 1/2, 3/2\) resonances was found near to lithium-like \(W^{7+}\) \([9]\). In the E1 approximation of radiation fields, that is, setting \(p_1 = p_2 = p'_2 = 0\) and \(L_1 = L_2 = L'_2 = 1\) in Eq. (8), the linear polarization of the second-step \(\gamma_2\) photons in the decay (9) can be parametrized by

\[
P_1(\theta) = \frac{3 \sin^2 \theta (\frac{1}{4} T_2 + \sqrt{10} T_3) A_2}{(1 - 3 \cos^2 \theta) (\frac{1}{4} T_2 + \sqrt{10} T_3) A_2 - 5 (2 T_1 + T_2)},
\]

(10)

if the photons are emitted in the scattering plane \((\theta, 0)\), where \(\theta\) denotes the polar angle with regard to the quantization \((z)\) axis. In this expression, we utilized the shorthand notations \(T_1 = |M_{1/2}^{1/2}|^2 |M_{3/2}^{1/2}|^2 / \Gamma_{1/2},\ T_2 = |M_{1/2}^{3/2}|^2 |M_{3/2}^{3/2}|^2 / \Gamma_{3/2},\ \text{and}\ T_3 = \Re (M_{1/2}^{1/2} M_{3/2}^{1/2} M_{1/2}^{3/2} M_{3/2}^{3/2} h_{1/2, 3/2})\) with the reduced E1 amplitudes \(M_{1/2}^{1/2} \equiv \langle 1s2s2p J || H(\gamma_1(E1)) || 1s2p^2 J_i = 1/2 \rangle\) and \(M_{3/2}^{1/2} \equiv \langle 1s2s2s J_f = 1/2 || H(\gamma_2(E1)) || 1s2s2p J \rangle\) for the first- and second-step radiative transitions.
Figure 2. Linear polarization of the second-step $\gamma_2$ photons as functions of the emission polar angle $\theta$. Results are shown for lithium-like W$^{71+}$ ions residing initially in the $1s2p^2 J_i = 3/2$ level and for four combinations of the alignment $A_2$ and the level-splitting $\Delta\omega$ (a.u.): -1 and 0.1 (black solid line), -1 and 0.3 (blue dashed line), 1 and 0.1 (red dash-dotted line) as well as, 1 and 0.3 (magenta dotted line).

2.3. Computation of transition amplitudes

Eq. (10) traces back the linear polarization of the $\gamma_2$ photons to the computation of the reduced transition amplitudes $M_{\gamma_1}J$ and $M_{\gamma_2}J$ for $J = 1/2, 3/2$. Indeed, these amplitudes occur rather frequently in atomic theory and have thus been implemented in various atomic codes [14, 15, 16]. Here, we follow our previous work [9] and use the same reduced amplitudes as before obtained within the multiconfiguration Dirac-Fock (MCDF) method [16, 17].

3. Results and discussion

Detailed calculations of the statistical tensors and the Stokes parameters of the second-step photons $\gamma_2$ have been carried out for lithium-like W$^{71+}$ ion in process (9), but by leaving the level-splitting of the two $1s2s2p$ $J = 1/2, 3/2$ overlapping resonances as the unknown variable. In particular, the same E1 transition amplitudes are applied as in Ref. [9]. While these amplitudes depend only weakly on the exact transition energies and on the nuclear charge, accurate computations of the level-splitting are difficult near to the crossing of the levels along the isoelectronic sequence. Therefore, any significant dependence of the linear polarization of the $\gamma_2$ photons upon the level-splitting $\omega_{1/2,3/2}$ may help determine such small splittings of the two $1s2s2p$ $J = 1/2, 3/2$ overlapping resonances.

Figure 2, for example, displays the degree of linear polarization (10) of the second-step $\gamma_2$ photons as functions of the polar angle $\theta$. Results are shown for different alignments $A_2 = \pm 1$ of the initial $1s2p^2 J_i = 3/2$ level and for two selected level-splittings $\Delta\omega$ of the overlapping $1s2s2p$ $J = 1/2, 3/2$ intermediate resonances. As seen from this figure, a rather strong (linear) polarization of the $\gamma_2$ photons occurs for emission angles perpendicular to the quantization axis, i.e., perpendicular to the incoming electrons that align the initial $1s2p^2 J_i = 3/2$ level. For given splittings of the two intermediate resonances, moreover, the linear polarization appears to be quite sensitive to the initial alignment $A_2$, not only to its magnitude but also to the sign.
Figure 3. Linear polarization of the second-step $\gamma_2$ photons as functions of the level-splitting $\Delta\omega$. Results are shown for photons that are emitted perpendicular to the quantization axis ($\theta = 90^\circ$) and for four supposed alignments $A_2$ of the initial $1s2p^2 J_i = 3/2$ level: $A_2 = -1.0$ (black solid line), -0.5 (blue dashed line), 0.5 (magenta dotted line), and 1.0 (red dash-dotted line).

of this alignment. Different alignments of the initial level may occur due to different excitation mechanisms as mentioned above. Obviously, the linear polarization of the $\gamma_2$ photons strongly depends also on the level-splitting itself, which makes it interesting for some further analysis.

The linear polarization of the $\gamma_2$ photons has been found most sensitive to the initial alignment and to the level-splitting for emissions under $\theta \approx 90^\circ$. In Figure 3, we therefore show for these photons how the degree of linear polarization depends on the level-splitting $\Delta\omega$ of the two $1s2s2p J = 1/2, 3/2$ resonances. Similar to the angular distribution and the photon-photon correlation function of the emitted x-rays in Ref. [9], a strong (lifetime-induced) effect upon the linear polarization of the $\gamma_2$ photons is found for small level-splittings of, say, $\Delta\omega \lesssim 0.2$ a.u. $\approx 5.4$ eV. Since the degree of linear polarization can be measured quite easily nowadays for a wide range of photon energies by using the techniques of Compton polarimetry [18], such accurate polarization measurements on the $\gamma_2$ photons may be used to explore the level-splitting of HCIs.

4. Conclusion
In conclusion, general expression has been derived for the linear polarization of the x-ray photons that are emitted in two-step radiative cascades via two (or more) overlapping intermediate resonances. Applying the framework of the density matrix theory, we have analyzed how the level-splitting of these intermediate resonances affects the polarization of the (2nd-step) x-ray photons. Calculations are performed for the $1s2p^2 J_i = 3/2 \rightarrow 1s2s2p J = 1/2, 3/2 + \gamma_1 \rightarrow 1s^22s J_f = 1/2 + \gamma_1 + \gamma_2$ radiative cascade along the lithium isoelectronic sequence, for which a level crossing appears near to the W$^{71+}$ ions. A remarkably strong polarization signal of the second-step $\gamma_2$ photons is found for initially aligned ions residing in the $1s2p^2 J_i = 3/2$ level as function of the level-splitting $\Delta\omega$, and especially for small splittings $\Delta\omega \lesssim 0.2$ a.u. $\approx 5.4$ eV.

We therefore conclude that accurate polarization measurements may open an alternative route for determining small level-splittings in HCIs.
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References
[1] Surzhykov A, Litvinov Y, Stöhlker Th and Fritzsche S 2013 Phys. Rev. A 87 052507
[2] Wu Z W, Surzhykov A and Fritzsche S 2014 Phys. Rev. A 89 022513
[3] Fritzsche S, Surzhykov A and Stöhlker Th 2009 Phys. Rev. Lett. 103 113001
[4] Wu Z W, Jiang J and Dong C Z 2011 Phys. Rev. A 84 032713
[5] Fritzsche S, Surzhykov A, Gumberidze A and Stöhlker Th 2012 New J. Phys. 14 083018
[6] Surzhykov A, Fritzsche S, Gumberidze A and Stöhlker Th 2002 Phys. Rev. Lett. 88 153001
[7] Weber G, Bräuning H, Surzhykov A, Brandau C, Fritzsche S, Geyer S, Hagmann S, Hess S, Kozhuharov C, Märtin R, Petridis N, Reuschl R, Spillmann U, Trotsenko S, Winters D F A and Stöhlker Th 2010 Phys. Rev. Lett. 105 243002
[8] Weber G, Bräuning H, Surzhykov A, Brandau C, Fritzsche S, Geyer S, Grisenti R E, Hagmann S, Hahn C, Hess R, Hess S, Kozhuharov C, Kühnel M, Märtin R, Petridis N, Spillmann U, Trotsenko S, Winters D F A and Stöhlker Th 2015 J. Phys. B 48 144031
[9] Wu Z W, Kabachnik N M, Surzhykov A, Dong C Z and Fritzsche S 2014 Phys. Rev. A 90 052515
[10] Blum K, 1981 Density Matrix Theory and Applications (New York: Plenum)
[11] Balashov V V, Grum-Grzhimailo A N and Kabachnik N M 2000 Polarization and Correlation Phenomena in Atomic collisions (New York: Kluwer Academic)
[12] Kabachnik N M, Fritzsche S, Grum-Grzhimailo A N, Meyer M and Ueda K 2007 Phys. Rep. 451 155
[13] Wu Z W, Dong C Z and Jiang J 2012 Phys. Rev. A 86 022712
[14] Parpia F A, Fischer C F and Grant I P 1996 Comput. Phys. Commun. 94 249
[15] Gu M F 2008 Can. J. Phys. 86 675
[16] Fritzsche S 2012 Comput. Phys. Commun. 183 1525
[17] Grant I P, 2007 Relativistic Quantum Theory of Atoms and Molecules: theory and computation (New York: Springer)
[18] Jörg H, Hu Z, Bekker H, Blessenohl M A, Hollain D, Fritzsche S, Surzhykov A, Crespo López-Urrutia J R, Tashenov S 2015 Phys. Rev. A 91 042705