Polarization studies on the dielectronic recombination hypersatellite x–ray lines

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Abstract. The dielectronic recombination of heavy ions has been studied theoretically within the framework of the density matrix theory and the multiconfiguration Dirac–Fock approach. Emphasis was placed especially on the (linear) polarization of the characteristic x–ray emission and how it is affected by the non–dipole terms in the expansion of the electron–photon interaction operators. In particular, it is found that the interference between the leading electric–dipole (E1) and higher—electric and magnetic—multipole channels may significantly enhance the degree of linear polarization of the Kα hypersatellite lines. Detailed calculations for such a multipole–mixing effect are performed for the decay of the doubly–excited L3/2L3/2 resonances following the dielectronic recombination of (initially) hydrogen–like uranium U⁹¹⁺ ions.

1. Introduction
In the dielectronic recombination (DR), a free electron is captured by an ion under the simultaneous excitation of an (initially bound) electron, thus, producing a multiply excited ion state that may stabilize itself under photon emission. For many years, this resonant capture of free (or quasi–free) electrons has attracted much attention both, by experiment and theory, since it provides a unique tool for studying relativistic, quantum electrodynamical (QED) and many–body effects on the structure and dynamics of few–electron, heavy ions [1, 2, 3]. While, in the past, these studies have mainly dealt with the total DR rates, much of today’s interest is focused on the angular–resolved properties of the characteristic x–ray emission following the resonant electron capture. For the K – LL dielectronic recombination of initially hydrogen–like uranium U⁹¹⁺ ions, for example, the angular distribution of the (hyper–)satellite Kα1,2 lines have been recently measured at the GSI facility in Darmstadt [4, 5]. When compared with theoretical predictions based on Dirac’s theory [6, 7], these measurements reveal important information on the magnetic corrections to the electron–electron interaction as well as the mixing of different multipoles in the expansion of the radiation field.

Beside the angular–resolved measurements, polarization studies on the DR characteristic radiation provide an alternative and very promising route for a systematic analysis of the relativistic and retardation effects in the electron–electron and electron–photon interactions and in the presence of strong electromagnetic fields. During the last few years such investigations became feasible owing to the recent advancements in the design of position–sensitive solid–state detectors [8]. Therefore, the application of these x–ray detectors for analyzing the linear polarization of the characteristic emission from heavy ions is presently discussed, and this
will lead very likely to a new kind of electron-ion collision experiments at the GSI facility in Darmstadt in forthcoming years.

In this contribution, we apply the density matrix theory together with the multiconfiguration Dirac–Fock approach in order to predict the polarization properties of the DR hypersatellite lines. Although the basic theory, which is presented in Sections 2 and 3, can be utilized for the (polarization) analysis of any bound–bound transition, and independent of the particular shell structure of the ions in their initial and final state, here we restrict ourselves to the decay of the \( L_{3/2}L_{3/2} \) resonances in helium–like \( U^{90+} \) uranium ions. For these ions, the two \( 2p_{3/2}2p_{3/2} : J = 0, 2 \) levels belonging to the \( L_{3/2}L_{3/2} \) group are well isolated from any other doubly–excited \( LL \) resonances, allowing thus their exclusive population in ion–electron collision experiments. Moreover, only the \( J = 2 \) level can be aligned and may, hence, give rise to the emission of polarized \( K\alpha_1 \) \( (2p_{3/2}2p_{3/2} : J = 2 \rightarrow 1s_{1/2}2p_{3/2} : J = 1, 2) \) photons. In Section 4, we describe how the (degree of) linear polarization can be computed for the \( K\alpha_1 \) radiation and how it is modified by the interference of the dominant electric–dipole (E1) with other, higher–multiple channels in the coupling of the radiation field. Finally, a short summary of our results is given in Section 5.

2. Theoretical background

Not much has to be said about the basic formalism for studying the dielectronic recombination of few–electron relativistic ions. During the last two decades this formalism has been widely applied to investigate not only the total DR rates but also the angular distribution and polarization of the satellite radiation [6, 7, 9, 10]. For the analysis of these—angle– and polarization–dependent—properties, one usually treats the dielectronic recombination as a two–step process: a resonant electron capture that is followed by the radiative stabilization of the ions. Within this two–step approach, it is then convenient to make use of the density matrix formalism [11, 12] in order to express the magnetic sublevel population of the intermediate (doubly–excited) ionic states in terms of the alignment parameters \( A_{kq} \). Using the standard techniques of angular momentum algebra, the evaluation of the alignment parameters can be traced back to the DR reduced matrix elements \( \langle \alpha_d J_d || V || \alpha_0 J_0, l_j : J_d \rangle \) that describe the formation of the resonance \( |\alpha_d J_d\rangle \) due to the interelectronic interaction between the bound electrons in the initial state \( |\alpha_0 J_0\rangle \) and the free electron (see Refs. [7, 10] for further details):

\[
A_{kq}(\alpha_d J_d) = \delta_{q0} \frac{1}{(2J_d + 1)N} \sum_{l' j' j} (-1)^{J_d + J_0 - 1/2} \langle l, l', j, j' | 1/2 \rangle \langle l' 0 | k 0 \rangle \left\{ \begin{array}{ccc} j & l & 1/2 \\ j' & k & \end{array} \right\} \langle \alpha_d J_d || V || \alpha_0 J_0, l_j : J_d \rangle \langle \alpha_d J_d || V || \alpha_0 J_0, l' j' : J_d \rangle^* .
\] (1)

Here, we have supposed that neither the ion nor the electron are polarized, and that the quantization (\( z \)–axis) is chosen along the incoming electron momentum as seen within the rest frame of the ion. In Eq. (1), moreover, \( N = \sum_{l j} \langle \alpha_d J_d || V || \alpha_0 J_0, l_j : J_d \rangle^2 \), \( \langle l' 0 | k 0 \rangle \) is the Clebsch-Gordan coefficient, \( [a, b, ...] \equiv (2a + 1)(2b + 1)... \), and we use the standard notation for the Wigner 6j symbols.

The alignment parameters (1) are known to obey several properties. In particular, the parameter \( A_{k0}(\alpha_d J_d) \) is nonzero only if \( k \) is even and satisfies the condition \( k \leq 2J_d \). Therefore, the magnetic sublevel population of the doubly–excited states with \( J_d = 1 \) is described by a single parameter \( A_{20}(\alpha_d J_d = 1) \), while two parameters \( A_{20}(\alpha_d J_d = 2) \) and \( A_{40}(\alpha_d J_d = 2) \) are required for all resonances with \( J_d = 2 \).

Owing to the alignment of the excited ion as produced in course of the resonant electron capture, the subsequent photon emission is in general anisotropic and linearly polarized. Indeed, both the angular and polarization properties of the (hyper–)satellite photons are closely related...
to the sublevel population of the excited ionic state $|\alpha_d J_d\rangle$ and, hence, to the parameters $A_{k0}$. For a given $|\alpha_d J_d\rangle \rightarrow |\alpha_f J_f\rangle$ transition, for example, the degree of linear polarization of the emitted x-ray photons can be expressed as:

$$P_L(\theta) = \frac{\sum_{k=2,4,...} A_{k0} \left( D_{k-2}^0(0,\theta,0) + D_{k}^0(0,\theta,0) \right) g_k(\alpha_d J_d, \alpha_f J_f)}{1 + \sum_{k=2,4,...} A_{k0} f_k(\alpha_d J_d, \alpha_f J_f) P_k(\cos \theta)}$$

(2)

where $P_k(\cos \theta)$ denotes a Legendre polynomial of order $k$, $D_{k,q}^m(0,\theta,0)$ a Wigner’s D–function, and where $\theta$ refers to the angle between the propagation direction of the emitted photons and the quantization axis. In addition to the alignment parameters $A_{k0}$, there appear the so–called structure functions $f_k(\alpha_d J_d, \alpha_f J_f)$ and $g_k(\alpha_d J_d, \alpha_f J_f)$ in Eq. (2) which purely depend on the given bound-state transition of the ions. In general, these structure functions contain the matrix elements of different multipole components as they arise in the expansion of the electron–photon interaction operator [13]; they are given by:

$$f_k(\alpha_d J_d, \alpha_f J_f) = \frac{\sqrt{2J_d + 1}}{2} \sum_{L p L' p'} i^{L+J_d+J_f} (-1)^J + J_f + k + 1 \left[ L, L', L'' \right]^{1/2} \langle L 1 L' - 1 | k 0 \rangle \times \left\{ \begin{array}{c} L \\ J_d \\ J_f \end{array} \right\} \left\{ \begin{array}{c} L' \\ J_d \\ J_f \end{array} \right\} \langle \alpha_d J_d || H(\gamma(pL)) || \alpha_f J_f \rangle^* \times \langle \alpha_d J_d || H(\gamma(p'L')) || \alpha_f J_f \rangle \left[ \sum_{L p} \langle \alpha_d J_d || H(\gamma(pL)) || \alpha_f J_f \rangle^2 \right]^{-1},$$

(3)

and

$$g_k(\alpha_d J_d, \alpha_f J_f) = \frac{\sqrt{2J_d + 1}}{2} \sum_{L p L' p'} i^{L+J_d+J_f} (-1)^J + J_f + k + 1 + p' \left[ L, L', L'' \right]^{1/2} \langle L 1 L' 1 | k 2 \rangle \times \left\{ \begin{array}{c} L \\ J_d \\ J_f \end{array} \right\} \left\{ \begin{array}{c} L' \\ J_d \\ J_f \end{array} \right\} \langle \alpha_d J_d || H(\gamma(pL)) || \alpha_f J_f \rangle^* \langle \alpha_d J_d || H(\gamma(p'L')) || \alpha_f J_f \rangle \times \left[ \sum_{L p} \langle \alpha_d J_d || H(\gamma(pL)) || \alpha_f J_f \rangle^2 \right]^{-1},$$

(4)

if all the allowed multipoles are taken into account, and where $\langle \alpha_d J_d || H(\gamma(pL)) || \alpha_f J_f \rangle$ denotes the reduced matrix element for the particular magnetic ($p = 0$) or electric ($p = 1$) transition of order $L$ [14].

Equations (2)–(4) represent the most general form of the linear polarization of the characteristic radiation following the resonant electron capture. They include especially the summation over all the multipoles ($pL$) of the radiation field that are allowed owing to the parity and angular momentum selection rules. If several multipoles are allowed for a given transition, one of them often dominates the radiative decay. In many cases, therefore, the summation over the multipole components of the radiation field can be restricted to just a single term which results in a significant simplification of Eqs. (2)–(4). For electric dipole (E1) radiation, for example, the degree of linear polarization is given by the well–known formula [12]:

$$P_{E1}^E(\theta) = \sqrt{3 \over 2} {A_{20} g_{E1}^E} (\alpha_d J_d, \alpha_f J_f) \sin^2 \theta \over 1 + {A_{20} f_{E1}^E} (\alpha_d J_d, \alpha_f J_f) P_2(\cos \theta)$$

(5)
where the structure functions
\[ f_{E1}^{E1}(\alpha_dJ_d, \alpha_fJ_f) = -\sqrt{\frac{2}{3}} g_2^{E1}(\alpha_dJ_d, \alpha_fJ_f) = (-1)^{1+J_d+J_f} \sqrt{\frac{3(2J_d+1)}{2}} \left\{ \begin{array}{ccc} 1 & 1 & 2 \end{array} \right\}, \]

coincide with the anisotropy parameter \( \alpha_{2h}^{ph} \) as introduced earlier in Ref. [12]; \( f_2(\alpha_dJ_d, \alpha_fJ_f; E1) \equiv \alpha_{2h}^{ph} \). As seen from this equation, the structure function for the electric–dipole case does not depend on the bound–bound reduced transition amplitudes and, hence, on the nuclear charge \( Z \) of the ion.

3. Computations

As seen from the formalism above, the computation of the polarization properties of the DR hypersatellite radiation can be traced back to the reduced matrix elements \( \langle \alpha_dJ_d || V || \alpha_0J_0, l_j : J_d \rangle \) and \( \langle \alpha_dJ_d || H_{\gamma}(pL) || \alpha_fJ_f \rangle \) for the resonant electron capture and the multipole radiative transitions, respectively. Matrix elements of this or similar type occur frequently in atomic structure studies and have therefore been considered in various approaches. In the calculations below, we made use of the multiconfiguration Dirac–Fock (MCDF) method which has been found a versatile tool to account for the relativistic and many–body effects in high–\( Z \) ions and which is implemented in the RATIP computer program [15, 16]. This program facilitates now the computation of the DR cross sections, alignment parameters and polarization characteristics within a distorted–wave approximation and includes, moreover, a complete multipole decomposition of the electron–photon interaction as well as the full operator \( V = V^{\text{Coulomb}} + V^{\text{Breit}} \) for the electron–electron interaction.

4. Results and discussion

After this short discussion of the basic formulas for the resonant electron capture and the subsequent radiative decay, we are ready now to analyze the effects of multipole–mixing on the linear polarization of the dielectronic recombination hypersatellite lines for ions from the helium isoatomic sequence. In the present work, we shall restrict ourselves to the formation of the \( 2p_{3/2}2p_{3/2} : J = 0, 2 \) resonances following the \( K = L_{3/2}L_{3/2} \) DR of initially hydrogen–like uranium \( \text{U}^{91+} \). From these two intermediate levels, only the resonance with \( J = 2 \) may be aligned and, hence, may give rise to a linearly polarized photon emission. As seen from Eqs. (2)–(4), the degree of this linear polarization is determined by the two parameters \( A_2 \) and \( A_4 \), which characterize the magnetic sublevel population of the \( 2p_{3/2}2p_{3/2} : J = 2 \) state and which take the values 1.116 and 1.249, respectively, as well as by the structure functions \( f_j \) and \( g_k \) that account for the interference between different allowed decay channels. The explicit form of these functions

\[ f_2 = \sqrt{2} \sqrt{\frac{3}{2}} g_2^{E1}(\alpha_dJ_d, \alpha_fJ_f) = (-1)^{1+J_d+J_f} \sqrt{\frac{3(2J_d+1)}{2}} \left\{ \begin{array}{ccc} 1 & 1 & 2 \end{array} \right\}, \]

\[ g_2^{E1} = \sqrt{\frac{2}{3}} \]
and, hence, the strength of the multipole–mixing effects depend of course on the particular bound–bound transition. In order to study this dependence, Fig. 1 displays the (degree of the) linear polarization for the two $K\alpha_1$ hypersatellite lines $2p_{3/2}2p_{3/2} : J = 2 \rightarrow 1s_{1/2}2p_{3/2} : J = 1$ (left panel) and $2p_{3/2}2p_{3/2} : J = 2 \rightarrow 1s_{1/2}2p_{3/2} : J = 2$ (right panel) for helium–like $U^{90+}$ ions following the $K - L_{3/2}L_{3/2}$ DR. Two different approximations are shown in this figure: while the dashed line refers to the electric–dipole approximation (i.e., when the contributions of all the higher multipoles are neglected for a particular line), the solid line represents the degree of linear polarization $P_L$ as defined by Eq. (2).

Moreover, since the DR of high–Z ions is usually measured in collision with electrons and low–Z atoms [5], the linear polarization in Fig. 1 is presented for angles as measured in the laboratory system (i.e. the rest frame of the target). As seen from this figure, the multipole–mixing affect the polarization properties of two hypersatellite lines rather differently. While, for the $J = 2 \rightarrow J = 1$ transition, the non–dipole effects give rise to only a minor change in the shape of the linear polarization $P_L(\theta)$, the degree of polarization is remarkably enhanced for the $J = 2 \rightarrow J = 2$ line and, especially, for $\theta = 62^\circ$ that corresponds to an angle of 90° in the frame of the projectile. At this particular angle, we expect an enhancement of the linear polarization from 0.56 in the E1 approximation to 0.65 if all the (higher) multipoles are taken into account.

Unfortunately, a direct measurement of the multipole–mixing effects is not that simple in practice for (high–Z) ions from the helium-like sequence. For $U^{90+}$ ions, for example, the two fine–structure components $2p_{3/2}2p_{1/2} : J = 2 \rightarrow 1s_{1/2}2p_{3/2} : J = 1, 2$ of the $K\alpha_1$ cannot (so easily) be resolved by the currently available x–ray detectors as these lines with transition energies 101.9 and 102.0 keV are separated from each other by only 70 eV about.

In present–day experiments, therefore, only a superposition of the two fine–structure lines with their corresponding branching fractions can be observed. However, since the $J = 2 \rightarrow J = 1$ and $J = 2 \rightarrow J = 2$ components are polarized in perpendicular directions to each other, such a superposition will lead to a complete depolarization of the resulting $K\alpha_1$ line as seen from Fig. 2. But although these multipole–mixing effects might be difficult to resolve with current detector technology, the rapid progress in the field of position and energy–sensitive x–ray detectors may facilitate such measurements already in the near future, for instance at the future Facility for Antiproton and Ion Research [17].

**Figure 2.** Degree of linear polarization of the $2p_{3/2}2p_{3/2} : J = 2 \rightarrow 1s_{1/2}2p_{3/2} : J = 1$ (dashed line) and $2p_{3/2}2p_{3/2} : J = 2 \rightarrow 1s_{1/2}2p_{3/2} : J = 2$ (dotted line) fine–structure transitions together with their average (solid line) if the two line components are not resolved explicitly. Results are shown for the DR into hydrogen–like $U^{90+}$ ions and only for the full account multipole mixing effects.

5. **Summary and outlook**

In summary, the linear polarization of the $K\alpha_1$ hypersatellite radiation has been explored for the helium–like $U^{90+}$ ions as produced in course of the $K - L_{3/2}L_{3/2}$ dielectronic recombination. In this study, emphasis was placed on the effects which arise from the higher non–dipole terms in the expansion of the electron–photon interaction. It is shown that the interference between the multipole components can enhance the (degree of the) linear polarization of the $2p_{3/2}2p_{3/2} : J = 2 \rightarrow 1s_{1/2}2p_{3/2} : J = 2$ fine–structure transition, and that the effect can be as
large as 16 % if the photons are emitted perpendicular to the beam direction. However, this rather strong effect may remain hidden in the x–ray spectrum if the individual fine–structure components of the Kα₁ hypersatellite line cannot be resolved experimentally. — We therefore hope that this theoretical analysis will stimulate the further development of high–resolution polarization detectors for hard x–rays and will thus allow a much more detailed analysis of the relativistic and non–dipole effects on the resonant electron capture of high–Z, few–electron ions and their subsequent radiative stabilization.

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