Theoretical progress in studying the characteristic x–ray emission from heavy few–electron ions

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Abstract. Recent theoretical progress in the study of the x-ray characteristic emission from highly-charged, few-electron ions is reviewed. These investigations show that the bound–state radiative transitions in high–Z ions provide a unique tool for better understanding the interplay between the structural and dynamical properties of heavy ions. In order to illustrate such an interplay, detailed calculations are presented for the Kα\textsubscript{1} decay of the helium–like uranium ions U\textsuperscript{90+} following radiative electron capture, Coulomb excitation and dielectronic recombination processes.

1. Introduction

Different processes that are known to occur in relativistic collisions of heavy, few-electron ions with atomic or electronic targets lead to the production of excited ionic states. In the high-Z domain, the de-excitation of these states then usually results in the emission of one (or several) x-ray photons until the ground state is reached. The investigation of this characteristic x–ray emission has recently attracted much theoretical and experimental interest since it may improve our understanding of the electronic structure and dynamical behaviour of heavy atomic systems [1, 2]. A series of measurements have been carried out, especially at the GSI storage ring in Darmstadt, in order to analyze the angular–resolved radiation from the bound–state transitions in helium–like uranium U\textsuperscript{90+} ions [3, 4, 5]. Being performed differential in photon emission angle, these experiments appeared to be very sensitive to electron–electron and electron–photon interactions in the strong–field domain.

It is well known, however, that the angle–differential properties of the characteristic radiation usually depend on both, the structure of the ions and the way how the excited ionic states were formed originally [6, 7]. In order to interpret correctly the GSI experimental data on the x–ray emission from heavy projectiles, following relativistic ion–atom collisions, one needs to be able to describe the interplay between the structure and dynamics in course of the “excitation–and—decay” processes. For high–Z, few–electron ions, moreover, such a description should account for the relativistic and many–body effects.
In this contribution, we shall summarize the results from our recent theoretical studies on the production of excited ionic states and their subsequent radiative decay. Emphasis in this short review will be placed on the angular properties of characteristic Kα1 emission from helium–like uranium U⁹⁰⁺ ions. In Section 2, we first discuss the emission which follows the radiative electron capture (REC) into the 1s²p₃/₂ excited ionic states. In particular, we argue that the isotropy of the Kα₁ (1s²p₃/₂¹3P₁₂ → 1s²¹S₀) line, reported in Refs. [4, 5], results from a mutual compensation of the strongly anisotropic ¹P₁ → ¹S₀ electric dipole (E1) and ³P₂ → ¹S₀ magnetic quadrupole (M2) fine–structure components. In contrast to REC, no compensation arises for the radiative decay following Coulomb excitation since the latter process leads to an almost exclusive population of the 1s²p₃/₂¹P₁ fine–structure level. Results of our multi–configuration Dirac–Fock (MCDF) calculations for the magnetic sublevel population of this state and, hence, anisotropy of the subsequent 1s²p₃/₂¹P₁ → 1s²¹S₀ radiation are displayed in Section 3. Beside the radiative electron capture and Coulomb excitation, in Section 4 we also discuss the angular properties of the Kα₁ hypersatellite (HS) photons following the K – LL dielectronic recombination (DR) of initially hydrogen–like U⁹¹⁺ ions. In this Section, emphasis is placed especially on the effects of higher (non–dipole) contributions to the electron–photon interaction in the bound–state transitions. Finally, a brief summary of our theoretical results is given in Section 5.

2. Kα₁ decay following radiative electron capture: The fine–structure effects

During the last two decades, a number of experiments have been performed at the GSI storage ring in order to investigate various charge transfer processes in relativistic ion–atom collisions. In the radiative electron capture, for example, a free (or quasi–free) electron is captured into a bound state of the projectile ion, accompanied by the simultaneous emission of a recombination photon. If such a capture proceeds into some excited state, the residual ion will decay towards some lower–lying level under the emission of characteristic radiation. Angular properties of this characteristic emission have been the subject of intense experimental and theoretical studies for many years [3]. For example, several measurements have been performed to explore the electron capture into the 1s₁/₂²p₃/₂¹3P₁₂ states of (initially) hydrogen–like U⁹¹⁺ uranium ions and its subsequent Kα₁ (¹3P₁₂ → ¹S₀) decay [4]. This bound–bound transition gave rise to an almost isotropic angular distribution of the characteristic radiation, quite in contrast to what is expected from a "one–electron" model for which the Lyman–α₁ (²p₃/₂ → ¹s₁/₂) decay following REC into (initially) bare ions exhibits a strong angular dependence [8].

In order to understand the qualitatively different behaviour of the Lyman–α₁ and Kα₁ angular–dependent emission, a detailed theoretical analysis has been carried out within the framework of the density matrix theory. In this framework, the population of the excited ionic
states and their subsequent decay are treated as two steps, well separated in time. In the first step, the radiative electron capture usually leads to an alignment of the resulting (excited) ion which is described by means of so–called alignment parameters $A_k$. The properties of the decay photons, which are emitted in the second step, are then closely related to these alignment parameters. That is, the angular distribution of the characteristic radiation is given in general by [7, 9]:

$$ W(\theta) \sim 1 + \sum_k \beta_k P_k(\cos \theta), $$

where the anisotropy parameters $\beta_k$ are uniquely defined by the alignment $A_k$ and by the total angular momenta of the initial and final ionic states. For example, the anisotropy parameters of the $1s^2 2p_{3/2}^1 P_1 \rightarrow 1s^2 1S_0$ electric dipole (E1) and $1s^2 2p_{3/2}^3 P_2 \rightarrow 1s^2 1S_0$ magnetic quadrupole (M2) transitions read as:

$$ \beta_2 \left( 1P_1 \rightarrow 1S_0 \right) = \frac{1}{\sqrt{2}} A_2(J = 1), $$

and

$$ \beta_2 \left( 3P_2 \rightarrow 1S_0 \right) = -\sqrt{5/14} A_2(J = 2), $$

respectively. Apart from the second–rank parameter $\beta_2$, the anisotropy of the $3P_2 \rightarrow 1S_0$ radiation is also described by the forth–rank parameter $\beta_4$. For the REC into fast, high–Z projectiles, however, this parameter appears to be very small and, therefore, its contribution to the angular distribution of the decay photons M2 can be neglected.

As seen from Eqs. (1)–(3), the angular dependence of the subsequent photon emission is described by the Legendre polynomials $P_2(\cos \theta)$, weighted by the alignment parameters $A_2$ and some geometrical factors, that arise with different signs for the decay of the $1P_1$ and $3P_2$ states. Therefore, as long as the $1P_1 \rightarrow 1S_0$ and $3P_2 \rightarrow 1S_0$ transitions are not resolved experimentally, their – measured – superposition (Kα1 line) may exhibit an (almost) isotropic behaviour even if the individual components of this line are strongly anisotropic. By performing a more detailed analysis we have found that the angular dependence of the Kα1 radiation of helium–like ions follows the typical $\sim 1 + \beta_2 P_2(\cos \theta)$ shape, but with an overall anisotropy parameter [10]:

$$ \beta_{2 \text{eff}}(K\alpha_1) = N_{J=1} A_2(J = 1) \frac{1}{\sqrt{2}} - N_{J=2} A_2(J = 2) \sqrt{5/14}, $$

which depends on both, the alignment parameters $A_2(J = 1)$ and $A_2(J = 2)$ and the weight factors $N_{J=1}$ and $N_{J=2}$, respectively. These weights describe the contribution of the individual $1P_1 \rightarrow 1S_0$ and $3P_2 \rightarrow 1S_0$ fine–structure transitions to the overall Kα1 and are given by the relative population of the $1, 3P_{1,3}$ excited states. We have performed these calculations within the Multiconfiguration Dirac–Fock.

**Figure 2.** Total excitation cross sections (left panel) and alignment parameters (right panel) of the $1s^2 2p_{3/2}^1 P_1$ (solid line) and $1s^2 2p_{3/2}^3 P_2$ (dashed line) states of helium–like uranium U$^{90+}$. 
Beside the radiative electron capture, the Coulomb excitation of few–electron ions in collision with atoms and molecules also leads to the formation of excited ionic states. Again, these excited states are very likely aligned and associated with an anisotropic angular distribution and non–zero polarization of the subsequent decay radiation. In the past, the angle– and polarization–resolved analysis of such a characteristic radiation has been of ongoing interest owing to its importance for the diagnostics of high-temperature laboratory and astrophysical plasmas [11]. In particular, a number of experiments have been performed at the GSI storage ring in order to investigate the population of the 1s 2p3/2 ionic states following Coulomb excitation of helium–like U90+ projectiles in collision with N2 target molecules [4]. In contrast to the REC, this excitation process was found to result in a strongly anisotropic Kα1 radiation, and, hence, has initiated a more detailed analysis in order to account for the collision dynamics of the helium–like projectiles.

In Ref. [12], the Coulomb excitation of few–electron heavy ions in relativistic collisions with low–Z target atoms (or protons) has been recently explored by us within the framework of the first–order perturbation theory and combined with multiconfiguration Dirac–Fock (MCDF) computations. Special emphasis was placed on the effective parameter \( \beta_2^{\text{eff}}(K\alpha_1) \) which reflects the anisotropy of the Kα1 decay radiation. While the general expression (4) for this parameter does not depend on the particular excitation process, its numerical values are different if evaluated for the radiative electron capture and Coulomb excitation. For the latter process, our MCDF calculations clearly indicate that the \( K \rightarrow L_3 \) excitation of helium–like uranium ions results in an almost selective population of the 1s 2p3/2 1P1 ionic state as it was observed earlier in Ref. [13]. The total cross section for this singlet state is at least 50 times larger than the population cross section for the 1s 2p3/2 3P2 level [cf. left panel of Fig. 2]. Such a selective population leads to the fact that only 1s 2p3/2 1P1 state contributes to the characteristic Kα1 radiative whose anisotropy parameter:

\[
\beta_2^{\text{eff}}(K\alpha_1) \approx A_2(J = 1) \frac{1}{\sqrt{2}},
\]

is easily obtained from Eq. (4) by taking \( N_{J=1} = 1 \) and \( N_{J=2} = 0 \).

As seen from Eq. (5), the anisotropy of the Kα1 radiation following Coulomb excitation of the helium–like projectiles is directly related to the alignment of the 1s 2p3/2 1P1 state. Therefore,
been placed on the four levels a full multipole decomposition of the electron–photon interaction [15]. Special emphasis has recently re–considered the radiative decay of the doubly–excited ionic states to include these—non–dipole effects—have not been taken into account in the previous case studies, we line might be caused by the higher (non–dipole) channels in the bound–bound transitions. Since not been resolved until today.

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4K α 1 HS / Kα 2 HS intensity ratio

Observation angle (deg)

Figure 4. Intensity ratio of the Ko1/Ko2 HS lines for helium–like uranium following the K – LL DR. Calculations are performed within the E1 approximation (dashed line) as well as by accounting of all allowed multipole channels (solid line) and are compared with experimental data (filled circles) by Ma and co–workers [5].

a series of MCDF computations have been carried out to analyze this alignment for the K–shell excitation of uranium U^{90+} projectiles with energies in the range 10 ≤ \( T_p \) ≤ 600 MeV/u. The results of these calculations are shown in the right panel of Fig. 2 and indicate that the parameter \( \mathcal{A}_2(1^1P_1) \) is large and negative for low–energy collisions with \( T_p \leq 200 \) MeV/u. This refers to a predominant population of the \( M_J = 0 \) magnetic substate and therefore to an alignment, i.e. an electron density that is directed perpendicular to the beam. In fact, such a result is consistent with the classical picture in which the transferred orbital angular momentum is found perpendicular to the collision direction. For the higher collision energies, however, the classical picture is no longer valid due to the increasing role of relativistic and magnetic effects. These effects result in an ion alignment along the beam direction and subsequently in large positive values of the parameter \( \mathcal{A}_2(1^1P_1) \) [cf. right panel of Fig. 2].

The strong energy dependence of the alignment parameter \( \mathcal{A}_2(1^1P_1) \) results in qualitatively different emission patterns of the Ko1 radiation following Coulomb excitation in (relatively) slow and fast ions–atom (ion–electron) collisions. For example, as seen from Fig. 3, while the large positive parameter \( \mathcal{A}_2(1^1P_1) = 0.28 \) for \( T_p = 600 \) MeV/u clearly favors a co–linear photon emission along the beam direction, a remarkable Ko1 emission perpendicular to this direction can be observed for the decay of 1s 2p_{3/2} 1^1P_1 state produced with alignment \( \mathcal{A}_2(1^1P_1) = -0.49 \) at the energy \( T_p = 100 \) MeV/u.

4. Ko1 decay following dielectronic recombination: Multipole–mixing effects

Until now we have discussed the angular properties of the Ko1 photons following the radiative electron capture and Coulomb excitation of heavy, few–electron ions. During recent years, moreover, special interest has been paid also to the radiative decay of the doubly–excited resonances produced in course of the K – LL dielectronic recombination of (finally) helium–like U^{90+} ions. In the experiments by Ma and coworkers [5], for example, the angular distributions of the Ko1,2 hypersatellite and satellite lines have been measured and compared with the theoretical predictions [14] based on Dirac’s relativistic theory. Although a reasonable agreement between experiment and theory was found for most groups of lines, a rather remarkable discrepancy remained for the angular distribution of the Ko1 hypersatellite lines that arise from the decay of the \( L_{1/2}L_{3/2} \) resonances. For this line group, the theoretically predicted anisotropy of the Ko1 HS underestimates the observations by more than a factor of two [5, 14], a discrepancy that has not been resolved until today.

As it was already argued in Ref. [5], the observed stronger anisotropy of the Ko1 hypersatellite line might be caused by the higher (non–dipole) channels in the bound–bound transitions. Since these—non–dipole effects—have not been taken into account in the previous case studies, we have recently re–considered the radiative decay of the doubly–excited ionic states to include a full multipole decomposition of the electron–photon interaction [15]. Special emphasis has been placed on the four levels \( 2s_{1/2} 2p_{3/2} : J = 1, 2 \) and \( 2p_{1/2} 2p_{3/2} : J = 1, 2 \) which belong to
the $L_{1/2}L_{3/2}$ resonant group and on their subsequent radiative decay. In particular, we have studied the non electric–dipole effects on the fine–structure characteristic transitions in helium–like uranium $U^{90+}$ ions. We have shown that the interference between the allowed multipole components of the electron–photon interaction can easily decrease or enhance the anisotropy of individual fine–structure transitions by more than a factor of six [15].

A direct comparison of the calculated and measured angular distributions for individual $K\alpha_1$ fine–structure HS lines is presently impossible because of several restrictions that are inherent in existing relativistic collision experiments. Apart from the uncertainty in the central energy and energy profile of the ion beam, there are difficulties associated with the Compton profile of the target electrons as well as with the relatively low resolution of the x–ray detectors. Therefore, in order to understand the experimental data on the $K\alpha_1$ HS decay of four unresolved $L_{1/2}L_{3/2}$ resonances, the various fine–structure transitions belonging to the $K\alpha_1$ line have to be summed incoherently by using the calculated branching ratios and the population cross sections for the doubly–excited $2s_{1/2}2p_{3/2}$ and $2p_{1/2}2p_{3/2}$ states. Resulting angular distribution is presented in Fig. 4 together with the experimental data by Ma and co–workers [5]. As seen from this figure, the multipole–mixing effects result in about a 30 % enhancement of the anisotropy of the $K\alpha_1$ line and, hence, in a better agreement with the experimental results if compared to the theoretical predictions obtained within the E1 approximation only.

5. Conclusion

In conclusion, the recent theoretical progress in studying the characteristic emission from few–electron, heavy ions has been reviewed. Special attention was paid to the angular distribution of the $K\alpha_1$ x–rays following radiative as well as dielectronic recombination of (initially) hydrogen–like $U^{91+}$ and Coulomb excitation of helium $U^{90+}$ uranium projectiles. Together with the experimental data, our calculations demonstrate that the angle-resolved x-ray spectroscopy provides a sensitive tool for studying the relativistic and many-body effects on the structure and dynamics of high-Z, few–electron ions.

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