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Angular and polarization analysis of x-rays emitted from highly-charged, few-electron ions

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Abstract. The recent theoretical progress in studying the x-ray emission from highly-charged, few-electron ions is reviewed. These case studies show that relativistic, high- Z ions provide a unique tool for better understanding the interplay between the electron-photon and electron-electron interactions in strong fields. Most naturally, this interplay is probed by the radiative capture of a (quasi-) free electron into the bound states of projectile ions, and by varying the charge state and the energy of the projectiles. For the capture into initially hydrogen- and lithium-like ions, here we summarize the recent results for the angular distribution and polarization of the recombination photons as well as the subsequent K_α emission, if the electron is captured into an excited state of the ion.

1. Introduction

During the last decade, new (types of) collision experiments have been carried out with high- Z ions and with different target materials owing to the recent advances in heavy-ion accelerators and detection techniques. Hereby, one of the main goals in studying the structure and dynamics of simple atomic systems is to understand the photon-matter interaction in the largely unexplored domain of relativistic collision energies and strong nuclear fields. Among several other processes, in particular the radiative electron capture (REC) of target electrons into the bound states of fast-moving projectile ions has attracted much recent interest [1, 2], because it enables one to explore the interplay between the electron-photon and electron-electron interactions in the presence of strong fields. In addition, the knowledge of the REC cross sections is important also for the design of novel accelerators and ion storage rings since, for relativistic energies, this charge-transfer process is known to be dominant and leads to the loss of ions from the beam.

In recent experiments at the GSI storage ring, emphasis was placed especially on the analysis of the x-rays which are emitted in course of the electron capture or the subsequent decay of the ions, if the electrons were captured first into an excited state. From the angular distribution and polarization of the emitted photons, for example, valuable information was obtained about the relativistic and magnetic-interaction effects [3, 4] as well as the multipole-mixing in the coupling of high- Z ions to the radiation field [5]. Up to the present, however, most of the angle- and polarization-resolved experiments have been performed for the REC into initially bare ions and were found in very good agreement with computations, based on Dirac's equation and the density matrix theory [2, 5, 6, 7, 8]. For the capture into *few-electron* ions, first measurements

were carried out only recently [9, 10] but are expected to provide additional information about the interplay of the electron–photon and electron–electron interactions. Experiments along these lines are currently planned at GSI and are to be performed during the next few years.

In this contribution, we shall therefore summarize the results from our recent investigations on the electron capture into high- Z , hydrogen- and lithium-like ions. Emphasis in this short review will be placed on the angular and polarization properties of the recombination photons as well as the (subsequent) characteristic K_α radiation. Since the properties of the emitted x-ray photons are best described in the framework of the density matrix theory, in the next section we briefly discuss the basic features of this theory and how it enables one to relate the properties of the emitted radiation to the many-electron amplitudes for the coupling of the ions to the radiation field. These amplitudes are later utilized in Sections 3 and 4 to analyze the angle and polarization properties of both the observed REC and K_α photons. The promise of these case studies for a better understanding of the dynamics of high- Z ions and for developing new experimental techniques are summarized in section 5.

2. Use of the density matrix to allow a simple access to the properties of the emitted radiation

Since the density matrix approach has been frequently applied for studying the polarization and correlation phenomena in atomic collisions and, in particular, for the radiative electron capture, we shall restrict ourselves to a rather short account of its basic expressions. For all further details on this theory, we refer the reader to the literature [11, 12, 13, 14]. Within the density matrix formalism, the state of a physical system is characterized by means of statistical operators $\hat{\rho}$ which describe a single system or an ensemble of equally prepared collision systems in either a pure quantum state or in a mixture of different states with any given degree of coherence. The great benefit of using the density matrix theory is that it enables one to ‘accompany’ such an ensemble through the collision process, and without loss of quantum–mechanical information. That is, if one starts from a given initial state of the system as described by the operator $\hat{\rho}_i$, all information about the interactions resides in the (so-called) *transition operators* \hat{R} , and the final state operator follows simply from the well-known relation

$$\hat{\rho}_f = \hat{R} \hat{\rho}_i \hat{R}^+. \quad (1)$$

In practice, of course, the particular form of operator \hat{R} depends on the process under consideration. Moreover, by having the final state matrix $\hat{\rho}_f$, the result of any measurement can be predicted by applying the corresponding (set of) ‘detector operators’, \hat{P} , and by taking the trace over $\hat{P} \hat{\rho}_f$. Hereby, the detector operators describe the set-up and the efficiency of the detectors in a particular experiment.

For the REC into few-electron heavy ions, the theory has been worked out in detail in Refs. [12, 13]. In this case, the initial state is given by a free electron with asymptotic momentum p and spin projection m_s as well as by the few-electron ion in the state $\alpha_f J_i M_i$ with well-defined angular momentum J_i and its projection M_i . If, for the sake of brevity, we here consider a spin-less nucleus, the initial-state density operator of the combined system ‘ion+electron’ can be written simply as the tensor product $\hat{\rho}_i = \hat{\rho}_e \otimes \hat{\rho}_i^{\text{ion}}$ of the statistical operators of the two subsystems. After the (first) interaction with the radiation field, the electron is then captured by the ion to form the bound state $\alpha_f J_f M_f$, while the emitted photon is described in terms of the wave vector \mathbf{k} and its helicity λ , that is the spin projection along the direction of propagation. For the electron capture, moreover, the operator $\hat{R} = \sum_{i=1}^N \boldsymbol{\alpha}_i \mathbf{u}_\lambda \exp i\mathbf{k} \mathbf{r}_i$ describes the (sum of the) electron–photon interaction and where \mathbf{u}_λ denotes the polarization vector of the outgoing photon.

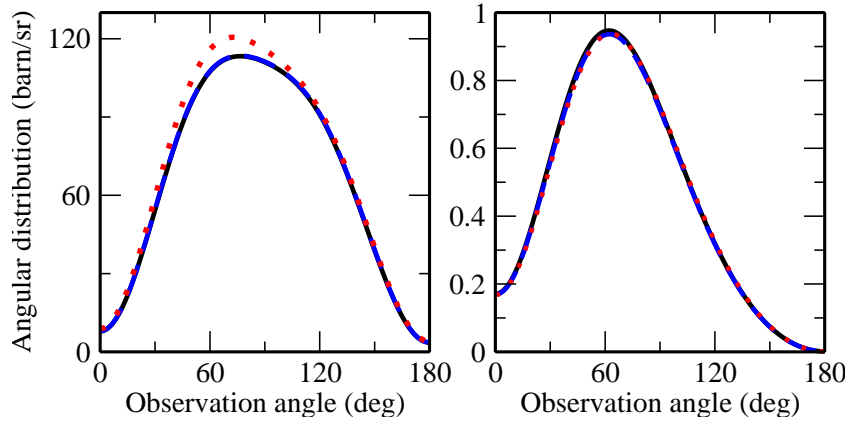


Figure 1. Angle-differential cross-sections for the radiative electron capture into the $1s^2 2s^2 \ ^1S_0$ ground state of (finally) beryllium-like uranium U^{88+} ions with projectile energy 2.18 MeV/u (left panel) and 218 MeV/u (right panel). Results from an independent particle model (---) with a proper effective charge, adapted for the projectile energy 218 MeV/u, are compared with those from MCDF calculations in Coulomb (---) and Babushkin gauge (—); taken from Ref. [19].

Using Eq. (1) with the statistical and interaction operators from above, all the properties of both the photon and the residual ion, can be derived rather easily. For instance, if we wish to determine the angular distribution of the recombination photons as a function of the emission angles $\mathbf{n} = (\theta, \phi)$ with a detector, which is sensitive to the energy but not the polarization of the photons, the detector operator is

$$\hat{P}_{\mathbf{n}} = \sum_{\lambda M_f} |\mathbf{k}\lambda\rangle \langle \alpha_f J_f M_f | \langle \alpha_f J_f M_f | \langle \mathbf{k}\lambda | \quad (2)$$

and, hence, the angular distribution of the REC photons

$$W(\theta, \phi) = \text{Tr}(\hat{P}_{\mathbf{n}} \hat{\rho}_f) = \frac{1}{2(2J_i + 1)} \sum_{m_s \lambda M_i M_f} |M_{if}(M_i, m_s, M_f, \lambda)|^2. \quad (3)$$

In this expression, the $M_{if}(M_i, m_s, M_f, \lambda) = \langle \alpha_f J_f M_f, \mathbf{p} m_s | \hat{R} | \alpha_i J_i M_i, \mathbf{k} \lambda \rangle$ denote the (many-electron) free-bound transition amplitudes which form the *building blocks* for the computation of most of the REC properties. In the calculations below, the multiconfiguration Dirac-Fock (MCDF) method [15, 16] has been applied to generate the wave functions for both the initial $\langle \mathbf{r}_1, \dots, \mathbf{r}_{N-1} | \alpha_i J_i M_i \rangle$ and final $\langle \mathbf{r}_1, \dots, \mathbf{r}_N | \alpha_f J_f M_f \rangle$ bound states. Moreover, the REC amplitudes $M_{if}(M_i, m_s, M_f, \lambda)$ were obtained by using the REC component of the RATIP program [15] which facilitates the computation of the (REC) cross sections and alignment parameters within a distorted-wave approximation.

3. Electron capture into hydrogen-like and lithium-like ions

3.1. Angular distribution of the REC photons

First experiments on the capture into few-electron ions have been performed only recently by Bednarz and co-workers [17] who measured the angular distribution of the x-ray photons for the

capture into hydrogen-like, helium-like, and lithium-like uranium. To analyze the importance of the interelectronic effects, a series of computations have been performed by us [12, 19] for the capture into the K- and L-shells of heavy, few-electron ions and for a rather wide range of projectile energies. In Figure 1, for example, we display the angle-differential cross sections for the L-shell capture into the $1s^2 2s^2 \ ^1S_0$ ground state of (initially) lithium-like U^{89+} ions. These cross sections were calculated for projectile energies from 1 to about 500 MeV/u and are shown above for the two selected energies 2.18 MeV/u and 218 MeV/u, respectively. Results from multiconfigurational computations in Coulomb and Babushkin gauge are compared with the data from an independent-particle approximation (IPA), in which a single Slater determinant was utilized together with hydrogen-like orbitals and by making use of the DIRAC program [20]. In these IPA calculations, the effective charge was set to $Z_{\text{eff}} = Z - 1$ to ensure a good agreement with the MCDF computations for 218 MeV/u and at all larger projectile energies. Over the whole range of projectile energies, excellent agreement (within about the thickness of the curves) was found between the Babushkin and Coulomb gauge which, in the nonrelativistic limit, correspond to the length and velocity gauge, respectively.

There are virtually no differences between the MCDF and independent-particle model computations at large and medium energies, say up to about $T_p = 100$ MeV/u (or for an electron energy of $T_e \geq 50$ keV within the laboratory frame). These results are in agreement with Bednarz and co-workers [17] who found their observed cross section insensitive with regard to interelectronic interactions. As seen from Fig. 1, however, deviation between the one- and many-electron computations become visible for slow projectiles with 2.18 MeV/u, leading to a (small) shift of the angular distribution as well as a decrease of the total cross-section by about 5 % for this projectile energy. Even larger effects may be expected therefore if the projectiles are further decelerated towards a zero kinetic energy as it might be realized by means of electron-beam ion traps (EBIT) or the future GSI facility. Indeed, the deceleration of the ion beams is currently one of the central goals at GSI, and with the hope to bring them down to rest within the HITRAP project [18].

3.2. Linear polarization of the REC photons: A tool for measuring the spin-polarization of heavy ion beams

Owing to the recent progress in the detector techniques, a new generation of x-ray polarization measurements have become feasible during the last few years. In a recent experiment at the GSI storage ring, for instance, a strong linear polarization was found within the reaction plane for the K-shell capture into initially bare uranium ions U^{92+} [4], and in excellent agreement with earlier theoretical predictions [6, 7]. Further polarization measurement for the REC into few-electron ions are currently under way and will reveal information about the effects of the electron-electron interaction, since the polarization of the REC photons is known to be sensitive to the many-electron amplitudes $M_{if}(M_i, m_s, M_f, \lambda)$. This direct dependence is quite in contrast to the angle-differential and total REC cross sections which always include the average over the spin states or, in addition, even over the angles of the emitted REC photons.

Apart from studying the elementary interactions in strong fields, however, the polarization properties of the K-REC radiation have attracted recent interest because they are sensitive also to the spin polarization of both, the electrons and ions, which are involved in the capture process. For this reason, the measurement of the linear polarization of K-REC can be utilized as a valuable tool for ‘observing’ the (degree of the) polarization of the ion beams in storage rings, if compared to a reliable theory [21]. The use of polarized ion beams has been discussed for a long time for studying, for example, spin-dependent nuclear interactions [22] or parity nonconservation (PNC) effects in highly charged ions [23, 24].

To investigate the polarization transfer from the ions to the (polarization) properties of the emitted radiation, we analyzed the linear polarization of the K-REC photons if (unpolarized)

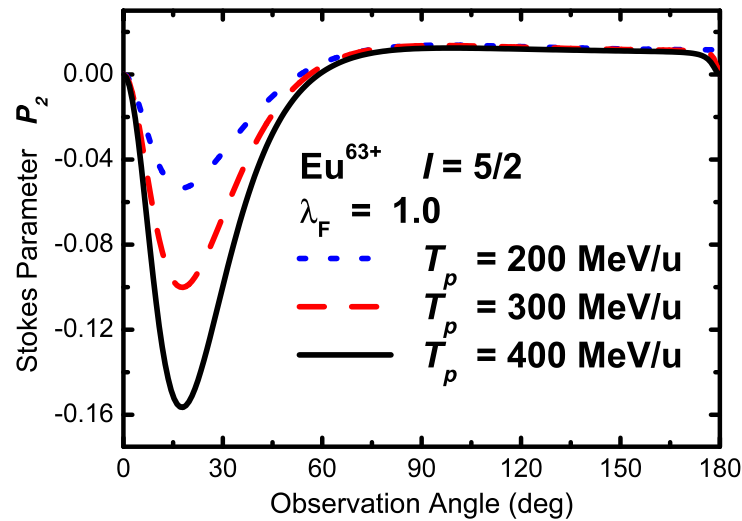


Figure 2. The Stokes parameter P_2 of the photons which are emitted in the electron capture into the K-shell of completely polarized hydrogen-like europium ions. See text for discussion.

electrons are captured into the ground state of spin-polarized hydrogen-like heavy ions [21]. As usual, here the polarization of the recombination photons is described in terms of the Stokes parameters. Experimentally, these parameters can be determined quite easily by measuring the intensities of the light I_χ under various angles with respect to the reaction plane. While the parameter $P_1 = (I_0 - I_{90})/(I_0 + I_{90})$ is obtained from the intensities *within* and *perpendicular* to the reaction plane, the parameter P_2 follows from a similar intensity ratio, taken at $\chi = 45^\circ$ and $\chi = 135^\circ$, respectively.

It is worth to note here that the two Stokes parameters, P_1 and P_2 , behave very differently with regard to the (degree of) spin polarization of the initially hydrogen-like projectiles. While the parameter P_1 *does not depend* on the polarization of the ion beam, the second Stokes parameter P_2 appears to be *direct proportional*

$$P_2(\theta) \propto \lambda_F \cdot f(\theta) \quad (4)$$

to the polarization of the ion beam, if this is defined by

$$\lambda_F = \sum_{M_F} n_{F,M_F} M_F / F, \quad (5)$$

and where n_{F,M_F} denotes the population of the magnetic sublevels and F , M_F the total angular momentum and its z -projection for a given hyperfine level of the hydrogen-like ions: $\mathbf{F} = \mathbf{I} + \mathbf{J}$. By measuring the Stokes parameter P_2 , therefore, the polarization properties of a heavy ion beam at storage rings can be obtained quite easily if the angular function $f(\theta)$ is reliably known from theory. Figure 2 displays the parameter P_2 for the radiative electron capture into the ground state of completely polarized ($\lambda_F \equiv 1$) hydrogen-like europium ions and for projectile energies in the range $200 \text{ MeV/u} \leq T_p \leq 400 \text{ MeV/u}$. As seen from this figure, a particular strong effect is found for the photons emitted under $\theta = 18^\circ$ with respect to the ion beam, where the second Stokes parameter decreases from the $P_2 = -0.05$ for $T_p = 200 \text{ MeV/u}$ to almost -0.16 for $T_p = 400 \text{ MeV/u}$.

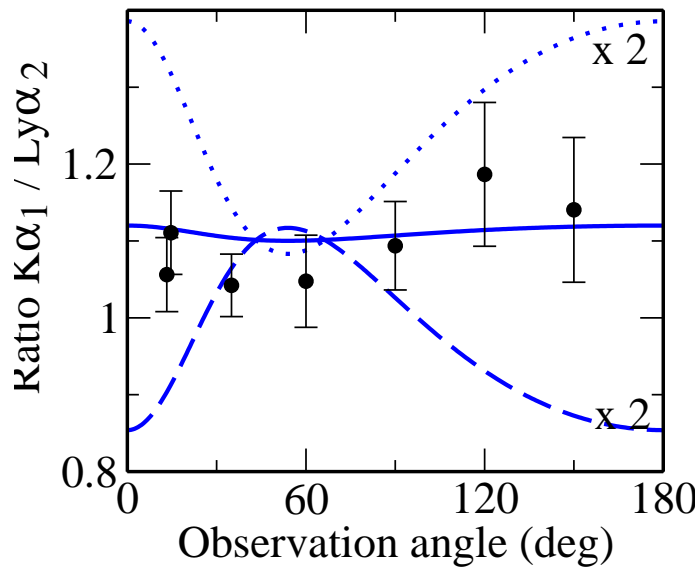


Figure 3. Angular distributions of the $K\alpha_1$ radiation of helium-like uranium following the REC into hydrogen-like U^{91+} ions at the projectile energy $T_p = 220$ MeV/u. Experimental data (solid points) are compared with theoretical results (solid line) for the $K\alpha_1$ emission from the $1s2p$ 1P_1 and 3P_2 levels. In addition, the individual contributions from the $^1P_1 \rightarrow ^1S_0$ (dashed line) and $^3P_2 \rightarrow ^1S_0$ transitions (dotted line) are shown, each multiplied by a factor of 2. All the data are normalized with respect to the intensity of the isotropic Lyman- α_2 radiation following the capture into bare U^{92+} ions, cf. Ref. [25].

4. Nearly isotropic K_α emission from helium-like uranium: A signature of the fine-structure

If the electron is captured not into the ground but some excited state, the ion will decay towards some lower-lying level under the emission of characteristic radiation. The investigation of this characteristic photon emission has attracted recent interest, both from the experimental and theoretical side, since it may help improve our understanding of the population dynamics of heavy ions. For example, several experiments were performed in order to investigate the electron capture into the $1s_{1/2}2p_{3/2}$ 1P_1 and 3P_2 states of (initially) hydrogen-like U^{91+} uranium ions and their subsequent $K\alpha_1$ ($^{1,3}P_{1,2} \rightarrow ^1S_0$) decay [9]. For the capture into hydrogen-like uranium, an almost *isotropic* angular distribution of the $K\alpha_1$ radiation was found, quite in contrast to the observations for the Lyman- α_1 ($2p_{3/2} \rightarrow 1s_{1/2}$) of hydrogen-like uranium, i.e. for the REC into initially bare ions, which exhibits a strong angular dependence [5].

In order to explain this qualitatively different ‘behaviour’ of the Lyman- α_1 and $K\alpha_1$ emission, a detailed theoretical analysis has been carried out in the framework of the density matrix theory. Within this approach, the $K\alpha_1$ emission is treated as an independent step, following the (prior) REC capture and population of the excited (sub-) levels. The radiative capture leads to an alignment of the (excited) ion which is typically described in terms of alignment parameters \mathcal{A}_k and which directly affect the subsequent characteristic photon emission. For example, the angular distribution of the $1s2p_{3/2}$ $^1P_1 \rightarrow 1s^2$ 1S_0 electric dipole (E1) and $1s2p_{3/2}$ $^3P_2 \rightarrow 1s^2$ 1S_0 magnetic quadrupole (M2) transitions can be expressed as

$$W_{E1}(\theta) \sim 1 + 1/\sqrt{2} \mathcal{A}_2(J=1) P_2(\cos\theta) \quad (6)$$

and

$$W_{M2}(\theta) \sim 1 - \sqrt{5/14} \mathcal{A}_2(J=2) P_2(\cos \theta), \quad (7)$$

and where θ denotes the angle between the emitted $K\alpha_1$ photon and the beam direction. In these expressions, the parameters $\mathcal{A}_2(J=1,2)$ refer to the alignment of the 1P_1 and 3P_2 levels; for the 3P_2 , moreover, the fourth-rank parameter \mathcal{A}_4 occurs in the angular distribution but was found to be small for the REC into fast, high- Z projectiles and, hence, is neglected in Eq. (7) above.

As seen from the distributions (6) and (7), the angular dependence of the subsequent photon emission is given by the (shape of the) Legendre polynomials $P_2(\cos \theta)$, weighted by the alignment parameters \mathcal{A}_2 , and together with some geometrical factors. For the 1P_1 and 3P_2 levels, in particular, these factors have different signs and, hence, lead to a cancellation in the angular dependence [13]. Therefore, as long as the $^1P_1 \rightarrow ^1S_0$ and $^3P_2 \rightarrow ^1S_0$ transitions are *not resolved* individually by the experiment, a more or less isotropic $K\alpha_1$ radiation is found even if the individual components of this line are strongly anisotropic. In Figure 3, the angular distribution of the $K\alpha_1$ decay (solid line) is displayed for the collision energy $T_p = 220$ MeV/u and indicates an almost isotropic behaviour, in perfect agreement with the experimental data. In general, however, the angular distribution of the $K\alpha_1$ radiation depends on both, the level structure and the alignment, and it will change along the isoelectronic sequence or if a different population (excitation) mechanism is considered for the 1P_1 and 3P_2 levels.

5. Conclusions

In conclusion, the recent theoretical (and experimental) progress in studying the electron capture into few-electron high- Z ions has been reviewed. Emphasis was placed on the angular and polarization characteristics of the x-ray photons which are emitted in course of the electron capture and the subsequent stabilization of the ions. Together with the experimental data, our calculations demonstrate that the angle- and polarization resolved x-ray spectroscopy provides a sensitive tool for studying the many-body effects on the structure and dynamics of high- Z , relativistic ions. As argued above, moreover, the measurement of the K-REC polarization may be utilized also to derive the polarization properties of the ion beam, if compared to a reliable theory. This may help in applying spin-polarized ions beams in atomic and nuclear physics experiments in the future.

Apart from the independent measurement of the REC and characteristic ($K\alpha$) radiation, a further challenge arises today from photon-photon coincidence experiments in the x-ray region and the study of angle-angle correlations. When compared to the individual steps in the photon emission, indeed, such x-x coincidence measurements are expected to be even more sensitive to many-body relativistic and polarization effects. A first theoretical analysis of the angle-angle correlation function for the capture into bare ions has been carried out recently [26] and is planned to be extended towards other x-x coincidences and for the capture into few-electron ions.

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