Towards a fast calculator for the radiation characteristics of radiative recombination and radiative electron capture

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Abstract. The radiative capture of free electrons (radiative recombination) and bound electrons (radiative electron capture) are among the most important charge changing processes for fast, highly-charged ions. While total cross sections can be obtained by an approximate formula with reasonable accuracy, the estimation of angular distributions and polarization properties of the emitted radiation requires a fully relativistic treatment that is numerical expensive. Therefore we recently started the development of a fast calculator for these radiation characteristics. The program is based on a grid of rigorously calculated data points for free-electron capture into bare ions, between which interpolation is performed to obtain radiation characteristics for specific collision systems. Also capture into few-electron systems is taken into account in an approximate way. We present first results from this development.

1. Introduction

The capture of electrons into bound states of ions is of significant importance for both experiment and theory in the fields of atomic and plasma physics as well as for astrophysics. The capture process is called radiative if it is accompanied by the emission of a photon that carries away the sum of the binding energy of the final state and the incident electron kinetic energy. If the initial electron is considered as free, the capture process is referred to as radiative recombination (RR) [1], being the time-reversal of the photoeffect [2], whereas the capture of a bound electron is called radiative electron capture (REC) [3, 4, 5]. The RR process is relevant for understanding the characteristics of hot plasmas [6, 7] being present in astronomical objects or in laboratory devices, for example electron beam ion traps and fusion devices, and it determines the charge change-induced beam losses in electron coolers [8, 9, 10]. On the other hand, REC is a prominent charge-changing process for fast, highly-charged ions interacting with dedicated target materials or with residual gas being present in the beam lines of accelerators and storage rings [11]. Moreover, when low- to medium-Z targets and heavy, highly-charged projectile ions are considered, the to-be-captured electrons can be treated as free particles having a momentum distribution equal to the one of the bound target states. This so-called impulse approximation reduces the REC description to the RR cross section folded with the incident electron momentum distribution. Consequently, both the REC and the RR processes, as well

as the photoeffect, can be treated within the same theoretical framework. This fact gave rise to several REC measurements aiming for a deeper insight into the photoeffect while exploiting the advantageous experimental conditions present for the time-reversed process, see [5] and references therein.

For ongoing highly-charged ion studies at the experimental storage ring (ESR) and for future experimental campaigns planned at the CRYRING@ESR [12] and the high-energy storage ring (HESR) of the FAIR facility [13], a precise knowledge of REC characteristics in a broad range of collision energies from about 1 MeV/u up to 5 GeV/u is highly desirable. While total cross sections for RR and REC can be obtained by an approximate formula with reasonable accuracy [14] up to roughly 1 GeV/u, the estimation of angular distributions and polarization properties of the emitted radiation requires a fully relativistic treatment that is non-trivial and numerical expensive [15, 16]. Tabulated values for RR total and angular differential cross sections covering a broad range of projectile atomic number Z and collision energy E were published by Ichihara and Eichler [17, 18]. However, the grid points of this data set are too sparse to allow interpolation with a good accuracy. Moreover, the photon linear polarization, that attracted interest only recently due to the introduction of novel hard x-ray polarimeters [19, 20, 21, 22], is not addressed at all. Thus, we started the development of a fast and precise calculator for the differential cross section and linear polarization of radiation arising in the RR and REC processes. This calculator is based on a dense grid of rigorously calculated RR data points for the recombination into bare ions, between which interpolation is performed to obtain data for the collision systems of interest. Recombination into few-electron systems is taken into account in an approximative way. Finally, as described above, the capture of bound electrons is treated within the impulse approximation by folding the RR cross sections with the electron momentum distribution of the target electrons. In this report we present first results for the RR cross sections generated by our code, which is in the following referred to as the REC calculator (RECAL).

2. Radiative Recombination

Differential cross sections and linear polarization values of the RR photons are calculated using the algorithms provided by Fritzsche and Surzhykov which are part of the DIRAC toolkit, see [23, 24] and references therein for details. For first test calculations, we generated a RR data base of capture into bare projectiles for the $1s_{1/2}$ to $3d_{5/2}$ orbitals with atomic numbers $Z = 1, 7, 18, 36, 54, 66, 79$, and 92 and more than 100 kinetic energies between 2 MeV/u and 1 GeV/u (1.1 keV to 548.6 keV electron kinetic energy). The accuracy of the RR calculation is mainly determined by the accuracy of the continuum wavefunction representing the initial state of the incident electron, which is described by a series expansion in terms of partial waves. A careful choice of the number of partial waves, defined by $\nu = 2\kappa_{\max}$, with $\kappa_{\max}$ being the maximum number for the Dirac angular momentum to be taken into account, is of particular importance. More precisely, a too small choice of $\kappa_{\max}$ may lead to truncation errors, while, on the other hand, a too large value increases significantly computation time (approximately scaling with $\kappa_{\max}^3$) and eventually leads to an explosion of numerical errors due to the rapid oscillations of the radial part of the continuum wavefunction. With a proper choice of $\kappa_{\max}$ an uncertainty on the percent level can be reached for the parameter range concerned in this work.

The RR photon characteristics for a specific projectile and collision energy are obtained from an interpolation between the rigorously calculated data points using a method proposed by Akima [25]. To verify the quality of this procedure, in Fig. 1 the angular differential cross section for photons stemming from the recombination into the ground state and the $2p_{3/2}$ orbital of bare lead ions (Z=82) are compared to reference calculations published in [18]. For RR into the $1s_{1/2}$ orbital and electron kinetic energies lower than 300 keV (equals 547 MeV/u projectile energy) nearly perfect agreement is found, while an increasing deviation is seen for higher collision energies. This due to the fact that the proper $\kappa_{\max}$ number increases with higher energies and

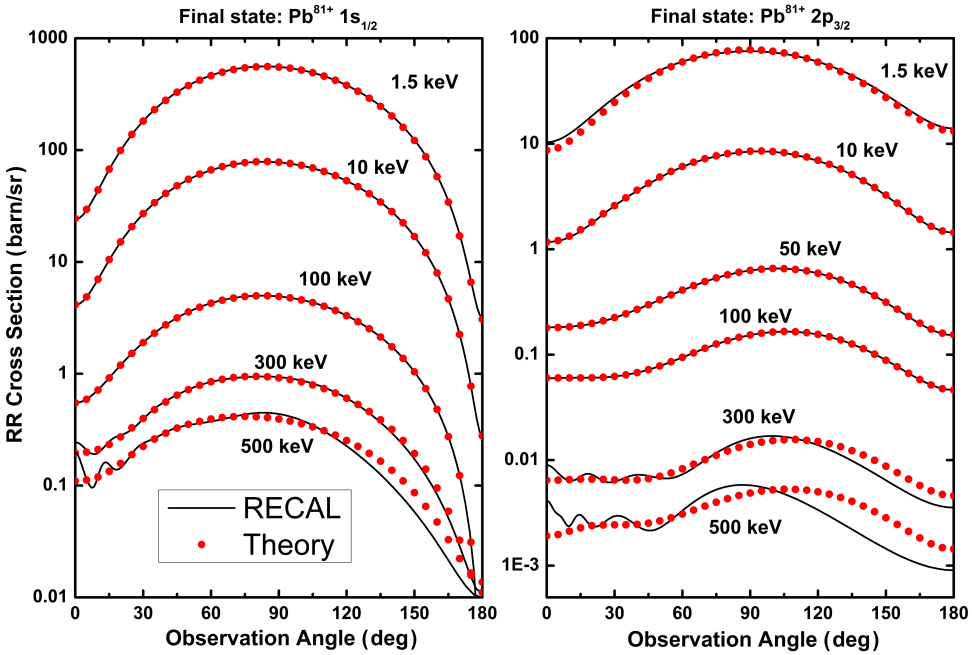

Figure 1. Angular differential radiative recombination cross section into the $1s_{1/2}$ and the $2p_{3/2}$ of bare lead ions for various collision energies. Fully relativistic calculations are compared to RECAL predictions. An increasing deviation at high collision energies is seen due to an improper choice of $\kappa_{\max}$ for the underlying RR data base of the RECAL calculator, see text for details.

in our first attempt we failed to chose large enough $\kappa_{\max}$ values for the relativistic regime of collision energies. Moreover, for RR into the $2p_{3/2}$ orbital, also at the lowest collision energy a small deviation between rigorous calculations and RECAL predictions is found in Fig. 1. We are still investigating if this feature is also due to a wrong maximum partial wave number or if it is caused by an improper interpolation along the Z axis. Here one has to stress that depending on $\kappa_{\max}$ the rigorous calculation for a single collision energy and a single final orbital may take up to a few hours of computation time on a standard desktop computer. We are currently performing systematic test calculations to obtain a map of optimum $\kappa_{\max}$ values as a function of the collision energy, final electron state and projectile Z. Therefore, we compare the obtained radiation characteristics to reliable reference calculations such as the data published in [17, 18]. As mentioned above, for the linear polarization of RR/REC photons no tables with references values are available, so here we rely on the convergence of the polarization characteristics with increasing $\kappa_{\max}$ as the only criterion.

So far only recombination into finally hydrogen-like ions was considered. However, there is the need to have RR/REC cross sections with a reasonable precision also for few-electron systems. It was previously shown that for few-electron, heavy ions and collision energies above a few MeV/u the RR process can be approximated with a single-electron model using an appropriate effective nuclear charge Z_{eff} as in that case the electron-electron interaction is very small compared to the interaction of each electron with the nuclear charge [26]. Effective Z values for the RECAL code were determined from a table of successive ionization potentials originally compiled for the SUK program that is applied for electron beam ion trap simulations [27, 28].

In Fig. 2 we compare the RECAL results for RR into initially hydrogen-like and lithium-like uranium ions to rigorous multi-configuration Dirac Fock (MCDF) calculations presented

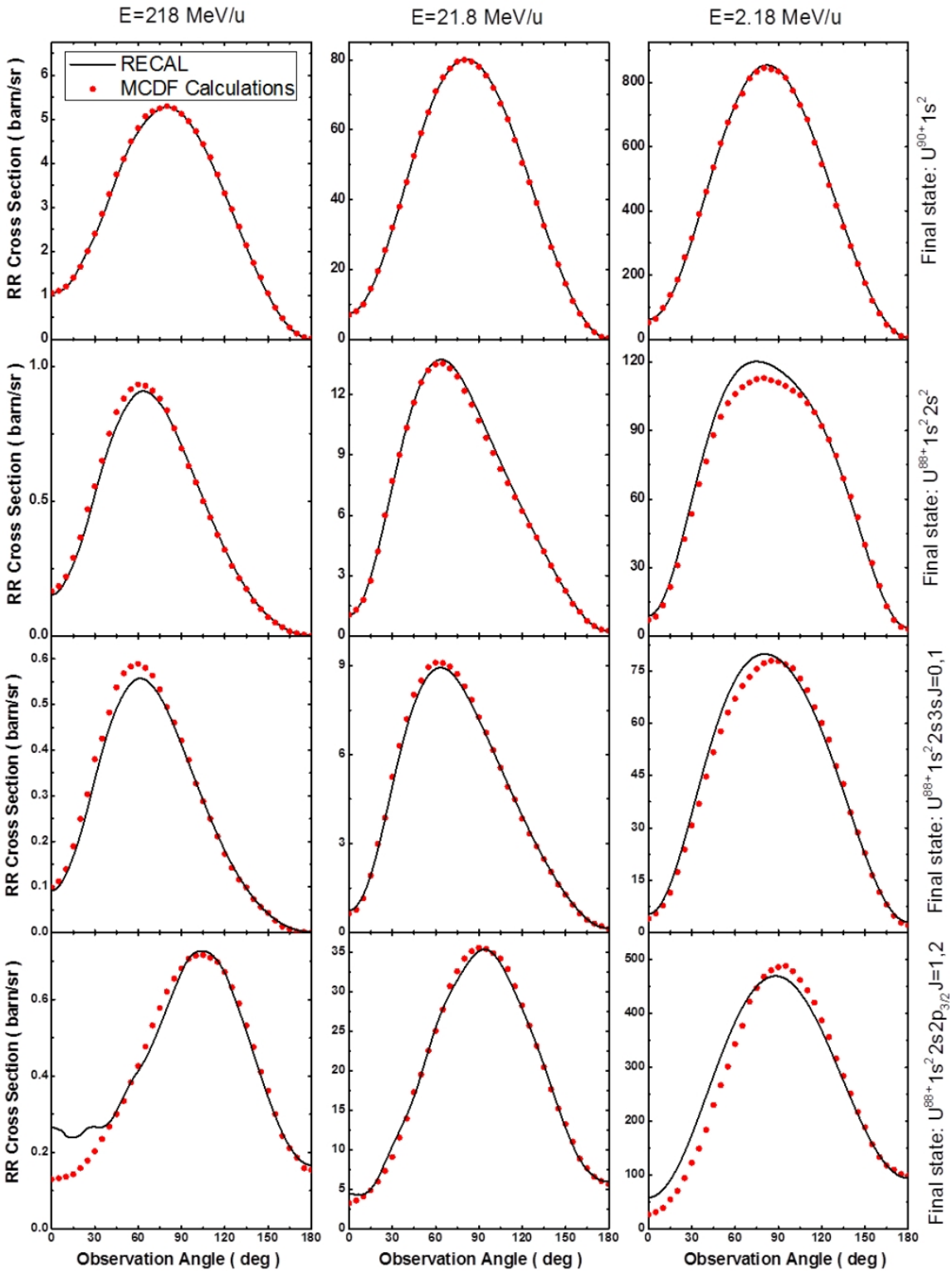

Figure 2. Angular differential radiative recombination cross section into hydrogen-like (final state: helium-like) and lithium-like (final state: beryllium-like) uranium ions for various collision energies. Rigorous MCDF calculations [26] are compared to RECAL predictions. Good agreement is found for the medium collision energy, while for the low and the high energy data significant deviations are seen for the finally beryllium-like system.

in [26] (results from Coulomb and Babushkin gauges were averaged). Note that the theory cross sections for recombination into neighboring J-levels of the $1s^2 2s3s$ and the $1s^2 2s2p_{3/2}$ configurations were summed up to allow a comparison to the RECAL predictions which rely on a single-electron data base. However, in many cases these levels differ only by a few eV and are hardly resolved by standard solid-state x-ray detectors. For recombination into the ground state of initially hydrogen-like uranium RECAL matches the theory values with good agreement. In this case one can expect that the huge binding energy of the final state suppresses any significant electron-electron interaction during the capture into the projectile. In contrast, for the initially lithium-like system only for a moderate collision energy of 21.8 MeV/u good agreement is found, while for the low and the high energy data significant deviations are seen. A possible explanation is that for low collision energies the electron-electron interaction can not be neglected. On the other hand at high energies the chosen $\kappa_{\max}$ might be too small as at least for the $1s^2 2s2p_{3/2}$ configuration and at observation angles below 30° an artefact due to a wrong $\kappa_{\max}$ value is visible in the RECAL data.

3. Summary

We presented first results from a fast calculator for the radiation characteristics of the RR and REC processes. Such a tool will be helpful for the planning and interpretation of energetic ion-atom collision experiments at the new FAIR facility as well as for ongoing heavy ion studies at GSI. A comparison to rigorously calculated data shows in general a reasonable agreement. However, significant deviations are observed for parameters where the underlying data base of the calculator was produced using improper values for the maximum number of partial waves $\kappa_{\max}$ for the series expansion representing the incident electron. A systematic study is needed to determine valid $\kappa_{\max}$ values throughout the full parameter range of interest.

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