PROCEEDINGS OF SCIENCE

Calculation of Radiative Recombination Rates for Hydrogen-Like Ions at High-Z

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We report on the calculations of radiative recombination (RR) rate coefficients for very low, in the range of a few meV, relative electron–ion energies. The rate coefficients are derived for bare lead ions colliding with free electrons in a rigorous relativistic manner, in which all multipoles of electron-photon interaction under the inclusion of retardation effects are taken into account. We demonstrate that the measurements of absolute rate coefficients at electron cooler devices are really sensitive to the high Rydberg states, as well as to the transverse electron temperature $kT_\perp$ and the longitudinal electron temperature $kT_\parallel$.

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1. Introduction

Electron-ion recombination processes play a significant role in the determination of the ionization-recombination balance of highly charged ions both in electron-ion beam colliding experiments and in high-temperature laboratory and astrophysical plasmas. Motivations for studying these processes include an understanding of fundamental processes in reactions of free electrons with ions, and the determination of corresponding cross sections and rate coefficients for use in models of energy transport phenomena and plasma diagnostics.

The main and the simplest recombination mechanism in bare ions is the radiative recombination (RR) or radiative electron capture (REC), in which a free electron or quasi-free target electron is transferred via the photon interaction to the final bound atomic state. For incoming ions that carry one or more electrons, dielectronic recombination (DR) is also a possible channel [1]. In the case of hydrogen-like (H-like) ions at high-Z, excitation of the $1s$ electron requires a large amount of energy and the DR resonances start at a relatively large impact energy. With the tightly bound $1s$ electron of H-like heavy ions and electron beam temperature of a few meV or a few eV in electron cooler devices [2], however, we are far away from fulfilling the required resonance condition.

For ongoing atomic structure studies with highly-charged ions at the electron cooler of CRYRING@ESR storage ring [3], radiative recombination is the most dominant electron-ion recombination mechanism for the systems considered here. In this report, we present the first results for the RR rate coefficients generated by our code [4], which will be an important tool exploring the origin of the so-called rate enhancement observed up to now only for total RR rates [5].

2. Radiative recombination

In the nonrelativistic dipole approximation, the calculations of RR cross section were given by Stobbe's and Burgess's procedure evaluating the electric dipole matrix elements [6, 7]. However, the cross sections given in nonrelativistic treatment are not valid for high photon and hence electron binding energies, since these approximations for total and sometimes even for differential cross sections are not what one should expect [8]. The exact evaluation of the relativistic photoelectric or, inversely, the RR cross section requires a partial-wave expansion of the Coulomb-Dirac wave functions for the bound and for the continuum states modified for the finite nuclear size. This means that closed-form expressions can no longer be derived, and one has to resort to numerical methods. Detailed formulations exist since a long time which can be found in [9].

In figure 1 we display the RR cross sections as predicted by the exact treatment in comparison with the Stobbe approximation for the subshells of Pb^{82+} up to principle quantum number $n = 8$ at relative electron-ion energy of 2.6 meV. A sizeable difference in the total angular momentum quantum number j-sensitive cross sections within 30% is observed, in particular for s-states. The statistical weights considered for the Stobbe's calculations of j-sensitive cross sections are responsible for these discrepancies. This means that even for $n = 8$, relativistic effects in Pb^{82+} survive or, possibly, retardation effects (high powers in kr of photon field) play a role, owing to tighter binding. The pronounced deviation of the Stobbe theory from the rigorous treatment indicates the importance of introducing relativistic corrections, if one would like to apply nonrelativistic theory for RR cross section calculations for each low-lying bound state, i.e. states with $n \leq 10$.

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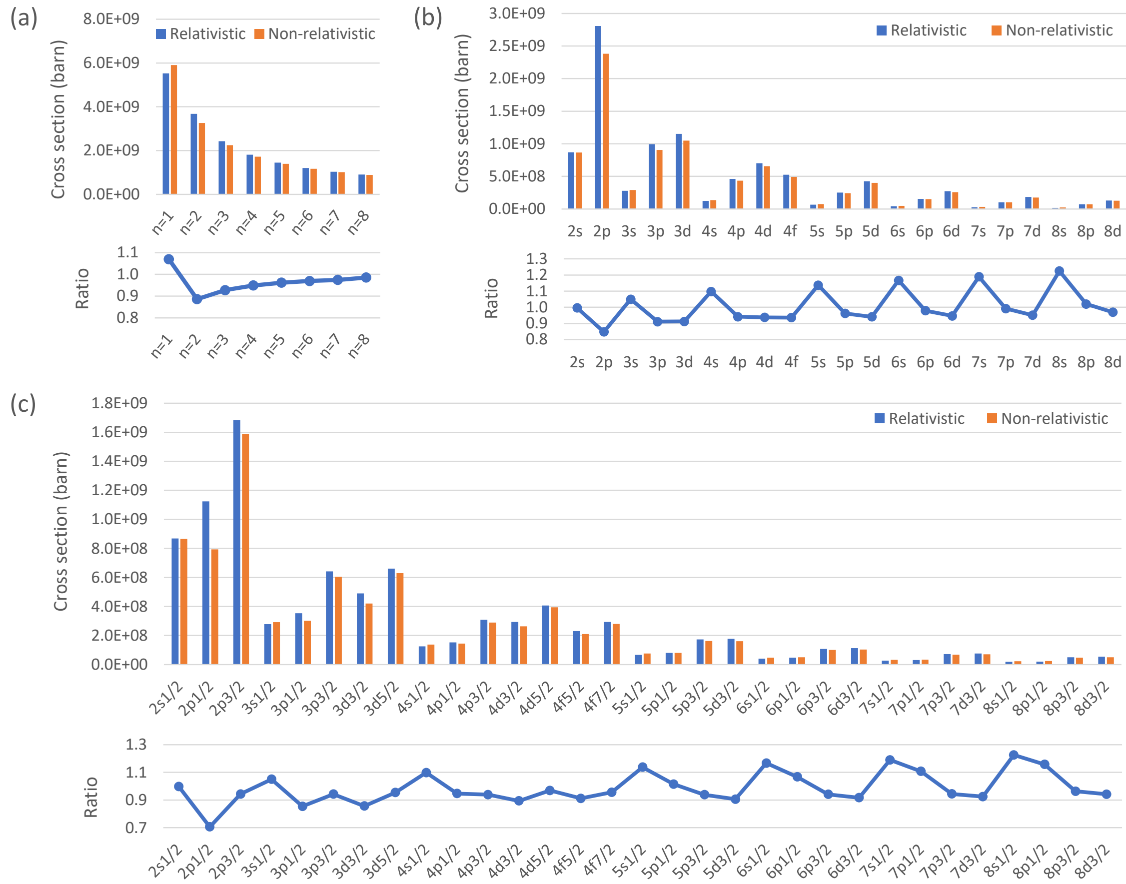

Figure 1: The RR cross sections as predicted by the exact treatment in comparison with the Stobbe approximation (non-relativistic) for the subshells of Pb^{82+} up to $n = 8$ at relative electron-ion energy of 2.6 meV. In each sub-figure the deviation of both approaches is depicted.

At electron cooler devices, in practice, when an electron beam has some velocity distribution $f(\mathbf{v})$, introducing an integrated quantity namely the rate coefficient α_{nl} instead of the RR cross section σ_{nl}, defined for a fixed electron velocity, appears to be more reasonable. The relation between the cross section σ_{nl} and the rate coefficient α_{nl} is given in a mathematical form of

$$\alpha_{nl} = \langle v\sigma_{nl}(\mathbf{v})\rangle = \int v\sigma_{nl}(\mathbf{v})f(\mathbf{v})d^3v. \tag{1}$$

For the velocity distribution, the cooler electron beam usually is described in terms of an anisotropic Maxwell-Boltzmann distribution (also called a normalized flattened distribution) characterized by effective longitudinal $kT_\parallel$ and transverse $kT_\perp$ beam temperatures [10], as

$$f(\mathbf{v}) = \left(\frac{m_e}{2\pi}\right)^{3/2} \frac{1}{kT_\perp(kT_\parallel)^{1/2}} \exp\left[-\left(\frac{m_e v_\perp^2}{2kT_\perp} + \frac{m_e v_\parallel^2}{2kT_\parallel}\right)\right]. \tag{2}$$

Quite generally, the effective electron beam temperatures in the projectile frame are characterized by the convolution of the electron and ion beam velocity distributions in the form of $(kT_{e\parallel}, kT_{e\perp})$

and $(kT_{i\parallel}, kT_{i\perp})$, respectively, and they are given by

$$\begin{aligned} kT_{\parallel} &= kT_{e\parallel} + \frac{m_e}{M} kT_{i\parallel} \\ kT_{\perp} &= kT_{e\perp} + \frac{m_e}{M} kT_{i\perp}, \end{aligned} \quad (3)$$

where k is the Boltzmann constant, M and m_e are the ion and electron masses, respectively.

3. Results and discussions

For the realistic experimental conditions, the electron beam temperature of $kT_{\perp} = 2.6$ meV and $kT_{\parallel} = 52$ μeV was achieved at the electron cooler of CRYRING@ESR [3], where bare or few-electron ions could recombine with free electrons of continuum states. Figure 2 depicts the state selective total rate coefficients for radiative recombination into Pb^{82+} at the electron cooling temperature as a function of principal and angular momentum quantum number (n, l). As can be seen that the main contribution to the rate coefficients is given by the small l states, as is to be expected. However, due to the small relative velocity between projectiles and electrons, the contribution from high Rydberg states might have a significant contribution to the total rate coefficient.

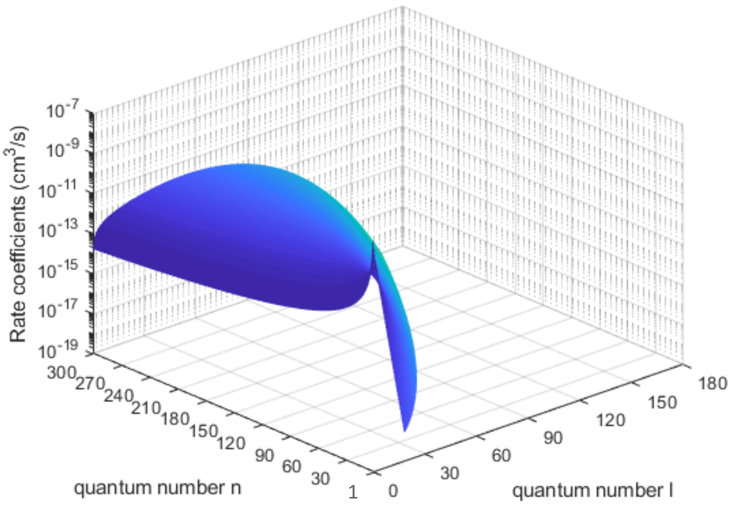

Figure 2: State selective (n, l) rate coefficients calculated for radiative recombination into bare lead ions for flattened electron velocity distribution with $kT_{\perp} = 2.6$ meV and $kT_{\parallel} = 52$ μeV.

In figure 3 we vary the principle quantum number n from $n = 10$ to $n = 300$ to show the changes of magnitude in total rate coefficient. As can be seen that the n-RR contribution to the total rate coefficient increases rapidly until $n = 50$, because in radiative recombination much higher n-states contribute to the recombination rates, which scale as $1/n$, as it is revealed in the figure that the occupation of K-shell population decrease from 32% (corresponding to $n = 10$) to 14% when the magnitude reaches saturation at $n = 300$. Thus, the recombination into these high levels is crucial for the study of characteristic projectile x-rays resulting from the radiative cascade of these electrons to the low-lying subshells.

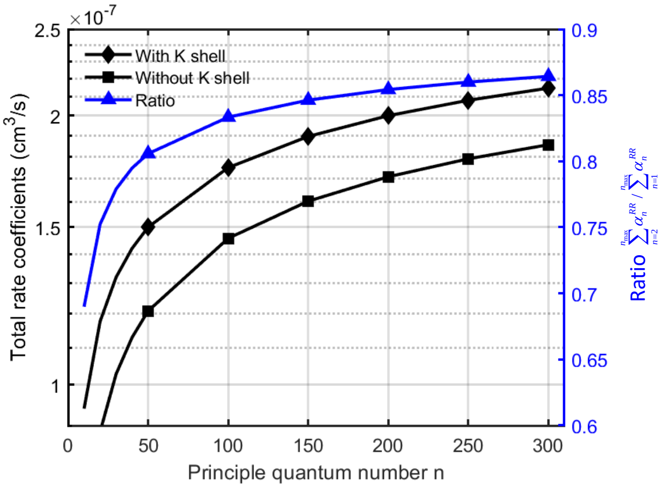

Figure 3: The total rate coefficient calculated for radiative recombination into bare lead ions is displayed as a function of the principle quantum number n. The ratio $\sum_{n=2}^{n_{max}} \alpha_n^{RR} / \sum_{n=1}^{n_{max}} \alpha_n^{RR}$ reveals that the rate coefficient is sensitive to the population distribution of high Rydberg states.

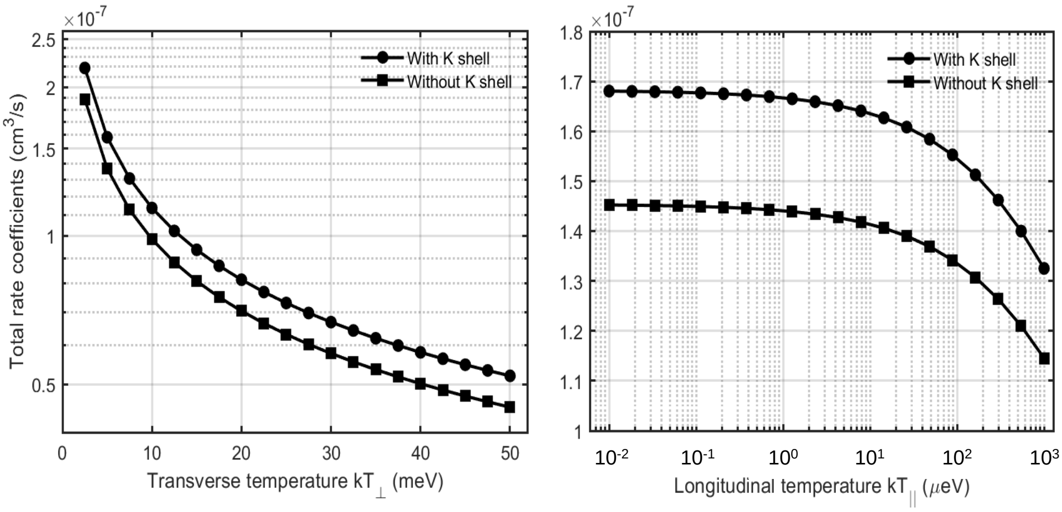

Figure 4: The radiative recombination rate coefficient is plotted [left] as a function of the transverse temperature $kT_\perp$ with a fixed longitudinal temperature $kT_\parallel = 50$ μeV, and [right] as a function of the longitudinal temperature $kT_\parallel$ with a fixed transverse temperature $kT_\perp = 5$ meV for nuclear charge $Z = 82$. Here, n up to $n = 300$ is included in the calculations.

From this point of view, it would be interesting to investigate the dependence of rate coefficients on the longitudinal $kT_\parallel$ and transverse $kT_\perp$ electron beam temperatures for electron-ion merged-beam experiments at electron cooler devices. The contributions from $\sum_{n=1}^{n_{max}} \alpha_n^{RR}$ and $\sum_{n=2}^{n_{max}} \alpha_n^{RR}$ to the total rate coefficient are depicted in figure 4, and both cases show similar decreasing behavior of rate coefficient that scales as $1/E_{rel}$ (relative collision energy $E_{rel} = \sqrt{(kT_\perp)^2 + (kT_\parallel)^2}$) [10]. At low relative electron-ion collision energies, the principle quantum number $n = n_{max} = 300$ is included in the calculations, and we found no more than 15% of projectile x-rays are from K-shell free electron capture. One may expect that the characteristic x-ray radiations stemming from cascade feeding from high n-states would be registered at the low-energy part of the spectrum (e.g. Balmer series), which is typical for the experiments in the storage ring utilizing an electron cooler as a target of free electrons [3]. Furthermore, it is worth mentioning that the smaller is $kT_{\parallel}$ with respect to the transverse temperature $kT_{\perp}$, the influence of the longitudinal temperature on the total rate coefficients is tiny, i.e. the latter seems to be constant as a function of the longitudinal temperature $kT_{\parallel}$ for $kT_{\perp}/kT_{\parallel} > 10^4$.

4. Conclusions

We present here the first results from a simulation program for the radiation characteristics of the RR processes. Such a tool will facilitate the studies of rate enhancement phenomenon for recombination in electron cooler devices. In the near future, one may aim at the high-precision x-ray spectroscopy experiments at the CRYRING@ESR electron cooler measuring both state-selective and total rate coefficient for bare ions at high-Z interacting with low-energy electrons.

Acknowledgments

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References

[1] Y. Hahn, *Electron–ion recombination processes—an overview*, *Rep. Prog. Phys.* **60** (1997) 691–759

[2] H. Poth, *Electron cooling: Theory, experiment, application*, *Phys. Rep.* **196** (1990) 135–297

[3] B. Zhu *et al.*, *X-ray emission associated with radiative recombination for* Pb^{82+} *ions at threshold energies*, *Phys. Rev. A* **105** (2022) 052804

[4] B. Zhu and Th. Stöhlker, *Radiative recombination studies for bare lead ions interacting with low-energy electrons*, *Atoms* **11** (2023) 2

[5] W. Shi *et al.*, *Recombination of* U^{92+} *ions with electrons*, *Eur. Phys. J. D* **15** (2001) 145–154

[6] M. Stobbe, *Zur quantenmechanik photoelektrischer prozesse*, *Ann. Phys.* **399** (1930) 661–715

[7] A. Burgess, *Tables of hydrogenic photoionization cross-sections and recombination coefficients*, *Mem. R. Astron. Soc.* **69** (1965) 1–8

[8] O. Brinzanescu, J. Eichler, A. Ichihara, T. Shirai and Th. Stöhlker, *Comparison between the nonrelativistic dipole approximation and the exact relativistic theory for radiative recombination*, *Phys. Scr.* **T80** (1999) 324–325

[9] J. Eichler and Th. Stöhlker, *Radiative electron capture in relativistic ion–atom collisions and the photoelectric effect in hydrogen-like high-Z systems*, *Phys. Rep.* **439** (2007) 1–99

[10] M. Pajek and R. Schuch, *Radiative recombination of bare ions with low-energy free electrons*, *Phys. Rev. A* **45** (1992) 7894–7905