Theoretical study on electron impact excitation and recombination of highly charged ions

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Abstract. Electron impact excitation and recombination are the most essential atomic processes. A systematical study on these processes will be helpful for both the understanding of atomic excited structures and the modeling of various plasma properties. Recently, based on the GRASP92/2K and RATIP packages in the frame of MCDF method, some new programs, such as REIE06 for electron impact excitation (EIE), RERR06 for radiative recombination (RR) and REDR06 for dielectronic recombination (DR), have been developed by our group. In this paper, some selected applications of these programs are reviewed.

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1. Introduction

Collisions of electrons with atoms and ions including excitation and recombination are the most essential and important atomic processes. The studying of these collision processes can enhance our understanding of the basis natures of quantum-physics and provide knowledge about the structure and the dynamics of atomic systems. These process are also important in astrophysical and fusion plasmas, which strongly affects both the charge state distribution and the photo emissions. Furthermore, the accurate cross sections are widely required for calculating of ionization balance and spectral line intensities in the diagnostics of various plasmas. In recent years, with the development of experimental techniques, for example, electron beam ion traps (EBIT) [1–14], merged electron-ion beams energy-loss (MEIBEL) [15–17], atom trap-based [18], synchronous photon detection [19], radiation trapping [20], Storage Ring [21, 22] etc., various electron-impact excitation and recombination cross sections have been measured with a very high accuracy.

On the theoretical side, during the last two decades, several different theoretical methods have been developed including distorted-wave approximation (DW) [23–29], R-matrix method [30–38], close-coupling (CC) method [39–44] etc. The R-matrix and CC methods are known to be very accurate for neutral atoms and lowly charged ions, but they are also computational expensive and limited to low collision energies often, the DW method is mainly used for highly ionized heavy ions. The DW method

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is regarded as an easier and more effective method for producing a large amount of data of cross sections.

Recently, based on the multi-configuration Dirac-Fock (MCDF) method and the corresponding packages GRASP92/2K [45, 46] and RATIP [47], some new relativistic distorted wave programs, such as REIE06 [48,49] for electron impact excitation (EIE), RERR06 [50] for radiative recombination (RR) and REDR06 [51] for dielectronic recombination (DR), have been developed by us. By using these programs, a series of collision processes have been studied systematically [48–58]. As examples, the direct EIE processes of Ne-like ions, resonant EIE processes of Ba$^{46+}$ ions, the effects of Breit interactions on the EIE processes, DR processes of highly charged iodine ions, radiative electron capture (REC) of U$^{89+}$, and the quantum interference between RR and DR were briefly reviewed in this report.

2. Direct electron impact excitation of Ne-like ions

![Figure 1. The electron impact excitation cross sections of Ne-like ions from the ground state $2p^6$ J=0. The incident electron energy is 5 times of threshold.](image_url)

The atomic structures and dynamic processes of Ne-like ions have been an interesting subject in theory, experiment and applications. As shown in our previous studies on the energy level structure and transition properties, some pairs of levels with the same parity and J cross each other in some particular Z regions and result in very strong configuration interactions [59]. For example, in the wavefunction components of the $(2p_{1/2}3s_{1/2})_1$, the contribution from the $(2p_{3/2}3d_{3/2})_1$ arrives by 29% at Z $\sim$ 51, and the contribution from the $(2p_{5/2}3d_{5/2})_1$ arrives by 40% at Z $\sim$ 55. These mixtures result in dramatically increase and decrease of the corresponding transition probabilities in the crossing regions. Furthermore, these crossings will also cause a series of changes of the corresponding EIE cross sections. In Fig. 1, the EIE cross sections of Ne-like ions from the ground state $2p^6$ J=0 to the levels with J=1 are shown, where the incident electron energy is 5 times of threshold. From this figure, we
can see that the cross sections to the $(2p_{1/2}^{-1}3s_{1/2})_1$ state rises rapidly to a maximum near $Z = 55$, and the cross sections to the $(2p_{3/2}^{-1}3d_{5/2})_1$ decrease to a minimum near $Z = 55$. But the cross sections to the other excited states change smoothly with the increasing of the atomic number. Consequently, as shown in Fig. 2, the ratio of line intensities of $(2p_{3/2}^{-1}3d_{5/2})_1 \rightarrow 2s^22p^6 \, ^1S_0$ (called 3C line) and $(2p_{3/2}^{-1}3d_{5/2})_1 \rightarrow 2s^22p^6 \, ^1S_0$ (called 3D) lines of Ne-like ions, which has been widely used to diagnose the temperature and density of the astrophysical plasmas [60], changes dramatically at the $Z = 55$ rather than the trend at the range of $Z = 24-47$ [60].

![Figure 2](image.png)

**Figure 2.** The ratio of the collision strength of 3C and 3D lines as a function of $Z$. The incident electron energies are 1.5, 2.0, 5.0, 8.0 and 10 times of the threshold. The experimental data from Marrs et al. [14]

3. Resonant electron impact excitation of Ne-like $Ba^{46+}$ ions

The resonant excitation processes are also very important channels in some special EIE processes, and can be described as

$$e^-(\varepsilon_i) + A^{q+} \rightarrow A^{**(q-1)+} \rightarrow A^{*q+} + e^-(\varepsilon_f),$$

where one bound electron is excited and meanwhile the incident electron is captured to form a doubly excited state, and then followed by an autoionization to an excited final state. In the isolated resonance approximation, the resonant excitation contributions can be added to the direct excitation.

In Fig. 3, the EIE cross sections from the ground state $2p^6 \, J = 0$ to the magnetic sublevels of the level $2p^53s \, J=2$ of neonlike $Ba^{46+}$ are displayed, and both the direct excitation and resonant excitation contributions from the $4l5l'$, $4l6l'$ and $5l5l'$ are included. The resonance structures can be clearly identified from the figure. In the energy ranging from 5 keV to 5.2 keV, the indirect contribution from the $4l5l'$ resonances are dominant and the cross section will enhance more than two times compared with the direct excitation. In the earlier EBIT experiment [61], it was

\[ \text{Figure 3.} \]
Figure 3. The electron impact excitation cross sections of neonlike Ba$^{46+}$ from the ground state $2p^6$ J=0 to the specific magnetic sublevels $M_f$ of the level $2p_{3/2}3s_{1/2}$ J=2 as a function of the incident electron energy.

found that the M2 emission was enhanced by more than 50% in the energy range due to resonance excitation. In addition, in Ref. [62], the 46l and 55l contribution were thought too small to be seen in a plot of total line intensity, but both of them were observed in the high-resolution polarization measurement.

By using these calculated cross section data, the polarization degree of this emission line following the EIE can be obtained further. In Fig. 4, the calculated polarization degree of M2 line are compared with the experimental measurements of Takács et al. [62]. The present results were shifted to left 130eV for considering the space charge effects in the experiment [62]. It can be seen that if only the direct impact excitation were considered in the calculations, the negative polarization degree increases from 10% to 13% smoothly with increasing of electron energy, which agree with the experiment of Takács et al. [62] very well. The averaged polarization degree of $-12 \pm 10\%$ also agrees with the assumption of $-5\pm10\%$ by Beiersdorfer et al. [61] at the considered energy range. The resonance excitations result in the sharp change of polarization degree, especially for the energy ranging from 5keV to 5.3 keV, where the contribution of the double excited states 4l5l is dominant. At the energy near 5 keV, the negative polarization degree were largely enhanced to -22%, and at the energy near 5.1 keV the polarization effects were decreases strongly, which agree with the experiments excellently. However, at the energy near 5.25 keV, there is a strongly decrease of polarization in the experiment, but could not be reproduced by the theory. For the energy from 5.3 keV to 5.6 keV, where the 46l resonance series is dominant, the change of polarization is relatively small because of relatively small resonance excitation contributions. However, when the energy is larger than 5.6 keV, the effects of the 55l resonance excitation on the polarization are very obviously. There are two
Figure 4. Linear polarization degree of neonlike Ba$^{46+}$ M2 line ($2p_{3/2}^13s_{1/2}^1$) → $2p^6 J = 0$ as a function of the incident electron energy. Solid line represents the present work; dashed lines represent Takács et al. [62]'s calculations which considered the cascade scheme. The experimental data from Takács et al. [62] are given as solid circles.

peaks with the obvious decreasing polarization for the energy close to 5.8keV, and one of them was measured by Takács et al. [62]. For the energy near 5.75keV, the polarization were increased to -26%, which were not measured by experiment because of the limited energy points. Comparing with Takács et al. [62]'s calculations with cascade scheme, It is found that the cascade effects may play a relatively small role.

4. Breit interaction effect of inner-shell EIE of highly charged Be-like ions

The effects of Breit interactions on the electron collision processes are very important, and have been studied for many years [63–66]. In this work, the influence of Breit interaction on specific magnetic sublevel excitation cross sections and the degree of linear polarization for the transition line of Be-like Mo$^{38+}$, Nd$^{56+}$, and Bi$^{79+}$ ions,

$$\varepsilon e + 1s^22s^2 → 1s2s^22p_{1/2}(J = 1) + e' e → 1s^22s^2(J = 0) + h\nu,$$

(1)

are demonstrated.

In Fig. 5, the degree of linear polarization as functions of incident electron energy for the Be-like Mo$^{38+}$, Nd$^{56+}$, and Bi$^{79+}$ ions are presented. As can be found that both the degrees of linear polarization with and without the Breit interaction increase sharply with increasing of incident electron energy before starting to decrease at higher energy region. And when the incident electron energies are greater than about 2 times of the threshold energies, the degree of linear polarization without the Breit interaction decreases very slowly, however, the degree of linear polarization with the Breit interaction decreases rapidly. This same pattern of an increase in the
Figure 5. The degree of linear polarization of transition line $1s2s^22p_{3/2}^1J = 1\rightarrow 1s^22s^22p_{3/2}^1J = 0$ for the Be-like Mo$^{38+}$, Nd$^{56+}$, and Bi$^{79+}$ ions as functions of incident electron energy in threshold units. R represents the value with inclusion of only the Coulomb interaction, and RB represents the one with the Breit interaction included.

degree of linear polarization after the threshold energy followed by a steady decrease was apparent in the intermediate coupling calculations for He-like Fe ion reported by M. K. Inal et al. [67] and in the distorted-wave calculations for several other He-like ions reported by K. J. Reed et al. [68]. It is found that the Breit interaction makes the degree of linear polarization decrease at given incident electron energies, and the contribution of the Breit interaction on the degree of linear polarization is more and more important with increasing of incident electron energy. For example, the Breit interaction even causes a change of the sign of the linear polarization for the Be-like Nd$^{56+}$, and Bi$^{79+}$ ions at about 4.5 and 3.5 times of the threshold energy, respectively. It is also found that the contribution of the Breit interaction on the degree of linear polarization is more and more important with increasing of atomic number at given incident electron energies, which is quite similar with the case in DR process [66]. However, an opposite trend is found for the EIE and DR spectra.

5. DR of highly charged iodine ions

Recently, the KLL DR spectra of open 2$l$ shell of highly charged ions has gained great attraction both in experiment and theory [69–72]. We have also studied such DR processes of highly charged carbon, argon, krypton, iodine, xenon, mercury and uranium [73–75]. As an example, here the results for highly charged iodine ions are shown below.

In Fig. 6, the theoretical DR spectra and Watanabe et al.’s experimental spectra [69] are presented. Where the theoretical DR resonant position was shifted
around 420 eV to match with the experimental result. Comparison of the present DR spectra with the EBIT experiment shows a good agreement for both the amplitude of the cross section and the line shape.

Table 1. Total DR resonant strengths (10$^{-19}$ cm$^2$ eV) of He-like to C-like iodine ions in the KLL resonance region. Experimental uncertainties are listed in parentheses.

| Iodine ions | Theory | Experiment |
|-------------|--------|------------|
|             | Our work [73] | Kavanagh [70] | Watanabe [69] | Kavanagh [70] | Zhang [72] |
| He-like     | 3.41   | 3.62       | 4.27(39)      | 3.62(22)      | 3.14       |
| Li-like     | 2.32   | 2.40       | 2.91(26)      | 2.51(18)      | 2.14       |
| Be-like     | 1.83   | 2.19       | 2.39(22)      | 2.03(20)      | 1.77       |
| B-like      | 1.18   |            | 1.49(14)      |               | 1.12       |
| C-like      | 0.59   |            | 0.764(76)     |               | 0.58       |

Table 1 further lists the calculated total strengths for KLL DR processes into He-like to C-like iodine ions. For comparison, several different theoretical and experimental results are also given. As shown in Table 1, the present calculated total KLL strengths for each different charged iodine ion are smaller than Watanabe's experimental result [69] in 2007 by about 20%, but only smaller than Kavanagh's latest experimental result [70] in 2010 by about 7.7%. In addition, the old experimental results of Watanabe et al. [69] were corrected further by Zhang et al. [76]. The corrected results agree very well with ours for Be-, B- and C-like ions.

6. REC in collision of U$^{89+}$ with N$_2$

Radiative electron capture (REC) is the most dominant electron-capture channel in fast encounters of heavy ions with light target atoms or molecules. If the kinetic energy
of the electron in the projectile system greatly exceeds the initial binding energy in the target atoms or molecules, one may disregard the latter, so that REC is equivalent to radiative recombination (RR) for highly charged projectiles with free electrons. In REC, the captured electron is removed from the target atoms or molecules and during the transfer the electron-projectile interaction is accompanied by the interaction with the electromagnetic field; thus photons are emitted during the capture. By using the RERR06 program, we have studied the RR process of the H- and Li-like uranium and highly charged gold [56–58]. As an example, here the results of the RR for Li-like uranium ions are shown below.

The present calculations are compared with the experimental spectra at ESR in GSI [77]. Fig. 7(a) shows the experimental spectra associated with the electron capture from the outgoing charge state of U^{88+} ion. In the figure, the observed radiation is dominated by the radiative electron capture (REC) into the L, M, and up to S shells of the projectile. The broader profile results from the distribution of the electron momentum projection along the direction of the projectile target N_2. The theoretical REC and the related RR spectra in the projectile frame are shown in Fig. 7(b) and (c).

From the Fig. 7, firstly, it is found that with decreasing photon energy the loosely bound electron in the target is captured into the L-shell, M-shell, and up to S-shell by the highly charged Li-like uranium. Secondly, the REC cross sections for capture into L-shell, M-shell, and up to S-shell decrease gradually, i.e. less probabilities for capture into higher shells. It also shows that the energies become closer to each other and approach to the ionization limit of the projectile. As seen in Fig. 7, a good agreement between the experimental and theoretical results is obtained when we considered the eight shells mentioned above, and the five marked peaks can be clearly designated by the dominant RR lines. Furthermore, the spectra for radiative cascades can also be simulated very well using the multi-step model [56].

7. Quantum interference between RR and DR processes

In principle, the entire photorecombination processes including RR and DR must interfere due to the same initial and final atomic states, where the two processes are not separated each other in practice. The two amplitudes, the RR under emission of a photon and the DR where the excited intermediate state is stabilized through radiative emission at identical energy, can interfere eventually.

In past decades, there are many theoretical works on providing an unified description of RR and DR, such as the unified treatment of RR and DR with coupled-channel analysis [78], R-matrix code based on the close-coupling equations [79] and an approach based on projection-operator and resolvent-operator methods [80–84] and so on.

Here, the interference effects between the direct and resonant photorecombination (i.e. radiative and dielectronic recombination) from the ground state 1s \(^{2}S_{1/2}\) of H-like Ar\(^{17+}\) ions via doubly excited 2s\(^{2}\) \(^{1}\)S\(_{0}\), 2s2p \(^{3}\)P\(_{0,1,2}\), \(^{1}\)P\(_{1}\) and 2p\(^{2}\) \(^{3}\)P\(_{0,1,2}\), \(^{3}\)D\(_{2}\), \(^{1}\)S\(_{0}\) resonances of He-like Ar\(^{16+}\) ions are presented in Fig. 8 by using Fano parameterization technique. As comparison, the individual spectra from RR and DR processes are also included. The results indicate that the interference effects are remarkable at some resonances and strongly influence on the intensity of the wing of nonresonant background in the photorecombination of H-like Ar\(^{17+}\) ions through the comparison between the final Fano and total RR-DR spectra. This interference effect
Figure 7. Projectile x-ray spectra for 98 MeV/u U\(^{89+}\) → N\(_2\) collisions (a) measured coincidence with electron capture (U\(^{88+}\)) [77], (b) REC spectra simulated by folding the initial electronic momentum distribution in the cross section for radiative recombination and (c) calculated RR cross sections to identify the contribution of the RR processes, including the relevant Doppler shift in (b) and (c). For comparison, the two spectra have been normalized to the maximum peak of the respective REC, and the spectra in the following sections have also been normalized in this way.

Figure 8. Theoretical RR, DR and the total cross sections for H-like Ar\(^{17+}\) ions via the 2\(l\)2\(l\)' resonances to the 1s2\(l\) of He-like Ar\(^{16+}\) ions.

...are expected to be observed in future experiment with a high resolution [85].
8. Conclusion

In summary, during recent years, some new programs, like REIE06 for electron impact excitation, RERR06 for radiative recombination and REDR06 for dielectronic recombination etc., have been developed in the frame of distorted wave approximation. By combining these programs with the widely used GRASP92/2K and RATIP packages, atomic/ionic structures and various collision dynamic cross sections can be treated uniformly to include the effects of relativistic, electron correlation and Breit interaction. As their application, the direct EIE process and the resonant EIE process of Ne-like ions, the Breit interactions on the EIE process of Be-like ions, DR of highly charged iodine ions, REC process of collision of U^{89+} with N\textsubscript{2} and the quantum interference between RR and DR have been studied in details. Good agreements between available experiments and other calculations were found. In addition, using these programs, resonance, polarization even interference effects can also be dealt.

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