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Dominance of the radiative cascades in the cross section and circular polarization of x-ray radiation

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Abstract

The radiative cascade typically appears as a somewhat small correction to the direct impact process. We demonstrate here, however, that for the longitudinally-polarized electron impact excitation of highly charged ions, radiative cascades may play a significant role that can change the cross section and circular polarization of the emitted x-ray radiation qualitatively. This conclusion is verified by taking the $1s^2$ $(J=0) \rightarrow 1s2s_{1/2}$ $(J=1)$ excitation of He-like Fe^{24+}, Ge^{30+}, Mo^{40+}, Ag^{45+}, and W^{72+} ions as examples. For these ions, the dominant cascade channels from high-lying levels 1 snp (n = 2, 3, 4, 5, 6) will strongly dominate the direct excitation process and greatly modify the $M_f = -1$ magnetic sublevel cross sections, as well as leading to a considerable change in the expected circular polarizations of the x-ray emission pattern.

Keywords: radiative cascades, circular polarization, cross section

1. Introduction

Apart from its fundamental importance, the polarization of x-ray radiation from highly charged ions undergoing collisions with an electron beam has practical implications in various kinds of plasmas [1, 2], in astrophysics, and in fusion devices. When compared with other observables, the polarization helps to reveal many details about both the dynamical process and the magnetic sublevel population, and, in fact, can provide new insight and a promising route for studying the *e–e* and *e–p* interactions in the presence of Coulomb fields [3–10].

An enormous amount of effort has been expended on studying the polarization properties of x-rays emitted from highly charged ions. Bostock *et al* [11] calculated the linear polarization of light emitted during the electron impact excitation (EIE) of Ba^+ ions using the relativistic convergent close-coupling method. Their results resolved the discrepancy between experimental and previous theoretical calculations. Reed *et al* [6] investigated relativistic effects on the linear polarization of radiation emitted from He-like and H-like ions and found that the nonrelativistic calculation fails to describe the polarization properties for high-*Z* ions at high energy. Chen *et al* [12] calculated the x-ray linear polarization resulting from the EIE of complex ions using the Breit–Pauli R-matrix method. They found the resonance effects in magnetic sublevel cross sections, which contribute to the energy dependence in the polarization. Fritzsche *et al* [13] demonstrated that the linear polarization of the x-ray radiation is very sensitive to the Breit interaction (BI). Dipti *et al* [14] reported a series of results for the polarization for tungsten ions using the fully relativistic distorted-wave (RDW) method. There are also many other publications on the polarization of the emitted x-ray radiation [15–25].

Up to now, most studies have concentrated on linear polarization, while little attention has been paid to circular polarization. As is known, the two polarizations are different parameters, with different definitions experimentally and different formulas theoretically. Compared with the linear polarization, the circular polarization of decay products following collisions provides a more detailed test of the theoretical methods and interactions in the collision dynamics [16]. However, due to the formidable experimental difficulties, quantitative information about circular polarization is still limited and far from satisfies the needs of practical applications. A systematic calculation of the circular polarization properties of the characteristic x-rays was attempted by Inal *et al* [15–17], and also, more recently, by us [19, 20]. In these studies, some higher-order physical effects such as BI and relativistic effects during the direct impact process were reported. Although cascade effects in the calculation were mentioned [15, 17], to our knowledge, there has been no systematic work regarding their contributions to the cross sections and circular polarization properties of x-ray radiation.

The purpose of the present work is to investigate the radiative cascade effects on the cross section and circular polarization of the emitted radiation through direct excitation of ions by a longitudinally-polarized electron beam, taking the $1s^2(J=0) \rightarrow 1s2s_{1/2}(J=1)$ excitation of highly charged He-like ions as an example. Usually, the radiative cascade is a correction to the direct impact process, and hence its contribution to the cross section/polarization is relatively small. For instance, Inal *et al* [18], Hakel *et al* [26], and Chen *et al* [27] calculated the $1s2s_{1/2}(J=1) \rightarrow 1s^2(J=0)$ transition line of He-like Fe^{24+} ions, and found that the cascade effects may create a small amount of linear polarization. Bostock *et al* [24] estimated that the cascade corrections lead to about 10% depolarization of the radiation for the Lyman-α_1 line of H-like Fe^{25+} ions. Wu *et al* [25] showed that the cascade cross section for the 3d → 5f excitation of Cu-like to Se-like gold ions is less than the direct cross section by almost four orders of magnitude. There are also many experimental reports regarding the cascade contributions to the EIE cross section of metastable levels [28, 29], where the contributions were found to be ⩽10%.

In this study, the longitudinally-polarized EIE cross sections and the circular polarization properties of the x-ray radiation for the $1s2s_{1/2}(J=1) \rightarrow 1s^2(J=0)$ transition line of He-like Fe^{24+}, Ge^{30+}, Mo^{40+}, Ag^{45+}, and W^{72+} ions are investigated using the fully RDW method [19, 23, 30], in which both the relativistic and the BI effects are considered. The cascade contributions from high-lying levels $1snp$ ($n = 2, 3, 4, 5, 6$) to the direct excitation and radiative de-excitation processes are discussed in detail. The rest of this paper is organized as follows. In section 2, a short description of the theoretical method is given. In section 3, the cascade effects on the magnetic sublevel cross sections and the circular polarization of the subsequent x-ray radiation are discussed. Finally, we conclude with a brief summary in section 4.

2. Theory

2.1. Cross section

The RDW method, which is used for calculating the direct longitudinally-polarized EIE cross sections, has been described in detail in our previous paper [20]. Here, only an additional brief description of the method is presented. In [20] the collision matrix element is given by

$$R(\gamma_i, \gamma_f) = \left\langle \Psi_{\gamma_f} \right| \sum_{p,q,p<q}^{N+1} \left(V_C + V_B\right) \left| \Psi_{\gamma_i} \right\rangle, \tag{1}$$

in which V_C/V_B denotes the Coulomb/BI operator, and $\Psi_{\gamma_i}/\Psi_{\gamma_f}$ denotes the initial/final state wave-functions of the impact system, expressed as [30]

$$\Psi_{\gamma_t} = \frac{1}{(N+1)^{1/2}} \sum_{p=1}^{N+1} (-1)^{N+1-p} \sum_{M_t,m} C\left(J_t j M_t m; JM\right) \times \Phi_{\beta_t J_t}\left(x_p^{-1}\right) u_{\kappa m \varepsilon}(x_p), \tag{2}$$

Here $\Phi_{\beta_t J_t}$ (t = i, f) are the target-ion wave functions, generated using the atomic structure package GRASP92 [31], and $u_{\kappa m\varepsilon}$ is the Dirac spinor for a continuum electron, produced by the component COWF of the RATIP package [32]. x_p/x_p^{-1} denotes the space and spin coordinates of the electron p/other electrons than p.

For low-density plasmas ($Ne \leqslant 10^{-16} cm^{-3}$), the excitation cross section σ, taking account of radiative cascade, can be written as [18, 24]

$$\sigma\left(\beta_i J_i M_i - \beta_f J_f M_f\right) = \sigma_{dir}\left(\beta_i J_i - \beta_f J_f M_f\right) + \sigma_{cas}\left(\beta_i J_i - \beta_f J_f M_f\right) \tag{3}$$

in which σ_{dir} is the direct excitation cross section, σ_{cas} is the cascade cross section, given by [18, 24]

$$\sigma_{cas}\left(\beta_i J_i - J_f M_f\right) = \sum_{M_k} \sigma_{dir}\left(\triangle_i J_i - \triangle_k J_k M_k\right) \times \left(C^{J_f 1 J_k}_{M_f M_k - M_f M_f}\right)^2 \times \sum_{\triangle_k, J_k} R\left(\triangle_k J_k - \triangle_f J_f\right) \tag{4}$$

where $R(\triangle_k J_k - \triangle_f J_f)$ is the branching ratio for the level-to-level transition. In the present work, we only consider the electric dipole cascade transitions. Magnetic dipole and quadrupole transitions are neglected because they have very small branching ratios for the level-to-level transitions.

2.2. Circular polarization of x-ray emission

For the decay from the $J = 1$ to the $J = 0$ level, the maximum degree of circular polarization $P_c(\theta = 0)$, given by [17], is

$$P_c(\theta = 0) = \frac{I_{\sigma^+} - I_{\sigma^-}}{I_{\sigma^+} + I_{\sigma^-}} = \frac{\sigma_1 - \sigma_{-1}}{\sigma_1 + \sigma_{-1}}, \tag{5}$$

in which σ_1/σ_{-1} is the $M_f = 1/M_f = -1$ magnetic sublevel cross section. Furthermore, the angular distribution of the circular polarization $P_c(\theta)$, given by [15], is

$$P_c(\theta) = \frac{2(\sigma_1 - \sigma_{-1}) cos\,\theta}{2\sigma_0\, sin^2\,\theta + (\sigma_1 + \sigma_{-1})\left(1 + cos^2\,\theta\right)} \tag{6}$$

where σ_0 is the $M_f = 0$ magnetic sublevel cross section, and θ the angle between the incident electron beam and the observation direction.

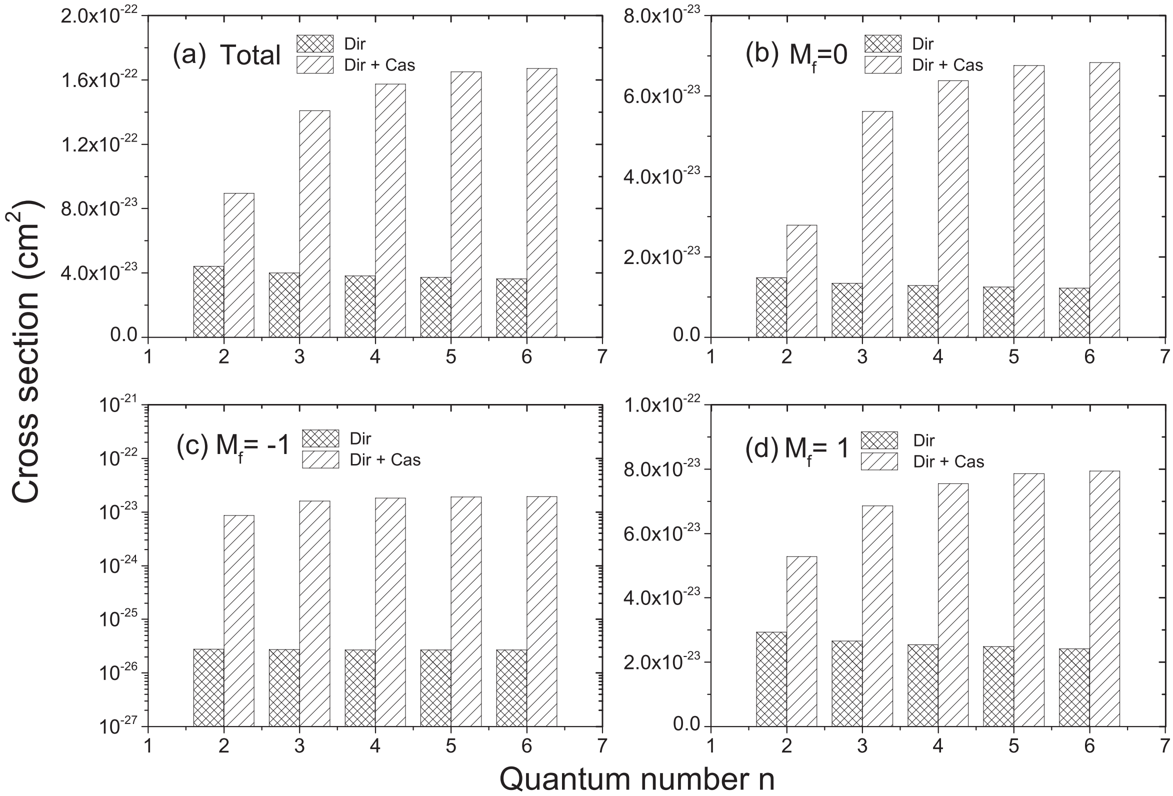

Figure 1. Longitudinally-polarized EIE cross sections from the ground state to the individual magnetic sublevels of the excited state $1s2s_{1/2}$ ($J = 1$) of highly charged He-like Fe^{24+} ions as a function of the quantum number n. Dir represents the direct results without cascade contributions, and Dir + Cas the results with the latter included. Here, the incident energy is 7870, 8290, 8485, 8590, and 8700 eV for 1 snp, $n = 2$, 3, 4, 5, and 6, respectively.

3. Results and discussion

We first investigate the longitudinally-polarized EIE and radiative de-excitation processes of He-like Fe^{24+} ions. An accuracy check of our method (taking He-like Fe^{24+} ions as an example) has been described in our previous work [20], so it is not performed here. In figure 1, the cross sections from the ground state $1\,s^2$ ($J = 0$) to the magnetic sublevels of the $1\,s_{1/2}2\,s_{1/2}$ ($J = 1$) level for longitudinally polarized EIE of He-like Fe^{24+} ions are displayed, and both the direct and cascade cross sections are included. In this figure, the cascade contributions from the different high-lying 1 snp ($n = 2$, 3, 4, 5, 6) levels can be clearly identified. It can be seen that the cascades from the 1 snp ($n = 2$, 3, 4) levels dominate the total cross section, while the contributions of the $n = 5$ and 6 levels are relatively small. This is to be expected, because lower levels have relatively larger excitation cross sections. For example, for an incident energy ranging from 6700 eV (threshold energy) to 7870 eV, the 1s2p levels dominate the cascade contributions and enhance the total cross section to $\geqslant$ 102% compared with the direct excitation. For the energy range from 7881 to 8290 eV (threshold for the $n = 4$ singly excited states), the radiative cascades from 1s3p levels are turned on. These effects on the total cross section are found to be $\geqslant$ 250%. For the energies at 8485, 8590, and 8700 eV, the cascade contributions of the 1 snp ($n = 2$, 3, 4), 1 snp ($n = 2$, 3, 4, 5), and 1 snp ($n = 2$, 3, 4, 5, 6) levels are about 311, 342, and 358% of the total cross section, respectively. Moreover, from figure 1(a), we can see that the total cross section converges very quickly at a small quantum number n. However, with increasing incident energy, the convergence becomes much slower and levels up to $n = 6$ are needed when the energy is larger than 8700 eV. In principle, excitations up to a very large n will contribute to the cross section, yet in reality contributions from higher $n \geqslant 7$ prove to be trivial, due to the fact that their direct cross sections are very small. For example, according to our preliminary estimates, the cascade contributions of the 1 snp ($n = 2 \to 9$) and ($n = 2 \to 15$) levels are about 364% and 369% to the total cross section, respectively.

A similar remarkable cascade effect is also predicted for the $M_f = 0$ and 1 sublevel cross sections, as shown in figures 1 (b) and (d), respectively. The contributions of the 1 snp ($n = 2$), 1 snp ($n = 2$, 3), 1 snp ($n = 2$, 3, 4), 1 snp ($n = 2$, 3, 4, 5), and 1 snp ($n = 2$, 3, 4, 5, 6) levels to the cross sections are 80%, 158%, 197%, 217%, and 228% for the $M_f = 1$ sublevel, and are 88%, 317%, 396%, 438%, and 458% for the $M_f = 0$ sublevel, respectively. However, for the $M_f = -1$ sublevel (figure 1 (c)), there are some differences, that is, for the direct excitation process, the $M_f = -1$ sublevel only has a very small cross section and seems to be approximately constant, independent of the incident energy. The population ratios for $\frac{\sigma_1}{\sigma_{-1}}$ and $\frac{\sigma_0}{\sigma_{-1}}$ are about 1000 and 530 at an incident energy of 7870 eV (n = 2), respectively. When

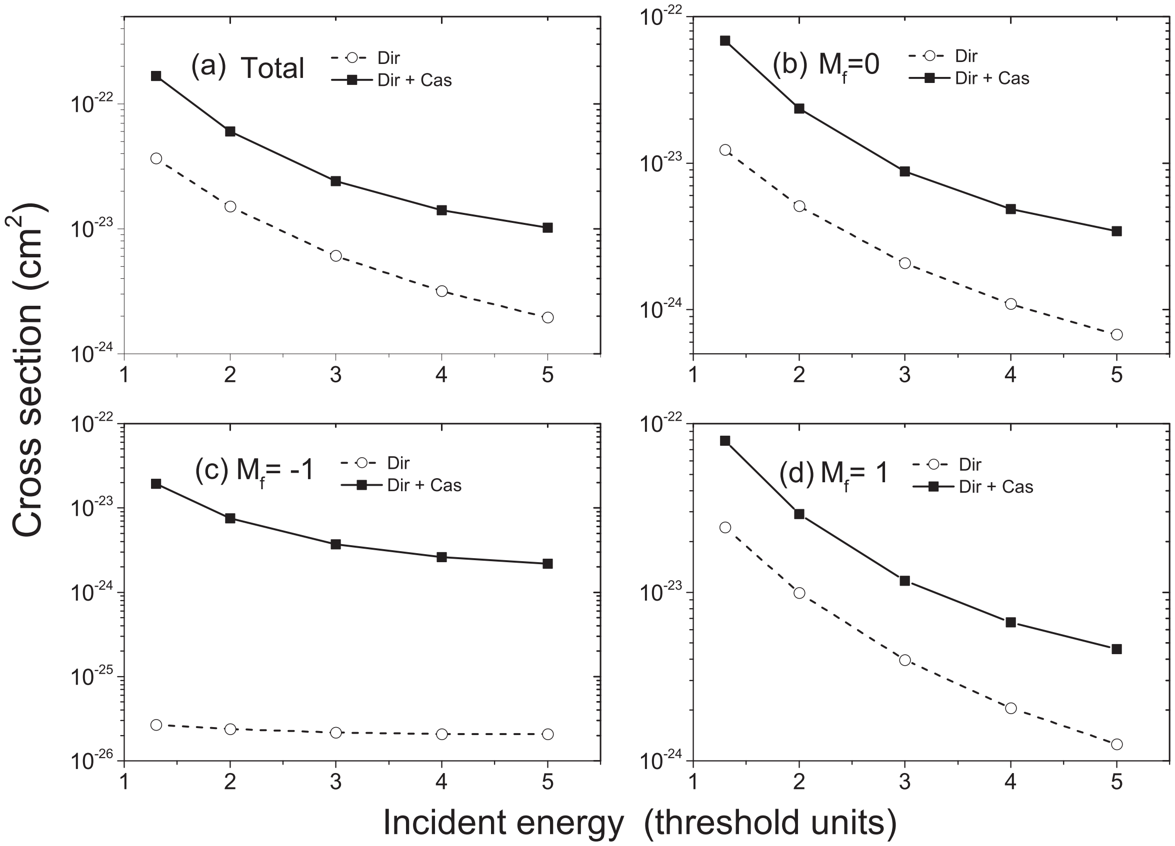

Figure 2. Longitudinally-polarized EIE cross sections from the ground state to the individual magnetic sublevels of the excited state $1s2s_{1/2}$ ($J = 1$) of highly charged He-like Fe^{24+} ions as a function of the incident energy. Here, Dir represents the direct results without cascade contributions, and Dir + Cas the results with the latter included.

the cascade process is considered, we find that its contribution to the cross sections of the $M_f = -1$ sublevel are very large. The cascade effects from the 1 snp ($n = 2$), 1 snp ($n = 2$, 3), 1 snp ($n = 2$, 3, 4), 1 snp ($n = 2$, 3, 4, 5), and 1 snp ($n = 2$, 3, 4, 5, 6) levels can alter the $M_f = -1$ cross section by as much as a factor of 310, 590, 670, 700, and 720, respectively. The population ratio for $\frac{\sigma_1}{\sigma_{-1}}$, due to the cascade, is found to be close to 6/4, which is much smaller than the ratio 1000/900 due to direct excitation at the incident energy of 7870 eV (n = 2)/8700 eV (n = 6).

Figure 2 shows the cross sections for longitudinally polarized EIE of He-like Fe^{24+} ions as a function of incident energy (in threshold units). In the calculations, the cascade contributions from high-lying 1 snp ($n = 2$, 3, 4, 5, 6) levels are included. Obviously, both the cross sections decrease monotonically in the same way as the incident energy increases. They decrease rapidly (slowly) near the threshold (higher-energy) region. The cascade effects on the $M_f = -1$ sublevel cross sections are very large, while for the total and $M_f = 1$ and 0 sublevel cross sections they are relatively small.

To discuss the cascade effects on the radiative de-excitation process, in figure 3, we show the cascade effects from the different high-lying 1 snp($n = 2$, 3, 4, 5, 6) levels on the circular polarization of x-ray radiation for the $1s_{1/2}2s_{1/2}$ ($J = 1$) → $1s^2$($J = 0$) line of He-like Fe^{24+} ions. For the decay following direct excitation, this transition line has a large

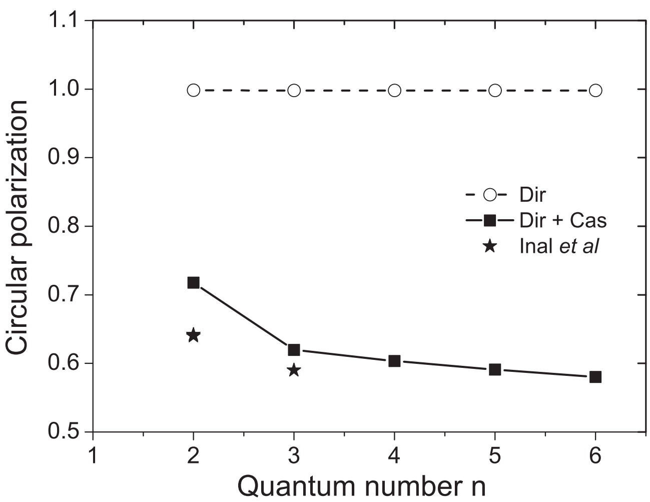

Figure 3. Circular polarization of the $1s2s_{1/2}$ ($J = 1$) → $1\,s^2$ ($J = 0$) line of He-like Fe^{24+} ions as a function of the quantum number n. Here, Dir represents the direct results without cascade contributions, and Dir + Cas the results with the latter included. The stars represent the semirelativistic results obtained by Inal *et al* [15].

value, is completely circularly polarized, and is approximately independent of the incident energy. When cascade effects are included, we can see that the cascade from the 1 snp($n = 2$)/($n = 2$, 3) levels in the energy range below the $n = 3/n = 4$ excitation threshold may reduce the circular polarization to

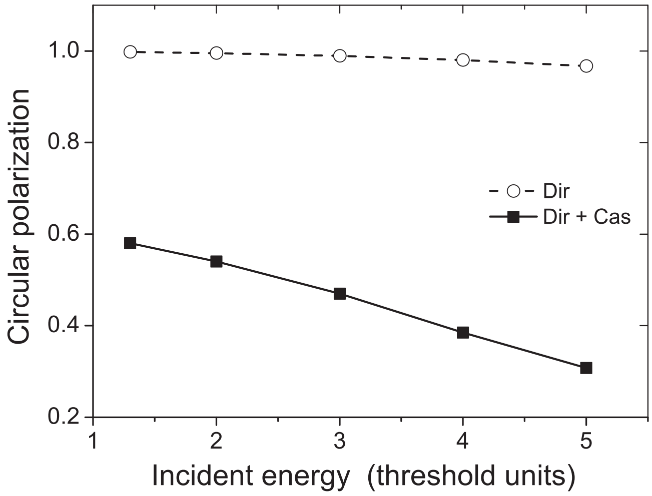

Figure 4. Circular polarization of the $1s2s_{1/2}$ $(J = 1) \rightarrow 1\,s^2$ $(J = 0)$ line of He-like Fe^{24+} ions as a function of the incident energy. Here, Dir represents the direct results without cascade contributions, and Dir + Cas the results with the latter included.

0.71/0.62. These results are about 10% larger than those of Inal *et al* [15], who used the semirelativistic method with cascades from the levels $n = 2$ and 3. The reason for these differences may be due to the relativistic effects in the structure calculation and the BI effects in the scattering calculation. As the energy increases, the cascades from high-lying $1\,snp(n = 2, 3, 4)$, $(n = 2, 3, 4, 5)$, and $(n = 2, 3, 4, 5, 6)$ levels are turned on, which will further reduce the circular polarization to 0.58, 0.55, and 0.53, respectively.

Figure 4 shows the circular polarization for longitudinally polarized EIE of He-like Fe^{24+} ions as a function of incident energy. In the calculation, the cascade contributions from high-lying $1\,snp$ $(n = 2, 3, 4, 5, 6)$ levels are included. It is obvious that this reduces the circular polarization, which decreases very slowly as the energy increases for the direct process, but decreases rapidly with inclusion of the cascade process. The effect on the circular polarization of $1s_{1/2}2s_{1/2}$ $(J = 1) \rightarrow 1\,s^2(J = 0)$ line is about 46%/70% at twice/five times the threshold energy. Furthermore, to illustrate these effects more clearly, figures 5 (a) to (d) show the θ-dependence of the circular polarization at an incident energy of 2, 5, 10, and 20 times the threshold energy, respectively. Obviously, the differences between the results with and without cascade effects included become increasingly pronounced as θ tends to 0^0 or 180^0. At 20 times the threshold energy, the cascade effects will decrease the circular polarization to nearly zero.

For other He-like ions, a general phenomenon is that the cascade process makes a relatively large contribution to the direct longitudinally-polarized EIE and radiative de-excitation processes. In figure 6, we show the circular polarizations with and without the cascade contribution as a function of incident energy for He-like Ge^{30+}, Mo^{40+}, Ag^{45+}, and W^{72+} ions.

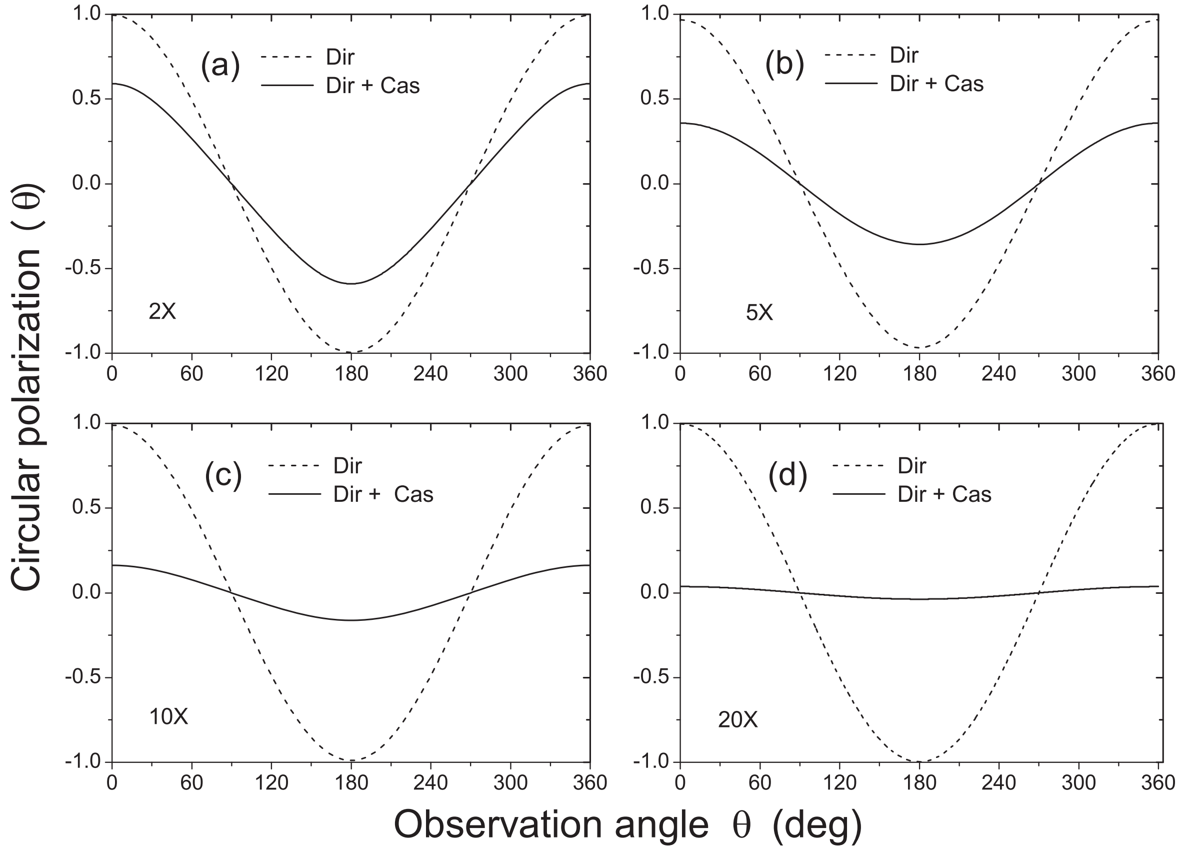

Figure 5. Angular distribution of the circular polarization for the $1s2s_{1/2}$ $(J = 1) \rightarrow 1s^2$ $(J = 0)$ line of He-like Fe^{24+} ions as a function of the observation angle for incident energies of: (a) 2, (b) 5, (c) 10, and (d) 20 times the threshold energy X. Here, Dir represents the direct results without cascade contributions, and Dir + Cas the results with the latter included.

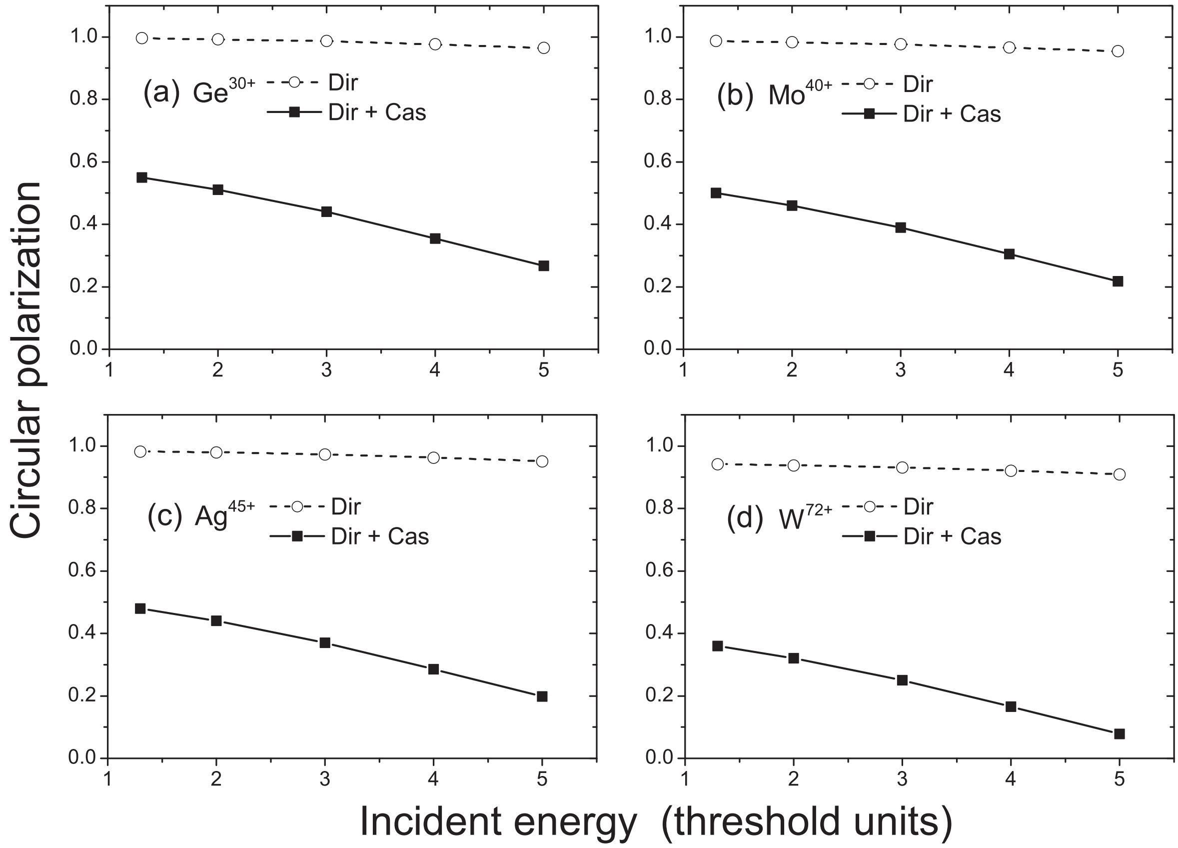

Figure 6. The same as in figure 4, but for He-like Ge^{30+}, Mo^{40+}, Ag^{45+}, and W^{72+} ions.

The effects can be easily seen for all the ions. Without the cascade contributions, the circular polarization is stabilized to a value of 0.98, and is nearly constant for all He-like ions from Fe^{24+} to W^{72+} ions, independent of the specific ion. When the cascade is included, the polarization decreases rapidly in the same manner as the incident energy increases. As the ionization state increases from Fe^{24+}, at four times the threshold energy the cascade effects on the circular polarization are 63.6%, 68.4%, 70.0%, and 82.1% for Ge^{30+}, Mo^{40+}, Ag^{45+}, and W^{72+} ions, respectively.

In the above calculations, we only considered the dominant cascade channels 1 s*np* ($n = 2, 3, 4, 5, 6$) levels. We did not include the cascade contributions from other excited states. Such levels may affect the cross section and circular polarization, and, thus bring into question the accuracy of the present longitudinally-polarized EIE cross section. However, after a preliminary estimate, we concluded that the contributions from the other (double) excited states are very small compared with their direct cross sections. Moreover, in some cases, the resonant EIE and the hyperfine structure may become significant in the calculation of the direct cross sections and circular polarization properties. For example, in the high temperature coronal plasma our RDW approach may work for excitations to low energy levels, because resonances make little contribution in this case. But, then resonances are likely to be important for highly excited levels. According to our preliminary calculations, in the present work, the resonance mainly comes from relatively high levels (1 s*nln*'*l*', *n*, *n*' $\geqslant 3$). The total resonance corrections to the polarization of the interest line are small when compared with the total cascade corrections. Estimating these physical effects is beyond the scope of this study and further calculations will be done in future work.

4. Summary

The detailed longitudinally-polarized EIE cross section and circular polarization of x-ray radiation for the $1s2s_{1/2}(J = 1) \rightarrow 1s^2(J = 0)$ transition line of He-like Fe^{24+} ions have been investigated theoretically using a fully RDW method. The cascade effects from high-lying 1 s*np* ($n = 2, 3, 4, 5, 6$) levels on the cross section and circular polarization, as well as the angular distribution of subsequent x-ray emission, have been discussed. Our results show that, for the longitudinally-polarized EIE of highly charged ions, the radiative cascades from the high-lying excited levels will strongly dominate the direct impact excitation and greatly enhance the cross section, as well as lead to a substantial change in the circular polarization of the radiation. This is a general phenomenon, and we demonstrate this conclusion by investigating the circular polarization of He-like ions such as Fe^{24+}, Ge^{30+}, Mo^{40+}, Ag^{45+}, and W^{72+} ions. For example, for the excitation of Fe^{24+} ions, the cascades can increase the total, $M_f = 1$, 0, and -1 sublevel cross sections by about 102%, 80%, 88%, and 31000%, respectively, at an incident energy of 7870 eV (n = 2). For the radiative de-excitation process, the cascade effects from high-lying 1 *snp* ($n = 2, 3, 4, 5, 6$) can reduce the circular polarization of x-ray radiation by about 46% and 70% at two and five times the threshold energy, respectively. We hope that the present results will stimulate interest in unidirectional spin-polarized electron collision experiments. We also hope that such strong effects will become feasible in experiments by measuring either the excitation cross sections or the circular polarization properties of the emitted x-ray radiation.

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