

Influence of Breit interaction on the polarization of radiation following inner-shell electron-impact excitation of highly charged berylliumlike ions

Zhong-Wen Wu, Jun Jiang, and Chen-Zhong Dong*

Key Laboratory of Atomic and Molecular Physics & Functional Materials of Gansu Province, College of Physics and Electronic Engineering, Northwest Normal University, Lanzhou 730070, People's Republic of China

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Electron-impact excitation cross sections from the ground state to the individual magnetic sublevels of the excited state $1s2s^22p_{1/2}J = 1$ for highly charged berylliumlike ions have been calculated by using a fully relativistic distorted-wave (RDW) method. The degrees of linear polarization of the corresponding radiations are obtained. It is found that the Breit interaction makes the linear polarization of radiations decrease, and this character becomes more evident with increasing of incident electron energy. For a given energy in threshold units, the linear polarization without the Breit interaction included increases very slowly as the atomic number increases, however, the linear polarization with the Breit interaction included decreases rapidly. These characteristics are very different from the conclusions for the linear polarization of the same radiations but formed by the dielectronic recombination process [Phys. Rev. Lett. **103**, 113001 (2009)], in which the Breit interaction makes the linear polarization increase, and the linear polarization with the Breit interaction included increases with increasing of the atomic number.

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I. INTRODUCTION

When the highly charged ions are excited by an electron beam or more generally by electrons with an anisotropic velocity distribution, the excited state populations for the magnetic sublevels are in a nonstatistical way. Then, the radiations emitted from these unequally populated sublevels are polarized to a lower level. The degree of linear polarization depends on the extent of deviation from the statistical populations of excited magnetic sublevels. So the degree of linear polarization can provide the information on both the incident electrons and excitation dynamics, based on which an important diagnostic tool has been developed to describe the electron anisotropy in laboratory and astrophysical plasmas. This innovative diagnostic tool has been successfully applied to laser produced plasmas [1–6], solar plasmas [6–8], Z pinches [9–12], and vacuum sparks [13].

During the last several decades, the degree of linear polarization of x-ray emission from highly charged ions colliding with an electron beam has been extensively investigated, both experimentally and theoretically. Henderson *et al.* [14] measured the degree of linear polarization of the x-ray emission for the heliumlike scandium ion. Later, some other experimental measurements were also published [15–24]. At the aspect of theoretical calculations, Y. Itikawa *et al.* [25] have studied the degree of linear polarization for the heliumlike Li, O, and the limit $Z \rightarrow \infty$ ions with a distorted-wave method. M. K. Inal *et al.* [26–31] have reported the degree of linear polarization for the heliumlike Sc, Fe, and lithiumlike Fe ions as well as for the sodiumlike Fe and U ions with the use of a distorted-wave method. T. Kai *et al.* [32–35] have investigated the degree of linear polarization for the magnesiumlike S, Ar, and Ca ions as well as for the heliumlike Be, C, O, Cl, Fe, Kr, Xe, and Cu ions by using Breit-Pauli R -matrix method.

Z. Q. Wu *et al.* [36] have calculated the degree of linear polarization for the heliumlike Ti, Fe, and U ions as well as for the lithiumlike Ti ion by a fully relativistic distorted-wave method. L. Sharma *et al.* [37] have studied the degree of linear polarization of the $ns_{1/2} - np_{1/2}$ and $ns_{1/2} - np_{3/2}$ resonance transitions for the singly charged $Mg^+(n = 3)$, $Ca^+(n = 4)$, $Zn^+(n = 4)$, $Cd^+(n = 5)$, and $Ba^+(n = 6)$ ions with the use of a fully relativistic distorted-wave theory. We [38] have calculated the degree of linear polarization of the magnetic quadrupole line of neonlike Ba ion by using a fully relativistic distorted-wave program. As we know, the relativistic effects and Breit interaction are very important for highly charged ions; they can significantly affect the cross sections and collision strengths for excitation to the specific magnetic sublevels. K. J. Reed *et al.* [39] have studied the relativistic effects on the degree of linear polarization for the highly charged hydrogenlike and heliumlike Si, Ti, Mo, Ba, Au, U, and the limit $Z \rightarrow \infty$ ions with a distorted-wave code, and M. H. Chen *et al.* [40] have investigated the relativistic effects on the degree of linear polarization for the hydrogenlike F, Ti, Ni, Mo, and U ions using the multiconfiguration Dirac-Fock model. They found that the degree of linear polarization of the resulting radiation is independent of atomic number Z in the nonrelativistic limit, but when the effects of relativity are taken into account, the polarization becomes markedly Z dependent. C. J. Fontes *et al.* [41] have calculated collision strengths for excitation of heliumlike Fe and Xe ions from the ground level to the specific magnetic sublevels of the excited states $1s2s^3S_1$, $1s2p^3P_1$, $1s2p^1P_1$, and $1s2p^3P_2$ for various electron-impact energies by using a relativistic distorted-wave method. It was found that the effect of inclusion of the generalized Breit interaction is very large for the Xe^{52+} ion and is even non-negligible for the Fe^{24+} ion. C. J. Bostock *et al.* [42] have calculated the degree of linear polarization of the Lyman- α_1 x-ray line emitted by the hydrogenlike Ti^{21+} , Ar^{17+} , and Fe^{25+} ions excited by the electron-impact process with the recently formulated relativistic convergent close-coupling

*dongcz@nwnu.edu.cn

(RCCC) method. They found that account of Breit relativistic corrections is important to resolve the discrepancy between experiment and theoretical calculations.

Recently, S. Fritzsche *et al.* [43] have investigated the Breit interaction on the degree of linear polarization of the x-ray emission radiated from the transition $1s2s^22p_{1/2}J = 1 \rightarrow 1s^22s^2J = 0$ for the highly charged berylliumlike I, Nd, Ho, W, Bi, and U ions following dielectronic recombination process, which can be described schematically by

$$\begin{aligned} \varepsilon e + 1s^22s &\rightarrow 1s2s^22p_{1/2}(J = 1) \\ &\rightarrow 1s^22s^2(J = 0) + h\nu. \end{aligned} \quad (1)$$

They found that the Breit interaction makes the degree of linear polarization of the corresponding lines increase, and the influence of the Breit interaction on the polarization becomes more and more remarkable with increasing of atomic number.

In this work, for the same transition line of the berylliumlike Mo^{38+} , Nd^{56+} , and Bi^{79+} ions but formed by inner-shell electron-impact excitation process, namely,

$$\begin{aligned} \varepsilon e + 1s^22s^2 &\rightarrow 1s2s^22p_{1/2}(J = 1) + \varepsilon' e \\ &\rightarrow 1s^22s^2(J = 0) + h\nu, \end{aligned} \quad (2)$$

the specific magnetic sublevel excitation cross sections and the degree of linear polarization of the transition line have been calculated by using a fully relativistic distorted-wave method. Additionally, the influence of the Breit interaction on the excitation cross sections as well as the degree of linear polarization have been discussed in detail. In Sec. II, the theoretical method is described. In Sec. III, the magnetic sublevel cross sections and the degree of linear polarization of the corresponding lines are discussed. Finally, some brief conclusions of the present work are given in Sec. IV.

II. THEORETICAL METHOD

In the present work, a recently developed fully relativistic distorted-wave (RDW) program REIE06 [38,44] is used to calculate the electron-impact excitation cross sections, where the target state wave functions are generated with the use of the atomic structure package GRASP92 [45] based on the multiconfiguration Dirac-Fock (MCDF) method, and the continuum electron wave functions are produced by the component COWF of the RATIP package [46] by solving the coupled Dirac equation in which the exchange effect between the bound and continuum electrons are considered. In this method, the z axis is chosen along the motion of the incident electron, and then the z component of the incident electron orbital angular momentum is zero, namely $m_i = 0$. In this case the electron-impact excitation cross section of the target ion from the initial state $\beta_i J_i M_i$ to the final state $\beta_f J_f M_f$ can be represented as [47,48]

$$\begin{aligned} &\sigma_{\varepsilon_i}(\beta_i J_i M_i - \beta_f J_f M_f) \\ &= \frac{2\pi a_0^2}{k_i^2} \sum_{l_i, l'_i, j_i, j'_i, m_{s_i}, l_f, j_f, m_f} \sum_{J, J', M} (i)^{l_i - l'_i} [(2l_i + 1) \\ &\quad \times (2l'_i + 1)]^{1/2} \exp[i(\delta_{\kappa_i} - \delta_{\kappa'_i})] C\left(l_i \frac{1}{2} m_{l_i} m_{s_i}; j_i m_i \right) \end{aligned}$$

$$\begin{aligned} &\times C\left(l'_i \frac{1}{2} m'_{l'_i} m_{s'_i}; j'_i m'_i\right) C(J_i j_i M_i m_i; J M) \\ &\times C(J_i j'_i M_i m_i; J' M) C(J_f j_f M_f m_f; J M) \\ &\times C(J_f j'_f M_f m_f; J' M) R(\gamma_i, \gamma_f) R(\gamma'_i, \gamma'_f), \end{aligned} \quad (3)$$

where the subscripts i and f refer to the initial and final states, respectively; ε_i is the incident electron energy in Rydberg; a_0 is the Bohr radius; C s are Clebsch-Gordan coefficients; R s are the collision matrix elements; $\gamma_i = \varepsilon_i l_i j_i \beta_i J_i J M$ and $\gamma_f = \varepsilon_f l_f j_f \beta_f J_f J M$, J , and M are the quantum numbers corresponding to the total angular momentum of the impact system, target ion plus free electron, and its z component, respectively; β represents all additional quantum numbers required to specify the initial and final states of the target ion in addition to its total angular momentum J and z component M ; $m_{s_i}, l_i, j_i, m_{l_i}$, and m_i are the spin, orbital angular momentum, total angular momentum, and its z component quantum numbers, respectively, for the incident electron e_i ; δ_{κ_i} is the phase factor for the continuum electron; κ is the relativistic quantum number, which is related to the orbital and total angular momentum l and j ; k_i is the relativistic wave number of the incident electron, it is given by

$$k_i^2 = \varepsilon_i \left(1 + \frac{\alpha^2 \varepsilon_i}{4} \right), \quad (4)$$

and α is the fine-structure constant. It turns out that the $R(\gamma_i, \gamma_f)$ are independent of M ,

$$R(\gamma_i, \gamma_f) = \langle \Psi_{\gamma_f} | \sum_{p,q,p<q}^{N+1} (V_{\text{Coul}} + V_{\text{Breit}}) | \Psi_{\gamma_i} \rangle, \quad (5)$$

where Ψ_{γ_i} and Ψ_{γ_f} are the antisymmetric $N + 1$ electron wave functions for the initial and final states of the impact systems, respectively, V_{Coul} is the Coulomb operator, and V_{Breit} is the Breit operator, which can be given by [45]

$$\begin{aligned} V_{\text{Breit}} &= - \frac{\alpha_p \cdot \alpha_q}{r_{pq}} \cos(\omega_{pq} r_{pq}) \\ &+ (\alpha_p \cdot \nabla_p)(\alpha_q \cdot \nabla_q) \frac{\cos(\omega_{pq} r_{pq}) - 1}{\omega_{pq}^2 r_{pq}}, \end{aligned} \quad (6)$$

where α_p and α_q are the Dirac matrices, and ω_{pq} is the angular frequency of the exchanged virtual photon.

The degree of linear polarization of the radiation emitted without detecting the scattered electron is then defined by [49]

$$P = \frac{I_{\parallel} - I_{\perp}}{I_{\parallel} + I_{\perp}}, \quad (7)$$

where I_{\parallel} and I_{\perp} are the intensities of photons with electric vectors parallel and perpendicular to the electron beam direction, respectively. If we assume that electron-impact excitation is the dominant mechanism for populating the upper magnetic sublevels, the degree of linear polarization for radiation from the $J = 1$ to the $J = 0$ line is given by [49]

$$P = \frac{\sigma_0 - \sigma_1}{\sigma_0 + \sigma_1}, \quad (8)$$

where σ_0 and σ_1 are the electron-impact excitation cross sections from the ground state to the magnetic sublevels $m_f = 0$ and $m_f = 1$ of the excited state, respectively.

TABLE I. Excitation energies (eV) from the ground state $1s^2 2s^2 J = 0$ to the excited state $1s 2s^2 2p_{1/2} J = 1$ for the berylliumlike Mo^{38+} , Nd^{56+} , and Bi^{79+} ions. The rows labeled by R and RB stand for the values with only the Coulomb interaction included and the Coulomb-plus-Breit interaction included, respectively.

	Mo^{38+}	Nd^{56+}	Bi^{79+}
R	17840	37674	76267
RB	17812	37587	76015

III. RESULTS AND DISCUSSIONS

In the calculations of wave functions and energy levels for the initial and final states, we use the configurations $1s^2 2s^2$, $1s 2s^2 2p$, and $1s^2 2p^2$. The contributions from the quantum electrodynamics (QED) corrections are also taken into account. In the calculations of cross sections, the maximal partial $\kappa = 50$ is included in order to ensure convergence. For the Coulomb calculations (labeled by R), we just use the Coulomb excitation energies and the Coulomb operator for the electron-impact matrix elements. For the Coulomb-plus-Breit calculations (label by RB), the Breit interaction is included in the calculations of the excitation energies and the electron-impact matrix elements. In Table I, the excitation energies from the ground state $1s^2 2s^2 J = 0$ to the excited state $1s 2s^2 2p_{1/2} J = 1$ for the highly charged berylliumlike Mo^{38+} , Nd^{56+} , and Bi^{79+} ions are listed. In order to emphasize the contribution of the Breit interaction on the excitation energies, we display two kinds of results with and without the Breit interaction included, respectively. From the table we can find the Breit interaction reduces the excitation energy by 28 eV, 87 eV, and 252 eV for the berylliumlike Mo^{38+} , Nd^{56+} , and Bi^{79+} ions, respectively, that is, the influences of the Breit interaction on the excitation energy are about 0.16%, 0.23%, and 0.33% for these highly charged ions, respectively. It is clear that the influence of the Breit interaction on the excitation energies for higher Z ions is more important.

For explaining the accuracy of the present calculations, the present calculated cross sections for excitation from the ground state to the magnetic sublevels of the excited states $1s 2s^2 2p_{1/2} J = 1$, $1s 2s^2 2p_{3/2} J = 1$, and $1s 2s^2 2p_{3/2} J = 2$

for the berylliumlike Mo^{38+} ion at incident electron energy of 20 keV are listed in Table II along with the available results [50]. In the calculations of the nonrelativistic cross sections, we select the speed of light 10000 a.u. [51] instead of the default value 137.036 a.u. in the subprogram RSCF92 of the main program GRASP92 [45] and our relativistic distorted-wave (RDW) program REIE06 [38]. By comparing the excitation cross sections in the nonrelativistic and relativistic cases (labeled by NR and R), we can find that the agreement is excellent for the two theoretical results. From the table we can also find that the influences of the relativistic effect and the Breit interaction on the cross sections for excitation to the different excited states are different. The influences of the relativistic effect on the cross sections for excitation to the $1s 2s^2 2p_{1/2} J = 1$ and $1s 2s^2 2p_{3/2} J = 1$ are very large. For example, the cross section for the magnetic sublevel $m_f = 0$ of the state $1s 2s^2 2p_{1/2} J = 1$ is altered by as much as a factor of 7, while the contributions of the Breit interaction on the cross sections are relatively small.

The total cross sections for the berylliumlike Mo^{38+} , Nd^{56+} , and Bi^{79+} ions are displayed in Fig. 1. It is found that both the total cross sections with and without the Breit interaction included decrease monotonically by the same pattern, each with increasing of incident electron energy; they decrease rapidly near the threshold energy and decrease slowly within a higher energy region. It is also found that the Breit interaction makes the total cross sections increase at all given incident electron energies.

Figure 2 shows the influence of the Breit interaction on the cross sections for excitation to the magnetic sublevels of the excited state $1s 2s^2 2p_{1/2} J = 1$ for the berylliumlike Mo^{38+} , Nd^{56+} , and Bi^{79+} ions. In the case of including only the Coulomb interaction, the cross sections for excitation to the sublevel $m_f = 0$ are significantly larger than the cross sections for the sublevels $m_f = \pm 1$ at given incident electron energies for the berylliumlike Mo^{38+} , Nd^{56+} , and Bi^{79+} ions. This character is quite similar with the conclusions of the electron impact excitation process for several heliumlike ions studied by K. J. Reed *et al.* [39]. In this case, the cross sections for excitation to the sublevel $m_f = 0$ increase within the energy range of about 1.8 times of the threshold energy before starting to decrease at higher incident electron energies, while

TABLE II. Total and magnetic sublevel cross sections (barns) for excitation from the ground state $1s^2 2s^2 J = 0$ to the magnetic sublevels of the excited state $1s 2s^2 2p_{1/2} J = 1$, $1s 2s^2 2p_{3/2} J = 1$, and $1s 2s^2 2p_{3/2} J = 2$ for the berylliumlike Mo^{38+} ion, the impact electron energy is 20 keV. The rows labeled by NR, R, and RB refer to the nonrelativistic, relativistic, and relativistic-plus-Breit interaction values, respectively.

Excited state	m_f	NR [50]	NR[Our]	R [50]	R[Our]	RB[Our]
$1s 2s^2 2p_{1/2} J = 1$	0	1.56	1.55	10.20	10.21	10.10
	± 1	5.09	5.01	6.83	6.78	7.39
	Total	11.74	11.58	23.86	23.78	24.87
$1s 2s^2 2p_{3/2} J = 1$	0	41.60	40.46	30.20	29.30	27.34
	± 1	9.83	9.60	8.40	8.16	7.73
	Total	61.26	59.66	47.00	45.62	42.81
$1s 2s^2 2p_{3/2} J = 2$	0	6.27	6.17	6.31	6.16	6.97
	± 1	5.09	5.02	5.15	5.04	5.16
	± 2	1.56	1.54	1.68	1.65	1.67
	Total	19.57	19.28	19.97	19.54	20.64

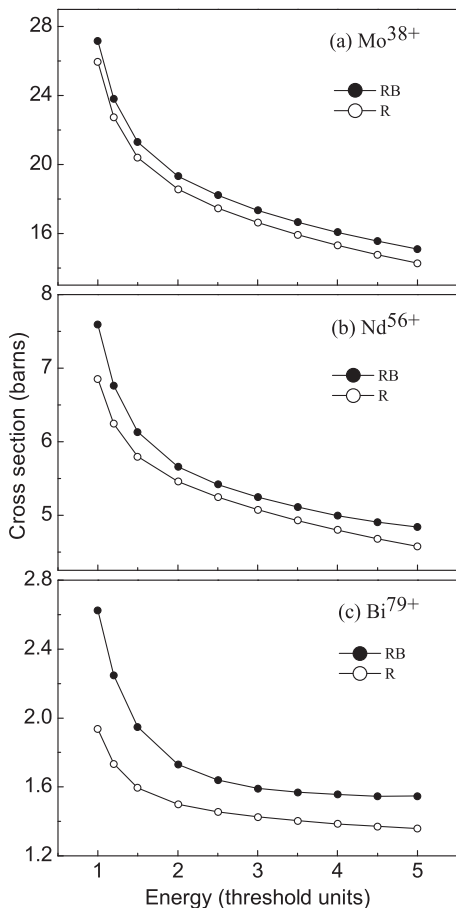


FIG. 1. Total electron-impact excitation cross sections (barns) for excitation from the ground state $1s^2 2s^2 J = 0$ to the excited state $1s 2s^2 2p_{1/2} J = 1$ for the berylliumlike Mo^{38+} , Nd^{56+} , and Bi^{79+} ions as functions of incident electron energy in threshold units. R represents the values with inclusion of only the Coulomb interaction, and RB represents the ones with the Breit interaction included.

the cross sections for excitation to the sublevels $m_f = \pm 1$ always decrease with increasing of incident electron energy. When the Breit interaction is taken into account, it is found that the Breit interaction makes the cross sections for excitation to the sublevel $m_f = 0$ decrease, however, it makes the cross sections for excitation to the sublevels $m_f = \pm 1$ increase at given incident electron energies for the berylliumlike Mo^{38+} , and Nd^{56+} ions, and the contributions from the Breit interaction become more and more evident with increasing of incident electron energy. But for the berylliumlike Bi^{79+} ion, there are some differences. For example, the two curves of cross sections for the sublevel $m_f = 0$ with and without the Breit interaction included cross each other at about 1.7 times the threshold energy. The cross sections for the sublevel $m_f = 0$ with the Breit interaction included always decrease with increasing of incident electron energy.

In Fig. 3, we show the degree of linear polarization as functions of incident electron energy for the berylliumlike Mo^{38+} , Nd^{56+} , and Bi^{79+} ions. Both the degrees of linear polarization with and without the Breit interaction included increase sharply with increasing of incident electron energy before starting to decrease at the higher energy region.

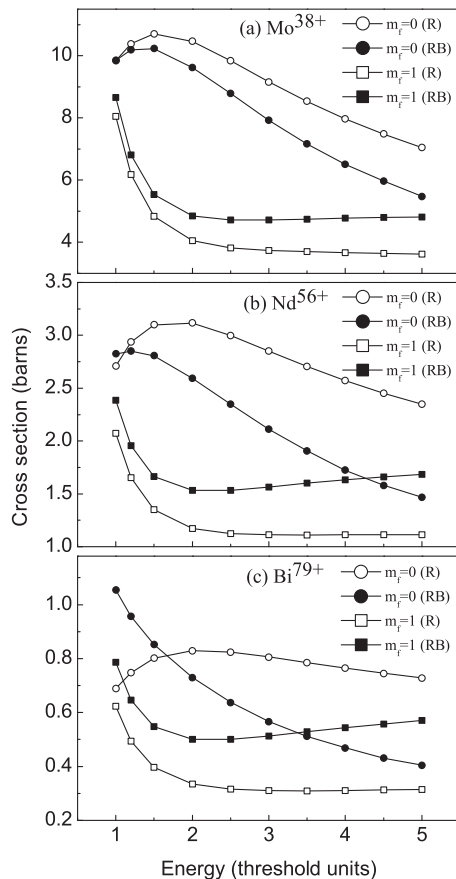


FIG. 2. Cross sections (barns) for electron-impact excitation from the ground state $1s^2 2s^2 J = 0$ to the specific magnetic sublevels $m_f = 0$ and $m_f = \pm 1$ of the excited state $1s 2s^2 2p_{1/2} J = 1$ for the berylliumlike Mo^{38+} , Nd^{56+} , and Bi^{79+} ions as functions of incident electron energy in threshold units. R represents the values with inclusion of only the Coulomb interaction, and RB represents the ones with the Breit interaction included.

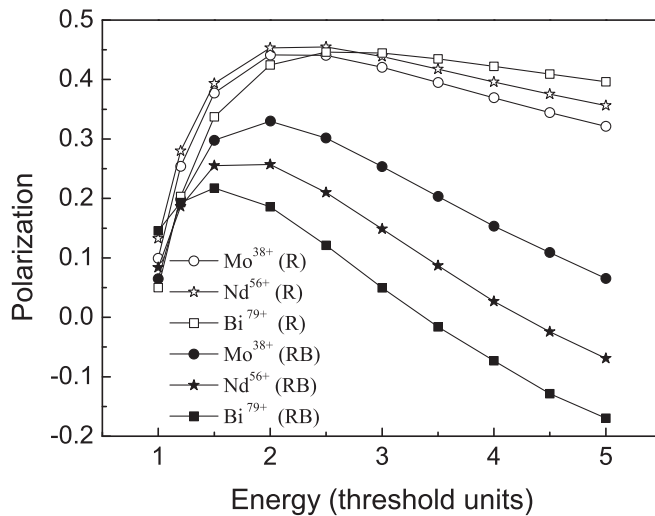


FIG. 3. The degree of linear polarization of the transition line $1s 2s^2 2p_{1/2} J = 1 \rightarrow 1s^2 2s^2 J = 0$ for the berylliumlike Mo^{38+} , Nd^{56+} , and Bi^{79+} ions as functions of incident electron energy in threshold units. R represents the values with inclusion of only the Coulomb interaction, and RB represents the ones with the Breit interaction included.

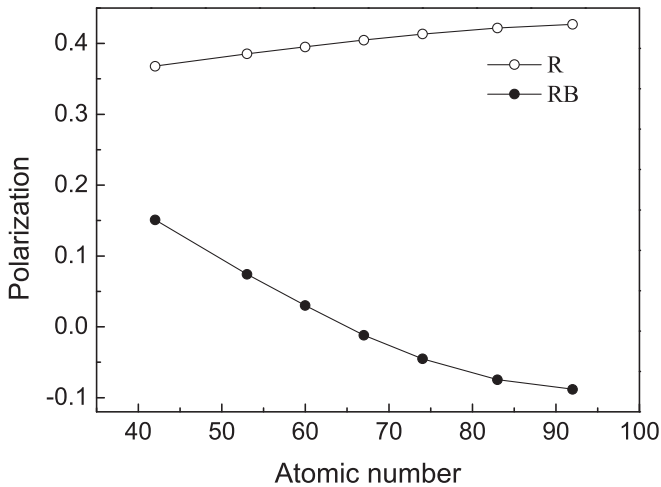


FIG. 4. The degree of linear polarization of the transition line $1s2s^22p_{1/2}J = 1 \rightarrow 1s^22s^2J = 0$ for the berylliumlike ions as functions of atomic number at incident electron energy is four times of threshold energy. R represents the values with inclusion of only the Coulomb interaction, and RB represents the ones with the Breit interaction included.

When the incident electron energies are greater than about 2 times of the threshold energies, the degree of linear polarization without the Breit interaction included decreases very slowly, however, the degree of linear polarization with the Breit interaction included decreases rapidly. This same pattern of an increase in the degree of linear polarization after the threshold energy followed by a steady decrease was apparent in the intermediate coupling calculations for heliumlike Fe ion reported by M. K. Inal *et al.* [26] and in the distorted-wave calculations for several other heliumlike ions reported by K. J. Reed *et al.* [39]. 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 berylliumlike Nd^{56+} , and Bi^{79+} ions at about 4.5 and 3.5 times the threshold energy, respectively. The reason can be seen clearly from the Fig. 2(b) and Fig. 2(c), that is, the cross sections for excitations to the sublevels $m_f = 0$ and $m_f = \pm 1$ with the Breit interaction included cross each other at about 4.5 and 3.5 times the threshold energy for the berylliumlike Nd^{56+} , and Bi^{79+} ions, 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 the atomic number at given incident electron energies.

In order to illuminate the dependence of the degree of linear polarization on the atomic number at given incident electron

energy more clearly, the degrees of linear polarization with and without the Breit interaction included as functions of the atomic number at 4 times the threshold energy are displayed in Fig. 4. It is found that the Breit interaction makes the degree of linear polarization decrease for all of the berylliumlike ions. It is also found that the degree of linear polarization with only the Coulomb interaction included increases very slowly as atomic number increases, and the degree of linear polarization with inclusion of the Coulomb plus Breit interaction decreases rapidly with increase of the atomic number. So the differences between the degrees of linear polarization with and without the Breit interaction included at the given energies become more evident with increasing of the atomic number. However, for the degree of linear polarization of the same lines but formed by the dielectronic recombination process [43], the situations are very different: The Breit interaction makes the degree of linear polarization increase, furthermore, the degree of linear polarization with the Breit interaction included increases with increasing of the atomic number.

IV. CONCLUSION

The cross sections for inner-shell electron-impact excitation to the magnetic sublevels $m_f = 0$ and $m_f = \pm 1$ of the excited state $1s2s^22p_{1/2}J = 1$ for highly charged berylliumlike ions are calculated by using a fully relativistic distorted-wave (RDW) method. These cross sections are employed in calculating the degree of linear polarization for the corresponding x-ray emission. The influence of Breit interactions on the cross sections and the degree of linear polarizations have been analyzed. It is found that the Breit interaction makes the cross sections for the magnetic sublevels $m_f = 0$ decrease, however, it makes the cross sections for the magnetic sublevels $m_f = \pm 1$ increase, and makes the total cross sections increase at given incident electron energies. It is also 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 becomes more and more evident with increasing of incident electron energy and atomic number, respectively.

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