Relativistic effects on angular distribution of Auger electrons emitted from Be-like ions following electron-impact excitation

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(Received 4 April 1994)

We have calculated the angular distribution functions for Auger electrons emitted from Be-like Mg, Fe, and Mo following $1s$-$2p$ excitation by electron impact. The calculations were carried out in intermediate coupling with configuration interaction using the relativistic distorted-wave and multiconfiguration Dirac-Fock methods. We found strong angular asymmetry for many transitions. We also found that relativistic effects can completely change the characteristics of the angular distribution for transitions which have many contributing partial waves, even for ions as light as Fe.

PACS number(s): 34.80.Kw, 32.80.Hd

I. INTRODUCTION

An atomic autoionizing state created by a beam of particles or photons is aligned in the direction of the incident beam if the total angular momentum of the excited state is greater than $\frac{1}{2}$. The x-ray or Auger electrons emitted by the aligned ions usually exhibit both anisotropic angular distribution and spin polarization [1]. For atoms with an innershell vacancy, the angular distribution of Auger electrons has been extensively investigated, both experimentally and theoretically [2]. The experimental work on the angular distribution of the resonant Auger electrons in rare gases [3,4] has revealed a large degree of angular anisotropy for many transitions. This unusually large angular anisotropy was later understood in light of theoretical work [5–8]. Furthermore, the effects of intermediate coupling have been found to alter the angular distribution parameters significantly for the M_{45} and N_{45} Auger transitions in Kr and Xe, respectively, [7,8].

Recently, we made a theoretical investigation of the relativistic effects on the polarization of line radiation emitted from He-like and H-like ions following electron-impact excitation [9]. We found that relativistic effects considerably alter the polarization and that the degree of polarization is markedly Z dependent. This contrasts sharply with the results from nonrelativistic calculations which indicate that the polarization should be independent of atomic number [10]. In this paper, we report calculations of the angular distribution of Auger electrons emitted from Be-like ions following $1s$-$2p$ excitation by electron impact. We made a systematic investigation of relativistic effects on the angular distribution of Auger electrons in Be-like ions of Mg, Fe, and Mo. We calculated the cross sections for excitation to the magnetic sublevels and the Auger anisotropy parameters in the nonrelativistic limit. We then repeated the calculations with relativistic effects included. The excitation cross sections were calculated using a relativistic distorted-wave code [11] and the Auger anisotropy parameters were evaluated using the multiconfiguration Dirac-Fock (MCDF) model [7,12,13].

II. THEORETICAL METHOD

In the present work, the resonant Auger decay is treated as a two-step process in which the interference between the resonant and direct ionization channels is ignored. As a result, the angular distribution parameter of the Auger electrons can be written as a product of two factors: the alignment parameter which depends on the ionization mechanism and the Auger decay anisotropy parameter which is related to the dynamics of the Auger decay [7,8,14]. Since the j-j coupling scheme is the natural coupling scheme for the relativistic atomic structure calculation, we employed this scheme in the basis functions and in the derivation of the angular-distribution function. The intermediate coupling in the MCDF method can be implemented through configuration interaction.

For randomly oriented target atoms and unpolarized incoming particles, the angular distribution of the Auger electrons without detecting the spin polarization can be written as [7,15,16]

$$W(\theta)=\frac{W_0}{4\pi}\left[1+\sum_{\substack{L\geq 2\\ \text{even}}}\alpha_L A_{L0}P_L(\cos\theta)\right]. \tag{1}$$

Here, α_L is the Auger anisotropy parameter and A_{L0} is a statistical tensor with rank L and zero projection in Z axis describing the alignment of the decaying ion; W_0 is the total Auger rate and θ is the angle between the Auger electrons and the incident electron beam. The alignment parameter A_{L0} is given by

$$A_{L0}=\left[\sum_{M_i} P(J_iM_i)(-1)^{J_i-M_i}[L,J_i]^{1/2} \times \begin{pmatrix} J_i & J_i & L \\ M_i & -M_i & 0 \end{pmatrix}\right]\left[\sum_{M_i} P(J_iM_i)\right]^{-1}, \quad (2)$$

where $P(J_iM_i)$ is the cross section for excitation to the M_i magnetic sublevel of the autoionizing state with total angular J_i.

The Auger-decay anisotropy parameter α_L in Eq. (1) is the characteristics of a particular Auger transition, and can be expressed as [7,14]

$$\alpha_L=\sum_{\kappa,\kappa'}(-1)^{J_i+J_f-1/2}(i)^{(l-l')}\cos(\delta_\kappa-\delta_{\kappa'})[l,l',j,j',L,J_i]\begin{pmatrix} l' & l & L \\ 0 & 0 & 0 \end{pmatrix}\begin{Bmatrix} j & j' & L \\ l' & l & \frac{1}{2} \end{Bmatrix}\begin{Bmatrix} J_i & J_i & L \\ j' & j & J_f \end{Bmatrix} \times \langle J_fjJ_i\|V\|J_i\rangle\langle J_fj'J_i\|V\|J_i\rangle^* \left[\sum_{\kappa}|\langle J_fjJ_i\|V\|J_i\rangle|^2\right]^{-1}. \quad (3)$$

Here, $\kappa=(l-j)(2j+1)$ is the relativistic quantum number; l and j are the orbital and total angular momenta of the continuum electron; δ_κ is the phase shift; J_i and J_f are the total angular momenta of the initial excited state and the final bound state reached by Auger decay, respectively; $\langle J_fjJ_i\|V\|J_i\rangle$ is the reduced Auger matrix element and $[a,b,c,\cdots]=[(2a+1)(2b+1)(2c+1)\cdots]$ in Eqs. (2) and (3). The summation over κ in Eq. (3) includes the summations over l and j.

III. NUMERICAL CALCULATIONS

For a Be-like ion, the excitation-autoionization process via the $1s$-$2p$ excitation can be described schematically by

$$e+1s^22s^2\rightarrow 1s2s^22p+e\rightarrow 1s^22l+e+e\ . \quad (4)$$

The cross sections for excitation to the magnetic sublevels were calculated using a distorted-wave code developed by Zhang, Sampson, and Clark [11]. Configuration-interaction-type wave functions were used in the target structure calculations which were performed with a Dirac-Fock-Slater atomic structure code [17,18]. These codes can be used in a fully relativistic mode or in a nonrelativistic mode, and we made use of both of these modes in order to obtain the results necessary to study the relativistic effects. The calculated excitation cross sections were then used to compute the alignment parameter A_{L0} according to Eq. (2).

The Auger transition rates and reduced Auger matrix elements were evaluated from perturbation theory [12]. The energies and wave functions for bound states were calculated using the MCDF model with average-level scheme [12,13] in intermediate coupling with configuration interaction from the same complex. The continuum wave functions were generated by solving the Dirac-Fock equations in the final-state potential. The phase shifts in Eq. (3) were computed according to a procedure given by Zhang, Sampson, and Clark [11]. These reduced Auger matrix elements, Auger rates and phase shifts were then employed to calculate the Auger decay anisotropy parameters α_L according to Eq. (3). The corresponding nonrelativistic values were obtained by repeating the calculations with the velocity of light increased by a factor of a thousand to simulate the nonrelativistic limit.

IV. RESULTS AND DISCUSSION

We calculated the angular distribution parameters for the Auger transitions in Be-like Mg, Fe, and Mo following the $1s$-$2p$ excitation in collisions with a beam of electrons. In Table I we compare the relativistic and nonrelativistic cross sections for excitation from the ground state to magnetic sublevels for Mo^{38+} at an incident electron energy of 20 keV. While the cross sections for the $1s2s^22p$ $J=2$ states are only slightly changed by relativity, the cross sections for the $1s2s^22p$ $J=1$ states are altered by as much as a factor of 7.

In Table II, the alignment parameters A_{20} for Mg^{8+}, Fe^{22+}, and Mo^{38+} are listed. The alignment parameters are quite large ranging from -0.2 to -0.7 for Mo^{38+} in the relativistic case and 0.4 to -0.7 in the nonrelativistic values. As in the case of the excitation cross sections, the relativistic effects on the alignment parameters are quite important for the $1s2s^22p$ $J=1$ states but are rather small for the $1s2s^22p$ $J=2$ state. The higher-order alignment parameters A_{40} are three orders of magnitude smaller than A_{20} and are neglected in the present calculations.

TABLE I. Cross sections (barns) for excitation from the ground state to magnetic sublevels for Mo^{38+}. The incident electron energy is 20 keV. The rows labeled by R and N refer to the relativistic and nonrelativistic values, respectively.

Excited state		$m=0$	$m=1$	$m=2$
$1s2s^22p_{1/2}$ $J=1$	R	10.2	6.83	
	N	1.56	5.09	
$1s2s^22p_{3/2}$ $J=1$	R	30.2	8.40	
	N	41.6	9.83	
$1s2s^22p_{3/2}$ $J=2$	R	6.31	5.15	1.68
	N	6.27	5.09	1.56

TABLE II. The alignment parameters A_{20} for Mg^{8+}, Fe^{22+}, and Mo^{38+}. The incident electron energies are 5, 9, and 20 keV for Mg, Fe, and Mo, respectively. The columns labeled by R and N represent the results from the relativistic and nonrelativistic calculations, respectively.

	Mg^{8+}		Fe^{22+}		Mo^{38+}	
Excited state	R	N	R	N	R	N
$1s2s^22p_{1/2}\,J=1$	0.255	0.333	−0.062	0.427	−0.199	0.425
$1s2s^22p_{3/2}\,J=1$	−0.414	−0.408	−0.703	−0.712	−0.656	−0.733
$1s2s^22p_{3/2}\,J=2$	−0.395	−0.393	−0.499	−0.505	−0.485	−0.503

The effects of relativity on the Auger matrix elements can arise from changes in the energy, from shifts in wave functions, and from the Breit interaction. The net effect depends on the strengths and phases of each component and cannot be easily predicted. In Table III, the Auger-decay anisotropy parameters α_2 for Mg^{8+}, Fe^{22+}, and Mo^{38+} are compared. As in the case of resonant Auger transitions in neutral atoms [8], the Auger-decay anisotropy parameters are quite large for many transitions. In the nonrelativistic case, the α_2 values are very weakly dependent on atomic number Z. On the other hand, we note strong Z dependence for some transitions in the relativistic calculations. The effects of relativity drastically alter the α_2 values for transitions involving $1s2s^22p_{3/2}\,J=1$ initial state but have little influence on the $1s2s^22p_{3/2}\,J=2-1s^22l\,J=\frac{1}{2}$ transitions. For Auger transitions with only one contributing partial wave (e.g., $1s2s^22p_{3/2}\,J=2-1s^22s\varepsilon p_{3/2}$), the α_2 values are independent of the Auger matrix elements and phase shifts, and they are the same for all ions. For transitions with many contributing partial waves (e.g., $1s2s^22p_{3/2}\,J=1-1s^22p_{1/2}\varepsilon s,\varepsilon d_{3/2}$), the effects of relativity can change the α_2 values by an order of magnitude and can even change the sign of the α_2 values. These findings are consistent with the observations made for the resonant Auger transitions in neutral atoms [8].

In Figs. 1–7, the angular distribution functions $\overline{W}(\theta)\equiv 4\pi W(\theta)/W_0$ for relativistic and nonrelativistic cases are displayed as functions of angle θ. From these comparisons, the following observations can be made. (1) For the nonrelativistic case, the angular distributions show strong angular asymmetry for these transitions and are nearly independent of atomic number. (2) For transitions involving $1s2s^22p\,J=1$ states, the effects of relativity are significant. For example, the $1s2s^22p_{1/2}\,J=1-1s^22s$ transition for Fe^{22+} shows no angular dependence in the relativistic calculation but exhibits strong angular asymmetry in the nonrelativistic case. For the $1s2s^22p_{3/2}\,J=1-1s^22s$ transition in Fe^{22+} and Mo^{38+}, $\overline{W}(\theta)$ has a minimum at $\theta=90°$ in the nonrelativistic results but has a maximum in the relativistic results. (3) For the $1s2s^22p_{3/2}\,J=2-1s^22s$ transition, strong angular asymmetry is revealed, but the effects of relativity are rather trivial.

TABLE III. Auger-decay anisotropy parameters α_2 for Mg^{8+}, Fe^{22+}, and Mo^{38+}. Rows labeled by R and N represent the relativistic and nonrelativistic values, respectively.

Transition		Mg^{8+}	Fe^{22+}	Mo^{38+}
$1s2s^22p_{1/2}\,J=1-1s^22s$	R	0.706	0.695	0.703
	N	0.707	0.707	0.707
$1s2s^22p_{3/2}\,J=2-1s^22s$	R	−0.837	−0.837	−0.837
	N	−0.837	−0.837	−0.837
$1s2s^22p_{3/2}\,J=1-1s^22s$	R	−0.567	0.707	0.631
	N	−1.385	−1.414	−1.414
$1s2s^22p_{1/2}\,J=1-1s^22p_{1/2}$	R	−0.010	0.001	0.002
	N	−0.015	−0.011	−0.011
$1s2s^22p_{3/2}\,J=2-1s^22p_{1/2}$	R	−0.840	−0.854	−0.845
	N	−0.837	−0.837	−0.837
$1s2s^22p_{3/2}\,J=1-1s^22p_{1/2}$	R	−0.082	−0.205	−0.595
	N	−0.068	−0.051	−0.046
$1s2s^22p_{1/2}\,J=1-1s^22p_{3/2}$	R	0.120	0.117	0.141
	N	0.116	0.090	0.083
$1s2s^22p_{3/2}\,J=2-1s^22p_{3/2}$	R	−0.006	−0.009	−0.011
	N	−0.003	−0.002	−0.001
$1s2s^22p_{3/2}\,J=1-1s^22p_{3/2}$	R	−0.062	−0.023	−0.011
	N	−0.068	−0.051	−0.046

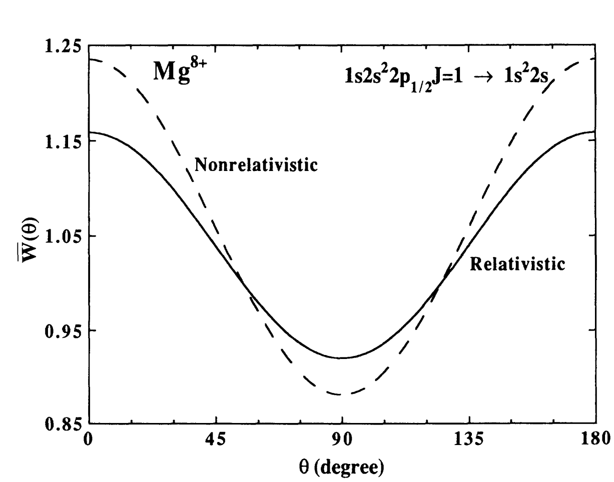

FIG. 1. Angular-distribution functions $\overline{W}(\theta)\equiv 4\pi W(\theta)/W_0$ for the $1s2s^22p_{1/2}\,J=1-1s^22s$ transition in Mg^{8+} as functions of θ. The solid curve indicates the relativistic results. The dashed curve represents the nonrelativistic values.

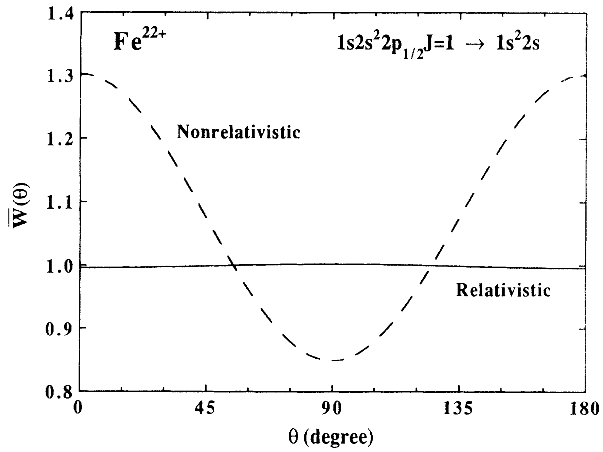

FIG. 2. The same as Fig. 1 but for Fe^{22+}.

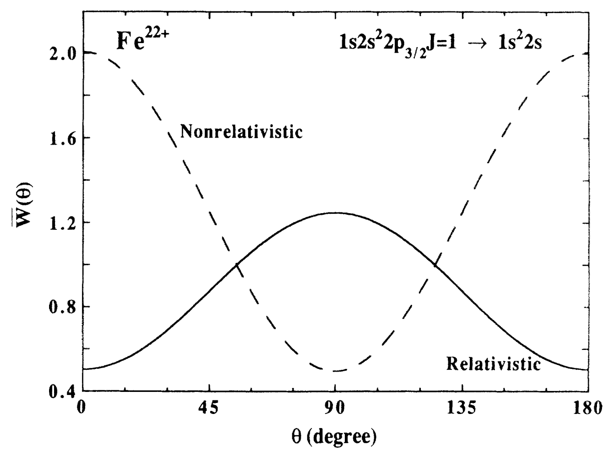

FIG. 5. The same as Fig. 4 but for Fe^{22+}.

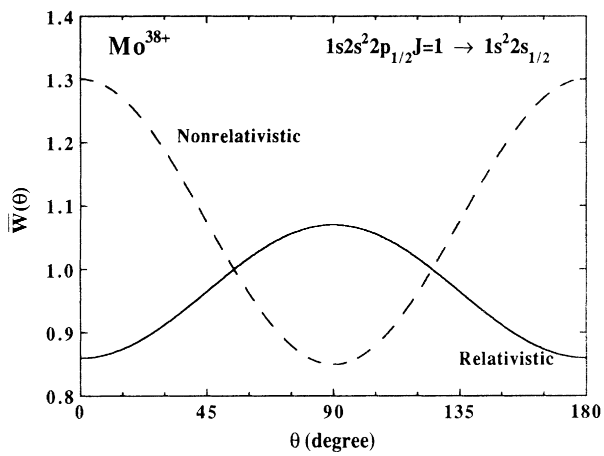

FIG. 3. The same as Fig. 1 but for Mo^{38+}.

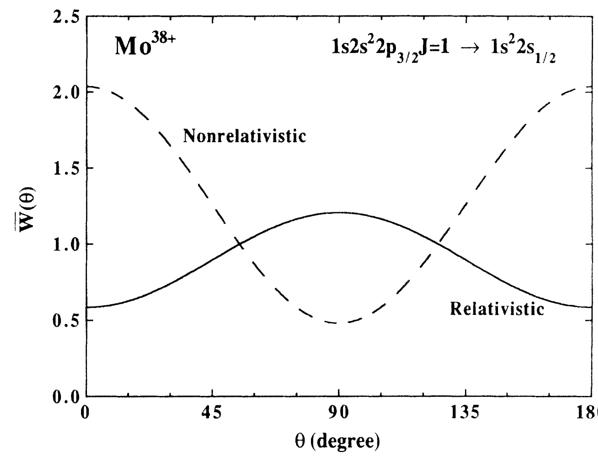

FIG. 6. The same as Fig. 4 but for Mo^{38+}.

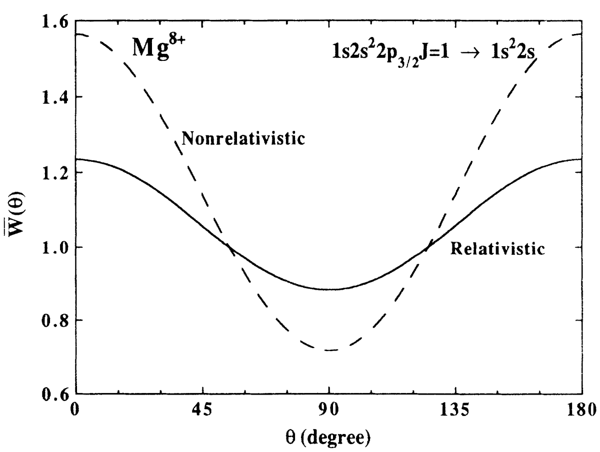

FIG. 4. Angular-distribution functions $\overline{W}(\theta)$ for the $1s2s^22p_{3/2}\,J=1-1s^22s$ transition in Mg^{8+} as functions of θ. The symbols are the same as in Fig. 1.

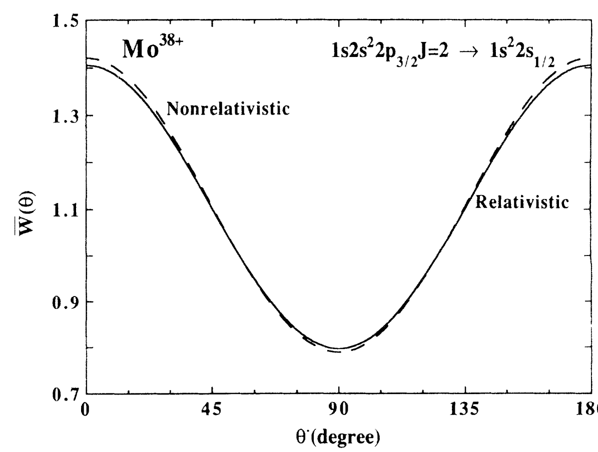

FIG. 7. Angular-distribution functions $\overline{W}(\theta)$ for the $1s2s^22p_{3/2}\,J=2-1s^22s$ transition in Mo^{38+} as functions of θ. The symbols are the same as in Fig. 1.

In summary, we have carried out multiconfiguration relativistic distorted-wave calculations for the angular distributions of Auger electrons emitted following $1s$-$2p$ excitation by electron impact for Mg^{8+}, Fe^{22+}, and Mo^{38+}. Strong angular asymmetry is found for many transitions. In the nonrelativistic limit, the angular distribution functions are independent of atomic number. We found, however, that the effects of relativity and intermediate coupling can completely alter the characteristics of the angular distribution for some transitions originating from the $1s2s^22p$ $J=1$ initial states.

ACKNOWLEDGMENTS

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

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