Effect of intermediate coupling on angular distribution of Auger electrons

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The Auger decay anisotropy parameter α_2 of angular distribution has been calculated for the M_{45}-NN transitions in Kr and M_{45}-NN and N_{45}-OO transitions in Xe atoms using the multiconfiguration Dirac-Fock model in intermediate coupling with configuration interaction. For transitions involving many contributing partial waves and leading to the strongly mixed final ionic states in intermediate coupling, the effects of relativity and spin-orbit interaction are found to be quite important for the calculations of α_2 values. The existing discrepancies between theory and experiment are largely removed by the present relativistic intermediate coupling calculations.

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I. INTRODUCTION

An atomic inner-shell vacancy created by a beam of particles or photons is aligned in the direction of the incident beam if the total angular momentum of the vacancy is greater than $\frac{1}{2}$. The x rays or Auger electrons emitted by the aligned ions usually exhibit anisotropic angular distribution and spin polarization [1]. The study of angular distribution and polarization of x rays or Auger electrons can provide more complete and fundamental information about the ionization and decay processes. Inner-shell ionization followed by Auger decay can be described as a two-step process if the post-collision interaction is neglected. 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 Auger decay dynamics.

In the past decade, many experiments [2–7] and theoretical works [2,8–14] were carried out to investigate the angular distribution and spin polarization of the Auger electrons. The most extensive theoretical calculations of Auger decay anisotropy parameter were done by Kabachnik and Sazhina [9,11] for many transitions with an initial $p_{3/2}$, $d_{3/2}$, or $d_{5/2}$ inner-shell vacancy in Kr and Xe atoms. These calculations were performed in *LSJ* coupling using the nonrelativistic Hartree-Slater (HS) wave function. Later, Kabachnik and co-workers extended their calculations to include the effect of many-electron correlations by using the random-phase approximation with exchange and the many-body perturbation theory (MBPT) [12]. Recently, a relativistic *jj* coupling calculation [13] was also performed by using the bound-state wave functions from Grant's multiconfiguration Dirac-Fock (MCDF) code [15].

Most of these existing theoretical calculations were carried out in *LSJ* coupling using hydrogenic, nonrelativistic Hartree-Fock (HF) or Hartree-Slater wave functions. The effect of intermediate coupling is usually ignored. At the present time, there still exist large discrepancies in the Auger decay parameter and polarization between different theoretical calculations and between theories and experiments.

In an attempt to resolve these discrepancies, we have carried out multiconfiguration Dirac-Fock [15,16] calculations of the Auger decay anisotropy parameter for the M_{45}-NN transitions in Kr and Xe atoms and N_{45}-OO transitions in xenon atoms. These calculations include the effects of relativity, intermediate coupling (IC), and configuration interaction. Nonrelativistic calculations in *LSJ* coupling were also performed for the purpose of comparisons with the results from the relativistic intermediate coupling calculations.

II. THEORY OF ANGULAR DISTRIBUTION OF AUGER ELECTRONS

For randomly oriented target atoms and unpolarized incoming particles or photons, the angular distribution of the Auger electrons can be obtained by multiplying the relative population $P(J_iM_i)$ of the magnetic sublevels of the atoms after ionization and the Auger decay probability $A(J_iM_i \rightarrow J_fM_f, \varepsilon\hat{\mathbf{k}}m_s)$ [14]:

$$W(\theta)=(2J_i+1)^{-1} \times \sum_{M_i} \sum_{M_f,m_s} P(J_iM_i)\,A(J_iM_i \rightarrow J_fM_f, \varepsilon\hat{\mathbf{k}}m_s)\ . \quad (1)$$

Here, J_iM_i and J_fM_f are the total and magnetic quantum numbers of the initial and final states, respectively; ε is the energy and m_s is the spin projection of the Auger electron; and θ indicates the angle between the direction $\hat{\mathbf{k}}$ of the Auger electron and the incident beam. Since the *jj* coupling basis set is the natural basis function for the relativistic intermediate-coupling calculation, the expression of Auger angular distribution is derived in terms of *jj* coupling scheme. Furthermore, we are only interested in the angular distribution. The spin polarization of the Auger electron is not treated here.

In the present work, the Auger transition probability is calculated from perturbation theory and the probability in a frozen-orbital approximation is given by [17]

$$A(J_iM_i \rightarrow J_fM_f, \varepsilon\hat{\mathbf{k}}m_s) = \frac{2\pi}{\hbar}|\Psi_f(J_fM_f,\varepsilon\hat{\mathbf{k}}m_s)|V|\Psi_i(J_iM_i)|^2 , \quad (2)$$

where Ψ_i and Ψ_f are the antisymmetrized many-electron wave functions and V is the two-electron interaction operator taken to be the Coulomb interaction. The outgoing Auger electron with definite energy ε and momentum $\mathbf{p}$ and spin can be written as superpositions of partial waves [18].

$$\phi^{(-)}_{\varepsilon\hat{\mathbf{k}}m_s} = \sum_{\kappa,m} i^l e^{-i\delta_\kappa}\Omega^+_{\kappa m}(\hat{\mathbf{p}})\chi_{sm_s}\phi_{\kappa m}(\mathbf{r}) \quad (3)$$

with

$$\phi_{\kappa m}(r) = \frac{1}{r}\begin{bmatrix} P_{\varepsilon\kappa}(r)\Omega_{\kappa m} \\ iQ_{\varepsilon\kappa}(r)\Omega_{-\kappa m}\end{bmatrix} \quad (4)$$

and

$$\Omega_{\kappa m} = \sum_{m_l,\mu} Y_{lm_l}(\theta,\varphi)\chi_{1/2\mu}\langle lm_l\tfrac{1}{2}\mu|l\tfrac{1}{2}jm\rangle . \quad (5)$$

Here, $\kappa=(l-j)(2j+1)$ is the relativistic quantum number; l and j are the orbital and total angular momentum of the continuum electron; δ_κ is the phase shift; $P_{\varepsilon\kappa}$ and $Q_{\varepsilon K}$ are the major and minor components of the radial wave functions which are normalized in energy.

After some algebra, the angular distribution without detecting the spin polarization can be written as [2,9]

$$W(\theta) = \frac{W_0}{4\pi}\left[1+\sum_{\substack{L\geq 2\\ \text{even}}}\alpha_L A_{L0}P_L(\cos\theta)\right] , \quad (6)$$

where the alignment parameter A_{L0} is given by

$$A_{L0} = \left[\sum_{M_i} P(J_iM_i)(-1)^{J_i-M_i}[L,J_i]^{1/2}\begin{pmatrix} J_i & J_i & L \\ M_i & -M_i & 0\end{pmatrix}\right]\left[\sum_{M_i}P(J_iM_i)\right]^{-1} \quad (7)$$

and the Auger decay anisotropy parameter α_L can be expressed as

$$\alpha_L = \sum_{\kappa,\kappa'}(-1)^{J_i+J_f-1/2}(-1)^{(l-l')/2}\cos(\delta_\kappa-\delta_{\kappa'})[l,l',j,j',L,J_i]^{1/2}\begin{pmatrix} l' & l & L \\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} j & j' & L \\ l' & l & \frac{1}{2}\end{Bmatrix}\begin{Bmatrix} J_i & J_i & L \\ j' & j & J_f\end{Bmatrix}$$

$$\times\langle J_fjJ_i||V||J_i\rangle\langle J_fj'J_i||V||J_i\rangle^*\left[\sum_\kappa|\langle J_fjJ_i||V||J_i\rangle|^2\right]^{-1} . \quad (8)$$

In Eqs. (6)–(8), W_0 is the total Auger decay probability per unit time, and θ is the polar angle with the incident beam direction chosen as the z axis; $P_L(\cos\theta)$ is the Legendre polynomial; $\langle J_fjJ_i||V||J_i\rangle$ is the reduced Auger matrix element; and

$$[a,b,c,\ldots]^{1/2} \equiv [(2a+1)(2b+1)(2c+1)\cdots]^{1/2} .$$

The summation over κ in Eq. (8) includes the summations over j and l. From Eq. (6), one can see that the angular distribution is axially symmetric and symmetric with respect to $\theta=90°$. For angular distribution to be anisotropic; the initial autoionizing state must be aligned. This can only occur for an ionic state with total angular momentum $J>\frac{1}{2}$ [2]. For an Auger transition with only one contributing partial wave, the anisotropy parameter is independent of phase shift and Auger radial matrix element [2].

The contribution to the angular distribution from $L\geq 4$ terms [Eq. (6)] is assumed to be small in the present work. Furthermore, if the inner-shell vacancy is created by photoionization, the L value is restricted to $L=2$ in the electric-dipole approximation. Hence, we will concentrate on the calculations of the Auger decay parameter α_2. The alignment parameter A_{20} will not be treated in this work.

III. NUMERICAL CALCULATIONS

In this work, we carried out relativistic intermediate-coupling calculations for the Auger decay parameter α_2 for the $M_{45}NN$ transitions of $_{36}$Kr and $_{54}$Xe and for the N_{45}-OO transitions of $_{54}$Xe. In the present MCDF calculations of reduced Auger matrix elements, an atomic state function for a state i with total angular momentum JM is constructed from the configuration state functions (CSF) denoted by $\phi(\Gamma_\lambda JM)$ [15]:

$$\Psi_i(JM) = \sum_{\lambda=1}^{n} C_{i\lambda}\phi(\Gamma_\lambda JM) . \quad (9)$$

Here n is the number of CSF's included in the expansion and $C_{i\lambda}$ are the mixing coefficients. The CSF functions are formed by taking linear combinations of Slater determinants of the Dirac bound-state orbitals which are similar to Eq. (4). The details for evaluation of reduced Auger matrix elements in the MCDF method have been presented in Ref. [16].

The energies and wave functions for bound states were calculated using the MCDF model with average-level scheme (MCDF-AL) [15]. In the MCDF-AL calculations, the orbital wave functions are obtained by minimizing the averaged energy of all the levels with equal

weight. The initial inner-shell vacancy states were calculated using a single configuration approximation. The final two-hole states were treated in intermediate coupling with configuration interaction from the same complex (e.g., all states from the double [*NN*] hole state were included in the same calculation). The mixing coefficients $C_{i\lambda}$ [Eq. (9)] were obtained by diagonalizing the energy matrix which includes Coulomb, transverse Breit interactions, and quantum-electrodynamic corrections [15].

The reduced Auger matrix elements were calculated using the bound-state wave functions corresponding to the initial hole state and the continuum wave functions generated by solving the Dirac-Fock equations in the final two-hole potential. The exchange interaction between the continuum and bound electrons is not taken into account. The phase shifts in Eq. (8) were computed according to a procedure outlined by Zhang, Sampson, and Clark [19]. The nonrelativistic values for α_2 in *LSJ* coupling were also obtained by repeating the MCDF calculations and increasing the velocity of light a thousandfold to achieve the nonrelativistic limit.

IV. RESULTS AND DISCUSSIONS

The Auger decay anisotropy parameter α_2 for the M_{45}-*NN* transitions of $_{36}$Kr, N_{45}-*OO*, and M_{45}-$N_{45}N_{45}$ transitions of $_{54}$Xe from the present work are compared with the previous theoretical predictions [11,12] and with experiments [4–7] in Tables I–III, respectively. In Table IV, the α_2 values from the present MCDF calculations for the M_{45}-N_1N_{45}, -$N_{23}N_{45}$, -$N_{23}N_{23}$, and -N_1N_{23} transitions of $_{54}$Xe are listed. In Tables I–IV, the final two-hole states are denoted by their dominant components in the *LSJ*-coupling basis functions which were obtained by coupling transformation. For the $J=2$ states in the ($N_{23}N_{45}$) and ($N_{45}N_{45}$) double-hole states of Xe (Tables III and IV), the spin-orbit mixing is rather severe. In order to provide unique identification, these states are also classified by their energies in ascending order.

The sensitivity of the α_2 values on the coupling scheme and atomic model can best be analyzed by classifying the Auger transitions into three different categories as stated by Kämmerling *et al.* [5]: (i) Auger transitions with only one partial wave permitted in any coupling scheme; (ii) Auger transitions with only one allowed partial wave in LS coupling but not in intermediate coupling; (iii) Auger transitions with several contributing partial waves in any coupling.

The Auger transitions leading to the final two-hole states with total angular momentum $J=0$ (e.g., M_{45}-$N_{23}N_{23}$ $^1S_0$, $^3P_0$; M_{45}-N_1N_{23} $^3P_0$) belong to the first category. The α_2 values of these transitions are independent of the dynamical properties of the Auger decay and can be considered as exactly known (e.g., $\alpha_2=-\sqrt{8/7}$ for M_5-$N_{23}N_{23}$ $^1S_0$ and -1 for M_4-$N_{23}N_{23}$ $^1S_0$). Hence, all the theoretical calculations give the same results for this class of transitions.

For the M_{45}-$N_{23}N_{23}$ $^3P_2$, M_{45}-$N_{45}N_{45}$ $^3P_2$, and N_{45}-$O_{23}O_{23}$ $^3P_2$ transitions, only one partial wave εd is allowed in *LS* coupling [category (ii)]. In *LSJ* coupling calculations, the contributions from the $\varepsilon d_{3/2}$ and $\varepsilon d_{5/2}$ partial waves are out of phase for transitions involving a $d_{3/2}$ initial hole state. This results in an exact cancellation and yields $\alpha_2=0$ [5]. A small nonzero α^2 value for

TABLE I. Auger decay anisotropy parameter α_2 for the M_{45}-*NN* transitions of $_{36}$Kr.

			Theory				
	Expt.		Present work		Kabachnik *et al.*		
Transition	a	b	IC	*LSJ*	HF[c]	MBPT[c]	HS[d]
M_5-$N_{23}N_{23}$ $^1S_0$			−1.069	−1.069			−1.069
M_5-$N_{23}N_{23}$ $^1D_2$	0.18±0.04		0.286	0.028			−0.099
M_5-$N_{23}N_{23}$ $^3P_0$			−1.069	−1.069			−1.069
M_5-$N_{23}N_{23}$ $^3P_1$			−0.742	−0.748			−0.748
M_5-$N_{23}N_{23}$ $^3P_2$	−0.31±0.06		−0.323	−0.382			−0.382
M_5-N_1N_{23} $^3P_2$		1.96±0.66	−0.762	−0.665	−0.63	−0.85	−0.622
M_5-N_1N_{23} $^3P_1$		1.74±0.83	−1.051	−1.002	−1.00	−1.03	−0.992
M_5-N_1N_{23} $^3P_0$			−1.069	−1.069			−1.069
M_5-N_1N_{23} $^1P_1$			−0.627	−0.704			−0.861
M_4-$N_{23}N_{23}$ $^1S_0$			−1.000	−1.000			−1.000
M_4-$N_{23}N_{23}$ $^1D_2$			0.154	0.026			−0.093
M_4-$N_{23}N_{23}$ $^3P_0$	−0.77±0.10		−1.000	−1.000			−1.000
M_4-$N_{23}N_{23}$ $^3P_1$			−0.817	−0.800			−0.800
M_4-$N_{23}N_{23}$ $^3P_2$	0.21±0.09		0.098	0.0			0.0
M_4-N_1N_{23} $^3P_2$		1.80±1.04	−0.865	−0.831	−0.82	−0.90	−0.807
M_4-N_1N_{23} $^3P_1$		1.79±1.03	−0.932	−0.833	−0.82	−0.92	−0.818
M_4-N_1N_{23} $^3P_0$			−1.000	−1.000			−1.000
M_4-N_1N_{23} $^1P_1$			−0.633	−0.658			−0.805

[a]From Ref. [5].
[b]From Ref. [4].
[c]From Ref. [12].
[d]From Ref. [11].

TABLE II. Auger decay anisotropy parameter α_2 for the N_{45}-OO transitions of $_{54}$Xe.

	Expt.		Theory				
			Present work		Kabachnik *et al.*		
Transition	KKS[a]	Carlson *et al.*[b]	IC	*LSJ*	HF[c]	MPBT[c]	HS[d]
N_5-$O_{23}O_{23}$ $^1S_0$	—[e]	—[e]	−1.069	−1.069			−1.069
N_4-$O_{23}O_{23}$ $^1S_0$	—[e]	—[e]	−1.0	−1.0			−1.0
N_5-$O_{23}O_{23}$ $^1D_2$	0.23±0.04		0.238	0.223			−0.592
N_5-$O_{23}O_{23}$ $^3P_1$	−0.77±0.17	−0.79	−0.736	−0.748			−0.748
N_5-$O_{23}O_{23}$ $^3P_0$	−1.07±0.10		−1.069	−1.069			−1.069
N_4-$O_{23}O_{23}$ $^1D_2$	0.05±0.06		0.086	0.210			−0.554
N_5-$O_{23}O_{23}$ $^3P_2$	−0.47±0.13		−0.257	−0.382			−0.382
N_4-$O_{23}O_{23}$ $^3P_1$	−0.73±0.11	−0.43	−0.831	−0.800			−0.800
N_4-$O_{23}O_{23}$ $^3P_2$	0.72±0.11	0.27	0.250	0.0			0.0
N_4-$O_{23}O_{23}$ $^3P_0$			−1.0	−1.0			−1.0
N_5-O_1O_{23} $^3P_0$			−1.069	−1.069			−1.069
N_4-O_2O_{23} $^3P_0$			−1.0	−1.0			−1.0
N_5-O_1O_{23} $^3P_1$			−1.064	−1.001	−0.96	−0.72	−0.986
N_4-O_1O_{23} $^3P_1$			−0.924	−0.862	−0.92	−0.88	−0.793
N_5-O_1O_{23} $^3P_2$			−0.738	−0.724	−0.81	−0.62	−0.570
N_4-O_1O_{23} $^3P_2$			−0.847	−0.845	−0.69	0.46	−0.792
N_5-O_1O_{23} $^1P_1$			−0.647	−0.750			−0.984
N_4-O_1O_{23} $^1P_1$			−0.683	−0.701			−0.920

[a]From Ref. [7].
[b]From Ref. [6].
[c]From Ref. [12].
[d]From Ref. [11].
[e]These lines were used to determine the alignment parameter in Ref. [7].

TABLE III. Auger decay anisotropy parameter α_2 for the M_{45}-$N_{45}N_{45}$ transitions of $_{54}$Xe.

Transition			Present work		Kabachnik *et al.*		
Initial	Final	Expt[a]	IC	*LSJ*	HF[b]	MBPT[b]	HS[c]
$^2D_{5/2}$	$^3F_2^{(1)}$		−0.222	0.0056	−0.02	−0.04	0.115
	$^3F_3$		0.331	0.332	0.32	0.30	0.412
	$^3F_4$	0.43±0.12	0.378	0.435	0.42	0.41	0.506
	$^1D_2^{(3)}$		−0.131	−0.178			−0.202
	$^3P_0$		−1.069	−1.069			−1.069
	$^3P_1$		−0.748	−0.748			−0.748
	$^3P_2^{(2)}$		−0.389	−0.382			−0.382
	$^1G_4$		−0.719	−0.685			−0.533
	$^1S_0$		−1.069	−1.069			−1.069
$^2D_{3/2}$	$^3F_2^{(1)}$		0.738	0.558	0.55	0.54	0.607
	$^3F_3$		0.432	0.430	0.42	0.40	0.493
	$^3F_4$		−0.826	−0.806	−0.82	−0.85	−0.608
	$^1D_2^{(3)}$		0.0503	−0.167			−0.189
	$^3P_0$		−1.0	−1.0			−1.0
	$^3P_1$		−0.799	−0.800			−0.800
	$^3P_2^{(2)}$		0.378	0.0			0.0
	$^1G_4$		−0.653	−0.640			−0.499
	$^1S_0$		−1.0	−1.0			−1.0

[a]From Ref. [4].
[b]From Ref. [12].
[c]From Ref. [11].

TABLE IV. Auger anisotropy parameter α_2 for the $M_{45}-N_{23}N_{45}$, $M_{45}-N_1N_{45}$, $M_{45}-N_{23}N_{23}$, and $M_{45}-N_1N_{23}$ transitions of $_{54}$Xe.

	Present theory			
	M_4		M_5	
Final state	IC	*LSJ*	IC	*LSJ*
$N_{23}N_{45}\ ^3F_2^{(3)}$	0.245	−0.159	−0.741	0.525
$^3F_3$	−0.162	−0.163	0.261	−0.145
$^3F_4$	−0.494	−0.488	−0.217	−0.223
$^1D_2^{(1)}$	0.587	0.723	0.212	0.773
$^3P_2^{(2)}$	0.528	0.839	−0.082 5	−0.740
$^3P_1$	−0.278	−0.913	−0.729	−0.740
$^3D_1$	0.088 7	0.804	−0.716	−0.739
$^3D_2^{(4)}$	0.758	0.758	−0.107	0.640
$^3D_3$	−0.203	−0.177	0.803	0.861
$^1P_1$	−0.124	−0.653	−0.691	−0.699
$^1F_3$	−0.173	−0.187	−0.229	−0.200
$N_1N_{45}\ ^3D_1$	0.0640	0.096 5	−0.998	−1.019
$^3D_2$	0.124	0.051 9	−0.210	−0.074 6
$^3D_3$	−0.822	−0.876	0.026 5	0.072 8
$^1D_2$	−0.221	−0.343	−0.366	−0.366
$N_{23}N_{23}\ ^3P_1$	−0.753	−0.800	−0.757	−0.748
$^3P_2$	−0.261	−0.001 2	−0.657	−0.382
$^1D_2$	−0.665	−0.714	−0.670	−0.763
$N_1N_{23}\ ^3P_1$	−0.335	−0.918	−0.893	−0.781
$^3P_2$	0.000 55	0.476	−0.713	−0.761
$^1P_1$	−0.832	−0.731	−0.826	−0.781

the $M_4N_{23}N_{23}\ ^3P_2$ transition in *LSJ* coupling in Xe atoms (see Table IV) is caused by the residual errors in the simulation of the nonrelativistic limit. The α_2 values for these transitions are very sensitive to the inclusion of the spin-orbit coupling. In fact, the contributions from εs and εg partial waves made possible by the spin-orbit interaction leads to nonzero results in α_2 for the $M_4-NN\ ^3P_2$ and $N_4-OO\ ^3P_2$ transitions (e.g., $\alpha_2=0.098$, 0.378, and 0.250 for the $M_4-N_{23}N_{23}\ ^3P_2$ in $_{36}$Kr, $M_4-N_{45}N_{45}\ ^3P_2$ and $N_4-O_{23}O_{23}\ ^3P_2$ in $_{54}$Xe, respectively). On the other hand, no strong cancellation occurs between contributions from $\varepsilon d_{3/2}$ and $\varepsilon d_{5/2}$ partial waves for the $M_5-NN\ ^3P_2$ and $N_5-OO\ ^3P_2$ transitions. Hence, the effect of spin-orbit coupling is much less significant for these transitions.

For transitions involving category (iii), such as $M_{45}-N_{23}N_{23}\ ^1D_2$, $M_{45}-N_{45}N_{45}\ ^3F_2$, $^1D_2$, and $N_{45}-O_{23}O_{23}\ ^1D_2$, many partial waves contribute to the calculations of Auger decay parameter in any coupling scheme. In addition, most of these final two-hole states are strongly mixed with the other $J=2$ states in the intermediate coupling. Thus, the α_2 values for this class of transitions can be significantly affected by the spin-orbit interaction. Some of these α_2 values change by more than a factor of 2 and some can even change sign (e.g., $\alpha_2=0.028$ in *LSJ* and 0.286 in IC coupling for the $M_5-N_{23}N_{23}\ ^1D_2$ in Kr; $\alpha_2=0.525$ in *LSJ* and −0.741 in IC for the $M_5-N_{23}N_{45}\ ^3F_2^{(3)}$ in Xe). Furthermore, the α_2 values for this category can be also quite sensitive to the choice of atomic model. As a result, different theoretical calculations can give quite different α_2 values in some cases, even if they are computed in the same coupling scheme. As an example, the present calculation in *LSJ* coupling using Hartree-Fock wave functions gives $\alpha_2=0.223$ for the $N_5-O_{23}O_{23}\ ^1D_2$ transition in Xe atom while the calculation done by Kabachnik *et al.* [11] using Hartree-Slater wave functions yields $\alpha_2=-0.592$.

For the Auger transitions with a pure final ionic state (e.g., $M_{45}-N_{23}N_{23}\ ^3P_1$ and $M_{45}-N_{45}N_{45}\ ^3F_3, ^3P_1$), the effects of relativity and spin-orbit coupling on the α_2 values are quite small in most cases (see Tables I–IV). The only exception in the present work is the α_2 value for the $M_4-N_1N_{23}\ ^3P_2$ transition in Xe. In the nonrelativistic *LSJ* coupling calculation, the Auger amplitude is dominated by the εp partial wave while the amplitude for εf partial wave is found to be as large as those for the εp partial wave in the relativistic intermediate-coupling calculation. The cancellation between the εp and εf amplitudes results in a very small α_2 value in the relativistic intermediate-coupling calculation.

From the comparisons made in Tables I–III, one can see that good agreement between the results from the present nonrelativistic calculations in *LSJ* coupling and the predictions from the HF model [12] has been attained. The agreement between the *LSJ* coupling results and the values from the HS calculations [11] is quite satisfactory except for a few cases that belong to category (iii). For the $N_4-O_{23}O_{23}\ ^1D_2$ and $N_5-O_{23}O_{23}\ ^1D_2$ transitions in Xe atoms, $\alpha_2=0.210$ and 0.223 from our nonrelativistic calculations while the HS model [11] yields

-0.554 and -0.592, respectively.

The α_2 values calculated by Lohmann [13] using the relativistic wave functions deviate considerably from the present MCDF intermediate-coupling results except for transitions leading to a sure final two-hole state or a state with total angular momentum $J=0$. These discrepancies are probably due to his use of jj coupling to describe the final two-hole states.

The Auger decay anisotropy parameters α_2 have recently been measured [4–7] for several transitions in Kr and Xe atoms by using either photon or electron impact. These experimental data have been found to disagree with the existing theoretical predictions [11,12] in many cases. These discrepancies have mostly been removed by our MCDF calculations including the effect of intermediate coupling. The experimental data of Hahn *et al.* [4] for the $M_{45}N_1N_{23}\,^3P_{1,2}$ transitions in Kr remain in disagreement with all the theoretical values. A recent many-body calculation [12] including the effect of electron correlation also fails to remove the discrepancies. However, recent experimental results from Merz and Semke [20] have given $\alpha_2=-0.83\pm0.44$ and -0.77 ± 0.25 for $M_4-N_1N_{23}\,^3P_2$ and $M_5-N_1N_{23}\,^3P_2$, respectively. These experimental data agree rather well with theories.

V. CONCLUSIONS

We have calculated the Auger decay anisotropy parameter α_2 of angular distribution for the M_{45}-NN transitions in Kr and M_{45}-NN and N_{45}-OO transitions in Xe using the MCDF method in intermediate coupling with configuration interaction. For transitions with exact cancellation in partial-wave contributions, the effects of relativity and spin-orbit interaction are found to remove this cancellation and to yield nonzero α_2 values. For cases involving many contributing partial waves and leading to the strongly mixed final two-hole states, the effects of intermediate coupling can change the α_2 values by more than a factor of 2 or even change sign. The existing discrepancies between experimental values and the theoretical results calculated in *LSJ* coupling are mostly removed by the inclusion of relativity and intermediate coupling.

Note added in proof. After this work was completed, N. M. Kabachnik, B. Lohmann, and W. Mehlhorn [J. Phys. B **24**, 2249 (1991)] reported α_2 values for the transitions L_3-$M_{23}M_{23}$ in Ar, M_{45}-$N_{23}N_{23}$ in Kr, and N_{45}-$O_{23}O_{23}$ in Xe atoms from the relativistic intermediate coupling calculations. Our results show similar intermediate coupling effects on α_2 values and general good agreement with the predictions from Kabachnik *et al.* Some minor discrepancies exist for a few transitions in categories (ii) and (iii).

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[1] W. Mehlhorn, Phys. Lett. **26A**, 166 (1968).
[2] B. Cleff and W. Mehlhorn, J. Phys. B **7**, 593 (1974); **7**, 605 (1974).
[3] E. Döbelin, W. Sandner, and W. Mehlhorn, Phys. Lett. **49A**, 7 (1974).
[4] U. Hahn, J. Semke, H. Merz, and J. Kessler, J. Phys. B **18**, L417 (1985).
[5] B. Kämmerling, V. Schmidt, W. Mehlhorn, W. B. Peatman, F. Schaefers, and T. Schroeter, J. Phys. B **22**, L597 (1989)
[6] T. A. Carlson, D. R. Mullins, C. E. Beall, B. W. Yates, J. W. Taylor, D. W. Lindle, and F. A. Grimm, Phys. Rev. A **39**, 1170 (1989).
[7] B. Kämmerling, B. Krässig and V. Schmidt, J. Phys. B **23**, 4487 (1990).
[8] E. G. Berezhko and N. M. Kabachnik, J. Phys. B **10**, 2467 (1977).
[9] N. M. Kabachnik and I. P. Sazhima, J. Phys. B **17**, 1335 (1984).
[10] K. Blum, B. Lohmann, and E. Taute, J. Phys. B **19**, 3815 (1986).
[11] N. M. Kabachnik and I. P. Sazhima, J. Phys. B **21**, 267 (1988).
[12] N. M. Kabachnik, I. P. Sazhima, I. S. Lee, and O. V. Lee, J. Phys. B **21**, 3695 (1988).
[13] B. Lohmann, J. Phys. B **23**, 3147 (1990).
[14] S. Flügge, W. Mehlhorn, and V. Schmidt, Phys. Rev. Lett. **29**, 7 (1972).
[15] I. P. Grant, B. J. McKenzie, P. H. Norrington, D. F. Mayers, and N. C. Pyper, Comput. Phys. Commun. **21**, 207 (1980).
[16] M. H. Chen, Phys. Rev. A **31**, 1449 (1985).
[17] W. Bambynek, B. Crasemann, R. W. Fink, H. U. Freund, H. Mark, C. D. Swift, R. E. Price, and P. V. Rao, Rev. Mod. Phys. **44**, 716 (1972).
[18] R. H. Pratt, A. Ron, and H. K. Tseng, Rev. Mod. Phys. **45**, 273 (1973).
[19] H. L. Zhang, D. H. Sampson, and R. E. H. Clark, Phys. Rev. A **41**, 198 (1990).
[20] H. Merz and J. Semke, in *X-ray and Inner-Shell Processes, Proceedings of the Fifteenth International Conference,* AIP Conf. Proc. No. 215 (AIP, New York, 1990), p. 719.