Effects of channel interaction, exchange, and relaxation on the angular distribution and spin polarization of Auger electrons from noble-gas atoms

J. Tulkki
Laboratory of Physics, Helsinki University of Technology, SF-02150 Espoo, Finland

N. M. Kabachnik*
Fakultät für Physik, Universität Bielefeld, 4800 Bielefeld, Germany

H. Aksela
Department of Physics, University of Oulu, SF-90570 Oulu, Finland
(Received 8 February 1993)

The angular anisotropy α_2 and spin polarization ξ_2 parameters have been calculated for Ar L_3MM, Kr $M_{4,5}NN$, Xe $N_{4,5}OO$, and Xe $M_{4,5}NN$ Auger transitions using the multichannel multiconfiguration Dirac-Fock method (MMCDF). The results of our MMCDF calculations are in good general agreement with experiment. We have also determined the separate contributions of the exchange, relaxation, and channel interaction to the angular anisotropy of the Auger process. We have shown that especially for Auger lines having at least two strong partial amplitudes corresponding to different values of the orbital angular momentum both the exchange and channel interaction can change the value of the α_2 parameter significantly and sometimes even change its sign. Because of the additional eigenchannel phase shifts the α_2 parameters are more sensitive to channel interaction than to the exchange. In contrast the relaxation has a small effect on the angular distribution of Auger electrons. A comparative study showed that the α_2 parameters are usually *less sensitive* to correlation than the branching ratios or even the total Auger rates. This was traced back to universal scaling of the modulus of transition amplitudes and to the existence of one dominating ionization channel in most transitions. The ξ_2 parameters were small for all strong Auger lines and exceedingly sensitive to all correlation effects.
PACS number(s): 32.80.Hd, 32.80.Fb

I. INTRODUCTION

The angular distribution of Auger electrons in the decay of ionic states with total angular momentum $j > 1/2$ is in general anisotropic [1]. The anisotropy is due to the alignment of the initial state of the Auger process during the primary ionization or excitation of inner-shell electrons by a directed beam of particles or photons. In a conventional two-step description of the Auger decay the degree of anisotropy is determined [2] by the products of the alignment parameters describing the polarization state of the decaying ion and the anisotropy parameters which characterize the intrinsic anisotropy of the particular Auger transition and which depend on Auger amplitudes. Recently it was realized that measurements of the Auger electron angular distributions as well as measurements of their spin polarization can provide a wealth of information on Auger decay dynamics [3]. This information is additional and more detailed than that obtained by standard measurements of the Auger electron energies and intensities.

In the past several years measurements of angular distributions for normal, satellite, and resonant Auger transitions in noble gases have been published [4 – 17]. There were also attempts to measure the spin polarization of Auger electrons [4, 10, 15]. These measurements stimulated a number of theoretical investigations [18 – 29].

Comparison of the results of the calculations with experiments and other calculations has revealed that angular anisotropy and spin polarization of Auger lines can be very sensitive to subtle details of the description of the decay dynamics. However, not all of the lines demonstrate such sensitivity. According to Kämmerling *et al.* [7] Auger transitions can be classified into three categories: (i) Auger transitions with only one allowed partial wave permitted in any coupling scheme, for example, transitions to the $J = 0$ final ionic states; (ii) Auger transitions with only one allowed partial wave in LS coupling; and (iii) Auger transitions with several contributing partial waves in any coupling scheme.

The transitions of the first category have the anisotropy parameters independent of the Auger amplitudes. The spin-polarization parameters of these Auger transitions are zero. As a rule the anisotropy of the transitions of second category, having single open channel in LS coupling, is weakly sensitive to the details of the atomic model if the atom can be well described in the LS approximation. There is also an exception to this rule: As one will see below there are transitions which are *isotropic* in LS coupling due to occasional cancellations of the contributions of $j = l \pm 1/2$ partial waves. The values of the anisotropy parameters for these transitions are very sensitive to the details in the description of continuum electron. Finally, the transitions of category (iii), with many contributing continuum channels, are in general very sensitive to the theoretical model and provide a good testing ground for different methods of calculating Auger amplitudes.

Comparison of the calculated anisotropy parameters with the experimental data for noble-gas Auger transitions shows that in general the agreement is satisfactory [24, 28]. However, there are some lines in Kr and Xe for which the agreement is still rather poor (see below). Discrepancies exists also between experimental data obtained by different groups. On the theoretical side all intermediate-coupling calculations neglected relaxation and channel-interaction effects. The continuum orbitals were optimized in a simple single-channel potential disregarding exchange interaction.

The importance of the relaxation and channel interaction for K Auger rates was discussed by Howat, Åberg, and Goscinski [30] and Howat[31] in lowest order. Later the channel interaction and relaxation effects have been studied using more advanced methods for several Auger spectra [32–35]. That the exchange effects in the continuum should be properly taken into account has been demonstrated earlier as well [36].

The observed large relaxation, channel interaction, and exchange effects in the Auger energies and line intensities have prompted us to study the influence of these correlation effects on the angular distribution and spin polarization of Auger electrons. In our calculations based on multichannel multiconfiguration Dirac-Fock method (MMCDF) [37] the many-electron effects are classified as initial ionic-state configuration interaction (IISCI), final ionic-state configuration interaction (FISCI), final continuum-state configuration interaction (FCSCI, also called channel interaction), and relaxation. In this work we concentrate on FCSCI, exchange, and relaxation effects. The IISCI that has been found to affect the Auger electron energies and the total transition rates [38] is neglected in the present calculations. We assume that its influence on the angular anisotropy of inner-shell Auger transitions in noble-gas atoms is fairly small.

In the next section we describe the theoretical approach and the computational approximations. In Sec. III we present and discuss the calculated α_2 and ξ_2 parameters for the L_3MM transitions in Ar, $M_{4,5}NN$ transitions in Kr, and $M_{4,5}NN$ and $N_{4,5}OO$ transitions in Xe. In Sec. IV we will compare the influence of various many-electron effects on the angular anisotropy with their influence on the branching ratios and on the total Auger rate.

II. THEORY AND CALCULATIONS

The following analysis of angular dependence and spin polarization of Auger electrons is based on a two-step treatment of Auger decay. Thus the excitation process is taken into account only in terms of polarization and alignment of the initial state of Auger decay. General expressions for the angular distribution of Auger electrons can be found elsewhere (see Ref. [3] for instance). These expressions are rederived and presented in the Appendix within the framework of MMCDF method. In the majority of cases studied experimentally the general formula [see (A24)] can be simplified by including only the first two terms in the expansion (A21) over the state multipoles. Note that in the photoinduced Auger process only these two terms contribute due to the dipole character of photoabsorption. The Auger electron angular distribution for either unpolarized or linearly polarized incoming photons is given by

$$\frac{dW_{J_i\to J_f}(\theta)}{d\Omega} = \frac{W^{(T)}_{J_i\to J_f}}{4\pi}[1+\alpha_2\mathcal{A}_{20}P_2(\cos\theta)] \tag{1}$$

where $W^{(T)}_{J_i\to J_f}$ is the total Auger rate between the initial and final ionic states having total angular momenta J_i and J_f, respectively. In Eq. (1) $\mathcal{A}_{20}$ describes the alignment of the initital state of the Auger decay, α_2 is the anisotropy parameter, and $P_2(\cos\theta)$ is a second Legendre polynomial. The angle θ gives the direction of the Auger electron wave vector with respect to the alignment axis of the ion. For unpolarized photons the axis of alignment is directed along the photon wave vector and for linearly polarized photons along the polarization vector of photons. The expressions for the total rate $W^{(T)}_{J_i\to J_f}$ and the α_2 parameter in terms of Auger amplitudes are presented in Eqs. (A23) and (A26).

The spin polarization of the Auger electron is perpendicular to the plane determined by the axis of alignment and the Auger electron wave vector and it is given by [3, 39]

$$P_\perp = \frac{\xi_2\mathcal{A}_{20}\sin 2\theta}{1+\alpha_2\mathcal{A}_{20}P_2(\cos\theta)} \tag{2}$$

where $\xi_2 = \sqrt{15/16}\beta_2$ and β_2 is determined by Eq. (A27). Note that we have used the same definition of parameter ξ_2 as in papers [3, 39], which differs by a factor of 3/2 from the definition used in Refs. [24, 29].

The α_2 and ξ_2 parameters were evaluated by adding the various many-electron effects stepwise into the wave functions and transition amplitudes. This made it possible to determine how each of them contributes to the anisotropy of Auger process. In order to analyze the effects of relaxation and FCSCI on Auger decay we need a generalization of Fano's [40] theory of autoionization by allowing for the nonorthogonality between the initial single-hole atomic-state function (ASF) $|\Psi_\gamma\rangle$, where $\gamma=\gamma_iJ_i$, and the final continuum $|\Phi^-_{\Gamma E}\rangle$ states [41]. Here $|\Phi^-_{\Gamma E}\rangle$ ($\Gamma=\Gamma_fJ_f\kappa EJ_i$) are N_c noninteracting MMCDF continua corresponding to the final ionic ASF $|\Psi_{\Gamma_fJ_f}\rangle$ and the continuum orbital $|\chi_{\kappa\varepsilon}\rangle$. The symmetry of the continuum electron is specified by the quantum number κ and the kinetic energy by ε. The total energy of the final state $E=E_f+\varepsilon$ is given with respect to the rest energy of the system. The MMCDF wave functions are calculated using a two-step procedure described in detail in Ref. [37] and also summarized briefly in the Appendix in Eqs. (A7)–(A10). The diagonalization of the discrete-continuum Hamiltonian [40] gives the full relaxation multichannel Auger amplitude

$$\langle\Psi_\gamma|H-E|\Phi^-_{\Gamma E}\rangle = \sum_{\alpha=1}^{N_c}\left[\langle\Psi_\gamma|H-E|\phi_{\alpha E}\rangle + \sum_{\beta=1}^{N_c}\mathrm{P}\int dE'\,\frac{\langle\Psi_\gamma|H-E|\phi_{\beta E'}\rangle\langle\phi_{\beta E'}|K|\phi_{\alpha E}\rangle}{E-E'}\right]Z^-_{\alpha\Gamma}. \tag{3}$$

In Eq. (3) H is the Hamiltonian of the ion and the Auger electron, P denotes the principal value, the K matrix is determined by FCSCI, and $Z^{-}_{\alpha\Gamma}$ includes the Dirac-Fock and multichannel phase shifts. The single-channel amplitudes are given by

$$\langle\Psi_\gamma|H-E|\phi_{\alpha E}\rangle = D_{\mu\nu} + D_\mu + D_0 \tag{4}$$

where the two-electron $D_{\mu\nu}$, one-electron D_ν, and constant operator D_0 parts are given by

$$D_{\mu\nu} \equiv \left\langle \Psi_\gamma \left| \sum_{\substack{i,j \\ i<j}} (1/r_{ij}) \right| \phi_{\alpha E} \right\rangle, \tag{5}$$

$$D_\mu \equiv \left\langle \Psi_\gamma \left| \sum_j h_j \right| \phi_{\alpha E} \right\rangle, \tag{6}$$

$$D_0 \equiv \langle\Psi_\gamma|E|\phi_{\alpha E}\rangle. \tag{7}$$

In Eq. (6) the single-particle operator h_j includes the kinetic energy, nuclear attraction, and spin-orbit interaction. In the discussion of the relaxation effect it is meaningful to split the two-electron amplitude into $D_{\mu\nu} = D^0_{\mu\nu} + \tilde{D}_{\mu\nu}$. The *principal* amplitude $D^0_{\mu\nu}$ includes a product of an overlap factor [42] and the dynamical two-electron matrix element $\langle\chi_{\beta_1}\chi_{\beta_2}|r_{12}|\chi_i\chi_A\rangle$ where $|\chi_x\rangle$, $x = \beta_1, \beta_2, i, A$, are the orbitals corresponding to the final and initial holes and the Auger electron. All other partial amplitudes in $D_{\mu\nu}$ resulting from permutations are called *conjugate* and denoted by $\tilde{D}_{\mu\nu}$. In calculations based on the use of the same bound orbitals in the initial and final states only the $D^0_{\mu\nu}$ remains in Eq. (4) with the overlap factor equal to one [35]. Although the relaxation and FCSCI effects should be included simultaneously, the relaxation and a weak FCSCI effect are approximately additive [35].

In all calculations we used a single-hole-configuration initial-state ASF. For the final ionic ASF we accounted for FISCI by always mixing all configuration-state functions (CSF's) that can be constructed by distributing the two final holes on the M, N, or O subshells. For instance, in the case of Xe $M_{4,5}NN$ Auger spectrum we obtain 35 possible final ASF's. These are associated in the case of the M_5 initial hole with 138 Auger emission channels including s, p, d, f, g, h, and i partial waves.

In our calculations we have neglected the FISCI of the final ionic double-hole configuration ns^0np^6, where n = 3, 4, and 5 for Ar, Kr, and Xe, respectively, with the triple-hole configurations $nsnp^4nd$ and $ns^2np^2nd^2$. Correspondingly the FISCI between the $nsnp^5$ and ns^2np^3nd configurations was also ignored. The CI between these double- and triple-hole configurations is particularly strong for the Xe $N_{4,5}O_1O_{2,3}$ and $N_{4,5}O_1O_1$ Auger lines [43]. The calculated transition energies of these lines are much smaller than the experimental values. A similar FISCI effect is found also in the final state of the Kr $M_{4,5}N_1N_1$ and $M_{4,5}N_1N_{2,3}$ [44] and Ar $L_{2,3}M_1M_1$ and $L_{2,3}M_1M_{2,3}$ transitions [45]. The CI with triple-hole configurations also gives rise to intense FISCI correlation satellites in the Auger spectrum and may also change the angular distributions of the main lines.

The continuum orbitals were calculated in jj-average field of the final ion, constructed using the generalized occupation numbers of final ionic CSF's [46]. In all calculations except in the one which excludes the exchange interaction the Lagrangian multipliers were included to orthogonalize the continuum orbital to the bound orbitals. Therefore to the Auger electron, there is asymptotically a doubly charged ionic field even when initial-state bound orbitals are used for the construction of the jj-average potential. In all calculations we used energies, which were obtained as a difference between separately optimized initial- and final-state ASF's (ΔSCF method).

The total Auger rates as well as branching ratios, angular distribution, and spin-polarization parameters of Auger lines were calculated in several approximations, based on different one-electron and many-electron wave functions. The four single-channel calculations are labeled by IE, I, RE, and FE and the multichannel calculation by FEMC in Tables I–VIII. In detail these results were obtained as follows.

IE: In this approximation the bound orbitals, optimized for the initial ionic state, were also used in the construction of the final-state many-electron wave function. The jj-average exchange interaction and the Lagrangian multipliers were included in the calculation of the continuum orbital. We call this the *nonrelaxed* approximation since effectively it assumes that the bound orbitals are frozen during the Auger decay.

I: The effect of exchange interaction between the continuum and bound electrons was studied by using the same bound orbitals as in the IE calculation, but by neglecting the exchange potential in the calculation of the continuum orbitals. The continuum orbitals were then Smith orthogonalized against the bound orbitals. The difference between results IE and I hence gives an estimate of the influence of exchange on the anisotropy of Auger decay. This approach is identical to that used by Chen [28]. The calculation of Kabachnik, Lohmann, and Mehlhorn [24] differs from our calculation I in three respects. First in their work only the np^4 (n = 3, 4, 5) parent configurations were used in the construction of the final ionic ASF's. This accounts effectively for intermediate coupling. Second the experimental transition energies were used, and third the Smith orthogonalization procedure was not applied to the continuum orbital.

RE: In this approximation the initial and final ionic ASF's were optimized separately and the resulting nonorthogonality was fully accounted for by evaluating D_0, D_μ, and $D_{\mu\nu}$ in Eq. (4) according to Löwdin's formalism [42]. Except for the different set of final-state orbitals and the use of Eq. (4) the IE and RE approximations have been obtained using identical computational procedures. Consequently the difference between these results is *entirely* assigned to *orbital relaxation* during the Auger decay.

FE: This calculation is identical to IE, but the bound orbitals which were optimized for the final ionic state were also used in the initial-state ASF. This approach has also been commonly used since it is based, in analogy to IE, on the use of an orthogonal set of one-electron

orbitals. Note that, according to first-principles neither approximation, IE nor FE, has any advantage over the other.

FEMC: In this calculation we include the exchange and channel interaction by using MMCDF wave functions in the final state. The computational method has recently been described by Tulkki *et al.* [37]. The MMCDF calculation of the Xe $N_{4,5}OO$ Auger spectrum has been discussed in detail by Mäntykenttä [47] and we have used the same MMCDF Auger amplitudes and phase factors to generate our α_2 and ξ_2 parameters. We calculated the MMCDF Ar L_3MM and Kr $M_{4,5}NN$ Auger rates using the same computational procedure as in the Xe $N_{4,5}OO$ case. For Ar the MCDF wave functions of the final ionic state were calculated by including ten CSF's obtained by distributing the two holes on the $3s$ and $3p$ subshells. In the multichannel calculation we included the corresponding 25 allowed ionization channels. For the Kr $M_{4,5}NN$ Auger spectrum the ten CSF's obtained from two holes on $4s$ and $4p$ subshells are associated with 25 (M_4) and 27 (M_5) channels. In all FEMC calculations the bound orbitals were optimized for the final state of the ion. Therefore the difference between our FE and FEMC results will directly gauge the influence of FCSCI.

III. ANGULAR ANISOTROPY: RESULTS AND DISCUSSION

Using the approach described above we have calculated the anisotropy parameter α_2 and spin-polarization parameter ξ_2 as well as the intensities for the L_3MM transitions in Ar, $M_{4,5}NN$ transitions in Kr, and $N_{4,5}OO$ transitions in Xe. In Table I we give the values of the α_2 parameter obtained in various approximations for $J_f = 2$ final ionic states. The identification of the transitions in LS-coupling scheme is traditional and corresponds to the leading component of the multiconfiguration wave function [48]. Table II includes only a few Auger lines corresponding to the largest absolute values of the ξ_2 parameter. Tables III–V include a comparison of our MMCDF α_2 parameters with previous calculations and experiments. The results for Xe M_5NN transitions are given in Table VI. Tables VII–VIII include the calculated intensities and total rates of Ar L_3MM and Kr $M_{4,5}NN$ Auger spectra in all approximations.

A. Comparison of calculated results

As pointed out in the Introduction, the α_2 and ξ_2 parameters are not sensitive to computational approxima-

TABLE I. Angular anisotropy parameter α_2 for selected Ar, Kr, and Xe Auger lines, corresponding to total final ionic angular momentum $J_f = 2$. Column I indicates single-channel results obtained by using intial-state bound orbitals and by excluding exchange interaction for the continuum orbital; IE is the same as I except that the exchange for the continuum electron has been included; FE is the same as IE, but based on the use of final-state bound orbitals; RE indicates single-channel values obtained with exchange and by using separately optimized initial- and final-state orbitals to account for relaxation according to Eq. (4); FEMC is the same as FE, but includes the interachannel interaction in the final state.

	Transition[a]		Approximation				
			I	IE	RE	FE	FEMC
Ar	$L_3M_{2,3}M_{2,3}$	$^3P_2$	0.789	0.789		0.788	0.787
		$^1D_2$	-0.483	-0.500		-0.522	-0.548
	$L_3M_1M_{2,3}$	$^3P_2$	0.048	0.042		0.037	0.007
Kr	$M_4N_{2,3}N_{2,3}$	$^3P_2$	0.088	0.105	0.112	0.108	0.095
		$^1D_2$	0.153	-0.036	-0.084	-0.103	0.224
	$M_4N_1N_{2,3}$	$^3P_2$	-0.866	-0.828	-0.822	-0.823	-0.839
	$M_5N_{2,3}N_{2,3}$	$^3P_2$	-0.323	-0.316		-0.309	-0.329
		$^1D_2$	0.252	-0.011		-0.091	0.419
	$M_5N_1N_{2,3}$	$^3P_2$	-0.765	-0.664		-0.657	-0.746
Xe	$N_4O_{2,3}O_{2,3}$	$^3P_2$	0.262	0.247	0.249	0.239	0.231
		$^1D_2$	0.083	-0.077	-0.109	-0.116	-0.116
	$N_4O_1O_{2,3}$	$^3P_2$[b]	-0.846	-0.750	-0.655	-0.603	0.051
	$N_5O_{2,3}O_{2,3}$	$^3P_2$	-0.257	-0.243	-0.241	-0.240	-0.385
		$^1D_2$	0.228	-0.029	-0.065	-0.078	0.094
	$N_5O_1O_{2,3}$	$^3P_2$[b]	-0.741	-0.671	-0.655	-0.663	-0.736

[a]The final ionic states are identified by giving the dominant LS term in the pertinent multiconfiguration ASF [48].

[b]These lines are very weak, see Ref. [47].

TABLE II. Spin-polarization parameter ξ_2 for selected Kr $M_{4,5}NN$ and Xe $N_{4,5}OO$ Auger lines. The selected lines have the largest ξ_2 values in FEMC approximation. The computational approximations are the same as in Table I.

	Transition		Approximation				
			I	IE	RE	FE	FEMC
Kr	$M_4N_{2,3}N_{2,3}$	$^3P_2$	-0.099	-0.254	-0.300	-0.313	0.095
	$M_4N_1N_{2,3}$	$^3P_2$	0.002	-0.0003	-0.0002	-0.0002	0.059
		$^3P_1$	-0.017	0.015	0.016	0.016	-0.271
	$M_5N_{2,3}N_{2,3}$	$^3P_2$	0.034	0.090		0.114	-0.064
	$M_5N_1N_{2,3}$	$^3P_2$	0.002	-0.005		-0.005	0.124
		$^3P_1$	0.0001	0.009		0.009	-0.215
Xe	$N_4O_{2,3}O_{2,3}$	$^3P_2$	-0.068	-0.275	-0.296	-0.296	0.040
	$N_4O_1O_{2,3}$	$^3P_2$	0.031	0.114	0.172	0.201	-0.282
		$^3P_1$	-0.298	-0.267	-0.144	-0.137	-0.091
	$N_5O_{2,3}O_{2,3}$	$^3P_2$	0.035	0.092	0.102	0.104	-0.100
	$N_5O_1O_{2,3}$	$^3P_2$	0.069	0.195	0.220	0.220	-0.070
		$^3P_1$	-0.071	-0.192	-0.225	-0.236	0.262

tions for all of the Auger lines. The most interesting cases in this respect are the transitions to the final ionic states with $J_f = 2$. For these transitions previous calculations predicted the largest influence of intermediate coupling [24, 28]. On the other hand, for some of these transitions there is also a discrepancy with experimental data.

The first two columns (I and IE) demonstrate the effect of exchange. For Ar the difference between the results I and IE is small (less than 5%) for strongly anisotropic lines. It is slightly larger for the almost isotropic $L_3M_1M_{23}$ $^3P_2$ transition. Small influence of exchange on the α_2 parameter in Ar is due to the large kinetic energy of emitted Auger electrons ($\sim$ 200 eV). A small exchange effect was also found (results without exchange not shown in Table VI) for the Xe $M_{4,5}NN$ transitions which also correspond to high kinetic energy (200–500 eV). This observation can be directly related to the one-electron Dirac equation of the continuum orbital. As the kinetic-energy term increases the exchange potential loses its significance.

A different situation occurs in Kr and Xe where the kinetic energy of Auger electrons is much smaller ($\sim$ 50 eV and $\sim$ 30 eV, respectively). Here the exchange is important and it can influence the angular anisotropy. In fact, the effect of exchange is dramatic for some of the lines. For example, for the $M_{4,5}N_{2,3}N_{2,3}$ $^1D_2$ transitions in Kr and for the $N_{4,5}O_{2,3}O_{2,3}$ $^1D_2$ transitions in Xe inclusion of the exchange leads to a change of the sign of the anisotropy. The results regarding the Kr $M_5N_{2,3}N_{2,3}$ $^1D_2$ line are especially illustrative. For this line a rather large positive value of the α_2 parameter, in good agreement with experiment (Table IV), was ob-

TABLE III. Angular anisotropy parameter α_2 for Ar L_3MM Auger transitions: a comparison of the present MMCDF results with experiment and earlier calculations. The last two columns give the spin-polarization parameter and the relative intensity I in percentage of the total MMCDF rate of 5.57 ma.u.

Transition		Experiment		Theory			
		a	b	ICDF[c]	This work		
					α_2	ξ_2	I (%)
$L_3M_{2,3}M_{2,3}$	$^3P_2$			0.795	0.787	−0.004	27.37
	$^3P_1$			−0.010	0.004	0.000	9.62
	$^3P_0$			−1.000	−1.000	0.000	2.52
	$^1D_2$	-0.48 ± 0.10	−0.41	−0.441	−0.548	0.004	31.91
	$^1S_0$			−1.000	−1.000	0.000	5.80
$L_3M_1M_{2,3}$	$^3P_2$				0.007	0.045	9.16
	$^3P_1$				−0.011	−0.214	2.01
	$^3P_0$				−1.000	0.000	0.02
	$^1P_1$				−0.041	0.000	10.28
	$^1S_0$				−1.000	0.000	1.30

[a]Sarkadi *et al.*, Ref. [11].

[b]Becker, Ref. [8].

[c] Intermediate coupling Dirac-Fock final ionic state, no exchange for the Auger electron, Kabachnik, Lohmann, and Mehlhorn, Ref. [24].

tained by Kabachnik, Lohmann, and Mahlhorn [24] and by Chen [28] without the exchange. However, when the exchange is included the α_2 of this line obtains a small negative value. This shows that the agreement was in a sense accidental.

A comparison of the results from the second and fourth columns (IE and FE) shows that the calculations with the one-electron orbitals obtained by optimizing the initial or final ionic state give almost identical results. Except for some weak lines and lines having a very small α_2 value the difference is smaller than a few percent. Therefore the α_2 parameter is relatively insensitive to the choice of the basis set.

The effect of relaxation is demonstrated by the column RE. These results were obtained by using separately optimized initial- and final-state orbitals and by accounting for the resulting nonorthogonality by employing the generalized Auger amplitude in Eq. (4). Comparing the results in the columns IE and RE one can see that relaxation affects the α_2 parameters only slightly. This conclusion is valid for all transitions studied in this work.

Finally we consider the effect of channel interactions. The last column (FEMC) in Table I shows the results of a calculation involving final-state orbitals, full exchange and full account of FCSCI as described in Sec. II and in the Appendix. The pure effect of FCSCI can be seen by comparing these results with those in the fourth column (FE), which were obtained in the identical way except that FCSCI was not included.

The largest FCSCI effects are obtained for the $M_{4,5}N_1N_{2,3}\ ^1P_1$ and $M_{4,5}N_{2,3}N_{2,3}\ ^1D_2$ in krypton and for the $N_5O_{2,3}O_{2,3}\ ^3P_2$, $^1D_2$ lines in xenon. For the Kr $M_{4,5}N_{2,3}N_{2,3}\ ^1D_2$ transitions the α_2 parameters have different signs in calculations with and without channel coupling. It is interesting that exchange and channel interaction affect the α_2 value in opposite directions: the former decreases the anisotropy whereas the latter increases it. The exchange and FCSCI partly compensate each other, so that the final α_2 value is only 50–70 % larger than the results obtained by disregarding both effects. For the $N_5O_{2,3}O_{2,3}\ ^1D_2$ transitions in Xe the situation is similar, but here the FCSCI is not as strong.

A strong FCSCI effect is also observed for the $M_5N_1N_{2,3}\ ^3P_2$ transitions in Kr and $N_{4,5}O_1O_{2,3}\ ^3P_2$ transitions in Xe. Earlier it was shown that for these lines the α_2 parameter calculated using many-body perturbation theory (MBPT) differs considerably from the corresponding Hartree-Fock result [21]. Although there is no simple relation between the *nonrelativistic LS*-coupling MBPT and MMCDF calculations, the large FCSCI effect, for these lines, in Table I is in qualitative agreement with MBPT result. The influence is especially strong for the Xe $N_4O_1O_{2,3}\ ^3P_2$ transition, but again the small line intensity makes the comparison somewhat inconclusive.

In Table II we present the results of calculations of the spin-polarization parameter ξ_2. In all transitions considered the ξ_2 parameter is extremely small, typically less than 0.01. The resulting polarization would be so small that it is not possible to observe it experimentally. Nevertheless, in order to demonstrate the sensitivity of the ξ_2 parameter to various dynamical effects we have chosen the transitions with the largest values of ξ_2. One can see

TABLE IV. Angular anisotropy parameter α_2 for Kr $M_{4,5}NN$ Auger transitions: a comparison of the present MMCDF results with experiment and earlier calculations. The last two columns give the spin-polarization parameter ξ_2 and the relative intensity in percentages of the total MMCDF rates 2.89 ma.u. and 2.93 ma.u. for M_4 and M_5 holes, respectively.

Transition		Experiment		Theory				
		a	b	ICDF[c]	MCDF[d]	This work		
						α_2	ξ_2	I (%)
$M_4N_{2,3}N_{2,3}$	$^3P_2$	0.21 ± 0.09		0.017	0.098	0.095	0.010	3.47
	$^3P_1$	-0.77 ± 0.10		−0.818	−0.817	−0.818	−0.005	6.09
	$^3P_0$			−1.000	−1.000	−1.000	0.000	1.07
	$^1D_2$			0.240	0.154	0.224	0.019	14.79
	$^1S_0$			−1.000	−1.000	−1.000	0.000	11.58
$M_4N_1N_{2,3}$	$^3P_2$		-1.02 ± 0.07		−0.865	−0.839	0.059	9.08
	$^3P_1$		-1.08 ± 0.07		−0.932	−0.895	−0.271	1.91
	$^3P_0$				−1.000	−1.000	0.000	0.33
	$^1P_1$		-0.77 ± 0.04		−0.633	−0.589	0.004	29.81
	$^1S_0$			−1.000	−1.000	−1.000	0.000	21.87
$M_5N_{2,3}N_{2,3}$	$^3P_2$	-0.31 ± 0.06		−0.303	−0.323	−0.329	−0.064	9.39
	$^3P_1$			−0.739	−0.742	−0.737	−0.009	3.69
	$^3P_0$				−1.069	−1.069	0.000	2.26
	$^1D_2$	0.18 ± 0.04		0.330	0.286	0.419	0.047	11.88
	$^1S_0$				−1.069	−1.069	0.000	7.79
$M_5N_1N_{2,3}$	$^3P_2$		-0.96 ± 0.07		−0.762	−0.746	0.124	5.01
	$^3P_1$		-1.20 ± 0.05		−1.051	−1.011	−0.216	5.55
	$^3P_0$				−1.069	−1.069	0.000	2.13
	$^1P_1$		-0.72 ± 0.04		−0.627	−0.569	0.028	30.91
	$^1S_0$				−1.069	−1.069	0.000	21.39

[a]Kämmerling, *et al.*, Ref. [7].

[b]Kämmerling *et al.*, Ref. [16].

[c]Intermediate-coupling Dirac-Fock final ionic state, no exchange for the Auger electron, Kabachnik, Lohmann, and Hehlhorn, Ref. [24].

[d]Multiconfiguration Dirac-Fock final ionic state, no exchange for the Auger electron, Chen, Ref. [28].

from Table II that the ξ_2 parameters are very sensitive to all many-electron effects and also to the choice of the one-electron orbitals. The relative change of the ξ_2 value calculated in different models is much larger than for the α_2 parameter.

B. Comparison with experiment

In Tables III–V we present the results of our MMCDF calculations for all transitions together with experimental data and some earlier calculations. Our results shown here correspond to FEMC approximation in Tables I and II, i.e., the most important effects of the exchange and channel interaction are taken into account, but not the relaxation effect, which on the basis of Table I does not influence the α_2 values much. Next we consider each Auger spectrum in more detail.

1. *Ar L_3MM transitions*

The present results (see Table III) are close to those of Ref. [24] and agree quite well with available experimental data. For the $L_3M_{2,3}M_{2,3}$ $^1D_2$ transition the absolute value of our result is somewhat larger than that of Ref. [24], however, the α_2 value is still compatible with experiment. Since the $L_3M_{2,3}M_{2,3}$ $^1D_2$ transition appears as a well-resolved intense peak in the experiment it is a suitable test to the theory. Note that for Ar the effects of exchange and channel interaction are rather small due to the relatively large Auger electron energy.

2. *Kr $M_{4,5}NN$ transitions*

For the transitions from the $3d_{3/2}$ hole state our results shown in Table IV are in good agreement with recent experimental data by Kämmerling *et al.* [7, 16]. However, both the present and earlier calculated anisotropies [24, 28] of the $M_4N_{2,3}N_{2,3}$ $^3P_2$ and all $M_4N_1N_{2,3}$ lines are slightly lower than the experimental values. The results for the M_5NN transitions fit the experimental data also well and are close to the previous calculations [24, 28]. The similarity of our results with the calculations excluding FCSCI and exchange is due to the strong compensation of these effects. In the case of $M_5N_{2,3}N_{2,3}$ transitions the comparison with experiment is most conclusive for the intense and well-separated $^1D_2$ and $^3P_2$ lines. All $M_{4,5}N_1N_{2,3}$ lines are well resolved in the experiment, which makes the determination of the α_2 parameters reliable. The discrepancy between theory and experiment for the $M_{4,5}N_1N_{2,3}$ $^1P_1$ lines might be related to FISCI involving the $4s^24p^34d$ triple-hole configurations.

TABLE V. Angular anisotropy parameter α_2 for Xe $N_{4,5}OO$ Auger transitions: a comparison of the present MMCDF results with experiment and earlier calculations. The last two columns give the the spin-polarization parameter ξ_2 and the relative intensity in percentages of the total MMCDF rates 5.16 ma.u. and 5.87 ma.u. for N_4 and N_5 holes, respectively.

Transition	Experiment			Theory				
	a	b	c	ICDF[e]	MCDF[f]	This work		
						α_2	ξ_2	I (%)
$N_4O_{2,3}O_{2,3}$								
$^3P_2$	0.72 ± 0.13	1.2 ± 0.2		0.156	0.250	0.231	0.040	2.72
$^3P_1$	-0.73 ± 0.11	-0.7 ± 0.1		−0.835	−0.831	−0.837	−0.022	8.40
$^3P_0$				−1.000	−1.000	−1.000	0.000	0.63
$^1D_2$	0.05 ± 0.06			0.055	0.086	−0.116	0.015	16.80
$^1S_0$					−1.000	−1.000	0.000	11.45
$N_4O_1O_{2,3}$								
$^3P_2$					−0.847	0.051	−0.282	0.36
$^3P_1$					−0.924	−0.779	−0.091	0.86
$^3P_0$					−1.000	−1.000	0.000	0.72
$^1P_1$					−0.683	−0.730	0.069	51.60
$^1S_0$					−1.000	−1.000	0.000	6.46
$N_5O_{2,3}O_{2,3}$								
$^3P_2$	-0.47 ± 0.13		-0.09 ± 0.10	−0.227	−0.257	−0.385	−0.100	10.80
$^3P_1$	-0.77 ± 0.17	-1.0 ± 0.2	-0.69 ± 0.10	−0.734	−0.736	−0.743	−0.008	3.89
$^3P_0$	-1.07 ± 0.10	-1.2 ± 0.2		−1.069	−1.069	−1.069	0.000	3.57
$^1D_2$	0.24 ± 0.10	0.31	0.30 ± 0.12	0.139	0.238	0.094	0.053	9.50
$^1S_0$					−1.069	−1.069	0.000	3.94
$N_5O_1O_{2,3}$								
$^3P_2$					−0.738	−0.736	−0.070	1.33
$^3P_1$					−0.924	−0.957	0.262	1.82
$^3P_0$					−1.069	−1.069	0.000	0.32
$^1P_1$					−0.647	−0.712	−0.003	59.86
$^1S_0$					−1.069	−1.069	0.000	4.96

[a] Kämmerling, Krässig, and Schmidt, Ref. [9].

[b] Becker [54].

[c] Whitfield *et al.*, Ref. [17].

[e] Intermediate-coupling Dirac-Fock final ionic state, no exchange for the Auger electron, Kabachnik, Ref. [24].

[f] Multiconfiguration Dirac-Fock final ionic state, no exchange for the Auger electron, Chen, Ref. [28].

3. Xe $N_{4,5}OO$ transitions

For the Xe atom the difference between the present and earlier calculations is considerably larger than for Ar and Kr (see Table V). The measurements show [9] that the decay of the $4d_{3/2}$ vacancy to the $O_{2,3}O_{2,3}$ $^3P_2$ final state is strongly anisotropic while the decay to the $O_{2,3}O_{2,3}$ $^1D_2$ final state is almost isotropic. Our calculation agrees qualitatively with the experiment, but for the former Auger line our and earlier calculations predict a considerably lower α_2 value than the experiment. For the transition to the $^1D_2$ final ionic state we obtain a small negative α_2 value whereas in Refs. [24, 28] a small positive value was obtained, in agreement with experiment. However, the calculated values are very sensitive to the computational model since they involve large partial amplitudes which almost cancel each other. The experimental determination of the anisotropy parameter is also rather difficult because the transition to the $^3P_2$ final state is rather weak and transitions to $^1D_2$ is strongly overlapping with the strong $N_5O_{2,3}O_{2,3}$ $^3P_2$ line. The results for the $N_4O_1O_{2,3}$ $^3P_2$ lines were very model dependent. The anisotropy of the decay of the $4d_{5/2}$ vacancy is well reproduced by the present calculation, except for the $N_5O_{2,3}O_{2,3}$ $^1D_2$ line. For this nearly isotropic line the calculated α_2 value is somewhat lower than the experimental one, which is accurate because the line is strong and well resolved. In analogy to Kr the discrepancies between theory and experiment may be related to the FISCI with the triple-hole configurations.

TABLE VI. Auger electron energies (E), relative line intensities (I), angular anisotropy parameter (α_2), and spin-polarization parameter (ξ_2) for Xe M_5NN Auger transitions. The results correspond to approximation IE described in Table I. The total M_5 Auger rates in various approximations were 24.14 ma.u. (I); 24.74 ma.u. (IE) and 21.87 ma.u. (FE). See text for further details.

Transition		E (eV)	I (%)	α_2	ξ_2
$M_5N_{4,5}N_{4,5}$	$^3F_4$ [a]	527.44	13.07	0.386	-0.011
	$^1D_2$	525.82	8.54	-0.226	-0.002
	$^3F_3$	525.64	5.18	0.336	0.021
	$^3P_2$	524.10	4.58	-0.371	-0.025
	$^3P_0$	523.33	1.85	-1.069	0.000
	$^3P_1$	523.00	3.00	-0.749	-0.000
	$^1D_2$	522.23	1.59	-0.124	0.092
	$^1G_4$	522.05	11.86	-0.710	0.003
	$^1S_0$	516.80	0.93	-1.069	0.000
$M_5N_{2,3}N_{4,5}$	$^3F_4$	440.86	4.43	-0.228	0.015
	$^1D_2$	438.67	2.30	0.205	0.007
	$^3F_3$	436.56	1.43	0.269	-0.058
	$^3D_2$	433.64	1.04	-0.095	0.036
	$^3P_1$	433.35	1.04	-0.721	-0.052
	$^3P_0$	433.11	0.00	-1.069	0.000
	$^3D_3$	430.98	5.76	0.788	0.041
	$^3D_1$	429.82	2.09	-0.732	0.007
	$^3F_2$	425.25	0.11	-0.754	-0.026
	$^3D_2$	422.46	4.19	-0.115	-0.018
	$^1F_3$	416.96	8.31	-0.256	-0.050
	$^1P_1$	416.22	0.34	-0.698	0.026
$M_5N_1N_{4,5}$	$^3D_3$	370.10	5.33	0.026	0.019
	$^3D_2$	369.23	3.72	-0.208	-0.040
	$^3D_1$	368.00	0.36	-1.000	0.040
	$^1D_2$	366.31	1.80	-0.391	0.059
$M_5N_{2,3}N_{2,3}$	$^3P_2$	343.01	1.28	-0.652	-0.307
	$^3P_0$	339.55	0.22	-1.069	0.000
	$^3P_1$	332.29	0.20	-0.757	-0.005
	$^1D_2$	326.53	3.73	-0.667	0.089
	$^1S_0$	315.51	0.01	-1.069	0.000
$M_5N_1N_{2,3}$	$^3P_2$	282.45	0.23	-0.736	-0.132
	$^3P_1$	276.52	0.32	-0.833	0.094
	$^3P_0$	269.75	0.004	-1.069	0.000
	$^1P_1$	259.44	1.10	-0.832	-0.011
$M_5N_1N_1$	$^1S_0$	206.55	0.03	-1.069	0.000

[a]For this line an experimental value of $\alpha_2 = 0.431 \pm 0.12$ has been reported by Hahn *et al.* [4].

4. Xe $M_{4,5}NN$

These transitions are induced by ionization of a rather deep inner shell of Xe and therefore the energy of Auger electrons is high. One can expect that for electrons having such a high kinetic energy the channel interaction and exchange effects must be small. Therefore we calculated the anisotropy and polarization parameters for these transitions only in single-channel approximations I, IE, and FE. Except for the weakest lines the branching ratios and the α_2 and ξ_2 parameters obtained in these three approximations are almost equal. Therefore we have given in Table VI (the M_4NN data not shown) only the results corresponding to the IE approximation together with the rare experimental data. Our calculated α_2 parameters are very close to those reported by Chen [28]. An exceptionally large value of ξ_2 is found for the $M_4N_1N_{2,3}$ $^3P_1$ line. Unfortunately, all strongly polarized transitions have a low intensity, which makes the experimental measurement of the polarization difficult. Experimental studies of the Xe $M_{4,5}NN$ spectra are, furthermore, hampered by the shift and broadening of the lines caused by the super Coster-Kronig decay of the final state.

IV. ANGULAR ANISOTROPY VERSUS BRANCHING RATIOS AS A PROBE OF CORRELATION EFFECTS

In the above discussion the influence of the exchange, relaxation, and FCSCI on the α_2 and ξ_2 parameters was studied without reference to the corresponding changes in the branching ratios or in the total Auger rate. In this section we will compare the sensitivity of the angular anisotropy and branching ratios to these many-electron effects. The unique feature of angle- and spin-resolved measurement is that it gives information about the phase differences between the transition amplitudes that cannot be obtained from the total Auger rate or from the branching ratios. However, according to Eqs. (A10) and (3) the multichannel phase shifts η_Γ also influence the branching ratios because of the incoming-wave boundary condition. Note that the multichannel phase shifts were neglected in earlier lowest-order studies of FCSCI [30, 41].

TABLE VII. Calculated and experimental Ar L_3MM Auger energies and intensities. The columns are labeled as in Table I. The experimental intensities have been normalized to the theoretical percentage intensity of the $L_3M_{2,3}M_{2,3}\ ^1D_2$ line. Therefore the experimental intensities do not sum up to 100%.

Transition		Energy (eV)		Intensity (%)				
		Theory	Expt.	I	IE	FE	FEMC	Expt.[a]
$L_3M_{2,3}M_{2,3}$	$^3P_2$	207.18	205.2	28.66	27.87	26.22	27.37	21.0
	$^3P_1$	207.04	205.1	9.36	9.09	9.27	9.63	9.3
	$^3P_0$	206.98	204.9	3.25	3.18	2.46	2.52	0.4
	$^1D_2$	205.07	203.5	29.03	29.19	30.23	31.91	31.9
	$^1S_0$	203.25	201.1	6.01	6.31	6.46	5.80	8.4
$L_3M_1M_{2,3}$	$^3P_2$	189.88	191.1	10.29	10.10	9.80	9.16	7.5
	$^3P_1$	189.75		2.42	2.38	2.10	2.01	
	$^3P_0$	189.68		0.01	0.01	0.001	0.02	
	$^1P_1$	182.03	187.4	9.75	10.33	11.44	10.28	5.8
$L_3M_1M_1$	$^1S_0$	165.07	178.0	1.21	1.53	2.03	1.30	4.8
Total rates (ma.u.)				6.91	6.88	5.10	5.57	4.4±0.4[b]

[a]Reference [55].
[b]Reference [53].

In order to make the relation of the α_2 and ξ_2 parameters to the transition amplitudes and their relative phases explicitly visible we rewrite Eqs. (A26) and (A27) as

$$\alpha_2 \sim N^{-1}\sum_{\kappa,\kappa'} B_{\kappa\kappa'}A_\kappa A_{\kappa'}\cos(\Delta_{\kappa\kappa'}), \tag{8}$$

$$\xi_2 \sim N^{-1}\sum_{\kappa,\kappa'} C_{\kappa\kappa'}A_\kappa A_{\kappa'}\sin(\Delta_{\kappa\kappa'}). \tag{9}$$

In Eq. (8) $B_{\kappa\kappa'}$ and $C_{\kappa\kappa'}$ are geometrical factors and $A_\kappa = |\langle\Psi_{\gamma_i J_i}\|H_I\|\Phi^-_{\Gamma_f J_f \kappa E J_i}\rangle|$ is the absolute value of the transition amplitude. The phase difference $\Delta_{\kappa\kappa'}$ between channels having Auger electron quantum numbers κ and κ' includes the Coulomb phase shifts σ_κ, short-range phase shifts δ_κ, and the multichannel phase shifts η_Γ according to Eqs. (A10) and (3). The normalization factor is given by $N = \sum_\kappa |A_\kappa|^2$.

In the sum over angular momenta in Eq. (8) the product of partial amplitudes is proportional to the cosine of the phase difference. Therefore the α_2 parameters are not

TABLE VIII. Calculated and experimental Kr $M_{4,5}NN$ Auger energies and intensities. The columns are labeled as in Table I. The experimental intensities have been normalized to the theoretical percentage intensity of the $M_{4,5}N_{2,3}N_{2,3}\ ^1D_2$ lines. Therefore the experimental intensities do not sum up to 100%.

Transition		Energy (eV)		Intensity (%)					
		Theory	Expt.	I	IE	RE	FE	FEMC	Expt.[a]
$M_4N_{2,3}N_{2,3}$	$^3P_2$	57.23	56.7	2.96	1.33	1.16	1.07	3.47	2.9
	$^3P_1$	56.67	56.1	5.20	2.40	2.13	1.95	6.09	
	$^3P_0$	56.58		0.75	0.33	0.29	2.46	1.07	5.4
	$^1D_2$	55.07	54.9	16.92	12.49	12.13	11.87	14.79	14.8
	$^1S_0$	53.25	52.6	10.98	6.66	6.12	5.81	11.58	10.2
$M_4N_1N_{2,3}$	$^3P_2$	40.40	42.3	7.54	8.95	9.08	9.24	9.08	6.9
	$^3P_1$	39.93	41.9	1.08	1.14	1.12	1.16	1.91	1.2
	$^3P_0$	39.67		0.11	0.04	0.04	0.04	0.33	
	$^1P_1$	33.40	39.1	35.80	44.45	45.65	46.47	29.81	13.8
$M_4N_1N_1$	$^1S_0$	16.94	25.5	18.67	22.21	22.28	22.10	21.87	5.0
Total rates (ma.u.)				3.30	2.82	3.20	3.10	2.88	2.9±0.4[b]
$M_5N_{2,3}N_{2,3}$	$^3P_2$	55.93	55.4	8.26	3.68		3.01	9.39	10.9
	$^3P_1$	55.38	54.9	3.06	1.34		1.08	3.69	
	$^3P_0$	55.28		2.03	0.93		0.78	2.26	
	$^1D_2$	53.78	53.6	13.69	10.71		10.35	11.88	11.9
	$^1S_0$	51.96	51.3	7.79	4.79		4.12	7.79	9.7
$M_5N_1N_{2,3}$	$^3P_2$	39.10	41.1	3.71	4.18		4.30	5.01	4.0
	$^3P_1$	38.64	40.6	4.70	5.49		5.73	5.55	5.4
	$^3P_0$	38.37	40.4	1.71	2.03		2.10	2.13	2.0
	$^1P_1$	32.10	37.8	36.08	44.17		45.99	30.91	14.8
$M_5N_1N_1$	$^1S_0$	15.64	24.2	18.99	22.68		22.54	21.39	6.1
Total rates (ma.u.)				3.15	2.84		3.15	2.93	2.9±0.4[b]

[a]Reference [55].
[b]Reference [53].

influenced by correlation effects that scales the Slater integrals in the transition amplitudes by a constant factor if the relative phases remain unchanged or when there is one dominant transition amplitude. In the following we will consider several special cases in which this condition is approximately satisfied. We will not consider very weak lines or lines having a very small α_2 value because for these transitions the results are sensitive to all correlation effects making conclusions difficult. Since the ξ_2 parameters are proportional to sine of the phase difference the diagonal terms $\kappa = \kappa'$ are canceled in Eq. (9). Therefore ξ_2 is not stable against usually large many-electron effects in the weak partial amplitudes, which makes ξ_2 much more sensitive to correlation.

A. Influence of the orbital set

We start by considering the influence of the choice of one-electron orbitals. From Table VII we see that for Ar L_3MM transitions the total IE and FE rates are 6.88 and 5.10 ma.u., respectively. This gives a relative difference of 35% with respect to FE value. Still the changes in the branching ratios are much smaller except for the weakest lines. For the strong $L_3M_{2,3}M_{2,3}\ ^3P_2$ line the relative intensity differs by 6.3%. However, from Table I we see that corresponding change in the α_2 parameter is only 0.13%. This behavior can be related to the changes in the transition amplitudes and their relative phase shifts. The small changes in the branching ratios is explained by a *uniform scaling* of the squares of the Slater integrals appearing in the transition amplitudes by 25–30 %. The even smaller changes in the α_2 parameter are due to the fact that the $L_3M_{2,3}M_{2,3}\ ^3P_2$ line is dominated by the p_j $(j = 1/2, 3/2)$ transition amplitudes, whereas the d_j $(j = 3/2, 5/2)$ amplitudes are very small. The p_j $(j = 1/2, 3/2)$ partial waves have a very small phase difference in both approximations making the phase factor $\cos\Delta_{\kappa\kappa'}$ close to one. The common scaling factor of these partial amplitudes is then normalized out in Eq. (A26), leaving α_2 unchanged. For the Ar $L_3M_{2,3}M_{2,3}\ ^1D_2$ line the situation is different because now also the $d_{5/2}$ partial wave has a non-negligible partial amplitude. The interference between the d_j and p_j amplitudes gives rise to a somewhat larger change in the α_2 parameter. This indicates that the α_2 parameters are particularly insensitive to the choice of orbitals when only one orbital angular momentum value significantly contributes to the line strength. For the Kr $M_{4,5}NN$ and Xe $N_{4,5}OO$ Auger spectra the difference between the IE and FE total rates is much smaller than for the Ar L_3MM spectrum. Due to the substantially lower kinetic energy the scaling of these transition amplitudes is not uniform, but depends on the quantum numbers of the participating electrons. This is reflected in larger changes in the branching ratios. However, the changes in the corresponding α_2 parameters are still very small because of the normalization effect.

B. The relaxation effect

The dependence of relaxation on the principal and angular momentum quantum numbers of the initial and final holes and the Auger electron has been recently studied by Tulkki and Mäntykenttä [35]. This study makes a distinction between three basic cases.

(1) For Auger transitions corresponding to final holes in deep inner shells the *sudden approximation* is valid and the relaxation reduces all line strengths by a constant overlap factor. Accordingly the effect of relaxation on both the branching ratios and the angular dependence is very small.

(2) For high kinetic-energy (more than 300–400 eV) Auger transitions leading to double holes in the valence shell, the total rate and the branching ratios are practically not influenced by relaxation. The same applies to the corresponding α_2 parameters. For cases (1) and (2) the relaxation primarily implies an isotropic contraction of the electron density. A small effect on angular distribution is thus consistent with this general picture of the relaxation process.

(3) Low-energy valence-shell Auger transitions are subject to a more complicated relaxation effect [35]. In this case the overlap factor in the $D^0_{\mu\nu}$ amplitude in Eq. (5) is usually very close to one, but the Slater integrals in this partial amplitude may be modified by contraction or expansion of the one-electron orbitals. Also the conjugate amplitudes $\tilde{D}_{\mu\nu}$ as well as the kinetic energy D_μ and the constant D_0 amplitudes can all make an important contribution. As a result the relaxation can either *increase* or *decrease* the line strengths. This can lead to significant changes in the branching ratios [47]. When several partial waves having different orbital angular momenta contribute to an Auger line in category (3) the relaxation can also affect the angular anisotropy if one of the contributing partial waves is sensitive to the orbital-collapse phenomenon [49].

C. The exchange interaction

The comparison between the α_2 values obtained using single-channel amplitudes without exchange (I) and multichannel amplitudes with exchange (FEMC) suggests that with regard to the α_2 parameter the exchange and FCSCI effects partially compensate each other. The same holds true also for the total rates and branching ratios with a few exceptions. In the case of the spin-polarization parameters ξ_2 the compensation is less systematic. A separate comparative study of intrachannel interaction and exchange integrals is necessary to find out if this compensation is more universal.

The Kr $M_5N_1N_{2,3}\ ^1P_1$ (Table VIII) line demonstrates that one should not make too far reaching conclusions on the basis of calculations neglecting exchange interaction. The intensity of this line is increased substantially when exchange is taken into account, but it is reduced again by channel interaction. The corresponding α_2 values -0.632 (I), -0.685 (IE), and -0.569 (FEMC) behave qualitatively in the same way. The Kr $M_5N_1N_{2,3}\ ^1P_1$ Auger line involves the $p_{3/2}$, $f_{5/2}$, and $f_{7/2}$ partial waves. The branching ratios of the f_j, $j = 5/2, 7/2$, partial rate to the $p_{3/2}$ partial rate are 4.69 and 2.01 in I and FEMC calculations, respectively. Since the $f_{5/2,7/2}$

amplitudes dominate in both cases this dramatic change in the branching ratio results only in a small differences in the corresponding α_2 parameters. In contrast, the ξ_2 values pertaining to this line were found to be -0.0094 and 0.003 45 (not shown in Table II) for I and FEMC calculations, respectively. In spite of the smallness of these values they demonstrate that a calculation neglecting exchange interaction would obviously give very poor estimates for any variable that depends on the sine of the phase differences $\Delta_{\kappa\kappa'}$.

D. The influence of FCSCI

The FCSCI differs from the previous effects in that it changes the relative phases through the phase matrix in Eq. (A10). Nondiagonal terms (usually small for high kinetic energies) in $Z^{-}_{\alpha\Gamma}$ result in mixing of transition amplitudes in the multichannel amplitude in Eq. (3). Presumably the α_2 and especially the ξ_2 parameter would then be sensitive to this correlation effect. A comparative study of the effect of FCSCI on α_2 parameters and branching ratios and total rates shows, however, that again the relative changes in the α_2 parameters are typically smaller than the changes in the branching ratios. For the Auger transitions studied in this work the total rate is least sensitive to the FCSCI. As an example we consider the Kr $M_{4,5}N_{2,3}N_{2,3}\ ^3P_2$ transitions. FCSCI increases the intensity of these lines by a factor of 3.4 and 3.1 for the M_4 and M_5 initial holes, respectively. In contrast the changes in the α_2 parameters are small. This can be traced back to the dominance of the $d_{5/2}$ partial wave making the α_2 parameter insensitive to changes in the absolute values of the transition amplitudes. Accordingly, the minor changes in α_2 of these lines are foremost due to the multichannel phase shifts. A counterexample showing a strong FCSCI effect both in the line strength and α_2 is provided by the Kr $M_{4,5}N_1N_{2,3}\ ^1P_1$ lines. Here both $p_{1/2}$ and $f_{5/2}$ ($p_{3/2}$ and $f_{7/2}$ for the M_5 hole) have large amplitudes. Therefore the large change in the intensity ratio of these channels is accompanied by a large change in the α_2 parameter. Note that the corresponding Xe $N_{4,5}O_1O_{2,3}\ ^1P_1$ transitions are governed by the f_j partial waves and therefore the changes of α_2 parameters are much smaller.

V. CONCLUSIONS

The angular anisotropy α_2 and spin-polarization ξ_2 parameters have been calculated for the L_3MM Auger transitions in Ar, $M_{4,5}NN$ transitions in Kr and Xe and $N_{4,5}OO$ transitions in Xe by MMCDF method. It is found that the α_2 values are insensitive to relaxation. The exchange and channel interactions are very important for low-energy Auger transitions in Kr and Xe. However, these two effects influence the α_2 values in opposite directions and partly compensate each other. For the high-energy Auger electrons (L_3MM in Ar and $M_{4,5}NN$ in Xe) the effects of exchange and channel interaction are much smaller and may in general be disregarded. The calculated values of the α_2 parameters agree well with the available experimental data. The spin-polarization parameter ξ_2, which determines the dynamical polarization, is found to be very small for the majority of transitions. We have found several lines with comparatively large spin polarization ($\xi_2 > 0.3$); however, all these lines are rather weak, which makes an experimental study of ξ_2 difficult. It is suggested that the use of circularly polarized photons to polarize the initial state of the Auger transition and the measurement of the resulting spin polarization of Auger electrons would be a more selective probe of the theory. Finally we have shown by a comparative study of α_2 parameters and branching ratios that due to various normalization and compensation effects the latter are as a rule more sensitive to many-electron effects. Large discrepancies between theory and experiment remain for the branching ratios of some Auger lines indicating that important many-electron effects such as the FISCI with the triple-hole configurations giving rise to correlation satellites are not included in our calculations.

ACKNOWLEDGMENTS

We thank M. H. Chen for information concerning his calculations of angular distributions and A. Mäntykenttä for putting the MMCDF Xe $M_{4,5}OO$ transition amplitudes at our disposal. We are grateful to T. Åberg, W. Mehlhorn, V. Schmidt, and B. Krässig for interesting and fruitful discussions. One of the authors (N.M.K.) gratefully acknowledges the hospitality of the Bielefeld University. This work was supported in Helsinki by the Academy of Finland and in Bielefeld by the Deutsche Forschungsgemeinschaft under Contract No. SFB216.

APPENDIX: RELATIVISTIC THEORY OF ANGULAR DISTRIBUTION AND SPIN POLARIZATION OF AUGER ELECTRONS

We have recently [37] described how various many-electron effects are included in the calculation of angle-integrated Auger rates using the MMCDF method. In this complementary appendix we describe the calculation of angular distribution and spin polarization of Auger electrons. In Ref. [37] we emphasized that the theoretical and computational methods utilized in the construction of the MMCDF wave functions are independent of the atomic ionization or scattering process under consideration. In analogy we will use the general density-matrix formalism to stress the close connection between angular distribution and spin polarization of Auger electrons and photoelectrons. The following results can also be easily generalized to allow for the one-step treatment of excitation and nonradiative decay of inner-shell-hole states within the framework of scattering theory [41].

In the construction of final-state many-electron wave functions we will use two kinds of one-electron continuum wave functions. The spherical one-electron states corresponding to definite values of energy, orbital angular momentum, total angular momentum, and its component in

a specified direction are given by

$$|\chi_{\varepsilon\kappa m}\rangle = \frac{1}{r}\begin{pmatrix} G_{\varepsilon\kappa}\Omega_{\kappa m} \\ iF_{\varepsilon\kappa}\Omega_{-\kappa m}\end{pmatrix}. \tag{A1}$$

In Eq. (A1) the large $G_{\varepsilon\kappa}$ and small $F_{\varepsilon\kappa}$ radial components of the four spinors are solutions of the nonlocal Dirac-Fock equation. The quantum number κ is defined by $\kappa = -2(j-l)(j+1/2)$ and the total energy of the electron by $E = (\varepsilon + c^2)^{1/2}$.

The angular part of the functions (A1) is given by the two-component spinors

$$\Omega_{\kappa m} = \begin{bmatrix} \langle l\, m - \frac{1}{2}s\, \frac{1}{2}|jm\rangle Y_{l\, m-1/2} \\ \langle l\, m + \frac{1}{2}s - \frac{1}{2}|jm\rangle Y_{lm+1/2}\end{bmatrix}. \tag{A2}$$

The spherical states (A1) are energy-normalized according to $\langle\chi_{\varepsilon\kappa m}|\chi_{\varepsilon'\kappa' m'}\rangle = \delta(\varepsilon - \varepsilon')\delta_{\kappa\kappa'}\delta_{mm'}$ and asymptotically the radial components are given by

$$G_{\varepsilon\kappa} = \left(\frac{\varepsilon + 2c^2}{\pi c^2 p}\right)^{1/2} \cos[\, pr - (l+1)\pi/2 + y\ln 2pr + \sigma_\kappa + \delta],$$

$$F_{\varepsilon\kappa} = -\left(\frac{\varepsilon}{\pi c^2 p}\right)^{1/2} \sin[\, pr - (l+1)\pi/2 + y\ln 2pr + \sigma_\kappa + \delta] \tag{A3}$$

where $\sigma_\kappa = (l+1)\pi/2 - \arg\Gamma(\gamma + iy) + \eta - 1/2\pi\gamma$ and δ is the phase shift coming from the short-range non-Coulombic part of the central field potential. In Eq. (A3) y , γ, and η are given by

$$\begin{aligned} y &= Z(\varepsilon + c^2)/c^2 p, \\ \gamma &= (\kappa^2 - Z^2/c^2)^{1/2}, \\ e^{2i\eta} &= -\frac{[\kappa - iyc^2/(\varepsilon + c^2)]}{\gamma + iy} \end{aligned} \tag{A4}$$

where Z is the charge of the ion.

The spherical states (A1) are used in the construction of the final-state many-electron wave functions corresponding to a fixed value of total angular momentum of the ion and continuum electron. In contrast, an ionized electron propagating in a fixed direction in space is most conveniently described by means of helicity states. These solutions of the one-electron Dirac-Fock equation correspond to a fixed asymptotic value of the electron wave vector $\mathbf{p}$ and the component of spin in the direction of the wave vector (helicity). The helicity operator is given by $\frac{1}{2}\boldsymbol{\Sigma}\cdot\mathbf{n}$ where $\mathbf{n} = \mathbf{p}/|\mathbf{p}|$ and $\boldsymbol{\Sigma}$ is constructed from the Pauli spin matrices

$$\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma}\end{pmatrix}. \tag{A5}$$

The helicity states can be expressed in terms of the spherical states (A1) as

$$|\chi_{\mathbf{p}\mu}\rangle = \left(\frac{c^2}{\mathrm{p}(\varepsilon + \mathrm{c}^2)}\right)^{1/2} \times \sum_{j,l,\nu}\left(\frac{2l+1}{4\pi}\right)^{1/2} \exp[-i(\sigma_\kappa + \delta)]i^l \times \langle l0\tfrac{1}{2}\mu|j\mu\rangle D^{(j)}_{\mu,\nu}(\phi,\theta,0)^*|\chi_{\varepsilon\kappa\nu}\rangle. \tag{A6}$$

In the rotation matrix $D^{(j)}_{\mu\nu}$ [50] the angles θ and ϕ specify the direction of $\mathbf{p}$ with respect to the laboratory frame. The helicity states (A6) are normalized according to $\langle\chi_{\mathbf{p}\mu}|\chi_{\mathbf{p}'\mu'}\rangle = \delta(\mathbf{p} - \mathbf{p}')\delta_{\mu\mu'}$.

In the transition matrix elements the one-electron continuum states (A1) or (A6) are coupled and antisymmetrized with the ionic ASF to give the total many-electron wave function. The multiconfiguration ASF's of the final (f) and initial (i) ionic state are in general given as a linear superposition

$$|\Psi_\beta\rangle = \sum_{\alpha=1}^{N_s} C^\beta_\alpha |\psi_\alpha\rangle \tag{A7}$$

of the N_s, $s = (i, f)$, ionic configuration-state functions $|\psi_\alpha\rangle$. In Eq. (A7) we have for brevity combined the quantum numbers $\beta_s J_s M_s$, $s = (i, f)$, into one index β. The multiconfiguration single-channel state is defined as a properly coupled antisymmetrized product

$$|\phi_{\beta_f J_f \kappa E J M}\rangle = \mathcal{A}\{|\Psi_{\beta_f J_f}\rangle|\chi_{\kappa\varepsilon}\rangle\}, \tag{A8}$$

where the total energy $E = E_f + \varepsilon$ is given with respect to the total rest energy of the system. In Eq. (A8) the angular momentum of the ion is denoted by J_f and the total angular momentum of the ion and Auger electron by J, respectively. The spherical incoming-wave normalized multiconfiguration multichannel wave functions $|\Phi^-_{\Gamma_f J_f \kappa E J M}\rangle$ are obtained by diagonalizing the total Hamiltonian in the subspace (A8). The details of the computational approach has been given in Ref. [37] and hence we only give the final result of the diagonalization ($\Gamma = \Gamma_f J_f \kappa J M$)

$$|\Phi^-_{\Gamma E}\rangle = \sum_{\alpha=1}^{N_c}\left(|\phi_{\alpha E}\rangle + \sum_{\beta=1}^{N_c} \mathrm{P}\int \frac{|\phi_{\beta E'}\rangle\langle\phi_{\beta E'}|K|\phi_{\alpha E}\rangle}{E - E'}dE'\right) Z^-_{\alpha\Gamma}. \tag{A9}$$

where the K matrix describes the coupling between the N_c ionization channels. The incoming-wave boundary condition is accounted for by the phase factor

$$Z^-_{\alpha\Gamma} = \sum_{\Lambda=1}^{N_c} U_{\alpha\Lambda}\cos\eta_\Lambda \exp(-i\eta_\Lambda) U_{\Gamma\Lambda}\exp(-i\delta_\Gamma) \tag{A10}$$

where the multichannel phase shifts δ_Γ and the vector components $U_{\alpha\Lambda}$ are obtained by diagonalizing the K matrix on the energy shell [37].

The many-electron helicity states are obtained in analogy to (A6) as a linear combination of spherical waves (A9).

$$|\Phi^-_{\Gamma_f J_f M_f \mathbf{p}\mu}\rangle = \left(\frac{c^2}{p(\varepsilon+c^2)}\right)^{1/2} \sum_{j,l} \exp(-i\sigma_\kappa) i^l \langle l 0 \tfrac{1}{2}\mu | j\mu\rangle \left(\frac{2l+1}{4\pi}\right)^{1/2} \times \sum_{J,M'} \langle J_f M_f j\mu | J M_f+\mu\rangle D^{(J)}_{M' M_f+\mu}(\phi,\theta,0)^* |\Phi^-_{\Gamma_f J_f \kappa E J M'}\rangle. \quad \text{(A11)}$$

Here $\Gamma_f J_f$ specifies the final ionic ASF. The total energy $E = E_f + \varepsilon$, where $\varepsilon = \sqrt{c^4 + c^2|\mathbf{p}|^2} - c^2$. The magnetic quantum numbers M_f and μ are given with respect to the detector frame whereas the quantum number M' of the spherical states is given with respect to the laboratory frame. The detector frame is obtained from the laboratory frame by first rotating it around the z axis by an angle ϕ and by a subsequent rotation by θ around the new y axis. Both rotations are counterclockwise when looking down the rotation axis toward the origin. The many-electron states (A9) and (A11) are normalized in the same way as the corresponding one-electron states (A1) and (A6). Note that the definitions (A9)–(A11) imply that in the single-channel case $Z_{\alpha\Gamma} = \delta_{\alpha\Gamma}\exp(-i\delta_\Gamma)$.

We will now use wave functions (A9) and (A11) to obtain transition rates, angular distributions, and spin polarizations of Auger electrons. In the following we assume a two-step treatment of the Auger decay. We simplify the derivation by neglecting the lifetime broadening and assuming an ideal energy resolution which allows for a distinction between each Auger line corresponding to a pair of initial and final ionic ASF's. In the real experiment this means resolving the different fine-structure components of the Auger lines. The lifetime broadening and finite energy resolution can be taken into account afterwards by taking appropriate weighted averages of the following results.

We define the density matrix $\boldsymbol{\rho}^{(f)}$ and density operator $\hat{\rho}^{(f)}$ in terms of the helicity states (A11) by

$$\hat{\rho}^{(f)} = \sum_{\Lambda\Lambda'} \langle\Phi^-_{\Lambda'}|\rho^{(f)}|\Phi^-_\Lambda\rangle |\Phi^-_{\Lambda'}\rangle\langle\Phi^-_\Lambda| \quad \text{(A12)}$$

where Λ stands for quantum numbers $(\Gamma_f J_f M_f \mathbf{p}\mu)$. The sum is taken over all final states on the energy shell $E = E_i = E_f + \varepsilon$. Thus (A12) also implies an integration over the direction of $\mathbf{p}$. The diagonal elements $\langle\Phi^-_\Lambda|\rho^{(f)}|\Phi^-_\Lambda\rangle$ of the density matrix give the relative probability that after the Auger decay the ion will be found in a state characterized by the quantum numbers Γ_f, J_f, and M_f and that the Auger electron has a wave vector $\mathbf{p}$ and helicity μ.

In the following we make a distinction between two kind of spectroscopic experiments. We first consider measurements which aim at determining the relative probability that the system ion plus Auger electron is in a specified subspace of the total "energy shell" (A11) after the decay process. We define the detector operator $\hat{F}$ (also known as detector efficiency operator [52])

$$\hat{F} = \sum_{\substack{\Lambda \\ \text{(obs states)}}} |\Phi^-_\Lambda\rangle\langle\Phi^-_\Lambda| \quad \text{(A13)}$$

where the sum is taken over those final states that are observed in the experiment. The relative probability of detecting the system in subspace (A13) is then given by

$$W = \mathrm{Tr}[\boldsymbol{\rho}^{(f)}\mathbf{F}]/\mathrm{Tr}[\boldsymbol{\rho}^{(f)}]. \quad \text{(A14)}$$

In (A14) $\hat{F}$ effectively projects out the relevant part of the density matrix.

As an example we consider angle-resolved measurement of Auger electrons which resolves the fine structure but leaves the asymmetry of the final ion and the helicity undetected. The detector operator is then given by

$$\hat{F}_A = \sum_{M_f \mu} |\Phi^-_{\Gamma_f J_f M_f \mathbf{p}\mu}\rangle\langle\Phi^-_{\Gamma_f J_f M_f \mathbf{p}\mu}| \quad \text{(A15)}$$

and the angular distribution of the selected Auger line is obtained by inserting (A15) into (A14).

In the second kind of experiment one determines an expectation value of a physical variable. The physical variable may be associated with the Auger electron only (spin polarization) or the ion (alignment in the final ionic state). The expectation values are again defined for the observed subset of the energy-allowed final states. Assuming that the final states to be observed in the experiment are specified by the detector operator $\hat{F}$ the expectation value of an operator $\hat{X}$ is given by

$$\langle X\rangle = \mathrm{Tr}[\boldsymbol{\rho}^{(f)}\mathbf{X}\mathbf{F}]/\mathrm{Tr}[\boldsymbol{\rho}^{(f)}\mathbf{F}]. \quad \text{(A16)}$$

As an example consider the measurement of the component of the spin-polarization vector perpendicular to the scattering plane. The matrix representation of $\hat{P}_\perp$ in the space of the helicity states in (A15) is given by

$$\mathbf{P}_\perp = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \text{(A17)}$$

and the spin polarization is obtained from $P_\perp = \mathrm{Tr}[\boldsymbol{\rho}^{(f)}\mathbf{P}_\perp\mathbf{F}]/\mathrm{Tr}[\boldsymbol{\rho}^{(f)}\mathbf{F}]$.

In both measurements (A14) and (A16) the final-state density matrix is needed in the calculation of the trace of matrices. The final-state density matrix is connected to the initial-state density matrix by

$$\boldsymbol{\rho}^{(f)} = \mathbf{T}\boldsymbol{\rho}^{(i)}\mathbf{T}^\dagger \quad \text{(A18)}$$

where $\mathbf{T}$ is the transition matrix [51] $T_{i,f} = \langle\Psi_{\gamma_i J_i M_i}|H_I|\Phi^-_{\alpha_f J_f M_f \mathbf{p}\mu}\rangle$. Here H_I denotes the static electron-electron interaction or its generalization $H - E$ according to Eq. (4) and possibly also the Breit interaction. Using $dE = (c^2 p/E)dp$ it follows from (A18) that the total Auger rate in atomic units is

$$W^{(T)}_{J_i \to J_f} = 2\pi \mathrm{Tr}[\boldsymbol{\rho}^{(f)}\mathbf{F}_T] = 2\pi \mathrm{Tr}[\mathbf{T}\boldsymbol{\rho}^{(i)}\mathbf{T}^\dagger\mathbf{F}_T]. \quad \text{(A19)}$$

The detector operator $\hat{F}_T = \int \hat{F}_A d\Omega_{\mathbf{p}}$ includes a sum over all states on the energy shell $E = E_f + \varepsilon$. The angle-resolved differential rate is correspondingly given by

$$\frac{dW_{J_i\to J_f}(\theta,\phi)}{d\Omega} = 2\pi \mathrm{Tr}[\boldsymbol{\rho}^{(f)}\mathbf{F}_A] = 2\pi \mathrm{Tr}[\mathbf{T}\boldsymbol{\rho}^{(i)}\mathbf{T}^\dagger \mathbf{F}_A]. \tag{A20}$$

For Auger decay the initial state only includes electrons and we can thus write the initial-state density matrix in terms of the statistical tensors [52]. Since it is assumed that the experiment resolves all initial-state ASF's, the normalized, $\mathrm{Tr}[\boldsymbol{\rho}^{(i)}] = 1$, initial-state density matrix describes the population of magnetic sublevels corresponding to the total initial-state angular momentum J_i. We can expand the density operator as

$$\hat{\rho}^{(i)} = \sum_{K,Q} \mathcal{A}_{KQ} \hat{T}^{(K)}_Q \tag{A21}$$

where

$$\hat{T}^{(K)}_Q = (2J_i+1)^{1/2} \sum_{M,M'} (-1)^{J_i - M'} \langle J_i M \; J_i - M' | KQ\rangle \times |\Psi_{\gamma_i J_i M}\rangle\langle \Psi_{\gamma_i J_i M'}|. \tag{A22}$$

The total and angle-differential Auger rates can now be obtained as an expansion over the state multipoles by inserting Eqs. (A21) and (A22) in Eqs. (A19) and (A20), by inserting the helicity states (A11) in the detector operators, and summing over the magnetic quantum numbers. The spin polarization $P_\perp$ is correspondingly obtained from Eq. (A16) by using the matrix (A17). Assuming that the initial state has been excited by unpolarized photons we obtain the well-known results

$$W^{(T)}_{J_i\to J_f} = \frac{2\pi}{2J_i+1} \sum_\kappa |\langle \Psi_{\gamma_i J_i} \| H_I \| \Phi^-_{\Gamma_f J_f \kappa E J_i}\rangle|^2, \tag{A23}$$

$$\frac{dW_{J_i\to J_f}(\theta,\phi)}{d\Omega} = \frac{W^{(T)}_{J_i\to J_f}}{4\pi}\left(1 + \sum_{K=2\ (\mathrm{even})} \alpha_K \mathcal{A}_{K0} P_K(\cos\theta)\right), \tag{A24}$$

$$P_\perp = \left(\sum_{K=2\ (\mathrm{even})} \beta_K \mathcal{A}_{K0} \bar{P}^1_K(\cos\theta)\right) \times \left(1 + \sum_{K=2\ (\mathrm{even})} \alpha_K \mathcal{A}_{K0} P_K(\cos\theta)\right)^{-1} \tag{A25}$$

where in dipole approximation only $K = 2$ is allowed. In Eqs. (A24) and (A25) $P_K(\cos\theta)$ and $\bar{P}^1_K(\cos\theta)$ are the standard Legendre polynomial and normalized associated Legendre functions, respectively [50].

The angular anisotropy parameter α_2 is given by

$$\alpha_K = \frac{1}{N}(-1)^{J_i+J_f-1/2} \sum_{l,l',\,j,j'} [\,l,l',j,j',J_i]^{1/2} \langle l0l'0|K0\rangle \begin{Bmatrix} J_i & J_i & K \\ j & j' & J_f \end{Bmatrix} \times \begin{Bmatrix} j & j' & K \\ l' & l & \frac{1}{2} \end{Bmatrix} \langle \Psi_{\gamma_i J_i} \| H_I \| \Phi^-_{\Gamma_f J_f \kappa' E J_i}\rangle \langle \Phi^-_{\Gamma_f J_f \kappa E J_i} \| H_I \| \Psi_{\gamma_i J_i}\rangle, \tag{A26}$$

$$N = \sum_\kappa |\langle \Psi_{\gamma_i J_i} \| H_I \| \Phi^-_{\Gamma_f J_f \kappa E J_i}\rangle|^2$$

and the spin polarization parameter by

$$\beta_K = \frac{\sqrt{12}}{N}(-1)^{J_i+J_f-1/2} \sum_{l,l',\,j,j'} (-1)^{1/2+l-j'} [l,l',j,j',J_i]^{1/2} \langle l0l'0|K0\rangle \begin{Bmatrix} J_i & J_i & K \\ j & j' & J_f \end{Bmatrix} \times \begin{Bmatrix} l & l' & K \\ \frac{1}{2} & \frac{1}{2} & 1 \\ j & j' & K \end{Bmatrix} \mathrm{Im}(\langle \Psi_{\gamma_i J_i} \| H_I \| \Phi^-_{\Gamma_f J_f \kappa' E J_i}\rangle \langle \Phi^-_{\Gamma_f J_f \kappa E J_i} \| H_I \| \Psi_{\gamma_i J_i}\rangle) \tag{A27}$$

where $[a,b,\ldots]^{1/2} = [(2a+1)(2b+1)\cdots]^{1/2}$. The results (A26) and (A27) are equivalent to the results of Kabachnik and Sazhina [3]. Above we assumed that the incoming photons are unpolarized and the angle θ is measured with respect to the photon wave vector. For linearly polarized photons the axis of alignment coincides with the direction of the electric-field vector. Therefore Eqs. (A26) and (A27) can be applied as such, but the angle θ is now measured with respect to the polarization vector of the incoming photons. Correspondingly $P_\perp$ now gives the component of the spin polarization perpendicular to the plane defined by the Auger electron wave vector and the polarization vector of photons.

* Permanent address: Institut of Nuclear Physics, Moscow State University, Moscow 119899, Russia.

[1] W. Mehlhorn, Phys. Lett. **26A**, 166 (1968).
[2] E. G. Berezhko and N. M. Kabachnik, J. Phys. B **10**, 2467 (1977).
[3] N. M. Kabachnik and I. P. Sazhina, J. Phys. B **17**, 1335 (1984).
[4] U. Hahn, J. Semke, H. Merz, and J. Kessler, J. Phys. B **18**, L417 (1985).
[5] T. A. Carlson, D. R. Mullins, C. E. Beall, B. W. Yates, J.

W. Taylor, D. W. Lindle, B. P. Pullen, and F. A. Grimm, Phys. Rev. Lett. **60**, 1382 (1988).
[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, V. Schmidt, W. Mehlhorn, W. B. Peatman, F. Schaefers, and T. Schroeter, J. Phys. B **22**, L597 (1989).
[8] U. Becker in *The Physics of Electronic and Atomic Collisions*, edited by A. Dalgarno, R. S. Freund, P. M. Koch, M. S. Lubell, and T. B. Lucatorto, AIP Conf. Proc. No. 205 (AIP, New York, 1989), p. 162.
[9] B. Kämmerling, B. Krässig, and V. Schmidt, J. Phys. B **23**, 4487 (1990); the error limits of the data presented in this work were later reconsidered by V. Schmidt and B. Krässig. Our Table V includes these revised data.
[10] H. Merz and J. Semke, in *X-ray and Inner-Shell Processes*, Proceedings of the X-90 Conference, edited by Invited Preventations, AIP Conf. Proc. No. 215 (AIP, New York, 1990), p. 719.
[11] L. Sarkadi, T. Vajnai, J. Palinkas, A. Köver, J. Vegh, and T. Mukoyama, J. Phys. B **23**, 3643 (1990).
[12] S. Ricz, J. Vegh, I. Kadar, B. Sulik, D. Varga, and D. Berenyi, Nucl. Instrum. Methods B **61**, 411 (1991).
[13] C.D. Caldwell, in *X-ray and Inner-Shell Processes*, Proceedings of the X-90 Conference (Ref. [10]), p. 685.
[14] S. Ricz, I. Kadar, V. A. Schegolev, D. Varga, J. Vegh, D. Berenyi, G. Hock, and B. Sulik, J. Phys. B **19**, L411 (1986).
[15] R. Kuntze, N. Böwering, N. Salzmann, and U. Heinzmann (unpublished).
[16] B. Kämmerling, B. Krässig, O. Schwarzkopf, J. P. Ribeiro, and V. Schmidt, J. Phys. B **25**, L5 (1992).
[17] S. B. Whitfield, C. D. Caldwell, D. X. Huang, and M. O. Krause, J. Phys. B **25**, 4755 (1992).
[18] N. M. Kabachnik and I. P. Sazhina, Opt. Spektrosk. **60**, 683 (1986) [Opt. Spectrosc. (USSR) **60**, 1106 (1986)].
[19] K. Blum, B. Lohmann, and E. Taute, J. Phys. B **19**, 3815 (1986).
[20] N. M. Kabachnik and I. P. Sazhina, J. Phys. B **21**, 267 (1988).
[21] N. M. Kabachnik, I. P. Sazhina, I. S. Lee, and O. V. Lee, J. Phys. B **21**, 3695 (1988).
[22] J. W. Cooper, Phys. Rev. A **39**, 3714 (1989).
[23] N. M. Kabachnik and O. V. Lee, Z. Phys. D **17**, 169 (1990).
[24] N. M. Kabachnik, B. Lohmann, and W. Mehlhorn, J. Phys. B **24**, 2249 (1991).
[25] B. Lohmann, J. Phys. B **23**, 3147 (1990).
[26] B. Lohmann, J. Phys. B **24**, 861 (1991).
[27] U. Hergenhahn, N. M. Kabachnik, and B. Lohmann, J. Phys. B **24**, 4759 (1991).
[28] M. H. Chen, Phys. Rev. A **45**, 1684 (1992); the small discrepancies between our results I in Tables I–VI and those obtained by Chen may be due to small differences in the optimization of bound orbitals or in the construction of the direct part of the jj-average potential for the continuum electron.
[29] B. Lohmann, J. Phys. B **25**, 4163 (1992).
[30] G. Howat, T. Åberg, and O. Goscinski, J. Phys. B **11**, 1575 (1978).
[31] G. Howat, J. Phys. B **11**, 1589 (1978).
[32] K. R. Karim and B. Crasemann, Phys. Rev. A **31**, 709 (1985), and references therein.
[33] S. Fritzsche, B. Fricke, and E.-D. Sepp, Phys. Rev. A **45**, 1465 (1992).
[34] S. Fritzsche and B. Fricke, Phys. Scr. **T41**, 45 (1992).
[35] J. Tulkki and A. Mäntykenttä, Phys. Rev. A **47**, 2995 (1993).
[36] M. H. Chen, B. Crasemann, M. Aoyagi, and H. Mark, Phys. Rev. A **18**, 802 (1978).
[37] J. Tulkki, T. Åberg, A. Mäntykenttä, and H. Aksela, Phys. Rev. A **46**, 1357 (1992).
[38] H. Kelly, Phys. Rev. A **11**, 556 (1975).
[39] N. M. Kabachnik, J. Phys. B **14**, L337 (1981).
[40] U. Fano, Phys. Rev. **124**, 1866 (1961).
[41] T. Åberg, and G. Howat, in *Encyclopedia of Physics*, edited by S. Flügge and W. Mehlhorn (Springer, Berlin, 1982), Vol. 31, p. 469.
[42] P. O. Löwdin, Phys. Rev. **97**, 1474 (1955).
[43] H. Aksela, S. Aksela, and H. Pulkkinen, Phys. Rev. A **30**, 865 (1984).
[44] H. Aksela, S. Aksela, and H. Pulkkinen, Phys. Rev. A **30**, 2456 (1984).
[45] K. G. Dyall and F. P. Larkins, J. Phys. B **15**, 2793 (1982).
[46] I. P. Grant, B. J. McKenzie, P. H. Norrington, D. F. Mayers, and N. C. Pyper, Comput. Phys. Commun. **21**, 207 (1980).
[47] A. Mäntykenttä, Phys. Rev. A **47**, 3961 (1993).
[48] K. G. Dyall, I. P. Grant, C. T. Johnson, F. A. Parpia, and E. P. Plummer, Comput. Phys. Commun. **55**, 425 (1989).
[49] A. F. Starace, in *Encyclopedia of Physics* (Ref. [41]), p. 1.
[50] A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, 1974).
[51] J. Tulkki and T. Åberg, J. Phys. B **13**, 3341 (1980); J. Tulkki, *ibid.* **17**, 3493 (1984).
[52] K. Blum, *Density Matrix Theory and Applications* (Plenum, New York, 1981).
[53] G. C. King and F. H. Read, in *Atomic Inner-shell Physics*, edited by B. Crasemann (Plenum, New York, 1985), p. 317.
[54] U. Becker (unpublished), data are taken from Ref. [24].
[55] Experimental data measured by H. Aksela, S. Aksela, and H. Pulkkinen using electron-beam excitation and high-resolution cylindrical mirror-type electron spectrometer. The Ar $L_{2,3}MM$ data are unpublished, Kr $M_{4,5}NN$ data are taken from Ref. [43].