Influence of the initial- and final-state configuration interaction on the anisotropy of the resonant Auger decay of Kr $3d^{-1}5p$ and Xe $4d^{-1}6p$ states

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The anisotropy of the resonant Auger decay of photon-excited Kr $3d^{-1}_{3/2,5/2}5p$ and Xe $4d^{-1}_{3/2,5/2}6p$ states has been studied by the multiconfiguration Dirac-Fock method. The calculations account for the configuration interaction both in the initial and in the final states of the Auger decay. For the nonresolved $nd^{-1}(n+2)p$ $(J=1)$ resonances ($n=3$ for Kr, and $n=4$ for Xe) the average intensities and the anisotropies of the Auger lines were calculated by weighing each partial rate by the pertinent Dirac-Fock photoexcitation probabilities. Our results show that, in addition to the initial- and final-state correlation, both the relaxation and the exchange interaction have a substantial effect on the anisotropy of these Auger spectra. For most Auger lines there is good agreement between our calculated β parameters and experimental values for the Kr and Xe $nd^{-1}_{5/2}(n+2)p$ photoexcitation resonances; there is also satisfactory agreement for the Kr $3d^{-1}_{3/2}5p$ and Xe $4d^{-1}_{3/2}6p$ resonant Auger spectra. However, the remaining notable discrepancies between theory and experiment indicate that important correlation effects are still omitted in our calculations. Discrepancies between different experimental results stress the need for further improvements on the experimental side.

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I. INTRODUCTION

Photoinduced resonant Auger transitions as well as normal Auger transitions result in anisotropic angular distribution of Auger electrons. The angular dependence of Auger emission is governed by the product of two factors characterizing the alignment of the initial state produced by incoming photon beam and the intrinsic anisotropy of the Auger decay. Although this anisotropy is well understood in general, there are Auger lines for which the anisotropy is highly sensitive to the intricate details of the atomic structure, thus prompting an elaborate theoretical study of the underlying many-electron dynamics. In particular the anisotropy of normal and resonant Auger decay has been found to depend critically on the final-ionic-state configuration interaction (FISCI) [1–7].

In the multiconfiguration Dirac-Fock (MCDF) method it is useful to distinguish between two different FISCI effects. The first contribution comes from the mixing of jj coupled configurations resulting from the same nonrelativistic parent. This kind of configuration interaction (CI) is governed by spin-orbit interaction and gives rise to intermediate coupling in the many-electron wave function. The coupling of angular momenta within the final ion and between the ion and the Auger electron will directly influence the space part of the wave function. Therefore the intrinsic anisotropy of Auger process is in general sensitive to intermediate coupling.

The second contribution to FISCI comes from the mixing of different nonrelativistic parent configurations. Although only a few calculations exist [8], we expect that the final-bound-state correlations involving an excitation of a pair of valence shell electrons to discrete levels should not have a prominent effect on the intrinsic anisotropy of Auger decay. In contrast the multiple-hole configurations that are energetically close to the primary two-hole configurations may give a large CI effect. In the Auger spectra discussed below this kind of CI could be exemplified by the strong coupling between $ns^{-2}(n+1)p$ and $ns^{-1}np^{-2}nd(n+1)p$ configurations which, however, will be the subject of a separate study.

The anisotropy of Auger emission may also be affected by the initial-state configuration interaction (ISCI). For normal Auger transitions in closed shell atoms the ISCI effect is usually weak and dominated, in analogy to photoionization [9], by pair excitations on the valence shell. For photoionization in rare gases it has been found that the initial-state correlations are prominent near threshold, suggesting that the effect of ISCI on Auger decay should be small except for lines corresponding to very low kinetic energies [9]. For resonance Auger spectra in closed

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shell atoms the ISCI is governed by the coupling between the inner shell hole and the excited spectator electron. For photon excitation the dipole allowed initial state of a resonant Auger transition in a closed shell atom can be specified by quantum numbers $(n_0 l_0 j_0)^{-1} n_p l_p j_p (J_i = 1)$. The key features of the ISCI can be summarized in this case as follows: (i) The spin-orbit coupling of the hole orbital dominates over core-spectator interaction, i.e., the fine structure components $j_0 = l_0 \pm 1/2$ are not mixed, and (ii) the core-spectator interaction is stronger than the spin-orbit coupling of the spectator electron and consequently the $j_p = l_p \pm 1/2$ states are mixed by ISCI and may strongly influence the characteristics of resonant Auger decay.

These conclusions are supported by intermediate coupling [4] and MCDF [6] calculations of the anisotropies of the Auger decay of Ar $2p_{3/2}^{-1}4s(J = 1)$ [6] and of Kr $3d_{5/2}^{-1}5p_{3/2}$ and Xe $4d_{5/2}^{-1}6p_{3/2}$ [4] resonances. The results of these calculations which included FISCI but either neglected ISCI entirely [4] or found it very small [6] were in good agreement with experimental data [10–15]. In contrast the ISCI is likely to be fundamentally important for the anisotropy of the Auger decay of Kr $3d_{3/2}^{-1}5p_{1/2,3/2}$ and Xe $4d_{3/2}^{-1}6p_{1/2,3/2}$ resonances. Previous calculations of these Auger spectra which were based on JK coupling model [3] and neglected the ISCI effect failed to reproduce the experimental data of Carlson *et al.* [10,11].

In this work we will study the ISCI and FISCI effects in Kr $3d^{-1}5p$ and Xe $4d^{-1}6p$ resonance Auger spectra by using several differently optimized orbital sets and by accounting for the photoexcitation probabilities whenever initial states are not resolved because of the lifetime broadening.

II. THEORY

The angular distribution of a normal or resonant Auger transition for either unpolarized or linearly polarized incoming photons is given by [5,16]

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

where $W_{i\to f}^T$ is the angle integrated rate for an Auger transition from initial state i to final state f. Here i and f stand for a complete set of quantum numbers needed to specify the pertinent atomic (ionic) states [5]. In Eq. (1) $\mathcal{A}_{20}$ describes the alignment of the initial state of the Auger decay and α_2 is the anisotropy parameter which characterizes the intrinsic anisotropy of the Auger decay and is determined by Eq. (A27) of Ref. [5]. The function $P_2(\cos\theta)$ is the second Legendre polynomial and θ is the angle between the directions of the Auger electron wave vector and the alignment axis of the ion. For a detailed theoretical analysis of the anisotropy of Auger emission within the multichannel multiconfiguration Dirac-Fock formalism see Ref. [5].

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 [17]

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

where $\xi_2 = \sqrt{15/16}\beta_2$ and where β_2 is determined by Eq. (A27) of Ref. [5].

In the experimental spectrum it is often not possible to resolve separate Auger lines corresponding to a well defined initial and final atomic (ionic) state. The fine-structure splitting caused by the coupling of the angular momenta of the final double-hole core and the spectator electron is not resolved. Moreover since the initial-state energy splitting of $nd_{3/2}^{-1}(n+2)p_{1/2,3/2}(J_i = 1)$ states (here and below it is always implied that $n = 3$ for Kr and $n = 4$ for Xe) is smaller than the half width of the $nd_{3/2}$ hole the experimental spectrum represents a superposition of Auger spectra coming from different initial states. Therefore Eq. (1) has to be averaged over the nonresolved initial and final states. In order to determine the corresponding average of the angle differential Auger rate we rewrite Eq. (1) as a differential cross section $d\sigma_{i\to f}/d\Omega = (\sigma_{i\to f}^T/4\pi)[1 + \beta_{i\to f} P_2(\cos\theta)]$. Here $\sigma_{i\to f}^T$ is the total cross section and $\beta = \alpha_2 \mathcal{A}_{20}$. The differential cross section corresponding to an experimentally resolved peak λ is given by

$$d\sigma(\lambda)/d\Omega = [\sigma^T(\lambda)/4\pi][1 + \beta(\lambda) P_2(\cos\theta)], \tag{3}$$

where $\sigma^T(\lambda) = \sum_{i,f\in\{\lambda\}} \sigma_{i\to f}^T$ and

$$\beta(\lambda) = \sum_{i,f\in\{\lambda\}} \sigma_{i\to f}^T \beta_{i\to f} \Big/ \sum_{i,f\in\{\lambda\}} \sigma_{i\to f}^T. \tag{4}$$

The sum in Eq. (4) is taken over the unresolved Auger lines which belong to the experimental peak λ. The cross section in Eq. (4) is given by $\sigma_{i\to f}^T = P_i W_{i\to f}^T$, where

$$P_i = \frac{N}{\Gamma_i} |\langle \Psi_0 \| \sum_\nu \boldsymbol{\alpha}_\nu \cdot \mathbf{A}_{\nu 1}^{(e)} \| \Psi_i \rangle|^2 \tag{5}$$

are the photoexcitation probabilities. In Eq. (5) N is the normalization constant, Γ_i is the initial-state lifetime, and $\boldsymbol{\alpha}_\nu \cdot \mathbf{A}_{\nu 1}^{(e)}$ is the relativistic (velocity-gauge) electron-photon interaction in dipole approximation. The single configuration ground-state wave function is denoted by Ψ_0 and the multiconfiguration excited-state wave function (the initial state of the Auger process) by Ψ_i. The $\beta(\lambda)$ is given in terms of the photoexcitation probabilities and Auger rates by

$$\beta(\lambda) = \sum_{i,f\in\{\lambda\}} P_i W_{i\to f}^T \beta_{i\to f} \Big/ \sum_{i,f\in\{\lambda\}} P_i W_{i\to f}^T. \tag{6}$$

The corresponding average of the anisotropy parameter $\alpha_2(\lambda)$ is obtained in analogy to Eq. (6). Note that both the photoexcitation probabilities and Auger transition rates appear as weights in Eq. (6). We found that, although the total Auger rates were almost equal for both initial $nd_{3/2}^{-1}(n+2)p_{1/2,3/2}$ states, the sum of partial Auger rates corresponding to the same experimentally resolved peak λ were not equal for both the

initial states.

Coherence effects (quantum beats) have been mentioned as potential a cause for the discrepancy between theory and experiment [3]. However, according to our estimates the spectral bandwidth of the photons $\Delta\omega \ll 1/\Delta T$, where ΔT is the typical pulse length in a storage ring. Thus the degree of coherence of light in the photon beam should be very low and consequently there is no transfer of coherence from the photons to the atom [18].

III. CALCULATIONS

A. General

The transition rates and the α_2, β, and ξ_2 parameters were calculated using a computer code described by us recently [8]. In this work we assume a two step description of Auger effect and neglect the direct transition amplitudes to the final states of the Auger decay. In all calculations the initial and final states of the atom (ion) were described by multiconfiguration wave functions accounting for the initial-state and final-ionic-state configuration interaction. For the initial state we used intermediate coupling by including three jj coupled configurations resulting from the nonrelativistic $nd^{-1}(n+2)p$ parent. For the final ionic state we included parent configurations $(n+1)p^{-2}(n+2)p$, $(n+1)s^{-1}(n+1)p^{-1}(n+2)p$, and $(n+1)s^{-2}(n+2)p$ and also the final states of participator transitions $(n+1)p^{-1}$ and $(n+1)s^{-1}$. Except for the initial state $nd_{5/2}^{-1}(n+2)p_{3/2}$, which is an almost pure jj coupled state, all other initial and final bound states are far from either the jj or the LS coupling limit and therefore the assignments given to them are intended only to serve as tags of the transitions. The interaction between continuum channels and the orbital relaxation taking place during Auger emission were neglected in the present calculations, although both these effects may give a nontrivial contribution to the intensity and angular distributions of Auger transitions discussed in this work [5,19,20]. For a detailed discussion of the numerical approach see Ref. [8].

The spectator orbital was always obtained in the same self-consistent field (SCF) calculation as the core orbitals. The continuum orbital was calculated in a jj average field of the core plus spectator electron and made orthogonal to the bound orbitals by Lagrangian multipliers. Thus the asymptotic field seen by the Auger electron corresponds to *singly* charged ion in contrast to the normal Auger decay.

B. Computational models

The effect of the choice of orbitals and the effect of exchange were studied by calculating the Auger spectra in the following approximations.

FE: In this approach the bound orbitals were optimized for the final ionic state. Note that even the mixing coefficients appearing in the initial-state multiconfiguration wave function were calculated by using final-state orbitals in the diagonalization of the initial-state Hamiltonian. The exchange interaction of the continuum and core electrons was fully taken into account. Particular advantage in the calculations making use of orbitals optimized for the final state is that they reproduce the experimental energy splitting and the order of lines much better than the calculation involving bound orbitals optimized for the initial state.

F: This approximation is identical to FE except that the exchange interaction was not included in the calculation of the continuum orbital. Accordingly the difference between FE and F indicates the effect of exchange interaction. The approximation F resembles closely the method used by Chen in Ref. [7] and the intermediate coupling calculation by Hergenhahn *et al.* [4]. Both works neglect the exchange interaction and also include a more limited configuration basis in the calculation of FISCI. In addition Hergenhahn *et al.* [4] used radial two-electron integrals taken from the transition amplitudes of the corresponding normal Auger spectrum in their work. This excludes the influence of the spectator electron on the Auger electron orbital and accordingly the phase shifts correspond to an asymptotic field of a *doubly* charged ion.

IE: In this approximation the bound orbitals optimized for the initial excited atomic state were used both in the initial- and in the final-state wave function. In analogy to FE the final-ionic-state mixing coefficients were determined by using the initial-state orbitals and the exchange was included for the continuum electron. In short the difference between calculations FE and IE comes exclusively from the different bound orbitals and therefore demonstrates at *qualitative* level the effect of orbital relaxation.

FEI: This approximation is equivalent to FE except that the initial-state *mixing coefficients* were obtained from the initial-state SCF calculation. This approach combines parts of the approximations IE and FE by involving different orbital basis in the calculation of mixing coefficients. These calculations were prompted by our observation that the mixing coefficients of the $nd_{3/2}(n+2)p_{1/2,3/2}$ initial states are rather sensitive to the choice of one electron orbitals.

Approximation FEI includes also some contribution coming from relaxation and it can therefore be considered more general than our other calculations. Therefore we have used FEI as a theoretical reference value in the comparison with experiment in Sec. IV. In contrast the comparison of FEI with other calculated results can be used to estimate the magnitude of various many-electron effects.

Note, however, that approximation FEI does not conserve the orthogonality of many-electron wave functions exactly. Therefore, in the comparison with experiment the discrepancies may be addressed not only to those correlation effects that were not included in the calculation of transition amplitudes but also to the incomplete treatment of nonorthogonality. The *ab initio* approach to overcome this imperfection would be to determine the orbitals and mixing coefficients for the initial and final states in separate SCF calculations and to include the

correction terms coming from the nonorthogonality of the one-electron orbitals in the transition amplitudes. Such a procedure has been described by us recently for the normal Auger decay [20].

C. Photoexcitation probabilities

The photoexcitation probabilities were calculated using a multiconfiguration Dirac-Fock computer program GRASP [21] and also by a photoabsorption code developed by us previously [22]. In GRASP the one-electron orbitals optimized for the initial state of the Auger transition were used both in the initial and final state of the photoexcitation amplitude. Our computer code is identical to GRASP, except that it makes use of separately optimized ground-state and excited-state orbitals and includes all partial photoexcitation amplitudes resulting from the nonorthogonality of one electron orbitals [22]. The photoexcitation amplitudes were calculated in dipole approximation and both in the velocity and length gauges. The branching ratios were gauge invariant within 1%.

IV. RESULTS AND DISCUSSION

A. General considerations

The photon energy region covered in the experiments includes for both Kr and Xe three photoexcitation resonances. The electronic states of these resonances can be described to a good approximation as a linear combination of *three* configuration-state functions (CSF's) $nd_{5/2}^{-1}(n+2)p_{3/2}$, $nd_{3/2}^{-1}(n+2)p_{1/2}$, and $nd_{3/2}^{-1}(n+2)p_{3/2}$, all corresponding to the dipole allowed total angular momentum $J = 1$. When the many-electron Hamiltonian is diagonalized in this CSF space one obtains three multiconfiguration Dirac-Fock eigenstates. The corresponding atomic state functions (mixing coefficients) are given in Table I. They were obtained with two different sets of the single-electron bound orbitals optimized for the initial atomic state (labeled I) or final ionic state (labeled F). One can see from Table I that the mixing coefficients for the states 2 and 3 depend strongly on the choice of the basis set. These coefficients influence the Auger transition amplitudes and thereby also the transition rates and anisotropy parameters, especially for the $nd_{3/2}(n+2)p$ excitations. From the physical point of view the basis set optimized for the initial state is preferential. Therefore we use in our theoretical reference values (FEI) mixing coefficients taken from columns I in Table I, even though the transition amplitudes are calculated by using orbitals optimized for the final state also in the initial-state wave function.

From the calculation involving bound orbitals optimized for the initial state the energy splitting between the resonance states 1 (lowest total energy) and 2 is 1.27 eV for Kr (1.97 eV for Xe) and the energy splitting between the resonances 1 and 3 is 1.30 eV for Kr (2.03 eV for Xe). The resonance 1 is separated from resonances 2 and 3 by an energy difference that is larger than the half width (see below) of the states. Therefore Auger electrons coming from initial state 1 can be, in an ideal experiment, resolved from Auger electrons coming from initial states 2 and 3. In contrast the energy difference between resonances 2 and 3 is much smaller than the half width. Therefore these resonances cannot be resolved in the experiment, but they are excited simultaneously with a population ratio that is governed by the photoexcitation probability given in Eq. (5). Thus for the resonances 2 and 3 we have to take a proper average using photoexcitation probabilities as weights according to Eq. (6) before the calculated results can be compared with experiment.

For both Kr and Xe the resonance Auger spectrum recorded at lower photon energy corresponds to resonance 1 in Table I. The atomic state functions (ASF) of this state is mainly described by the $nd_{5/2}^{-1}(n+2)p_{3/2}$ configuration with only a weak component of the $nd_{3/2}^{-1}(n+2)p_{1/2,3/2}$ configurations. Correspondingly the resonance Auger spectrum recorded at higher photon energy corresponds to simultaneous excitation of resonances 2 and 3. In spite of the strong mixing of jj coupled configurations the ASF 2 and 3 are still far from the LS coupling limit both for Kr and Xe.

The calculated half widths of the initial states are 0.085 eV and 0.19 eV for Kr and Xe, respectively. The calcu-

TABLE I. The mixing coefficients for the Kr $3d^{-1}5p$ $J = 1$ and Xe $4d^{-1}6p$ $J = 1$ initial-state ASF's. ASF's are numbered according to the descending binding energy. I denotes values obtained by using orbitals optimized for the initial state whereas F stands for values obtained by using orbitals optimized for the final ionic state.

Configuration		1		2		3	
		I	F	I	F	I	F
Kr	$3d_{5/2}^{-1}5p_{3/2}$	1.000	0.999	0.010	0.004	-0.007	-0.004
	$3d_{3/2}^{-1}5p_{1/2}$	-0.003	-0.016	0.796	0.503	0.605	0.864
	$3d_{3/2}^{-1}5p_{3/2}$	0.012	0.035	-0.605	-0.863	0.796	0.503
Xe	$4d_{5/2}^{-1}6p_{3/2}$	1.000	0.999	0.005	0.026	-0.008	-0.013
	$4d_{3/2}^{-1}6p_{1/2}$	-0.001	-0.008	0.887	0.680	0.462	0.736
	$4d_{3/2}^{-1}6p_{3/2}$	0.010	0.028	-0.462	-0.733	0.887	0.680

TABLE II. The relative intensities and angular anisotropy parameters α_2 for Kr $3d^{-1}5p$ $J = 1$ resonantly excited Auger spectrum. The values correspond to computational approximation FEI, which is described in the text. The initial states correspond to the eigenvectors (I) in Table I.

	Leading LS term in the final state	Final-state energy (eV)	Initial state 1		Initial state 2		Initial state 3	
			Rate	α_2	Rate	α_2	Rate	α_2
	$4p^5$							
1	$^2P_{3/2}$	0.00	0.74	-0.565	0.54	-0.323	0.12	-0.629
2	$^2P_{1/2}$	0.65	0.29	-0.726	0.39	-0.660	0.03	-0.136
	$4p^4(^3P)5p$							
3	$^4P_{5/2}$	15.26	0.59	0.703	0.55	0.698	0.11	0.318
4	$^4P_{3/2}$	15.32	0.17	-0.745	0.27	-0.379	0.04	-0.328
5	$^4D_{7/2}$	15.49	0.19	0.336	0.13	-0.073	0.24	-0.068
6	$^4P_{1/2}$	15.52	0.05	0.148	0.00	-0.094	0.01	0.141
7	$^2D_{5/2}$	15.54	0.38	0.701	0.12	-0.204	0.53	0.697
8	$^2D_{3/2}$	15.87	1.06	-0.565	0.21	-0.680	0.68	-0.549
9	$^2P_{1/2}$	15.98	0.32	-0.280	0.09	-0.498	0.01	0.147
10	$^4D_{5/2}$	16.03	0.07	0.522	0.53	0.670	0.85	0.665
11	$^2P_{1/2}$	16.04	0.14	-0.783	0.08	-0.739	0.10	-0.667
12	$^2P_{3/2}$	16.09	0.35	0.603	0.47	-0.284	0.11	0.665
13	$^4S_{3/2}$	16.25	0.15	0.500	0.05	-0.447	0.50	-0.657
14	$^4D_{3/2}$	16.35	0.27	-0.595	1.04	0.477	0.07	0.243
15	$^4D_{1/2}$	16.40	0.15	-0.195	0.05	-0.478	0.16	-0.536
	$4p^4(^1D)5p$							
16	$^2F_{5/2}$	17.51	0.26	0.562	3.60	-0.243	2.59	0.508
17	$^2F_{7/2}$	17.57	4.27	-0.199	1.50	0.597	2.62	0.597
18	$^2P_{3/2}$	17.78	3.68	-0.199	0.65	0.258	1.14	-0.022
	$4s^1$							
19	$^2S_{1/2}$	17.79	0.10	-0.027	0.12	0.195	0.02	0.110
	$4p^4(^1D)5p$							
20	$^2D_{5/2}$	17.90	1.60	0.563	2.02	0.405	2.49	-0.767
21	$^2D_{3/2}$	17.93	0.16	0.617	3.35	-0.525	1.78	-0.119
22	$^2P_{1/2}$	18.07	1.29	-0.848	0.63	-0.486	0.85	-0.458
	$4p^4(^1S)5p$							
23	$^2P_{1/2}$	19.52	0.00	0.171	3.49	-0.711	2.31	-0.699
24	$^2P_{3/2}$	19.53	3.70	-0.584	1.69	0.567	3.91	0.500
	$4s^14p^5(^3P)5p$							
25	$^4S_{3/2}$	31.90	0.04	-0.162	0.02	0.181	0.09	-0.545
26	$^4D_{7/2}$	32.20	0.83	0.707	2.44	0.707	4.26	0.707
27	$^4D_{5/2}$	32.25	0.50	-0.539	4.78	-0.565	3.47	-0.573
28	$^4D_{3/2}$	32.42	0.01	0.234	0.72	-0.567	0.10	-0.665
29	$^2D_{5/2}$	32.46	2.95	-0.585	1.57	-0.322	0.92	0.118
30	$^4D_{1/2}$	32.61	0.01	0.054	0.01	-1.167	0.01	-1.144
31	$^2P_{3/2}$	32.77	1.63	-0.577	0.08	-0.371	0.65	-0.624
32	$^4P_{5/2}$	32.81	2.48	-0.494	0.43	0.096	0.91	0.218
33	$^4P_{3/2}$	32.84	1.15	-0.615	0.22	-0.530	0.08	0.233
34	$^4P_{1/2}$	32.89	0.01	-1.412	0.01	-1.413	0.03	-0.325
35	$^2P_{1/2}$	32.99	0.01	0.285	0.00	0.356	0.00	-1.083
36	$^2D_{3/2}$	33.12	2.31	-0.575	0.08	-0.668	0.05	0.151
37	$^2S_{1/2}$	33.64	0.01	0.700	0.07	0.583	0.01	0.140
	$4s^14p^5(^1P)5p$							
38	$^2S_{1/2}$	39.15	1.98	-0.705	2.04	-0.249	0.29	-0.044
39	$^2D_{3/2}$	39.19	0.27	0.245	29.25	-0.537	10.24	-0.290
40	$^2D_{5/2}$	39.25	39.03	-0.375	12.92	0.666	22.47	0.670
41	$^2P_{1/2}$	39.45	1.33	-0.699	0.61	-1.385	2.08	-0.161
42	$^2P_{3/2}$	39.48	2.58	0.238	0.97	0.545	10.86	-0.803
	$4s^05p$							
43	$^2P_{1/2}$	55.68	0.00	-1.006	14.07	-0.709	8.13	-0.706
44	$^2P_{3/2}$	55.75	22.88	-0.557	8.14	0.548	14.06	0.559

TABLE III. The relative intensities and angular anisotropy parameters α_2 for Xe $4d^{-1}6p$ $J = 1$ resonantly excited Auger spectrum. The values correspond to computational approximation FEI, which is described in the text. The initial states correspond to the eigenvectors (I) in Table I.

	Leading LS term in the final state	Final-state energy (eV)	Initial state					
			1		2		3	
			Rate	α_2	Rate	α_2	Rate	α_2
	$5p^5$							
1	$^2P_{3/2}$	0.00	1.16	-0.642	1.04	-0.656	0.14	-0.310
2	$^2P_{1/2}$	1.30	0.50	-0.940	0.67	-0.647	0.09	-0.175
	$5p^4(^3P)6p$							
3	$^4P_{5/2}$	12.73	0.77	0.703	0.77	0.588	0.22	-0.163
4	$^4P_{3/2}$	12.73	0.16	-0.739	0.48	0.056	0.03	0.097
5	$^4D_{7/2}$	12.95	0.60	0.416	0.17	0.140	0.62	0.143
6	$^2D_{5/2}$	12.95	1.12	0.703	0.41	0.266	0.51	0.658
7	$^2S_{1/2}$	12.99	0.21	0.317	0.03	0.006	0.04	0.305
8	$^2P_{3/2}$	13.43	2.25	-0.729	0.14	-0.229	0.69	-0.840
9	$^2P_{1/2}$	13.81	0.17	-0.696	0.02	-0.712	0.04	-0.688
10	$^4P_{1/2}$	13.90	0.18	-0.165	0.03	-0.499	0.05	-0.229
11	$^2D_{3/2}$	13.94	1.36	-0.464	0.89	-0.502	0.13	0.012
12	$^4D_{5/2}$	14.11	0.05	0.133	0.74	0.680	2.73	0.683
13	$^4D_{3/2}$	14.22	0.52	-0.527	1.55	0.205	0.31	-0.553
14	$^4S_{3/2}$	14.29	0.61	0.379	0.46	-0.345	0.40	-0.548
15	$^4D_{1/2}$	14.37	0.45	-0.419	0.17	-0.598	0.10	-0.426
	$5s^1$							
16	$^2S_{1/2}$	15.05	0.21	-0.415	0.22	-0.396	0.05	0.260
	$5p^4(^1D)6p$							
17	$^2F_{5/2}$	15.19	0.15	0.619	6.55	0.039	2.65	0.649
18	$^2F_{7/2}$	15.32	5.17	-0.174	1.25	0.587	4.61	0.587
19	$^2P_{3/2}$	15.34	3.17	-0.124	2.45	-0.314	2.39	-0.178
20	$^2D_{3/2}$	15.60	0.90	0.391	4.98	-0.672	1.56	0.284
21	$^2D_{5/2}$	15.61	1.75	0.628	2.14	0.511	4.33	-0.698
22	$^2P_{1/2}$	15.76	1.70	-1.063	0.37	-0.355	1.73	-0.409
	$5p^4(^1S)6p$							
23	$^2P_{1/2}$	17.35	0.00	-0.092	7.15	-0.708	2.16	-0.698
24	$^2P_{3/2}$	17.40	3.20	-0.586	1.49	0.628	7.76	0.503
	$5s^15p^5(^3P)6p$							
25	$^4S_{3/2}$	26.78	0.03	0.575	0.03	0.625	0.01	0.163
26	$^4D_{5/2}$	27.05	0.02	-0.561	0.20	-0.539	0.06	-0.509
27	$^4D_{7/2}$	27.08	0.06	0.707	0.04	0.707	0.15	0.707
28	$^2P_{3/2}$	27.30	0.06	0.442	0.01	-0.470	0.00	0.302
29	$^4P_{5/2}$	27.32	0.25	-0.532	0.03	-0.335	0.06	-0.157
30	$^2P_{1/2}$	27.60	0.05	-0.097	0.03	-1.204	0.02	-1.236
31	$^4D_{3/2}$	27.90	0.09	-0.570	0.07	0.670	0.01	-0.180
32	$^4D_{5/2}$	28.04	0.68	-0.551	0.02	-0.154	0.04	-0.132
33	$^2D_{3/2}$	28.06	0.22	-0.478	0.00	0.689	0.13	0.659
34	$^4D_{1/2}$	28.07	0.03	0.495	0.01	-1.172	0.01	-0.332
35	$^2P_{1/2}$	28.20	0.09	-0.994	0.03	-1.407	0.10	-0.059
36	$^2D_{3/2}$	28.63	0.41	0.560	0.05	0.559	0.14	0.557
37	$^2S_{1/2}$	28.76	0.01	-1.245	0.21	0.072	0.01	-0.785
	$5s^15p^5(^1P)6p$							
38	$^2S_{1/2}$	33.11	2.61	-0.717	3.17	-0.500	0.60	-0.287
39	$^2D_{3/2}$	33.14	0.20	0.085	29.31	-0.503	5.46	-0.290
40	$^2D_{5/2}$	33.27	40.34	0.389	6.49	0.647	23.76	0.648
41	$^2P_{1/2}$	33.43	2.39	-0.697	1.26	-1.361	2.72	0.046
42	$^2P_{3/2}$	33.48	3.75	0.104	0.98	0.554	9.39	-0.585
	$5s^06p$							
43	$^2P_{1/2}$	46.84	0.00	-0.450	18.76	-0.710	5.07	-0.705
44	$^2P_{3/2}$	47.00	22.37	-0.560	5.13	0.549	18.79	0.559

lated half widths of all three initial states were almost equal and practically invariant of the orbital set used. The exchange effect instead had a large effect on the half width (total Auger rate): For the Xe $4d_{5/2}^{-1}6p_{3/2}$ line we obtained 0.192 eV in approximation FE and 0.289 eV in approximation F giving an exchange effect of 50.5 %. For Kr $3d_{5/2}^{-1}5p_{3/2}$ state the exchange effect in the total rate was correspondingly 16.2 %.

B. Calculated intensities and anisotropies of separate Auger transitions

In Tables II (Kr) and III (Xe) we list the rate and α_2 parameter for each $nd^{-1}(n+2)p$ Auger transition in FEI approximation. The values in Tables II and III correspond to transitions between a pair of initial and final spectroscopic states of the system. These data are given primarily for the future reference to make a comparison with high resolution experimental data possible. We calculated the α_2 parameters in Tables II and III also in the approximation F (data not shown for brevity) and found that they agree well with those obtained by Chen [7], except for a number of relatively weak lines which are known to be [5] especially sensitive to the details of numerical approach. Since also our β coefficients of experimentally observed Auger peaks in Tables V and VI agree in the approximation F well with those of Chen [7] we conclude that there is a good overall consistency between the present and Chen's [7] calculations.

In contrast there are large differences in the branching ratios between separate transitions in our FEI and Chen's [7] calculations. This is due to the relatively low kinetic energy of Auger electrons which makes the transition amplitudes very sensitive to approximations involved in the calculation of the continuum orbital and the phase shift.

The importance of many-electron effects is emphasized further in Table IV where we present the relative intensities of the Kr $3d_{5/2}^{-1}5p_{3/2}$ Auger peaks calculated in various approximations. The trends are very similar for xenon (not shown). The influence of the exchange and the orbital set on the branching ratios of separate Auger transitions is larger than their influence on the branching ratios of Auger peaks (each including several Auger transitions). It is remarkable, however, that the branching ratios of Auger peaks (Table IV) are still somewhat more sensitive to these many-electron effects than the β parameters of the corresponding Auger peaks (Table V).

TABLE IV. Calculated relative intensities of Kr $3d_{5/2}^{-1}5p_{3/2} \rightarrow 4p^5 5p$ Auger transitions. The approximations F, FE, and IE are explained in the text. The second column lists the final ionic states (FIS) that are included into each Auger peak (see Table II) .

Peak	FIS	F	FE	IE
1a	3,4	17.7	9.8	13.8
1b	5–7	11.6	7.6	15.5
1c	8,9	32.7	16.9	37.6
1d	10–12	12.1	6.9	7.1
1e	13–15	13.4	6.9	24.1
2a	16–18	100.0	100.0	100.0
2b	20–22	46.3	35.9	59.4
4	23,24	60.6	44.5	76.4

C. The $nd_{5/2}^{-1}(n+2)p_{3/2}$ resonance Auger spectra

1. Calculations

The calculated intensity weighted β coefficients for superpositions of Auger transitions corresponding to the experimentally observable peaks of the Kr $3d_{5/2}^{-1}5p_{3/2}$ resonance Auger spectrum are given in Table V and for the peaks of Xe $4d_{5/2}^{-1}6p_{3/2}$ resonance Auger spectrum in Table VI. In these tables we also give results of recent intermediate coupling calculations of Hergenhahn *et al.* [4] and Chen [7]. Note that the FEI and FE results in Tables V and VI are almost equal for the $nd_{5/2}^{-1}(n+2)p_{3/2}$ resonance since the ASF 1 includes only a negligible contribution of the other initial-state configurations (Table I).

The difference between calculations FE and IE in Tables V and VI is substantially larger than for the corresponding normal Auger transitions [5], underscoring the need for calculations taking full account of relaxation effect. The difference between FE and IE is mainly due to the changes in the final-ionic-state mixing coefficients,

TABLE V. Angular anisotropy coefficients $\beta = \mathcal{A}_{20}\alpha_2$ for Kr $3d_{5/2}^{-1}5p \rightarrow 4p^4 5p$ Auger transitions. Computational approximations IE, F, FE, and FIE have been explained in the text. The final ionic states included in each Auger peak are listed in Table IV.

Peak	Theory						Experiment	
	IE	F	FE	FEI	Ref. [4]	Ref. [7]	Ref. [15]	Ref. [11]
1a	-0.793	-0.567	-0.540	-0.535	-0.990	-0.66	-0.76(2)	-0.89
1b	-0.668	-0.925	-0.778	-0.773	-0.823	-0.88	-0.87(2)	-0.98
1c	0.894	0.784	0.699	0.705	0.801	0.83	0.77(6)	0.62
1d	0.792	-0.368	-0.309	-0.338	0.820	-0.12	0.04(5)	0.24
1e	0.444	0.452	0.268	0.277	0.467	0.42	0.31(6)	0.19
2a	0.128	0.116	0.240	0.247	-0.066	0.12	0.27(3)	-0.06
2b	-0.457	-0.011	0.048	0.043	-0.248	-0.06	0.05(3)	-0.12
4	0.807	0.835	0.795	0.825	0.759	0.84		0.73

TABLE VI. Angular anisotropy coefficients $\beta = \mathcal{A}_{20}\alpha_2$ for Xe $4d_{5/2}^{-1}6p \rightarrow 5p^4 6p$ Auger transitions. The second column lists the final ionic states (FIS) included in each Auger peak (see Table III). The approximations F, FE, FEI, and IE are explained in the text.

Peak	FIS	Theory						Experiment	
		IE	F	FE	FEI	Ref. [4]	Ref. [7]	Ref. [13]	Ref. [11]
1a	3,4	-0.836	-0.673	-0.647	-0.644	-0.976	-0.770	-0.60(3)	-0.88
1b	5–7	-0.824	-0.920	-0.817	-0.810	-0.726	-0.870	-0.90(2)	-0.93
1c	8	1.093	0.971	1.025	1.031	0.972	1.018	1.31(2)	0.82
2a	9–11	0.795	0.682	0.646	0.645	0.868	0.703	0.58(2)	0.26
2b	12–15	0.373	0.299	0.206	0.197	0.394	0.348	0.54(3)	0.16
3a	17–19	0.123	0.046	0.198	0.200	-0.048	0.039	0.23(2)	-0.02
3b	20–22	-0.012	0.034	0.121	0.117	-0.007	-0.007	0.33(5)	-0.09
5	23,24	0.810	0.817	0.801	0.828	0.753	0.847	0.83(5)	0.51

which also changed the energetic order of several Auger transitions. In some cases also the assignments based on LS symbols were altered, thus demonstrating the sensitivity of FISCI to the one-electron orbitals. The largest basis set dependence is found in the case of krypton 2b line for which all calculations except the one obtained with initial-state orbitals give a rather small anisotropy.

As can be seen by comparing columns F and FE in Tables V and VI, the effect of exchange on the anisotropy is rather large for both Kr and Xe. Because of the low kinetic energy the exchange terms make an important contribution to the effective potential seen by the Auger electron. The exchange interaction alters the β values especially for transitions involving several partial waves with partial amplitudes of comparable strength. In the final state of resonance Auger spectrum the total angular momentum is shared between the ionic core, spectator electron, and Auger electron. Therefore, in the case of resonance Auger transition the number of allowed partial waves of Auger electron is as a rule larger than in the case of normal Auger transition. This suggests that the resonance Auger spectra tend to be more sensitive to exchange effect than the corresponding normal Auger spectra.

2. Comparison with experiment

For both Kr and Xe our FEI β coefficients in Tables V and VI are in good general agreement with experiment [11,13,15]. For most lines the discrepancies between separate experiments are larger than the difference between our FEI result and experiment. The largest discrepancy between theory and experiment is found for the peak 1d in Kr $3d_{5/2}^{-1}5p_{3/2}$ spectrum (Table V). The α_2 values (approximation FEI) associated with Auger transitions 10–12 included in this peak (see Table II) agree well with those of Chen [7]. However, our branching ratios of these lines (not shown) are 1:2.5:6.0, respectively, whereas Chen obtained 1:2.1:2.3 (Table II in Ref. [7]), thus explaining the large difference between our -0.338 and Chen's -0.12 β value. That the latter value is closer to the experiment is, in light of these results, accidental.

The sensitivity of this Auger line to the choice of orbitals is also manifested by the large positive β value obtained in IE approximation. In the IE calculation both the branching ratios and the α_2 parameter of the transition 12 are very different from the FE results. The peak 1d illustrates the paradox that due to the sensitivity of branching ratios to correlation, the anisotropy of an Auger peak including several nonresolved transitions can in fact be more sensitive to correlation effects than the anisotropies of separate component transitions.

D. The $nd_{3/2}^{-1}(n+2)p_{1/2,3/2}$ resonance Auger spectra

1. Calculations

The β coefficients corresponding to Auger decay of the two unresolved $nd_{3/2}^{-1}(n+2)p_{1/2,3/2}$, $J = 1$ photoexcita-

TABLE VII. Angular anisotropy coefficients $\beta = \mathcal{A}_{20}\alpha_2$ for Kr $3d_{3/2}^{-1}5p \rightarrow 4p^4 5p$ Auger transitions. The approximations FE and FEI are explained in the text. The final ionic states included in each Auger peak are listed in Table IV. The different values for peak 2a in Ref. [15] originate from two different experiments.

Peak	Theory			Experiment	
	FE	FEI	Ref. [3]	Ref. [15]	Ref. [11]
1a	-0.656	-0.476	-0.002	-0.45(7)	-0.48
1b	0.126	0.077	-0.159	-0.18(17)	-0.20
1c	0.249	0.871	0.870	-0.50(9)	0.46
1d	-0.557	-0.237	-0.902	0.15(10)	0.14
1e	-0.330	-0.516	0.781	-0.41(8)	-0.26
2a	-0.292	-0.079	-0.264	-0.42(6),0.43(15)	-0.16
2b	0.331	0.310	0.140	0.24(7)	0.08
4	-0.243	0.386	0.030		0.49

TABLE VIII. Angular anisotropy coefficients $\beta = \mathcal{A}_{20}\alpha_2$ for Xe $4d_{3/2}^{-1}6p \rightarrow 5p^4 6p$ Auger transitions. The approximations FE and FEI are explained in the text. The final ionic states included in each peak are given in Table VI.

Peak	Theory			Experiment	
	FE	FEI	Ref. [3]	Ref. [11]	Ref. [14]
1a	-0.695	-0.540	-0.11		-0.8
1b	0.177	0.196	-0.143	-0.67(1a+1b)	0.2
1c	0.339	1.031	0.380	-0.38	-0.4
2a,2b	-0.034	0.425	-0.023	0.14	0.35
3a,3b	0.171	0.172	0	0.32	0.5
5	0.672	0.828	-0.024	0.89	1.0

tion resonances are given in Tables VII and VIII for krypton and xenon, respectively. Since the resonance Auger spectra coming from resonance states 2 and 3 (see Table I) are superimposed in experimental spectrum because of the lifetime broadening, these calculated spectra were averaged according to Eq. (6) before the comparison with experiment was made. The photoexcitation branching ratios between resonances 2 and 3 were obtained to be 19.2 and 20.1 for krypton using our own code and GRASP, respectively. For xenon the corresponding branching ratios were 310 and 287. The $nd_{3/2}^{-1}(n+2)p_{1/2,3/2}$ resonance Auger spectra are thus entirely dominated by initial state 2 in Table I. The results in Tables VII and VIII are based on branching ratios given by our own code.

The two $nd_{3/2}^{-1}(n+2)p_{1/2,3/2}$, $J=1$ initial states are strongly mixed according to the MCDF calculations (Table I). The ISCI depends decisively on the one-electron basis set used in the diagonalization of the Hamiltonian. In Tables VII and VIII the influence of ISCI is seen by comparing the β coefficients calculated in approximations FE and FEI, which differ only by the initial-state mixing coefficients as explained above. Our results show that the use of separately optimized orbitals has a dramatic effect on the calculated β values. The use of separately optimized orbitals improves the agreement with experiment (see below).

2. *Comparison with experiment*

Agreement between experiment and theory is fairly satisfactory especially for those Auger lines which are well resolved and for which the differences between the different experimental values are modest. For both krypton and xenon our results which are based on *ab initio* analysis of the initial-state populations and on the intermediate coupling present considerable improvement with regard to the previous jK coupling calculations of Hergenhahn *et al.* [3]. Our calculations reproduce the large negative anisotropy of the 1a peaks for Kr and Xe in Tables VII and VIII. Our negative FEI β value for krypton 1d line is still in disagreement with experiment, although even in this case there is a striking improvement over the previous calculation [3]. Note that the lines 1c, 1d, and 1e are separated only by about 0.2 eV from each other and thus they are not well resolved experimentally. Better agreement with experiment is obtained for well separated krypton lines 1a, 2a, 2b, and 4. The agreement between FEI results and experiment is also fairly good for xenon except for the very weak line 1c. Part of the discrepancy between theory and experiment can be addressed to the incomplete treatment of relaxation in FEI calculation. In contrast we expect that FISCI and other final-state correlation effects are a less probable source of error since these effects are also present in the $nd_{5/2}^{-1}(n+2)p_{3/2}$ spectra for which adequate agreement is achieved with experiment. The discrepancies between different experimental data are often very large and to judge the accuracy of different theoretical approaches one also needs improved experimental data.

E. Calculated spin polarization of Auger electrons in resonant Auger transitions

Some of the resonant Auger lines were found to have notably large values of spin polarization perpendicular to the plane defined by the axis of alignment and the Auger electron wave vector (so-called dynamical polarization). In Table IX we list the peaks having the largest spin-polarization parameters ξ_2. In analogy to normal Auger decay [5] we found that the spin-polarization parameters are rather sensitive to the computational approximation. In general the ξ_2 values are much larger than in the case of the corresponding normal Auger spectra. Note that the spin polarization is proportional to the product of the ξ_2 parameter and the degree of alignment which is very large $(-\sqrt{2})$ for the resonance photoexcitation. Therefore, for some of the resonant Auger transitions the dynamical polarization is large and its measurement is quite feasible.

TABLE IX. The peaks having the largest spin-polarization coefficients ξ_2 in the Kr $3d_{5/2}^{-1}5p_{3/2}$ and Xe $4d_{5/2}^{-1}6p_{3/2}$ resonant Auger spectra. The ξ_2 values correspond to approximation FE.

Kr $3d_{5/2}^{-1}5p_{3/2}$		Xe $4d_{5/2}^{-1}6p_{3/2}$	
Peak	ξ_2	Peak	ξ_2
1c	0.13	1b	0.10
2a	0.13	3a	0.09
2b	-0.42	3b	-0.23

V. CONCLUSIONS

In conclusion we have shown that the intensities and anisotropy of resonant Auger transitions following photoexcitation to Kr $3d^{-1}5p$ and Xe $4d^{-1}6p$ states are sensitive to both initial- and final-state configuration interaction. We have studied the influence of the one-electron orbital basis on the ISCI and FISCI effects and on the anisotropy of Auger emission. The difference between the results obtained by using relaxed and unrelaxed orbitals is related to the electronic relaxation taking place during Auger decay. We have found that the relaxation affects considerably the angular distribution of resonant Auger lines and it should be taken properly into account in future calculations.

It is shown that exchange effect, which was not included in all previous calculations, is significant for the angular anisotropy of considered resonant Auger transitions in Kr and Xe.

We have demonstrated that accurate calculations of the initial-state population has a dramatic effect on the anisotropy of the Auger decay of the $nd_{3/2}(n+2)p$ resonance, giving considerably better agreement with experimental data than previous calculations with a pure geometrical initial-state population.

We report dynamical spin-polarization values for a resonant Auger transitions. For some transitions we have found rather large values of spin polarization interesting for experimental investigation.

The overall agreement of our calculated anisotropy parameter with experiment is fairly good. In comparison with previous calculations the improvement is especially noticeable for the $nd_{3/2}(n+2)p$ resonances. However, some discrepancy remains between experiment and theory. One of the possibilities to improve the theoretical description of the process is to include simultaneously the initial- and final-state configuration interaction and full relaxation effect. This is not possible using the present version of our computer code. Our preliminary estimates indicate that inclusion of relaxation simultaneously with initial- and final-state configuration interaction and channel interaction in a single multichannel multiconfiguration Dirac-Fock calculation is feasible using present supercomputers. Therefore improving our present theoretical approach requires mainly extensive programming work. The accuracy of the present calculation is not good enough to determine if one of the experimental data sets is more accurate. Therefore further progress is also needed on the experimental side, especially in the case of $nd_{3/2}^{-1}(n+2)p_{1/2,3/2}$ resonance Auger spectra.

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