Coherence and correlation in the anisotropy of Ne *KL-LLL* satellite Auger decay

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The energies, intensities, and angular anisotropies of the Ne *KL-LLL* satellite Auger lines have been studied by the multiconfiguration Dirac-Fock method. In addition to the initial- and final-state correlation effects, we have studied the influence of the quantum beat effect on this Auger spectrum. Since the energy splitting of the Ne $1s^{-1}2p^{-1}\,{}^3P$ multiplet is much smaller than the lifetime broadening, the coherent excitation of these initial states by the in time and space localized electromagnetic pulse of the projectile has a drastic effect on the angular distribution of Auger electrons. To analyze this coherence effect we have generalized the theory of the angular distribution of Auger electrons to the case of coherent excitation of partially overlapping initial states. The results of our calculations are in good overall agreement with experiment. However, for a quantitative study of the influence of the coherence and the initial spin state on the anisotropy of these Auger lines new measurements with lower error limits are necessary.

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I. INTRODUCTION

The angular anisotropy of Auger electron emission has proven to be a selective probe of many-electron effects accompanying nonradiative decay of inner shell hole states in free atoms [1–3]. The angular anisotropy of electron emission is especially sensitive to the coupling of spin and orbital angular momenta in the initial and final bound states of Auger emission and, to a somewhat lesser extent, to dynamical effects like relaxation and final-state channel interaction. It provides complementary information about Auger decay amplitudes that cannot be obtained from conventional spectroscopic measurement of line intensities. In many cases the anisotropy coefficient is very sensitive to subtle details of the theoretical description of Auger decay. Recently angle-resolved electron spectroscopy has been used to study the satellite Auger transitions excited by ion [4,5] as well as electron [6] impact. In the latter case the satellite intensity was found to be isotropic, indicating that the alignment of the excited states produced by electron impact is small. On the contrary, in the experiments with ion beam excitation [4,5] a considerable anisotropy was observed. In the latter experiments the K Auger satellite spectrum in Ne was excited using different projectiles including H^+, Ne^{3+}, Ne^{10+}, Ar^{6+}, and Ar^{16+}, with an impact energy of 5.5 MeV/amu. A study of the Ne *KL-LLL* satellite Auger transitions showed that the double-vacancy states $1s^{-1}2p^{-1}$ produced in ion impact are largely aligned and the following satellite Auger decay was found to be anisotropic.

The first theoretical calculations of the anisotropy of the Ne Auger satellite emission were based on a pure LS-coupling scheme and the single-configuration Hartree-Fock approximation [5,7]. Accordingly, the influence of the electron spins was completely ignored in these works. Although the results of calculations were in qualitative agreement with experiment, they were not able to reproduce the experimental data quantitatively and failed, in particular, to reproduce the different measured anisotropies of the Auger transitions from $1s^{-1}2p^{-1}\,{}^3P$ and ${}^1P$ initial states. These calculations also neglected the coherence effect in the ${}^3P$ initial states.

Previous calculations of the anisotropy of the normal [8–10] and resonant [11–14] Auger transitions have shown that initial- and final-state configuration interaction is essential for a proper description of the Auger electron angular distribution. One can expect that for Auger satellites these correlation effects are even more prominent [15]. This has prompted us to make a more accurate analysis of the angular distribution of satellite Auger electrons by using the multiconfiguration Dirac-Fock (MCDF) method which has provided an adequate description of the anisotropy of normal and resonant Auger transitions [10,13,14]. Within the MCDF approach we

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have calculated the energies, decay rates and anisotropy parameters for all the KL-LLL satellite Auger lines in Ne.

As we shall show below, widths of the individual initial double-vacancy states are often comparable to or larger than their energy splitting. Therefore, the levels belonging to the same multiplet overlap strongly. Coherent excitation of overlapping atomic states by the electromagnetic pulse of the projectile localized in time and space leads to interference effects [16] which effectively diminish the anisotropy of the subsequent Auger decay. The general theory of the angular distribution of electrons from the decay of autoionizing states with an arbitrary ratio between the energy splitting of fine-structure levels and the natural level width was developed by Mehlhorn and Taulbjerg [17] and Bruch and Klar [18]. In the present paper we suggest a modification of the general expression for the angular distribution, which is more convenient for relativistic calculations. Our expression has the same standard form as that used in the case of a well resolved decaying state, but is applicable to a general case of overlapping fine-structure levels. In order to facilitate understanding of the final expression, we derive it in the next section using the density matrix and statistical tensor formalism. Details of the calculation will be described in Sec. III. The results and a comparison with experiment are presented in Sec. IV. Atomic units are used throughout unless otherwise indicated.

II. ANGULAR DISTRIBUTIONS OF AUGER ELECTRONS PRODUCED BY EXCITATION OF OVERLAPPING STATES

We discuss the Auger process in terms of the conventional two-step model disregarding the direct transitions to the final state. The anisotropy of the angular distribution of Auger electrons is determined by the alignment of the decaying state induced at the first stage (ionization) as well as by the anisotropy of the decay itself. In this paper we concentrate on the intrinsic anisotropy of satellite Auger decay. The problems of the alignment in multiple ionization will be discussed elsewhere [19].

Consider Auger decay (autoionization) of a group of overlapping ionic (atomic) levels, specified by the total angular momentum J and a set of other quantum numbers denoted by γ. The initial state of the ion can be in general described by the density matrix $\langle \gamma JM|\hat{\rho}|\gamma' J'M'\rangle$ or equivalently by a set of statistical tensors (state multipoles)

$$\rho^i_{kq}(\gamma J,\gamma' J') = \sum_{MM'} (-1)^{J'-M'} \langle JMJ'-M'|kq\rangle \times \langle \gamma JM|\rho|\gamma' J'M'\rangle . \tag{1}$$

The statistical tensors of the final state of the system (after Auger decay) are connected to $\rho^i_{kq}(\gamma J,\gamma' J')$ by

$$\rho^f_{kq}(\tilde{\gamma} J,\tilde{\gamma}' J') = \langle \tilde{\gamma} J\|V\|\gamma J\rangle \rho^i_{kq}(\gamma J,\gamma' J') \langle \tilde{\gamma}' J'\|V\|\gamma' J'\rangle^* , \tag{2}$$

where the reduced matrix elements $\langle \tilde{\gamma} J\|V\|\gamma J\rangle = \langle J_f(l\tfrac{1}{2})j : J\|V\|\gamma J\rangle$ describe the Auger decay. Here J_f is the final ionic state angular momentum, and l and j the orbital and total angular momenta of the Auger electron.

According to the standard prescription [20] the angular distribution of the Auger electron can be written as

$$W(\theta,\phi) = C \sum_{JJ'\kappa q} \rho^f_{kq}(J,J') \varepsilon^*_{kq}(J,J') , \tag{3}$$

where $\varepsilon_{kq}(J,J')$ is an efficiency tensor of the detector and C is a constant factor which is determined by the normalization convention for statistical tensors. We omit the quantum numbers $\tilde{\gamma}$ and γ here and below for brevity. The efficiency tensor can be written according to the general rules [20]. If the residual ion is not detected and the detector of electrons is not sensitive to their spin polarization we finally get

$$W(\theta,\phi) = \frac{C}{4\pi} \sum_{kqJJ'} A_k(J,J') \rho^i_{kq}(J,J') \times Y_{kq}(\theta,\phi) \sqrt{\frac{4\pi}{2k+1}} , \tag{4}$$

where

$$A_k(J,J') = (-1)^{J+J_f-1/2} \sum_{ll'jj'} \hat{l}\hat{l}'\hat{j}\hat{j}'\hat{J}\hat{J}' \langle l0l'0|k0\rangle \times \begin{Bmatrix} j & J & J_f \\ J' & j' & k \end{Bmatrix} \begin{Bmatrix} j & l & 1/2 \\ l' & j' & k \end{Bmatrix} \times \langle J_f(l\tfrac{1}{2})j : J\|V\|J\rangle \langle J_f(l'\tfrac{1}{2})j' : J\|V\|J'\rangle^* . \tag{5}$$

Here we abbreviate $\hat{a} = [2a+1]^{1/2}$, the spherical harmonics are denoted by Y_{kq}, and standard notations are used for the Clebsch-Gordan coefficients and 6-j symbols. Due to the parity conservation in Auger decay, the summation in Eq. (4) is carried out over even values of k only. Expression (4) is equivalent to the expression (6) of Mehlhorn and Taulbjerg [17].

If the excitation process is axially symmetric (nonpolarized projectile and target, only the Auger electron is detected) only zero-projection statistical tensor components are nonzero and expression (5) reduces to

$$W(\theta) = \frac{C}{4\pi} \sum_{kJJ'} A_k(J,J') \rho^i_{k0}(J,J') P_k(\cos\theta) \tag{6}$$

with $k = 0, 2, 4, \ldots$.

Now we take into account that the atom has been excited by fast particle impact. The collision time is much shorter than the characteristic time of the precession caused by the spin-orbit interaction. In this case one can argue [16] that the initial states have been excited coherently at a definite time ($t = 0$) and their subsequent evolution is described by the statistical tensors

$$\rho^i_{kq}(J,J';t) = \rho^i_{kq}(J,J';t=0) e^{-i\omega_{JJ'}t - \Gamma_{JJ'}t} , \tag{7}$$

where $\omega_{JJ'} = E_J - E_{J'}$ is the energy splitting, $\Gamma_{JJ'} = (\Gamma_J + \Gamma_{J'})/2$, and Γ_J is the total width of the level J. In

a noncoincidence experiment considered here, the time of excitation is not known. Consequently one has to average expression (7) over time. Substituting Eq. (7) in Eq. (6) and integrating over time we obtain the angular distribution of Auger electrons in a familiar form [21,22],

$$W(\theta) = \frac{W^{(T)}}{4\pi}\left[1 + \sum_k a_k P_k(\cos\theta)\right]. \tag{8}$$

Here $W^{(T)}$ is the total probability per unit time of Auger decay to the definite final state J_f, integrated over all emission angles. With appropriate normalization of the statistical tensors we can write

$$W^{(T)} = \sum_J W^{(T)}_{J\to J_f} = \sum_J P(J)\Gamma_{J\to J_f}/\Gamma_J\ , \tag{9}$$

where P_J is the probability of excitation of the state J, Γ_J is its total width, and $\Gamma_{J\to J_f} = \sum_{lj} |\langle J_f(l\tfrac{1}{2})j : J\|V\|J\rangle|^2$ is its partial width corresponding to the particular Auger transition. The anisotropy coefficient a_k is

$$a_k = \sum_{JJ'} A_k(J,J')\rho^i_{k0}(J,J';t=0)\frac{\Gamma_{JJ'}}{\omega^2_{JJ'}+\Gamma^2_{JJ'}} \times\left[\sum_J \hat{J}\rho^i_{00}(J,J;t=0)\Gamma_{J\to J_f}/\Gamma_J\right]^{-1}. \tag{10}$$

Expressions (8)–(10) are general and valid for any set of unresolved levels. Note that due to the coherent excitation of the overlapping states the anisotropy coefficients a_k cannot be factorized into a product of two factors, the first one describing the excitation and the second one the decay process, as in the case of an isolated excited state.

Now we consider a particular case where all levels J belong to the same multiplet $M(LS)$. Suppose that the excitation is independent of spins and in the ground state of the target atoms the spin is randomly oriented. Then the statistical tensors of the excited states may be expressed in terms of statistical tensors of the orbital angular momentum only:

$$\rho^i_{kq}(J,J';t=0) = \rho^i_{kq}(L,L)(-1)^{J'+L+S+k} \times\frac{\hat{J}\hat{J}'}{\hat{S}^2}\begin{Bmatrix} J & L & S \\ L & J' & k\end{Bmatrix}. \tag{11}$$

Substituting Eq. (11) into Eqs. (8)–(10) we obtain the angular distribution of Auger electrons from an unresolved multiplet M to the final state J_f as

$$W_{M\to J_f}(\theta) = \frac{W^{(T)}_{M\to J_f}}{4\pi}\left[1 + \sum_k \alpha_k^{M\to J_f}\mathcal{A}_{k0}(L,L) \times P_k(\cos\theta)\right], \tag{12}$$

where $\mathcal{A}_{k0}(L,L)$ is the alignment parameter characterizing the alignment of the orbital angular momentum: $\mathcal{A}_{k0}(L,L) = \rho_{k0}(L,L)/\rho_{00}(L,L)$. The anisotropy coefficient α_k for the whole multiplet has the form

$$\alpha_k^{M\to J_f} = \frac{1}{N}\sum_{JJ'} A_k(J,J')(-1)^{J'+L+S+k}\frac{\hat{J}\hat{J}'}{\hat{S}^2} \times\begin{Bmatrix} J & L & S \\ L & J' & k\end{Bmatrix}\frac{\Gamma_{JJ'}}{\omega^2_{JJ'}+\Gamma^2_{JJ'}}\ , \tag{13}$$

where $N = \sum_J \hat{J}^2\Gamma_{J\to J_f}/(\hat{L}\hat{S}^2\Gamma_J)$. The total probability of Auger decay is

$$W^{(T)}_{M\to J_f} = \sum_J P(L)\frac{\hat{J}^2}{\hat{L}^2\hat{S}^2}\frac{\Gamma_{J\to J_f}}{\Gamma_J}. \tag{14}$$

The anisotropy coefficients in Eq. (12) are factorized into parts determined by the excitation and decay processes. However, the physical meaning of the parameters is not the same as in the case of an isolated level [22]. The parameter $\alpha_k^{M\to J_f}$ is the average anisotropy of the multiplet, which depends on the widths and the energy splitting of the levels, and $\mathcal{A}_{k0}(L,L)$ is the alignment of the orbital angular momentum only. Note that the relation (11) is approximate. It means that at the excitation stage of the process we ignore the spin-orbit interaction, and therefore all states of the multiplet can be characterized by a definite orbital angular momentum. This approximation is used for calculating the alignment only. In the calculation of Auger amplitudes the spin-orbit interaction is fully taken into account.

For the singlet initial state $S = 0$, $J = J' = L$, and $\rho^i_{kq}(J,J';t=0) = \rho^i_{kq}(L,L)$. In this case expression (12) coincides with the usual one for an isolated excited state [22]. Analyzing experimental angular distributions, it is convenient to use transitions from a singlet state in order to obtain the experimental value of the alignment parameter $\mathcal{A}_{k0}(L,L)$ which may be used further in the analysis of the angular anisotropy of triplet states.

When the lines corresponding to the different states of the final multiplet are not resolved by experiment, Eq. (12) should be summed over all $J_f \in \{M_f\}$. The resulting angular distribution has the same form as Eq. (12) with

$$W^{(T)}_{M\to M_f} = \sum_{J_f\in\{M_f\}} W^{(T)}_{M\to J_f} \tag{15}$$

and

$$\alpha_k^{M\to M_f} = \sum_{J_f\in\{M_f\}} W^{(T)}_{M\to J_f}\alpha_k^{M\to J_f} \Big/ \sum_{J_f\in\{M_f\}} W^{(T)}_{M\to J_f}. \tag{16}$$

Next we discuss two limiting cases.

(i) $\Gamma_{JJ'} \ll \omega_{JJ'}$, i.e., nonoverlapping initial levels. In this case only terms $J = J'$ are significant and expression (12) transforms into an incoherent sum of contributions from the individual levels,

$$W_{M\to J_f}(\theta) = \sum_{J\in\{M\}} W_{J\to J_f}(\theta)$$
$$= \sum_{J\in\{M\}} \frac{W^{(T)}_{J\to J_f}}{4\pi}\left[1+\sum_k \alpha_k^{J\to J_f}\mathcal{A}_{k0}(J,J) \times P_k(\cos\theta)\right], \quad (17)$$

where $\mathcal{A}_{k0}(J,J) = \rho_{k0}(J,J;t=0)/\rho_{00}(J,J;t=0)$ and $\alpha_k^{J\to J_f}$ is determined by the known expression (see Ref. [22])

$$\alpha_k^{J\to J_f} = \frac{1}{\Gamma_{J\to J_f}}(-1)^{J+J_f-1/2}\sum_{ll'jj'}\hat{l}\hat{l}'\hat{j}\hat{j}'\langle l0l'0|k0\rangle \times\begin{Bmatrix} j & J & J_f\\ J & j' & k\end{Bmatrix}\begin{Bmatrix} j & l & 1/2\\ l' & j' & k\end{Bmatrix} \times\langle J_f(l\tfrac{1}{2})j : J\|V\|J\rangle\langle J_f(l'\tfrac{1}{2})j' : J\|V\|J'\rangle^*. \quad (18)$$

(ii) In the opposite limiting case $\Gamma_{JJ'} \gg \omega_{JJ'}$ there is complete overlap of the initial states. In this case one can neglect $\omega_{JJ'}$ in the denominator of Eq. (13). The general expression can still be simplified if we consider transitions to the final-state multiplet. Suppose that both initial and final states are well described by the LS-coupling scheme and ignore the spin-orbit interaction in the Auger electron continuum state. Then one can transform the matrix element of Auger decay to the matrix element in LS coupling:

$$\langle (L_fS_f)J_f,(l\tfrac{1}{2})j : J\|V\|(LS)J\rangle = \hat{J}_f\hat{j}\hat{L}\hat{S}\begin{Bmatrix} L_f & S_f & J_f\\ l & 1/2 & j\\ L & S & J\end{Bmatrix}\langle (L_fl)L\|V\|L\rangle . \quad (19)$$

Substituting Eq. (19) into Eqs. (5) and (10) and summing over all final states belonging to the multiplet M_f one can obtain after some angular momentum algebra an expression of the angular distribution of Auger electrons in LS coupling summed over the multiplets in the initial and final states:

$$W_{M\to M_f}(\theta) = \frac{W^{(T)}_{M\to M_f}}{4\pi}\left[1+\sum_k \alpha_k^{M\to M_f}\mathcal{A}_{k0}(L,L) \times P_k(\cos\theta)\right], \quad (20)$$

where

$$\alpha_k^{M\to M_f} = \frac{1}{N}\hat{L}(-1)^{L-L_f}\sum_{ll'}\hat{l}\hat{l}'\langle l0l'0|k0\rangle\begin{Bmatrix} L & L & k\\ l & l' & L_f\end{Bmatrix} \times\langle (L_fl)L\|V\|L\rangle\langle (L_fl')L\|V\|L\rangle^* \quad (21)$$

and the normalization is given by $N = \sum_l |\langle (L_fl)L\|V\|L\rangle|^2$. This formula is identical with that used in Refs [5–7] and it may be easily obtained from the general formula of Ref. [22], by ignoring spins.

III. CALCULATIONS

The energies and wave functions of the initial and final bound states were calculated by the multiconfiguration Dirac-Fock method (MCDF) [23]. All jj-coupled configurations that can be obtained from the nonrelativistic parent configurations $1s^{-1}(2s2p)^{-1}$ (initial state) and $(2s2p)^{-3}$ (final state) were included in the diagonalization of the Hamiltonian. The Auger decay amplitudes were calculated using one-electron orbitals optimized for the initial ionic state. The same bound orbitals were also used in the final-state multiconfiguration wave function, and therefore orbital relaxation was not accounted for in our calculations. The single-channel continuum states were constructed by generating the Auger electron continuum orbitals using a jj-average potential of the final ionic state. In the construction of this potential we used initial-state bound orbitals but changed the generalized occupation numbers to correspond to the final bound state [23]. Lagrangian multipliers were used to obtain orthogonality with bound orbitals and the jj-average exchange interaction between the Auger electron and the residual ion was fully taken into account. The details of the numerical procedure used in the MCDF code has been described recently by Tulkki *et al.* [10,24].

As shown by our calculations (see below), the splitting of the initial double-vacancy levels is of the same order as or even less than their natural width. Besides, the energy resolution of the experiment [5] was not sufficient to resolve the transitions to the fine-structure levels of the final multiplet. Therefore, we calculated the average intensity using expression (14) and average anisotropy parameters using expression (13) which were in addition averaged over the final states according to Eqs. (15) and (16).

IV. RESULTS AND DISCUSSION

A. Energies and intensities of satellite transitions

Energies and intensities of the KL-LLL Auger satellites in Ne have been measured in a number of experiments using electrons [6,25,26], protons, or heavier ions [27,28] for generating Auger transitions. A discussion of the consistency of the experimental results can be found in Ref. [28]. In Table I we show the experimental transition energies from two recent high-resolution measurements with electron beams [6] and ion beams [28]. In Ref. [6] the energies were measured relative to the $KL_{2,3}L_{2,3}$ ^1D diagram line. To obtain the absolute energies we used the energy of this line, 804.5 eV [29], which was also used in Ref. [28] for energy calibration. The results of the two measurements are in perfect agreement. There are several calculations of energies and intensities of Ne Auger satellites [15,30–32,26]. Practically all calculations of transition energies give very similar results, which are in good agreement with experimental data. In Table I we present our calculated energies which are in good agreement with experiment and previous calculations. The average difference between our results and corresponding results, for example, of the single-configuration DF cal-

TABLE I. Measured and calculated energies and branching ratios for selected Ne KL-LLL satellite Auger transitions. The initial-state configuration is $1s^1 2s^2 2p^5\ ^{1,3}P$.

Initial state	Final state	Energy (eV)			Branching ratios (%)			
		Experiment		Theory	Experiment		Theory	
		Ref. [28]	Ref. [6]	This work	Ref. [28]	Ref. [6]	Ref. [15]	This work
^3P	$1s^2 2s^0 2p^5\ ^2P$	730.95(2)	730.95(8)	730.09	10.8(3)	10.0(7)	9.6	11.05
	$1s^2 2s^1 2p^4\ ^2P$	751.41(3)	751.46(8)	751.80	8.7(3)	8.0(7)	9.0	11.17
	$1s^2 2s^1 2p^4\ ^2S$		754.48(12)	755.45		2.4(7)	2.3	2.8
	$1s^2 2s^1 2p^4\ ^2D$	759.62(9)	759.66(12)	760.93	14.3(5)	13.1(7)	11.6	13.94
	$1s^2 2s^1 2p^4\ ^4P$	768.32(8)	768.32(12)	770.99	6.8(2)	4.1(7)	4.9	5.36
	$1s^2 2s^2 2p^3\ ^2P$	783.29(1)	783.45(8)	786.18	16.4(5)	21.6(10)	21.8	18.42
	$1s^2 2s^2 2p^3\ ^2D$	785.86(2)	786.04(8)	788.35	43.0(4)	40.8(14)	40.8	37.25
	$1s^2 2s^2 2p^3\ ^4S$			793.77				0.001
^1P	$1s^2 2s^0 2p^5\ ^2P$	735.41(4)	735.42(8)	734.50	13.6(3)	10.0(10)	10.3	12.06
	$1s^2 2s^1 2p^4\ ^2P$	755.67(3)	755.83(8)	756.21	23.5(7)	23.5(10)	22.4	27.55
	$1s^2 2s^1 2p^4\ ^2S$			759.86				0.00
	$1s^2 2s^1 2p^4\ ^2D$	763.71(4)	764.1(2)	765.35	10.2(4)		0.0	0.00
	$1s^2 2s^1 2p^4\ ^4P$			775.38				0.00
	$1s^2 2s^2 2p^3\ ^2P$	787.84(2)	787.83(8)	790.59	18.4(7)	23.4(15)	23.5	20.05
	$1s^2 2s^2 2p^3\ ^2D$	790.46(1)	790.51(8)	792.76	34.0(10)	41.4(15)	43.9	40.34
	$1s^2 2s^2 2p^3\ ^4S$			798.24				0.00

culation [30] is 0.7 eV. Our calculated transition energies are slightly higher than the experimental ones. The average deviation is 1.56 eV (maximal 2.76 eV). Probably, inclusion of higher configurations, especially for the final three-L-vacancy state, would further improve the agreement. However this investigation was out of our scope.

The relative intensities are more sensitive to the details of the calculation. As was pointed out by Schmidt [15], for explanation of the relative intensities of Auger satellites it is essential to take into account configuration interaction in the final ionic state. In Table I we show some of the experimental results together with the earlier theoretical results and our own calculations. One can see that the relative intensities of satellites are also reproduced fairly well by our calculation. The agreement of our results with experiment is slightly better than in Ref. [15].

The total transition rates were calculated for all initial states. In particular, the initial state $1s2s^2 2p^5\ ^1P$ has the width 0.187 eV. The fine-structure components $^3P_0$, $^3P_1$ and $^3P_2$ of the initial state $1s2s^2 2p^5\ ^3P$ have the widths 0.204, 0.204, and 0.205 eV, respectively. On the other hand, the energy difference between the $^3P_0$ and $^3P_1$ states is 0.055 eV and between the $^3P_1$ and $^3P_2$ states it is 0.105 eV. The fine-structure levels overlap considerably and therefore coherent excitation may notably affect the angular distribution of the Auger electrons.

B. Angular anisotropy parameters

Table II shows experimental and theoretical anisotropy parameters α_2 for the Auger transitions from the $1s2s2p^5$ ^1P and ^3P initial states. The experimental values were obtained by reanalyzing the Auger electron spectra excited in Ne^{3+} + Ne collisions [5]. The fitting procedure included the change of the Auger line shape due to the post-collision interaction. The intensities of Auger lines measured at several ejection angles were fitted by expression (12) and the anisotropy parameters α_2 and the alignment $\mathcal{A}_{20}$ were determined. The alignment of the orbital angular momentum of the initial state $\mathcal{A}_{20}(L = 1)$ was obtained from the anisotropy of the $1s2s^2 2p^5\ ^1P \rightarrow 1s^2 2s^2 2p^3\ ^2D$ transition, which in both calculations (see Table II) has the same value $\alpha_2 = 0.707$. All other experimental α_2 values listed in Table II were obtained using this $\mathcal{A}_{20}$ value. The listed data are slightly different from those published in Ref. [5] due to the different line shape used in the analysis (see above). However, the difference is much less than the experimental errors.

The theoretical results presented in Table II are from Ref. [5] in pure LS coupling [Eq. (21)] and from our

TABLE II. Angular anisotropy parameters α_2, calculated from Eqs. (13) and (16), for some of the Ne KL-LLL satellite Auger transitions. The initial-state configuration is $1s^2 s^2 2p^5\ ^{1,3}P$.

Initial state	Final state	Expt.[a]	Theory	
			LS	MCDF
		Ref. [5]	Ref. [5]	This work
^3P	$1s^2 2s^0 2p^5\ ^2P$	−0.22(5)	0.000	0.005
	$1s^2 2s^1 2p^4\ ^2P$	0.62(20)	0.707[c]	0.574
	$1s^2 2s^1 2p^4\ ^2S$		−1.414[c]	−1.149
	$1s^2 2s^1 2p^4\ ^2D$	−0.31(6)	−0.141	−0.115
	$1s^2 2s^1 2p^4\ ^4P$	0.80(20)	0.707[c]	0.574
	$1s^2 2s^2 2p^3\ ^2P$	−0.75(20)	−0.511	−0.405
	$1s^2 2s^2 2p^3\ ^2D$	0.62(15)	0.707[c]	0.573
	$1s^2 2s^2 2p^3\ ^4S$			−0.384
^1P	$1s^2 2s^0 2p^5\ ^2P$	−0.14(3)	0.000	0.005
	$1s^2 2s^1 2p^4\ ^2P$	0.71(32)	0.707[c]	0.707
	$1s^2 2s^1 2p^4\ ^2S$		−1.414[c]	0.676
	$1s^2 2s^1 2p^4\ ^2D$	−0.16(3)	−0.141	−0.094
	$1s^2 2s^1 2p^4\ ^4P$			−0.510
	$1s^2 2s^2 2p^3\ ^2P$	−0.44(23)	−0.511	−0.498
	$1s^2 2s^2 2p^3\ ^2D$ [b]	0.707	0.707[c]	0.707
	$1s^2 2s^2 2p^3\ ^4S$			−0.503

[a]The data given here deviate slightly from those in Ref. [5] due to a different evaluation of experimental data.

[b]This line was used to determine the alignment of the initial state.

[c]These values are independent of the Auger amplitudes in the LS coupling.

MCDF calculations, which account for the partial overlap of the initial states [Eq.(13)]. First we note that in LS coupling the angular anisotropy is determined in a model-independent way for some transitions, marked with the superscript "c" in Table II. This is connected to the fact that for these transitions only one Auger emission channel is possible according to the momentum and parity selection rules. Note also that in this approximation the anisotropy parameters α_2 are equal for the ^3P and ^1P initial states because the spins are not involved in the alignment process and do not affect the Auger amplitudes. In the experiment there is a notable difference between the anisotropy of transitions corresponding to the ^3P and ^1P states. This difference is explained by the MCDF calculations in a natural way since the spin-orbit and spin-spin interactions are automatically included in this approach. The difference between the nonrelativistic LS coupling and our MCDF calculations is as a rule smaller than experimental error. More accurate experimental data are therefore necessary before a more definite comparison of different theoretical models can be made.

In general the agreement of our calculations with the experimental data is quite good. The only exception is the transitions to the $1s^22p^5\ ^2P$ level which according to the experiment show negative anisotropy, whereas in the calculation they are practically isotropic. The calculation slightly underestimates the anisotropy parameters for the transitions to the $1s^22s2p^4\ ^2D$ levels.

To study the interference effect it is interesting to compare results for satellite transitions from the ^3P state obtained in different approximations: complete overlapping of the fine-structure levels (LS coupling), partial overlapping, and nonoverlapping J levels of the multiplet (Table III). In the last case the contribution of the different levels of the multiplet were summed incoherently. All three cases were calculated using one and the same expression (13) for the angular anisotropy parameter. The case of complete overlapping was simulated by giving to the width Γ_J an artificially large value $\Gamma_J \gg \omega_{JJ'}$. The same method but with $\Gamma_J \ll \omega_{JJ'}$ was used to simulate the case of nonoverlapping initial fine-structure states. One can see from Table III that the effect of coherence is considerable. In some cases the α_2 parameter changes dramatically if one compares two limiting cases and even changes sign (see, for example, transitions to the final states $1s^22s2p^4\ ^2D_{3/2}$ and $^4P_{3/2}$). On the average the results for the real width $\Gamma_J = 0.2$ eV are closer to the complete overlapping limit than to the limit of nonoverlapping levels. Nevertheless, the difference between the LS-coupling limit and the real case is still large.

TABLE III. Anisotropy parameters α_2 for Auger decay of $1s2s^22p^5\ ^3P$ initial state. In addition to the values corresponding to the calculated half width $\Gamma = 0.20$ eV we also give the limiting values obtained by giving to the half width Γ_J in Eq. (13) an artificially large ($\Gamma_J \gg \omega_{JJ'}$) or small ($\Gamma_J \ll \omega_{JJ'}$) value.

Final state	$\Gamma_J \gg \omega_{JJ'}$	$\Gamma_j = 0.20$ eV	$\Gamma_J \ll \omega_{JJ'}$
$1s^22s^22p^3\ ^4S_{3/2}$	−0.489	−0.384	−0.096
$1s^22s^22p^3\ ^2D_{3/2}$	0.704	0.542	0.119
$1s^22s^22p^3\ ^2D_{5/2}$	0.707	0.594	0.247
$1s^22s^22p^3\ ^2P_{1/2}$	−0.508	−0.449	−0.236
$1s^22s^22p^3\ ^2P_{3/2}$	−0.496	−0.385	−0.090
$1s^22s^12p^4\ ^4P_{5/2}$	0.707	0.641	0.391
$1s^22s^12p^3\ ^4P_{3/2}$	0.707	0.456	−0.183
$1s^22s^12p^3\ ^4P_{1/2}$	0.707	0.611	0.372
$1s^22s^12p^3\ ^2D_{3/2}$	−0.141	−0.097	0.010
$1s^22s^12p^3\ ^2D_{5/2}$	−0.141	−0.127	−0.072
$1s^22s^12p^3\ ^2S_{1/2}$	−1.413	−1.149	−0.396
$1s^22s^12p^3\ ^2P_{3/2}$	0.707	0.603	0.270
$1s^22s^12p^3\ ^2P_{1/2}$	0.707	0.516	0.049
$1s^22s^02p^5\ ^2P_{3/2}$	0.006	0.007	0.006
$1s^22s^02p^5\ ^2P_{1/2}$	0.006	0.002	−0.007

V. CONCLUSIONS

We have calculated the energies, intensities, and anisotropy parameters of the Ne KL-LLL satellite Auger transitions by taking into account the initial and final configuration interaction within the framework of the multiconfiguration Dirac-Fock approximation. It has been shown that the initial double-hole states belonging to the same multiplet partially overlap. Therefore, the angular distribution of Auger electrons is affected by the coherent excitation of these levels in a collision process. A modification of the general formalism is developed for a description of the angular distribution of Auger electrons in the decay of partially overlapping resonances which is convenient for relativistic calculations of Auger amplitudes. Our MCDF calculations predict a large coherence effect in the anisotropy of the Ne KL-LLL satellite Auger spectrum. Due to the high error limits in the presently available experimental data, new, more accurate measurements are necessary before a quantitative verification of our theoretical results becomes feasible. On the theoretical side our work suggests the need for more extensive configuration-interaction calculations of the bound states and inclusion of the electronic relaxation effect.

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