5*p* photoemission from laser-excited cesium atoms

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Fine-structure resolved 5*p* photoemission spectra of Cs in the ground state and after laser excitation into the [Xe]6*p* $^2P_{1/2}$ and $6p$ $^2P_{3/2}$ states have been studied. The $5p^56p$ final states have been reached by the $5p^66s$ → $5p^56p$ conjugate shakeup process from ground-state atoms as well as by direct photoemission from laser-excited atoms. The laser-excited spectra can be well described with calculations based on the *jK*-coupling model. Calculations based on a multiconfiguration Dirac-Fock approach have been performed to investigate the deviations created by intermediate coupling from the pure *jK*-coupling scheme.

I. INTRODUCTION

Photoelectron spectroscopy is an effective method for studying the electronic structure of matter. Laser spectroscopy can be used to study specifically excited optical transitions of the valence electrons and gives detailed insight into the valence shell couplings. In this paper, we combine these two techniques to examine the photoemission of laser-excited cesium. A continuous wave laser has been used to selectively excite cesium atoms into a well defined electronic state. From this state we measured high-resolution photoemission spectra with synchrotron radiation. Similar experiments combining lasers and synchrotron radiation have already been performed in the early 1980s [1], but only recently the combination of lasers with third-generation, high-resolution synchrotron sources made it possible to study the fine structure of the spectra.

In the last two years, alkali-metal atoms [2–6] have been studied in combination of laser and synchrotron radiation. The direct and shakeup photoemission spectra have been studied for laser-excited sodium [2], rubidium [5], and potassium [6]. Shakedown spectra have been studied for laser-excited sodium [3]. Being the heaviest stable alkali-metal atom, cesium is an outstanding candidate for high-resolution photoemission studies. Even for the low binding-energy 5*p* electrons, the spin-orbit interaction is so strong that these states cannot be understood in the LS coupling approximation. The case of cesium differs considerably from rubidium [5] not only because of the stronger spin-orbit interaction but also because of the close lying open 4*f* shell. It is an interesting question whether the interaction between the 6*p* state and the 4*f* excited states plays a role in the explanation of the $5p^56p$ final states.

In the photoionization of ground-state cesium, the $5p^56p$ final states can be reached by a parity-changing shake process. These processes are generally referred to as conjugate shakeup and explained by a dipole excitation of the valence shell accompanied by a monopole photoemission of the inner shell electron. However, this process requires at least two active electrons and its intensity is therefore very low, thus it is difficult to obtain detailed information on the final states from this transition in experiment. We therefore use an alternative route to reach these final states. The atoms are laser-excited into each of the two $5p^66p$ $^2P_{1/2,3/2}$ states and then subsequently ionized. With this procedure, the $5p^56p$ final states are populated by direct photoemission. Thereby, the analysis of the spectra is considerably easier. By tuning the laser to the $6s_{1/2}$→$6p_{1/2}$ or the $6s_{1/2}$→$6p_{3/2}$ transition, we can choose two different initial states for this transition that lead to different relative intensities. It has been shown in laser-excited rubidium [5] that this procedure considerably increases the information on the final states.

II. EXPERIMENTAL SETUP

The spectra have been recorded using a modified Scienta SES100 electron spectrometer at the undulator beamline I411 [7,8] of the storage ring MAX II in Lund (Sweden). The photoelectrons have been recorded in the magic angle with respect to the electric-field vector of the synchrotron radiation. The spectral resolution has been determined to be 50 meV by fitting the final-state structure of atomic cesium to the measured spectrum. Atomic cesium vapor has been produced with a resistively heated oven at about 126 °C giving a vapor pressure of approximately 10^{-3} mbar in the crucible. The setup has been described in more detail in Ref. [9]. The atoms have been excited by a continuous-wave Ti:Sa laser tuned to the Cs $6s_{1/2}$→$6p_{1/2}$ and Cs $6s_{1/2}$→$6p_{3/2}$ transition at 894.3 and 852.1 nm, respectively. The laser beam entered the experimental chamber from a glass view port opposite to the entrance of the synchrotron radiation beam. The laser light was linearly polarized with an electric-field vector parallel to the electric-field vector of the synchrotron radiation. Other polarization directions have been used as well, but no change in the relative intensities due to polar-

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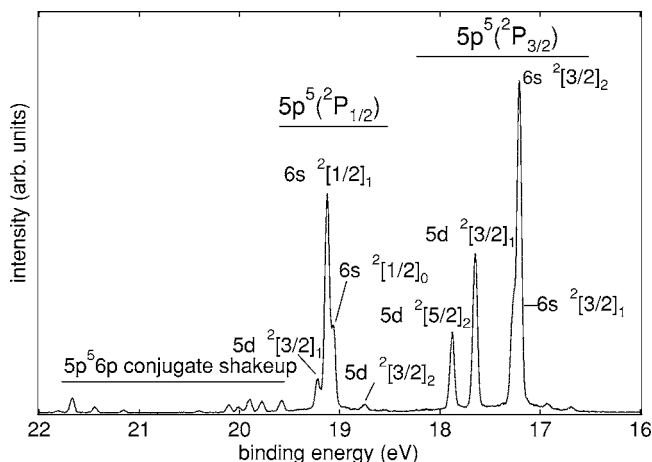
FIG. 1. The Cs $5p$ photoelectron spectrum. The spectrum shows the direct photoemission and the $6s \rightarrow 6p$ conjugate shakeup.

ization effects has been observed. In saturation and with good spatial alignment of the laser beam with respect to the synchrotron radiation beam, a fraction of up to 5% of the Cs atoms could be pumped into the excited state.

III. $5p$ PHOTOEMISSION

Figure 1 shows the Cs $5p$ photoemission spectrum. The spectrum can be divided into the direct photoemission lines between 17.0 and 19.4 eV and the $6s \rightarrow 6p$ conjugate shakeup lines between 19.4 and 22.0 eV. In the direct photoemission, final-state configuration interaction leads to the mixing of $5p^5 6s$ and $5p^5 5d$ electronic configurations. The binding-energy scale has been calibrated and the lines have been interpreted with the aid of optical data [10]. The direct photoemission lines split into two multiplets that are defined by the $5p$ hole total angular momenta $j=1/2$ and $3/2$. A similar observation in the $4p$ photoemission of atomic rubidium [5] showed that this configuration can be well explained within the jK-coupling scheme where the total angular momentum of the inner p hole couples to the spatial angular momentum of the valence electron to an intermedi-
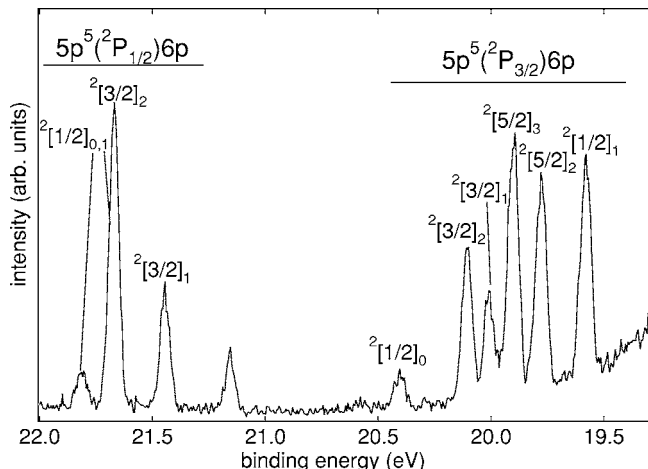

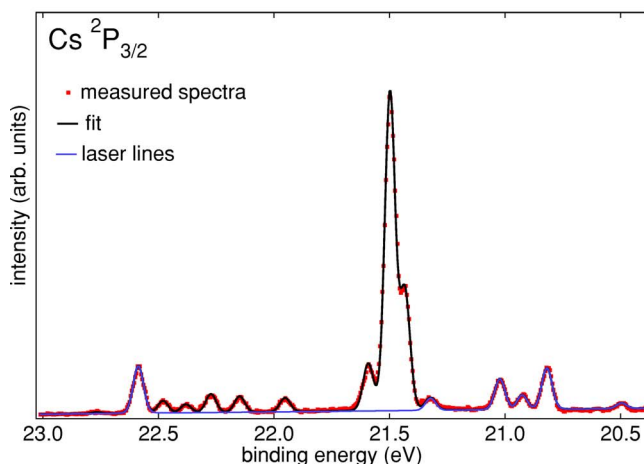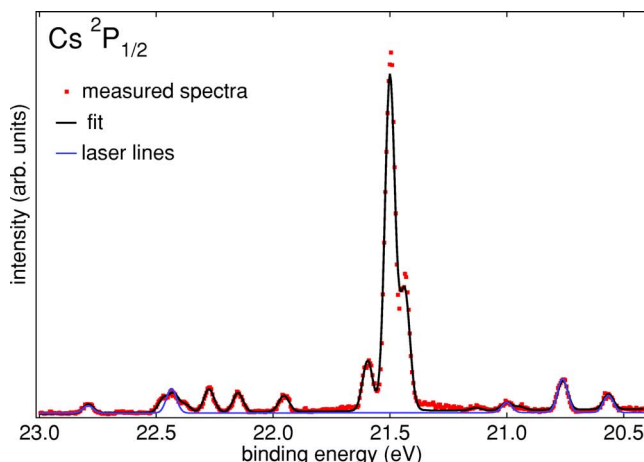FIG. 2. The $6s \rightarrow 6p$ conjugate shakeup spectrum.

FIG. 3. (Color online) Comparison of the Cs $5p^6 6p$ P_{J_0} $\rightarrow 5p^5 6p$ photoelectron spectra taken from two different initial states $^2P_{1/2}$ (upper panel) and $^2P_{3/2}$ (lower panel). The dots show the measured photoelectron signal, the black line gives a least-squares fit containing the structures from laser-excited and unexcited atoms, and the blue solid line plots the electron spectrum emerging from laser-excited atoms.

ate quantum number K_f. This quantum number finally couples with the valence electron spin to the total angular momentum J_f. The lines are assigned with the standard notation $^2[K_f]_{J_f}$.

Figure 2 shows a detailed view of the conjugate shakeup lines. In this spectrum a similar splitting into two group of lines for the $5p$-hole state with the total angular momenta $j=1/2$ and $3/2$ is visible. Two doublets for $j=1/2$ and three doublets for $j=3/2$ in the $5p^{-1}$ state can be seen. The spectrum resembles very much the conjugate shakeup in the $4p$ photoemission of rubidium [5]. Therefore, we will use the jK-coupling model, which explained the rubidium spectra well, as a first attempt to describe the excitation of these states from laser-excited cesium atoms.

IV. LASER-EXCITED Cs SPECTRUM

Figure 3 shows the $6p$ photoemission spectra of cesium comparing the two excitations $^2P_{1/2}$ (first panel) and $^2P_{3/2}$ (second panel). A least-squares fit to all cesium lines has
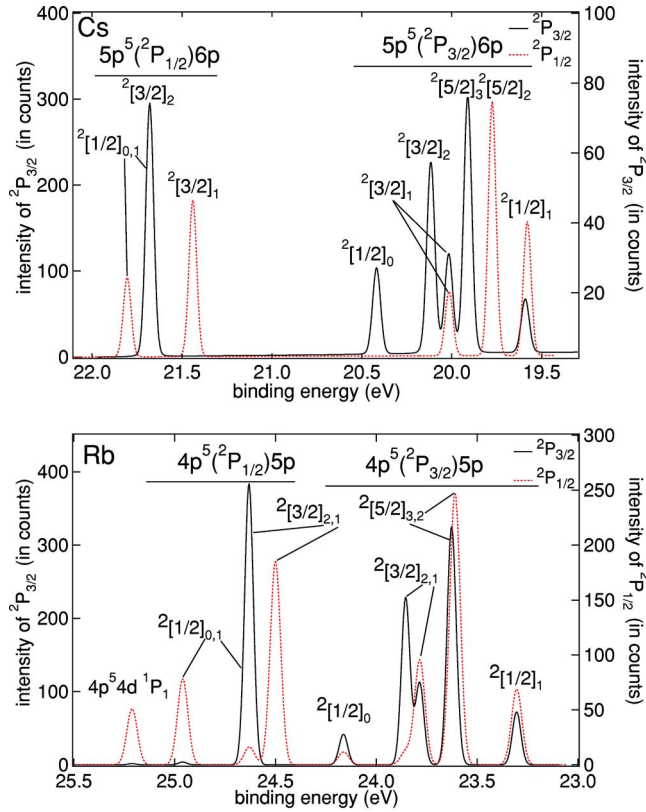
FIG. 4. (Color online) Comparison of the Cs $5p^6 6p$ $^2P_{J_0}$ $\rightarrow 5p^5 6p$ photoelectron spectra taken from two different initial states $^2P_{1/2}$ (red dashed line) and $^2P_{3/2}$ (black solid line) with the Rb $4p^6 5p$ $^2P_{J_0} \rightarrow 4p^5 5p$ photoelectron spectra [5] taken from two different initial states $^2P_{1/2}$ (red dashed line) and $^2P_{3/2}$ (black solid line).

been performed to obtain a spectrum from laser-excited cesium atoms only. The black line gives the fit to the measured data and the blue line shows the photoemission from the laser-excited state.

In Fig. 4, the electron spectrum emerging from the two different initial states $^2P_{1/2}$ (dashed red line) and $^2P_{3/2}$ (solid black line) has been plotted for comparison. The laser photon energy has been added to the binding energy in order to match the lines owing to the same final states. The lines clearly split up into two groups related to the spin-orbit splitting of the $5p$ subshell. The Cs $5p$ photoelectron spectra show a similar pattern like the Rb $4p$ photoelectron spectra [5], which are plotted for comparison into the lower panel of Fig. 4. For the $^2[3/2]$ and $^2[5/2]$ doublets, the line of a final state with a lower total angular momentum is more intense in the ionization from the $^2P_{1/2}$ state, the higher total angular momentum line is more intense in the ionization from the $^2P_{3/2}$ initial state. This pattern can be explained by a simple model. The difference between the initial states $5p^6 6p$ $^2P_{1/2}$ and $5p^6 6p$ $^2P_{3/2}$ is in the coupling of the spin to the orbital angular momentum of the valence electron. If we assume that the valence electron spin-orbit coupling is not changed during the photoemission, the initial state $5p^6 6p$ $^2P_{1/2}$ should lead to $^2[K]_{K-(1/2)}$ states and $5p^6 6p$ $^2P_{3/2}$ should lead to $^2[K]_{K+(1/2)}$ states. This conclusion agrees with the calcula-

TABLE I. Relative intensities of the experimental $5p$ photoemission spectrum for $^2P_{1/2}$ laser excitation.

Binding energy (eV)	Relative intensity (%)	Assignment
19.59	19.56	$5p^5(^2P_{3/2})6p$ $^2[1/2]_1$
19.78	36.22	$5p^5(^2P_{3/2})6p$ $^2[5/2]_2$
20.02	9.87	$5p^5(^2P_{3/2})6p$ $^2[3/2]_1$
21.46	22.53	$5p^5(^2P_{1/2})6p$ $^2[3/2]_2$
21.81	11.82	$5p^5(^2P_{1/2})6p$ $^2[1/2]_0$

tions based on the jK-coupling model that will be described later in this paper. Tables I and II summarize the final states that are excited in the experimental laser photoelectron spectra of Cs.

The cesium $5p$ photoelectron spectra deviate from the rubidium $4p$ photoelectron spectra [5] in the relative intensities (see Fig. 4). The line $5p^5(^2P_{3/2})6p$ $^2[1/2]_1$ for the $^2P_{1/2}$ initial state in the case of Cs (19.56%) is more intense than in the case of Rb (9.76%). For the $^2P_{3/2}$ initial state, the line $5p^5(^2P_{3/2})6p$ $^2[1/2]_0$ is more intensive for Cs (9.32%) than for Rb (3.56%). The latter observation gives insight into the origin of the deviations from the pure coupling model: There are only two final states with a total angular momentum of $J_f = 0$. These lines differ by the spin-orbit coupling of the core hole to a total angular momentum of $j = 1/2$ or $3/2$. The core-hole spin-orbit interaction for cesium is considerably larger than for rubidium. This is visible in the clear separation of the $j = 1/2$ and $3/2$ multiplets in Fig. 4. It leads to a weaker mixing of states that differ in the total angular momentum quantum number j of the core hole. This quantum number is therefore a better quantum number for describing the core-hole states in Cs than in Rb.

V. CALCULATIONS AND COMPARISON TO THE EXPERIMENT

To describe the spectra from laser-excited Cs, we will use two different approaches, namely an analytical jK-coupling model as given by Wernet and co-workers [11] and multiconfiguration Dirac-Fock (MCDF) calculations using the GRASP92 [12] code.

TABLE II. Relative intensities of the experimental $5p$ photoemission spectrum for $^2P_{3/2}$ laser excitation.

Binding energy (eV)	Relative intensity (%)	Assignment
19.59	6.04	$5p^5(^2P_{3/2})6p$ $^2[1/2]_1$
19.91	27.06	$5p^5(^2P_{3/2})6p$ $^2[5/2]_3$
20.02	10.78	$5p^5(^2P_{3/2})6p$ $^2[3/2]_1$
20.12	20.29	$5p^5(^2P_{3/2})6p$ $^2[3/2]_2$
20.42	9.32	$5p^5(^2P_{3/2})6p$ $^2[1/2]_0$
21.68	26.51	$5p^5(^2P_{1/2})6p$ $^2[3/2]_2$

In the jK-coupling model [13], the relative intensities for photoemission can be obtained using Eqs. (13), (15), and (17) from Ref. [11]. The total photoemission cross section is given by the parameter B_{000},

$$B_{000} = C_0(j, K_f, J_f) b_{000}, \qquad (1)$$

where

$$C_0(j, K_f, J_f) = \sqrt{3} \frac{\hat{J}_0^2 \hat{K}_f^2 \hat{J}_f^2}{\hat{l}_0^2} \begin{Bmatrix} J_0 & L_0 & S_0 \\ K_f & J_f & j \end{Bmatrix}^2 \qquad (2)$$

and

$$b_{000} = (|\langle \varepsilon s \| d \| 5p \rangle|^2 + |\langle \varepsilon d \| d \| 5p \rangle|^2). \qquad (3)$$

We have used $\hat{x} \equiv \sqrt{2x+1}$ and standard notation for the Wigner $6j$ symbol. L_0, S_0, and J_0 are the quantum numbers of the initial state $^2P_{J_0}$, and j is the total angular momentum of the core hole and couples with the valence orbital momentum L_0 to the resultant K_f. K_f couples with S_0 to the total final angular momentum J_f. In this approximation, the (relative) intensities of the photoemission lines are independent of the phases and relative amplitudes of the outgoing s-and d-symmetric electron waves. Only the sum of the squared amplitudes contributes to the intensities.

Beside the fact that the jK-coupling proved to be a good approximation for describing the photoemission of laser-excited rubidium, the analytical model has the advantage of giving a first insight into the involved quantum-mechanical couplings. However, to get a more complete picture of the photoemission process, intermediate coupling and configuration interaction has to be considered. In a second approach, we therefore calculated the spectra using the MCDF method. The relative photoionization cross sections have been evaluated using an approximate scheme where the ionization probability is determined by the weights of the initial-state parent configurations in the final ionic states. Within the MCDF scheme, this may be called a frozen configuration method, which has proven useful also in open-shell atoms (see, e.g., [14]). In terms of this approximation, the cross section becomes

$$Q_f(J_f) = \frac{1}{3} Q'_f(J_f) \int |\langle n_0 l_0 j_0 \| r C_1 \| \epsilon l' j' \rangle|^2 d\epsilon, \qquad (4)$$

where

$$Q'_f(J_f) = (2j_0 + 1) \left| \sum_{\nu\alpha} c_{f\nu} c_{0\alpha} \delta_{X_\nu Y_\alpha} \right|^2 \qquad (5)$$

is the reduced relative cross section. In Eq. (5), X_ν and Y_α refer to final and initial ionic state configurations, respectively, after decoupling the ionized orbital. The $c_{f\nu}$ and $c_{0\alpha}$ denote the associated mixing coefficients of the jj-coupled configuration state functions. The photoionization intensity estimates in this paper are based on Eq. (5), thus we have assumed that the single electron dipole amplitudes are the same for each final ionic state. The calculations were done using only configurations of the $5p^56p$ orbital occupations, which means that the model accounts for the intermediate
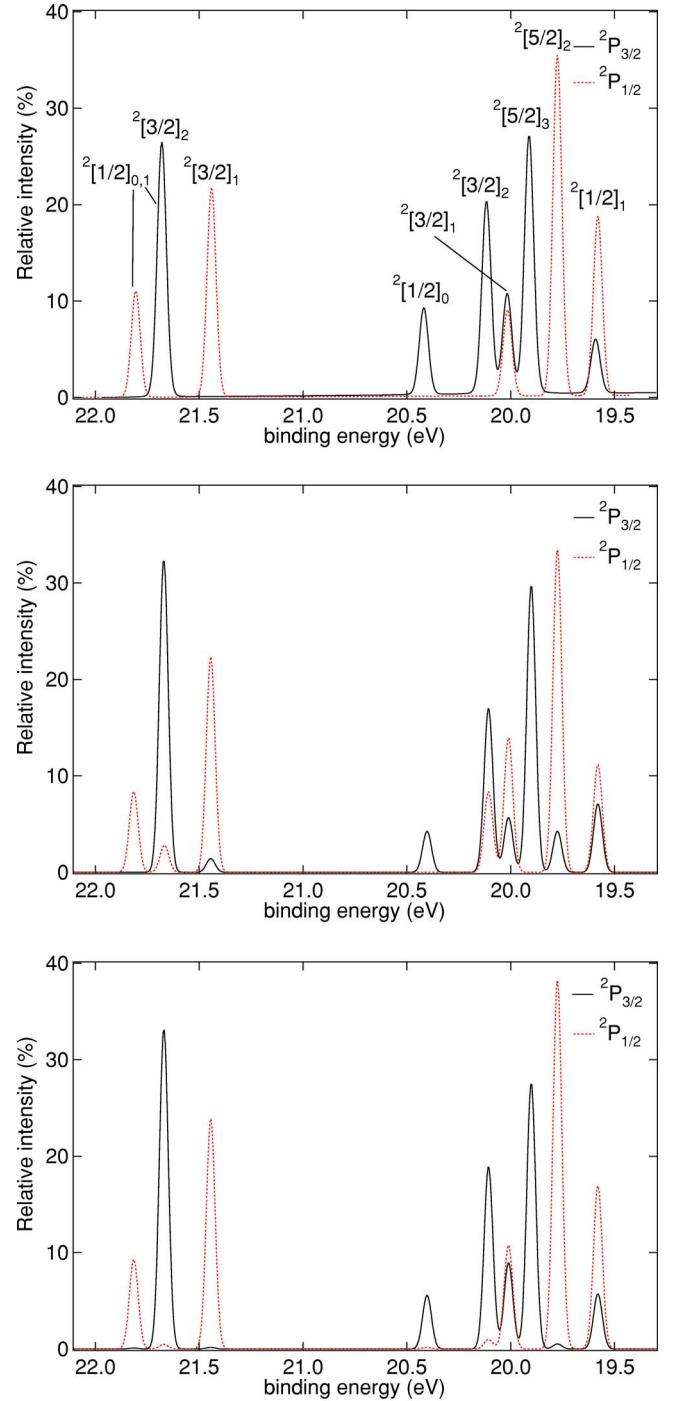

FIG. 5. (Color online). Comparison of the Cs $5p^66p$ $^2P_{J_0}$ $\rightarrow 5p^56p$ photoelectron spectra; experimental spectra (first panel), jK coupling (second panel), and MCDF calculations (third panel). The theoretical spectra are a convolution with a 50 meV Gaussian profile of the relative intensities.

coupling only, not for the mixing between different nonrelativistic configurations. In a separate MCDF calculation, $5p^54f$ and $5p^56p$ configurations were found not to mix, but differ in energy by about 4 eV.

Figure 5 shows the comparison of the experimental and theoretical Cs $5p^66p$ $^2P_{J_0} \rightarrow 5p^56p$ photoelectron spectra.

TABLE III. Relative intensities of the calculated $5p$ photoemission lines for $^2P_{1/2}$ laser excitation.

	Relative intensity		
(jK)	(MCDF)	(Expt.)	Assignment
11.11	16.80	19.56	$5p^5(^2P_{3/2})6p\ ^2[1/2]_1$
33.34	38.00	36.22	$5p^5(^2P_{3/2})6p\ ^2[5/2]_2$
0	0		$5p^5(^2P_{3/2})6p\ ^2[5/2]_3$
13.89	10.68	9.87	$5p^5(^2P_{3/2})6p\ ^2[3/2]_1$
8.33	0.99		$5p^5(^2P_{3/2})6p\ ^2[3/2]_2$
0	0.17		$5p^5(^2P_{3/2})6p\ ^2[1/2]_0$
22.21	23.67	22.53	$5p^5(^2P_{1/2})6p\ ^2[3/2]_1$
0	0.41		$5p^5(^2P_{1/2})6p\ ^2[3/2]_2$
2.78	0.08		$5p^5(^2P_{1/2})6p\ ^2[1/2]_1$
8.33	9.21	11.82	$5p^5(^2P_{1/2})6p\ ^2[1/2]_0$

TABLE IV. Relative intensities of the calculated $5p$ photoemission lines for $^2P_{3/2}$ laser excitation.

	Relative intensity		
(jK)	(MCDF)	(Expt.)	Assignment
6.94	5.66	6.04	$5p^5(^2P_{3/2})6p\ ^2[1/2]_1$
4.17	0.53		$5p^5(^2P_{3/2})6p\ ^2[5/2]_2$
29.16	27.32	27.06	$5p^5(^2P_{3/2})6p\ ^2[5/2]_3$
5.56	8.87	10.78	$5p^5(^2P_{3/2})6p\ ^2[3/2]_1$
16.67	18.75	20.29	$5p^5(^2P_{3/2})6p\ ^2[3/2]_2$
4.17	5.52	9.32	$5p^5(^2P_{3/2})6p\ ^2[1/2]_0$
1.38	0.17		$5p^5(^2P_{1/2})6p\ ^2[3/2]_1$
20.83	19.41	}26.51{	$5p^5(^2P_{1/2})6p\ ^2[3/2]_2$
11.11	13.68		$5p^5(^2P_{1/2})6p\ ^2[1/2]_1$
0	0.10		$5p^5(^2P_{1/2})6p\ ^2[1/2]_0$

The first panel shows the experimental spectra; the second and third panel show the theoretical spectra calculated with the jK-coupling model and the MCDF method, respectively. The energies for the theoretical spectra are taken from optical data [10]. Tables III and IV summarize the results that are presented in Fig. 5.

The theoretical spectra calculated with the simple jK-coupling model (second panel) are already in fairly good agreement with the experimental spectra. In particular, the above-mentioned relative intensities within the doublets resemble the experiment. However, there are some clear deviations from the experimental spectra. The theoretical spectra for the $^2P_{1/2}$ initial state show two lines, $5p^5(^2P_{3/2})6p\ ^2[3/2]_2$ and $5p^5(^2P_{1/2})6p\ ^2[1/2]_1$, which are not seen in the experiment. In the case of the $^2P_{3/2}$ initial state, the jK approach generates also two additional lines, $5p^5(^2P_{3/2})6p\ ^2[5/2]_2$ and $5p^5(^2P_{1/2})6p\ ^2[3/2]_1$, in clear disagreement with the experiment. Similar deviations have already been reported in the $5p$ photoemission spectrum of atomic rubidium [5]. The calculations based on the MCDF method (third panel) are in better agreement with the experiment than the predictions of the jK-coupling model. For both initial states $^2P_{1/2}$ and $^2P_{3/2}$, the additional lines created by the jK approach are considerably reduced.

According to the MCDF calculations, the states $5p^5(^2P_{3/2})6p\ ^2[3/2]_2$ and $^2[5/2]_2$ as well as the states $5p^5(^2P_{1/2})6p\ ^2[1/2]_1$ and $^2[3/2]_1$ mix. Also the states $5p^5(^2P_{3/2})6p\ ^2[1/2]_1$ and $5p^5(^2P_{3/2})6p\ ^2[3/2]_1$ mix strongly. Because of the mixing of the $J_f=2$ states, a part of the intensity of the $5p^5(^2P_{3/2})6p\ ^2[5/2]_2$ line is transferred to the line $5p^5(^2P_{3/2})6p\ ^2[3/2]_2$ in the case of the $^2P_{3/2}$ initial state. The situation is opposite for the $^2P_{1/2}$ initial state. The line $5p^5(^2P_{3/2})6p\ ^2[5/2]_2$ is getting intensity from the $5p^5(^2P_{3/2})6p\ ^2[3/2]_2$ line. The same holds also for the $J=1$ states; the $5p^5(^2P_{1/2})6p\ ^2[3/2]_1$ line is losing part of its intensity to the line $5p^5(^2P_{1/2})6p\ ^2[1/2]_1$ in the case of the $^2P_{3/2}$ initial state. In the case of the $^2P_{1/2}$ initial state, the $5p^5(^2P_{1/2})6p\ ^2[3/2]_1$ line is getting intensity from the $5p^5(^2P_{1/2})6p\ ^2[1/2]_1$ line. The sum intensity of the

$5p^5(^2P_{3/2})6p\ ^2[1/2]_1$ and $5p^5(^2P_{3/2})6p\ ^2[3/2]_1$ is also redistributed in MCDF predictions as compared to the jK-coupling model. When the mixing is included in the theory by MCDF calculations, a better correspondence with the experiment is obtained than in the case of the jK-coupling predictions. This indicates that the MCDF approach used correctly accounts for mixing.

The mixing of final states with different $5p$ hole angular momentum j is for all lines weaker than 2%. It thus can be stated that j is a good quantum number for the $5p$ hole state of atomic cesium. However, due to a considerable mixing of states that differ in K_f quantum number, the K_f cannot be considered as a good quantum number for describing the $5p$ hole states with a $6p$ excited electron in Cs.

VI. CONCLUSIONS

The $5p^56p$ final states of cesium ions have been reached by shakeup photoemission from the neutral ground state as well as by the combination of laser excitation and direct photoemission from two different excited states. The $5p^56p$ configuration strongly resembles the $4p^55p$ configuration of atomic rubidium [5]. It can be described fairly well within the jK-coupling scheme, although some of the line intensities deviate considerably from the jK coupling predictions. Therefore, the intermediate coupling of the states has been considered and the intensities have been calculated by a multiconfiguration Dirac-Fock approach. The deviations of the Dirac-Fock calculations from the jK-coupling predictions are due to intermediate coupling and configuration interaction was found not to play any role in the case of $5p^56p$ states of Cs. The K_f quantum number is losing its meaning in assigning the states, but j of the $5p$ hole remains a good quantum number.

ACKNOWLEDGMENTS

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