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H. P. Saha
University of Central Florida

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Photoionization of the $2p$ subshell of sodium atoms in ground and excited states

H. P. Saha

Department of Physics, University of Central Florida, Orlando, Florida 32816

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Photoionization cross sections and asymmetry parameters of photoelectrons resulting from ionization in the $2p$ subshell of excited-state $2p^6 3p^2 P_{3/2}$ and ground-state $2p^6 3s^2 S_{1/2}$ sodium atoms have been calculated using the multiconfiguration Hartree-Fock method over a large photon energy range. Calculations of relative intensities and branching ratios for leaving the positive ions in various final states corresponding to the main and satellite lines have been made and are compared with the available experimental measurements. It is found that there is a strong enhancement of the relative intensity of the shake-up satellite in the excited atom, in agreement with experimental observation. The asymmetry parameter β in the excited state agrees well with a recent experimental measurement made at a single photon energy. Further experimental work is needed to verify the theoretical results over a large photon energy range.

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I. INTRODUCTION

The problem of photoionization of inner-shell electrons has long been of interest to atomic physicists because of its sensitivity to electron correlation. Considerable progress has been made in recent years in inner-shell photoionization studies of both ground- and excited-state atoms. These advances are largely consequences of the increasing availability of vacuum ultraviolet and soft-x-ray synchrotron radiation sources, accompanied by refinements in electron detection techniques and coincidence spectroscopy.

The inner-shell photoionization from the excited state of atoms is of importance in certain hot regions such as stellar atmosphere and controlled thermonuclear research plasmas and is useful in understanding radiative recombination, the inverse process. Theoretically because the excited orbitals have a larger radius than the ground-state orbitals, the effect of the valence electron on inner-shell photoionization can be studied by promoting the outer electron to more and more excited orbitals. Essentially no experimental work exists for inner-shell photoionization of excited-state sodium atoms. Some time ago Wuilleumier and his co-workers [1,2] initiated experimental work on inner-shell photoionization of excited- as well as ground-state sodium atoms by combining the use of laser beam and synchrotron radiation. They measured the relative partial cross sections and asymmetry parameters. In 1989 Cubaynes *et al.* [1] measured the full photoelectron spectrum following ionization in $2p$ subshell of sodium atoms laser excited into the $2p^6 3p^2 P_{3/2}$ state. They observed that the most intense satellite corresponded to "shake-up" transitions of the valence electron, leaving the ion in the $2p^5 4p Na^+$ state. They determined the relative cross sections corresponding to the main line and to the satellite lines. Recently Pahler *et al.* [3], using a multidetection experimental setup, succeeded in measuring the angular distribution of inner $2p$ subshell electrons emitted in the direct photoionization of laser-excited sodium atoms. The great advan-

tage of this setup was that it made it possible to measure the emitted electron intensity simultaneously at several angles. This enabled them to determine the asymmetry parameter β of the direct $2p$ photoionization. They observed a strong variation for β between 47.5 and 105 eV photon energy. They also observed a strong enhancement of the correlation satellites and a decrease in the single photoionization cross section for $2p$ photoionization in the laser-excited sodium atoms, more pronounced in both cases than those obtained in their earlier measurement [1].

Although there have been a few theoretical predictions for $2p$ photoionization from the ground state of sodium atoms, there exists only one calculation for the $2p$ photoionization from the excited state. Chang and Kim [4,5] investigated the $2p$ photoionization of both ground and excited states using many-body perturbation theory. They presented results on cross sections and the angular distribution of the ejected photoelectron. They found that photoionization of the $2p$ subshell of the sodium atom with its valence electron either in its ground state or in the excited state is practically independent of the atomic orbit that the valence electron occupies. Isenberg *et al.* [6] performed calculations of the $2p$ photoionization of the ground state using a sophisticated many-body perturbation theory. They also calculated the asymmetry parameter describing the angular distribution of photoelectrons. There are also Hartree-Fock (HF) and Hartree-Slater (HS) calculations for the photoionization of the $2p$ electron from the ground state by Theodosiou and Fielder [7]. They calculated both cross sections and asymmetry parameters. Craig and Larkins [8] also investigated the $2p$ photoionization of the ground state in the relaxed Hartree-Fock approximation.

In spite of the calculations which exist, there are no theoretical results available for the contributions from the satellite lines to compare with the experimental predictions. Moreover, the photoionization cross section and asymmetry parameter results which exist do not cover a large energy range. We report here detailed calculations of the $2p$ -photoionization cross section and asym-

metry parameter for both the main and satellite lines, beginning with both the ground and excited states of the sodium atom. Our aims are to better understand the particular physics associated with the ionization of excited-state species and to test the experimental prediction. Our calculation uses the multiconfiguration Hartree-Fock (MCHF) method, employing procedures that allow optimization, at each kinetic energy of the electrons of the important core polarization effects on the continuum wave function as well as for the incorporation of target and ionic core configuration mixing effects. The main emphasis is to take into account electron correlation and core polarization effects *ab initio* in order to obtain accurate results and compare them with the recent experimental measurements.

II. THEORY

A. Photoionization cross sections

The photoionization cross section for absorbing a photon of energy $\hbar\omega$ from an initial state i to a final state f is given by

$$\sigma(\omega) = 4\pi^2 \alpha a_0^2 \omega \sum_{f,m} |\langle \psi_f | T | \psi_i \rangle|^2,$$

where α is the fine-structure constant and a_0 is the radius of the first Bohr orbit of the hydrogen atom. ψ_i and ψ_f represent the wave function describing the bound and free states of the atom. The summation runs over all of the final configuration and magnetic quantum numbers. The length and velocity forms of the dipole transition operator T are respectively given by

$$\mathbf{T}_L = \sum_{j=1}^n \mathbf{z}_j, \quad \mathbf{T}_V = \sum_{j=1}^n \frac{\nabla_j}{i\omega}.$$

If ψ_i and ψ_f are exact solutions of the same Hamiltonian equations, the length and velocity forms of the cross section will be identical.

B. Asymmetry parameter $\beta(\omega)$

The study of the angular distribution of electrons relative to the incident photon and/or polarization direction is a very powerful tool in extracting and separating geometrical and dynamical factors involved in the photoionization process. The angular distribution of photoelectrons detached from a subshell nl by light polarized in the $\hat{\mathbf{e}}$ direction is related to the differential cross section by the relation [10]

$$\frac{d\sigma(\omega)}{d\Omega} = \frac{\sigma(\omega)}{4\pi} [1 + \beta(\omega) P_2(\hat{\mathbf{e}}, \hat{\mathbf{k}})].$$

P_2 is the second-order Legendre polynomial whose argument is the cosine of the angle between the polarization vector $\hat{\mathbf{e}}$ and the direction of the outgoing electron $\hat{\mathbf{k}}$.

The angular distribution asymmetry parameter $\beta(\omega)$ can be obtained in a variety of ways. We shall use the angular-momentum-transfer formulation of Dill, Starace, and Manson [11,12] because this method is very useful

when the ionic configuration has several LS states and the final continuum configuration corresponding to each ionic state has several final LS states. In the LS -coupling approximation the total cross section and the asymmetry parameter $\beta(\omega)$ may be expressed as

$$\sigma(\omega) = \sum_{j_i, L_{cs}} \sigma(j_i)$$

and

$$\sigma(\omega)\beta(\omega) = \sum_{L_{cs}} \left[\sum_{j_i}^{\text{fav}} \sigma(j_i)_{\text{fav}} \beta(j_i)_{\text{fav}} - \sum_{j_i}^{\text{unf}} \sigma(j_i)_{\text{unf}} \right],$$

where

$$\mathbf{j}_i = \mathbf{L}_{cs} - \mathbf{L}_0.$$

$\mathbf{L}_0$ and $\mathbf{L}_{cs}$ are the orbital angular momentum of initial and final core states, respectively. $\sigma(j_i)$ and $\beta(j_i)$ are expressed in terms of the scattering amplitudes $S_l(j_i)$ for the photoionization process. $\mathbf{j}_i$ is the angular momentum transferred to the undetected fragments.

C. MCHF wave function for the continuum state

In the present calculation, the MCHF method as applied to continuum wave functions is used to compute the wave function of the final continuum state. The MCHF wave function for a continuum state may be expressed in a series of the form

$$\Psi(\gamma LS; N+1) = \sum_j^{m_c} a_j \Phi(\gamma_j L_c S_c; N) \phi_{kl} + \sum_i^m c_i \Phi(\gamma_i LS; N+1).$$

The method assumes that all the radial functions describing the core are fixed, along with the mixing coefficients a_j . Other bound-state radial functions responsible for electron correlation and core polarization, and represented by the second term in the wave-function expansion, may be determined variationally along with the radial function for the continuum electron. The method of constructing the various radial functions involves the solution of sets of coupled integro-differential equations of the form

$$\left[\frac{d^2}{dr^2} + \frac{2Z}{r} - \frac{l(l+1)}{r^2} \right] P_i(r) = \frac{2}{r} [Y_i(r)P_i(r) + X_i(r) + I_i(r)] + \sum_{i'} \varepsilon_{ii'} P_{i'}(r).$$

This is done by an iterative method, which has been described earlier [9]. The bound radial functions satisfy the boundary conditions

$$P_i(r) \xrightarrow{r \rightarrow 0} r^{l+1}, \quad P_i(r) \xrightarrow{r \rightarrow \infty} 0.$$

In this case the diagonal energy parameter ε_{ii} must be an eigenvalue of the integro-differential equation for non-

trivial solutions to exist and needs to be determined. The radial function of the continuum orbital satisfies the conditions

$$P_i(r) \xrightarrow{r \rightarrow 0} r^{l+1},$$

$$P_i(r) \xrightarrow{r \rightarrow \infty} \left[\frac{2}{\pi k} \right]^{1/2} \times \sin[kr - l\pi/2 + (q/k)\ln(2kr) + \sigma_l + \delta_l],$$

where σ_l is the Coulomb phase shift, $q = Z - N$ is the net charge of the ion, and $\varepsilon_{ii} = -k^2$, k^2 being the kinetic energy of the photoelectron.

III. COMPUTATIONAL PROCEDURE

In this study we consider the 2p-photoionization processes in the excited $2p^6 3p^2 P$ state as well as in the ground $2p^6 3s^2 S$ state of the sodium atom. Photoionization processes corresponding to the main line are described by

The 2p-ionization processes corresponding to the important shake-up satellite lines are given by

In addition to these processes the following conjugate shake-up processes are also considered in the present study:

All final LS states that are possible for dipole transition were also considered.

In the 2p photoionization from the $2p^6 3p^2 P$ and $2p^6 3s^2 S$ states, the electron-electron correlation and the dynamical core polarization effects are very important in both initial and final states. In the MCHF calculation, which considers the correlation and polarization effects very accurately, all the configurations contributing to the core polarization are included. The main emphasis is to take into account the dynamical core polarization effect *ab initio*. First of all, the 1s, 2s, and 2p radial functions are obtained from the HF calculation of the $2p^6 3s^2 S$ ground state of the atom. The MCHF method [13] for bound states was then used to obtain the wave functions for the initial excited states as well as ground-state wave

functions. The MCHF wave-function expansion for the initial $2p^6 3p^2 P$ excited state was over the set of 64 configuration states coupled to form a 2P term. These configurations were generated by the single replacement of 2s and 2p orbitals with excited orbitals 3s, 3p, 3d, 4s, 4p, 4d, 5s, and 5p responsible for dipole polarization. This initial-state wave function was obtained by the MCHF calculation varying eight bound orbitals simultaneously. The initial MCHF bound-state wave-function expansion for the $2p^6 3s^2 S$ state is over the 58 configurations coupled to form a 2S term. Again these configurations were formed with excited orbitals 3s, 3p, 3d, 4s, 4p, 4d, 5s, and 5p orbitals to replace the core orbitals 2s and 2p of the ground state. These excited orbitals were determined variationally by the MCHF method.

The final discrete ionic wave functions for main and satellite lines were calculated with 1s, 2s, and 2p orbitals from the ground state and the outer 3s, 3p, 3d, 4s, and 4p orbitals were determined variationally in the HF approximation. Since each ionic configuration has many LS states, the outer orbitals of the ion were determined separately for each LS state. The final continuum wave functions for the different final LS states corresponding to a specific ionic LS state were obtained using the MCHF method for continuum wave functions. For each final LS state separate MCHF wave function expansions were used. Again the configurations for each final LS state were generated by the single replacement of 2s and 2p core orbitals with excited orbitals responsible for the dipole transition. In this case the excited bound-state orbitals were optimized separately along with the continuum orbital simultaneously for each kinetic energy of the photoelectron. In all cases, the 1s, 2s, and 2p wave functions were kept fixed at the HF $2p^6 3s^2 S$ value.

IV. RESULTS

A. Photoionization cross section

1. Excited state

The beginning step in a MCHF calculation of this form is the determination of the energies of the states involved. This is a strong point of the MCHF technique applied to continuum fractions; it gives very reliable values of the energies involved. The threshold energies for each ionic LS state corresponding to each ionic configuration for both main and satellite lines were calculated from the difference between the excited-state and the ionic state energies and are compared with experiment [14], where available, in Table I. It is found that the present results agree reasonably well with experiment for both main and satellite lines.

There are six ionic states for the $2p^5 3p$ ionic configuration. These six ionic states form 18 final states when coupled to ks and kd photoelectrons. We calculated 18 partial cross sections for photon energies ranging from each threshold to 140 eV. By summing up the contributions of the partial cross sections corresponding to each ionic state, six partial cross sections were obtained. These six partial cross sections, when added together, give the total 2p-photoionization cross section for ioniza-

TABLE I. Comparison of threshold energies (a.u.) for $2p^6 3p^2 P_{3/2}$ excited state with experiment (where available). The experimental values are optical data taken from Ref. [14].

Configuration	Theory	Experiment
$2p^5 3p^3 D$	1.5165	1.4675
$^1 D$	1.5286	1.4749
$^3 P$	1.5304	1.4799
$^1 P$	1.5304	1.4781
$^3 S$	1.4930	1.4477
$^1 S$	1.5886	1.5190
$2p^5 4p^3 D$	1.7245	
$^1 D$	1.7280	
$^3 P$	1.7284	
$^1 P$	1.7284	
$^3 S$	1.7183	
$^1 S$	1.7486	
$2p^5 3d^3 F$	1.6857	1.6211
$^1 F$	1.6871	1.6231
$^3 D$	1.6904	1.6288
$^1 D$	1.6904	1.6281
$^3 P$	1.6828	1.6186
$^1 P$	1.6903	1.6233
$2p^5 3s^3 P$	1.3765	1.3207
$^1 P$	1.3972	1.3363

tion from the $2p^6 3p^2 P$ excited state. In this way we obtained total cross sections in both the length and velocity forms for the main and satellite lines. Figure 1 shows our MCHF results in both length and velocity forms for the main line as well as for the production of the shake-up satellite along with the theoretical data of Chang and Kim [4,5] as a function of photon energy. Chang and Kim calculated the $2p$ -photoionization cross section and asymmetry parameter with the valence electron in either the $2p^6 3p^2 P$ excited state or the $2p^6 3s^2 S$ ground state using many-body perturbation theory. As an experimental $2p$ -

FIG. 1. $2p$ -photoionization cross sections of Na atoms in the excited state: main line and shake-up satellite line as a function of photon energy. Results of Chang and Kim correspond to main line only.

photoionization cross section of excited $2p^6 3p^2 P$ is not available, we compared our results in the figure with the theoretical results obtained by Chang and Kim for $2p$ ionization from the excited state. Good agreement between length and velocity forms in our calculation is found for both main and satellite lines. The cross sections obtained by Chang and Kim seem too high compared to the present $2p$ main line cross sections and too low compared to the present total $2p$ cross sections (main line plus satellite).

2. Ground state

The threshold energies corresponding to each of the ionic states specific to ionic configurations for both main and satellite lines are obtained from the difference between the ground-state and the ionic state energies. These energies are presented in Table II, along with the experimental observations [14]. Good agreement is found between experiment and the present results.

In the $2p$ photoionization from the ground state there are two $^3 P$ and $^1 P$ ionic states which coupled with the continuum electron ks and kd to form four final LS states for the main line as well as for the satellite line. The MCHF expansions for the final continuum states consists of configurations generated by the single replacement of the core orbitals $2s$ and $2p$ with excited orbitals responsible for the dipole transition. These excited orbitals were optimized along with the continuum at each kinetic energy of the photoelectron. These initial- and final-state wave functions were then used to calculate $2p$ partial photoionization cross section corresponding to each of the final states. From these partial cross sections, photoionization cross sections for each of the ionic states were obtained, which, when added together, give the total $2p$ -photoionization cross section from the ground state. In Fig. 2 we show the $2p$ -photoionization cross section in length and velocity forms for both main and shake-up satellite lines. There is good agreement between the length and velocity forms of the present cross sections demonstrating that the present theoretical cross sections are reasonably accurate. The present results are also compared in the figure with results obtained by many-body

TABLE II. Comparison of threshold energies (a.u.) for $2p^6 3s^2 S$ ground state with experiment. The experimental values are optical data taken from Ref. [14].

Configuration	Theory	Experiment
$2p^5 3s^3 P$	1.4544	1.3980
$^1 P$	1.4751	1.4137
$2p^5 4s^3 P$	1.7626	1.7007
$^1 P$	1.7676	1.7069
$2p^5 3p^3 D$	1.5944	1.5449
$^1 D$	1.6065	1.5523
$^3 P$	1.6083	1.5572
$^1 P$	1.6083	1.5555
$^3 S$	1.5709	1.5251
$^1 S$	1.6665	1.5964

FIG. 2. 2p-photoionization cross sections of Na atoms in the ground state: main line and shake-up satellite line as a function of photon energy: —, MCHF (length); — —, MCHF (velocity); ···, MBPT (length) (Ref. [6]); ○○○○, relaxed Hartree-Fock (length) (Ref. [8]); ●●●●, relaxed Hartree-Fock (velocity) (Ref. [8]); △△△△, unrelaxed Hartree-Fock (length) (Ref. [7]); ▲▲▲▲, unrelaxed Hartree-Fock (velocity) (Ref. [7]).

perturbation theory by Isenberg *et al.* [6] for the main line only. Their length results show excellent qualitative agreement with our length results; quantitatively their results are higher. The results obtained by Craig and Larkins using a relaxed Hartree-Fock model for both main and satellite lines and by Theodosiou and Fielder using unrelaxed Hartree-Fock approximation for main line only are included in the figure for comparison. It is found that the present results for satellite lines agree extremely well with the relaxed Hartree-Fock calculations by Craig and Larkins. Their results for the main line also agree very well with the present results for photon energies from 80–140 eV whereas their results at the lower energies are slightly higher than the present results. The results obtained by Theodosiou and Fielder are higher than the present results.

It has been noted in the experimental results that one of the principal characteristics of 2p ionization from the excited state is the appearance of intense shake-up satellites. It is assumed that after 2p electron absorbs a photon and reaches the continuum *ks* or *kd*, the ionic electrons rearrange themselves due to the development of the new core potential. In this process the initial ionic orbitals relax in place or promote the outermost electron to an excited state via a monopole transition. In Fig. 3 we show the relative intensities of satellite lines with respect to the main lines corresponding to the 2p photoionization from the excited as well as ground state. The experimental values of Cubaynes *et al.* [1] are shown in the figure for comparison. Length and velocity results of the relative intensities from the excited and ground states agree very well. It is found that the relative intensity of the shake-up satellite is strongly enhanced in the excited-state photoionization by a factor of approximately 2.55, over that in the ground state. The reason for this enhancement is due to the fact that the 3p electron prefers to remain far away from the 2p core, as in the 4p

FIG. 3. Relative intensity of the shake-up satellites in the 2p photoionization of Na atoms in the excited and ground states as a function of photon energy: —, MCHF (length); — —, MCHF (velocity); ●●●●, experiment (Ref. [1]).

orbital, while the 3s electron follow the change of the core more closely than the 4s. The screening of the core is lowered more in the former case than in the latter. As a result the effect of the relaxation of the core is more for the 3p electron than for the 3s electron. Also the overlap of the 3p wave function with that of the 4p electron is larger than that of the 3s with the 4s electron. It is in accord with experiment that the shake-up satellite contribution is much higher in the excited-state photoionization than that in the ground state. There is excellent agreement with experiment [1] for the relative satellite contribution in the ground state. But we see that theoretical values depart significantly from experiment in the relative contribution of the satellite lines in excited-state photoionization. Further experimental measurement is necessary to clarify this discrepancy.

Figure 4 shows the ratio between the intensity of the 2p main lines in the excited and ground states as a function

FIG. 4. Branching ratios between the 2p-photoionization cross section (main lines) of excited and ground states of Na atoms as a function of photon energy: —, MCHF (length); — —, MCHF (velocity); ●●●●, experiment (Ref. [1]).

FIG. 5. Branching ratios between the $2p$ -photoionization cross section (main lines plus satellites) of excited and ground states of Na atoms as a function of photon energy: —, MCHF (length); — — —, MCHF (velocity); ●●●●, experiment (Ref. [1]).

of photon energy. Experimental ratios [1] are also shown in the figure for comparison. It is found that the present results agree well with the measurement within the error bars.

The ratios of the total cross sections obtained by summing up the main and satellite lines in the excited as well as in the ground state are shown in Fig. 5 as a function of photon energy. The length and velocity forms of the present result are in excellent agreement near the threshold, but they differ from each other slowly as a function of photon energy. The present results agree very well with experiment [1] from 90 to 140 eV photon energy. Near the threshold experimental results are slightly lower than the theoretical results. Again further experimental work is needed to verify the discrepancy between the theory and experiment. We also studied the relative intensity of the conjugate shake-up satellites with respect to the main line and found that their contributions are very small compared to those of the shake-up satellites and they are about the same in the excited and the ground states. They also decrease with photon energy. Thus their contribution to the total $2p$ cross sections does not alter the value shown in the figures to any great extent.

B. Asymmetry parameter $\beta(\omega)$

The asymmetry parameter $\beta(\omega)$ which determines the angular distribution of photoelectrons is a function of the photoionization matrix elements and of the continuum wave phase shifts. Physically, the nature of the angular distribution of the photoelectrons is determined by the angular structure of the continuum wave function representing the ejected electron. Our calculated results on the asymmetry parameter are displayed in Fig. 6 in the $2p^6 3p^2 P_{3/2}$ excited state together with theoretical results obtained by Chang and Kim [4,5]. Only one measurement [3] of the asymmetry parameter β from the excited state of the sodium atom exists. No measurements of β as a function of photon energy have been reported to

FIG. 6. $2p$ asymmetry parameter β of Na atoms in the excited state as a function of photon energy: —, MCHF (length); — — —, MCHF (velocity); ····, MBPT (Ref. [5]); ●●●●, experiment (Ref. [3]).

date. Pahler *et al.* [3] made the first measurement of the asymmetry parameter β for photoelectrons emitted from the $2p$ subshell of sodium atoms in a laser-excited state at the single photon energy of 55 eV. This experimental result is also plotted in the figure for comparison. It is found that present length and velocity results are in excellent agreement. The theoretical results obtained by Chang and Kim up to 68 eV using many-body perturbation theory show excellent qualitative agreement with the present result; quantitatively their results are slightly lower. The present result compares very well with the experimental measurement at 55 eV. However, a more detailed comparison between theory and experiment awaits further experimental measurements over a broad range of photon energies.

In Fig. 7 we present our calculated results on the asymmetry parameter for ionization of sodium atoms in the

FIG. 7. $2p$ asymmetry parameter β of Na atoms in the ground state as a function of photon energy: —, MCHF (length); — — —, MCHF (velocity); ····, MBPT (length) (Ref. [6]); ●●●●, MBPT (Ref. [5]); ▲▲▲▲, HS (Ref. [8]).

$2p^6 3s^2 S_{1/2}$ ground state along with theoretical results obtained by Isenberg *et al.* (MBPT), Chang and Kim (MBPT), and Theodosiou and Fielder (HS). There is excellent agreement between our length and velocity results. In the figure we plotted the length results of Isenberg *et al.* obtained using many-body perturbation theory. Their results agree very well with our present results except at energies very close to the threshold. Theodosiou and Fielder [7] calculated the asymmetry parameter $\beta(\omega)$ using the Hartree-Slater approximation. Their results also agree very well with our present results except at energies very close to the threshold, where their results are slightly higher. The theoretical results obtained by Chang and Kim using many-body perturbation theory are slightly lower than the present results.

V. CONCLUSION

Detailed theoretical calculations of the $2p$ -photoionization cross section and asymmetry parameter of the excited $2p^6 3p^2 P_{3/2}$ and ground $2p^6 3s^2 S_{1/2}$ states of the sodium atom corresponding to the production of the main and principal satellite lines have been made over an energy range from threshold to 140 eV using the multiconfiguration Hartree-Fock method for bound and continuum wave functions. We found a strong enhancement of the relative intensity of the satellite line in the excited state compared to that in the ground state. This enhancement is due to the fact that relaxation of the ionic core following inner-shell ionization leads to an overlap matrix element between the wave function of the shake-

up electron in the final state and the wave function of the valence electron in the initial state, which is found to be larger for the atom in the excited state than in the ground state. In the present investigation the relative intensity of the satellite lines in the excited state reaches about 55% of the main line whereas that in the ground state amounts to about 20% of the main line. A comparison with available experimental results shows good agreement in the relative intensities of the satellite lines in the excited and the ground states. The present calculation shows the capability of the MCHF method in the determination of the properties of inner-shell ionization of alkali-metal atoms. The present investigation points out the need for further experimental work, particularly studies that obtain photoionization cross sections and angular distribution parameters for main and satellite processes in both excited- and ground-state photoionization over a broader range of photon energies. Experimental measurement on this would be extremely useful in understanding the physics underlying the inner-shell ionization of all atoms in excited states.

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