DEPENDENCE OF SHAKE PROBABILITY ON NUCLEAR CHARGE IN Li-, Na- AND K-LIKE IONS

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Abstract

In sudden perturbation approximation, the probability of the shake-up process accompanying inner-shell ionization is calculated for the isoelectronic sequences of Li-, Na- and K-like ions in the ground and excited \textit{np} and \textit{nd} states. Numerical solutions of Hartree-Fock equations and hydrogen-like radial orbitals are used. Very large differences between the results of both approximations for all ions and strong dependences on ion charge are obtained at the beginning of the isoelectronic sequences.

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1. Introduction

A shake process accompanies inner-shell ionization of atoms and ions. It usually effects photoelectron \textsuperscript{1} \textsuperscript{2} and Auger electron \textsuperscript{3} \textsuperscript{4} \textsuperscript{5} spectra. In the case of shake-up or shake-off process, it describes the excitation \textsuperscript{6} or ionization \textsuperscript{7} of the second electron, respectively. The shake probability describes the relaxation of passive electrons and is also important for the single electron ionization cross section. It was obtained by Kupliauskiene \textsuperscript{8} \textsuperscript{9} \textsuperscript{10} that the shake probability should be taken into account even in the case of inner-shell ionization when spectator electrons saved their initial states. Then it describes the probability of spectator electrons to stay in their initial states.

A strong increase of the relative intensity of shake-up satellites in the inner-shell photoionization of excited Na atoms \textsuperscript{2} was explained by the change of the localization of valence electron
in the final state with respect to that in the initial state \([11, 8, 9]\). Very strong dependence of the calculated inner-shell ionization cross sections of alkaline atoms on the excited valence electron state was noticed not only in the case of photoionization \([8, 9, 12]\) but also for the ionization of atoms by electrons \([13, 14, 15]\). For neutral atoms and singly charged ions of the second and third rows, the probability of shake process accompanying inner-shell ionization was calculated in \([16]\), and very strong dependence on valence electron state was obtained. Enormous differences were found for low excited ns and np states between shake probabilities that were calculated using numerical solutions of Hartree-Fock equations (HF) and hydrogen-like (H-like) radial orbitals \([16]\). A simple two-parameter interpolation function for Z-dependences of shake-up probabilities per electron was presented by Kochur et al \([17]\) for atoms in the ground state.

The aim of the present work is the investigation of the dependence of shake probability for Li-, Na- and K-like ions on the ion charge and the state of valence electron because of the very strong sensitivity of the inner-shell ionization cross sections of Li-, Na- and K-like atoms on the valence electron state \([8, 9, 12, 15]\). The regularities of the shake probability passing from atoms to highly charged ions of these isoelectronic sequences are investigated.

The calculated shake probabilities can be used for searching strong relaxation effects in processes dealing with inner-shell ionization of excited atoms and ions by photons and electrons as well as for the Auger decay calculations in sudden perturbation approximation.

2. Description of calculations

The ionizing transition

\[
A^N+(nl^{l'+2}n'l') + \alpha \rightarrow A^{(N+1)+}(nl'^{l'+1}n''l') + e^- \tag{1}
\]

is investigated in the present work. Here \(nl = 1s, 2p, 3p\) for Li-, Na- and K-like ions, respectively, \(n' = n + 1\) for Li- and Na-like ions, \(n' = 4\) for s- and p-electrons and \(n' = 3, 4\) for d-electrons of K-like ions, \(l' = 0, 1, 2, n'' = n', n' + 1\), \(N\) is the charge of an ion, and \(\alpha\) stands for a particle or photon.

The shake probability can be expressed as:

\[
P(i' \rightarrow f) = |\langle i'|f\rangle|^2 \tag{2}
\]

where the wave function \(\langle i'|\) describes the ion in the intermediate state following ionization, in which spectator electrons remain in their initial states, with the radial orbitals of an atom, and \(|f\rangle\) is the wave function of an ion in the final state.
The calculations of shake probabilities (2) have been performed by using both numerical solutions of HF equations [18] obtained in the average-term approximation and hydrogen-like radial orbitals with effective nuclear charge \( Z = N + 1 \) and \( Z = N + 2 \) for ions in the initial and final states of the valence electron, respectively.

2. Results and discussion

The shake probabilities for single electron ionization (SPI) and shake-up (SPS) transition were calculated for Li-, Na- and K-like ions in the configurations \( nl^{l+2}n''l'' \), \( l'' = 0, 1, 2, n' = n + 1 \) for \( l' = 0, 1 \), and \( n' = n + 2 \) for Li-, \( n' = n + 1 \) for Na- and \( n' = n, n + 1 \) for K-like isoelectronic sequences in the case of d-electron. The final state of the ionized ions is \( n'' = n' + 1, n' + 2 \).

The values of the shake probabilities calculated by using both HF and H-like radial orbitals are presented in Fig. 1–2 for Li- and Na-like ions, respectively, and Table 1 for K-like ions. The values of shake probabilities for d-electrons calculated with H-like radial orbitals are not displayed in Fig. 1–2 because they are very close to those of HF approximation for Li- and Na-like ions.

The results of Fig. 1–2 and Table 1 demonstrate that SPI are smaller for d-electrons than those of s- and p-electrons. They increase with the decrease of the orbital quantum number from \( l'' = 2 \) down to \( l'' = 0 \). This tendency is independent of the charge of an ion. The values of SPI are much smaller than those at the beginning of all sequences investigated but rapidly increase up to one with growing ion charge \( N = 9, N = 8 \) and \( N = 6 \) for Li-, Na- and K-like ions, respectively.

At the beginning of each sequence under investigation the values of SPS are much larger than zero and decrease with increasing ion charge. The values of SPS become close to zero for ion charge a little less than the values of SPI which become close to one, i.e. 8, 7, and 5 for Li-, Na- and K-like ions, respectively. Thus, the values of SPS decrease more rapidly than those of SPI increase.

The values both of SPI and SPS calculated by using H-like radial orbitals with effective ion charge differ very much from those of HF calculation not only at the beginning of isoelectronic sequences but also for highly charged ions. They are similar to each other only for d-electrons in the case of Li- and Na-like ions. In the case of Li-like ions, the differences between the results of both approximations are less in comparison with those of Na- and K-like ions. In the case of K-like ions, the H-like calculations can not be used for the evaluations of shake probabilities even for highly charged ions (see table 1). The results of Table 1 show that the differences between
the values calculated with HF and H-like orbitals reach several times or even an order for both SPI and SPS probabilities.

Calculated values of the ratios of SPS and SPI for Li-, Na- and K-like isoelectronic sequences are presented in Fig. 3. Here white points in black background stand for the experimental ratios of shake-up and single electron photoionization cross sections in the case of Li, Na and K atoms. Experimental values of the ratio are chosen for large photon energies where sudden perturbation approximation is valid.

The results from Fig. 3 show that the agreement between calculated ratios of shake probabilities and measured shake-up and single electron photoionization cross sections is good. The values of the ratios decrease with increasing ion charge. The ratios for s- and p-electrons decrease while the number of core electrons increases. But the ratios for d-electrons in the case of K-like ions are larger than those of Na- and Li-like sequences. The ratios are larger at the beginning of the sequences, however, their decrease is more rapid for Li-like ions than for K-like ions.
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Table 1. Shake probabilities (2) (SPI and SPS) calculated by using HF and H-like (H) radial orbitals with $N + 1$ and $N + 2$ effective nuclear charges (1) for K-like ions in the 3p-electron ionization.

| $n l'$  | $n'' l'$ | Method | K  | Ca$^{+}$ | Sc$^{2+}$ | V$^{4+}$ | Mn$^{6+}$ | Co$^{8+}$ | Ni$^{9+}$ |
|---------|----------|--------|----|---------|---------|---------|---------|---------|---------|
| 4s 4s   |           | HF     | 0.84 | 0.94    | 0.97    | 0.98    | 0.99    | 0.99    | 0.99    |
|         |          | H      | 0.02 | 0.20    | 0.48    | 0.75    | 0.86    | 0.91    | 0.93    |
| 4s 5s   |           | HF     | 0.14 | 0.05    | 0.027   | 0.012   | 0.007   | 0.005   | 0.004   |
|         |          | H      | 0.67 | 0.69    | 0.41    | 0.17    | 0.085   | 0.051   | 0.042   |
| 4p 4p   |           | HF     | 0.73 | 0.90    | 0.95    | 0.98    | 0.99    | 0.99    | 0.99    |
|         |          | H      | 0.003 | 0.25   | 0.53    | 0.78    | 0.88    | 0.92    | 0.94    |
| 4p 5p   |           | HF     | 0.27 | 0.09    | 0.044   | 0.018   | 0.010   | 0.006   | 0.005   |
|         |          | H      | 0.69 | 0.63    | 0.37    | 0.15    | 0.077   | 0.047   | 0.038   |
| 3d 3d   |           | HF     | 0.16 | 0.90    | 0.98    | 0.99    | 1.00    | 1.00    | 1.00    |
|         |          | H      | 0.44 | 0.75    | 0.86    | 0.94    | 0.97    | 0.98    | 0.98    |
| 3d 4d   |           | HF     | 0.68 | 0.08    | 0.014   | 0.003   | 0.002   | 0.001   | 0.001   |
|         |          | H      | 0.54 | 0.24    | 0.12    | 0.05    | 0.026   | 0.016   | 0.013   |
| 4d 4d   |           | HF     | 0.027| 0.60    | 0.84    | 0.95    | 0.97    | 0.98    | 0.99    |
|         |          | H      | 0.02 | 0.39    | 0.64    | 0.84    | 0.91    | 0.94    | 0.95    |
| 4d 5d   |           | HF     | 0.47 | 0.33    | 0.13    | 0.04    | 0.02    | 0.012   | 0.01    |
|         |          | H      | 0.70 | 0.51    | 0.29    | 0.12    | 0.06    | 0.037   | 0.030   |
Figure captions:

Fig. 1. Shake probability vs nuclear charge for Li isoelectronic sequence in the case of the transition $nl^{l+2}(n + 1)l' \rightarrow nl^{l+1}n'l'$. Filled circles are for single electron ionization (SPI), diamonds are for shake-up process (SPS), solid line stands for $l' = 0$, dashed line is for $l' = 1$ and dotted line is for $l' = 2$, respectively. Triangles-dot up show single electron and triangles-dot down indicate shake-up probabilities calculated using hydrogen-like radial orbitals with effective nuclear charge $Z = N + 1$ and $Z = N + 2$ (1) for the initial and final states, respectively, and dashed-dot and dashed-dot-dot lines are for $l' = 0$ and $l' = 1$ electrons, respectively.

Fig. 2. Shake probability vs nuclear charge for Na isoelectronic sequence. Details are as in Fig. 1.

Fig. 3. The ratios of the probability of shake-up to that of single electron transition for Li- (filled circles), Na- (squares) and K-like (diamonds) isoelectronic sequences. Solid, dashed and dotted lines are for s, p and d electrons, respectively. The white dots in black background are experimental values of the ratios between shake-up and single electron photoionization cross sections for Li [19], Na [2] and K [1] atoms.
Figure 1
Figure 2

Na-like sequence
Figure 3