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Correlation effects for double K-shell vacancy production in lithium by fast charged projectile impact

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Abstract

Correlation effects are studied theoretically in case of the production of Li^+ S states with double K-shell vacancy in collision with 95 MeV/u Ar^{18+}, 60 MeV/u Kr^{34+} and 0.1–5.0 keV electron projectiles. Calculations with no correlations, or only initial- and only final-state correlations are performed in order to identify the main correlation contributions and to emphasize the role of correlated wavefunctions. The relative importance of the various first- and second-order mechanisms and the dependence of the cross sections on the sign of projectile charge are investigated, too. In most cases the obtained results are in reasonable agreement with the experimental data available.
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Ionization–excitation processes of inner-shell electrons in lithium atom are complex but feasible examples today for studying the effects of electron–electron correlations in atomic collisions. During recent years the formation process of K-shell vacant states in lithium by fast charged projectiles has been studied experimentally by Tanis et al. [1,2], and recently, new experimental data have been published concerning the double K-shell vacancy production [3]. These experimental results can be explained only if electron–electron interactions are considered in a proper way. In a previous study [4], single K-shell excitations of Li have been described successfully by applying correlated multiconfiguration Hartree–Fock (MCHF) wavefunctions for both the initial and final states. In the present paper a similar method is used in order to investigate the double K-shell vacancy production. In this case the final state of the system is a doubly excited Li^+ ion together with an electron

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in the continuum. Concentrating on final states with an overall S symmetry, our aim is to study the importance of the initial- and final-state correlations, to identify the main mechanisms which lead to the formation of hollow Li^+ ions and to analyze the dependence of cross sections on projectiles velocity and on their charge sign. The importance of the use of correlated wavefunctions is emphasized by comparing the corresponding results with those from non-correlated, single configuration calculations (NC).

In order to study ionization–excitation processes in Li atom, we have performed theoretical calculations based on the semiclassical impact parameter method described in [4]. For the inclusion of the bound-state electronic correlations, in our model MCHF wavefunctions are applied for bound electrons, while the interaction between the continuum electron and the residual ion is approximated by a mean-field potential. In this way, the bound-continuum interaction of the electrons are taken into account only partially.

The total ionization–excitation cross sections are obtained by integrating the square of the absolute value of the total amplitude (being a sum of the first- and second-order ones) over the impact parameter and the ejected electron momentum. In the first-order calculations MCHF wavefunctions are used with an orbital basis up to $n = 3$ for the representation of the ground state, and with an orbital basis $n = 2$ and $n = 3$ for the final and excited states. The basis sets are optimized separately for the initial and the final states, causing that electron orbitals for the two states are not orthogonal to each other. In these conditions one may obtain non-zero contribution in first-order for the two-electron process even if no correlation is taken into account (only the main determinant is considered for the initial and final states). In second-order computations only the main configurations are taken into account.

The method has first been used for studying the ionization–excitation of neutral lithium as produced by heavy ion projectiles. Table 1 presents the results for 95 MeV/u Ar^{18+} and 60 MeV/u Kr^{34+} projectiles in comparison with the experimental data from [2,5]. As expected, the second-order mechanisms appear to be negligible in case of Ar^{18+} projectiles where the z/v ratio (projectile charge over velocity) is small (0.3), but they become important for Kr^{34+} where the z/v ratio is higher (0.7). In order to study the importance of the different correlation types, first-order calculations which include either no correlations (NC), only initial-state correlations (IC) or only final-state correlations (FC) have been performed. Comparing these results with multiconfiguration calculations (MC) and experiments, one can conclude that, for the production of the $2s^2$ and $2p^2$ states both the initial- and final-state correlations play an important role in the ionization–excitation process. In case of the 2s3s states in contrast, the final-state correlation is less significant because the two electrons belong to two different shells, and because their interaction is therefore well described by a mean-field approximation (especially for the triplet case). Moreover, the listed results are in agreement with our expectations, because the use of correlated wavefunctions improves the theoretical results.

In order to obtain further insights into the role of correlations in atomic collisions, calculations have been performed for equivelocity electron and proton projectiles in the 0.1–5.0 keV electron energy range. In Fig. 1 cross sections as a function of projectile velocity are shown for different S final states. The contributions of the first- and second-order mechanisms are represented, and the total cross sections are compared with the available experimental data [3,5]. For these final S states, obviously, the first-order mechanisms are dominant, while the second-order processes become important only for the 2s3s ^1S state below 5 a.u. projectile velocity. For the $2p^2$ ^1S final state, the first-order term dominates the cross sections within the entire projectile velocity range while no direct second-order process contribute to this level. The dependence of ionization–excitation cross sections on the projectile charge sign becomes visible at low energies for singlet states where larger cross sections are obtained for proton projectiles.

The importance of the different mechanisms has been investigated also for 5 keV electron projectiles. The obtained results are listed in Table 2 from which we conclude that the S states are mainly formed by first-order shake-up processes

Table 1
Calculated cross sections (expressed in 10^{-20} cm^2) for double K-shell vacancy production in lithium induced by 95 MeV/u Ar^{18+} and 60 MeV/u Kr^{34+} projectiles in comparison with experimental data [2,5]

Projectile	State	First order				Second order	Theory	Exp.
		NC	IC	FC	MC			
95 MeV/u Ar^{18+} ($z/v \approx 0.3$)	$2s^2\ ^1S$	6.3	3.3	4.7	3.56	0.422	3.99	3.6
	$2p^2\ ^1S$	0	2.32	1.99	2.67	0.017	2.74	1.5
	$2s3s\ ^3S$	6.1	4.57	6.1	4.57	0.241	4.81	4.5
	$2s3s\ ^1S$	0.19	0.33	0.12	0.495	0.178	0.668	–
60 MeV/u Kr^{34+} ($z/v \approx 0.7$)	$2s^2\ ^1S$	33.3	18.1	24.9	18.6	13.7	32.4	25.4
	$2p^2\ ^1S$	0	12.2	10.5	14.3	0.502	15.6	20.7
	$2s3s\ ^3S$	32.9	24.5	32.9	24.5	7.80	32.3	31.2
	$2s3s\ ^1S$	1.0	1.79	0.66	2.68	5.67	8.29	–

Non-correlated, single configuration first-order results (NC) are listed separately along those including only initial-state correlations (IC) and only final-state correlations (FC).

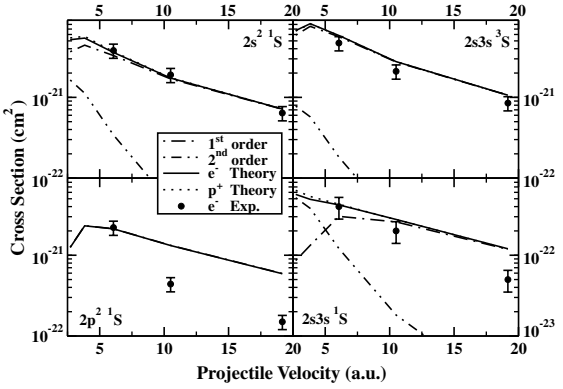

Fig. 1. Calculated ionization–excitation cross sections for S final states as a function of the electron/proton projectile velocity compared with experimental data [5].

(ionization by projectile–electron interaction followed by an excitation of an electron due to the rearrangement of electron density). The shake-off process, i.e. the excitation of an electron by the projectile and the subsequent ionization of a second electron due to electron rearrangement, is less important, but still not negligible. The comparison of the correlated results with non-correlated (NC) ones points out again the importance of the use of correlated wavefunctions. The calculated cross sections are in good agreement with the experiments.

In summary, calculations have been performed in this work in order to study the double K-shell vacancy S states of Li^+ produced from ground-state Li by 95 MeV/u Ar^{18+}, 60 MeV/u Kr^{34+} heavy ions and 0.1–5.0 keV electron (and equivelocity proton) projectiles. In most cases, the obtained cross sections show good agreement with the available experimental data. It was found that for the projectile velocities down to about 5 a.u., the ionization–excitation cross sections do not depend significantly on the charge sign of the projectile. This dependence becomes important only for low

Table 2
Calculated cross sections (expressed in 10^{-21} cm^2) for double K-shell vacancy production in lithium induced by 5 keV electron projectiles compared with experiments [5]

State	First order						Second order	Total	Exp.
	NC	IC	FC	MC	OFF	UP			
$2s^2\ ^1S$	1.32	0.81	0.99	0.71	0.047	0.634	0.005	0.717	0.64
$2p^2\ ^1S$	0	0.45	0.41	0.593	0.06	0.586	0.0001	0.59	0.15
$2s3s\ ^3S$	1.48	1.06	1.48	1.06	0.151	0.994	0.0027	1.06	0.85
$2s3s\ ^1S$	0.047	0.079	0.031	0.118	0.004	0.113	0.0018	0.12	0.05

First- and second-order contributions are listed separately. For the first-order results the various correlation effects are shown (as in Table 1), and moreover, the contributions of the shake-off (OFF) and the shake-up (UP) processes are listed separately.

projectile energies and for singlet S states. It can be concluded that both the initial- and final-state electron correlations have important contributions in formation of doubly K-shell vacant S states of lithium. For this reason the use of the correlated, multi-configuration wavefunctions is essential in these calculations.

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