Hyperspherical approach to double-electron excitation of He by fast-ion impact. IV. Excitation to the $(2l, 3l')$ and $(3l, 3l')$ manifolds by multiply-charged-ion impact

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Double-electron excitation processes to $(2l, 3l')$ and $(3l, 3l')$ manifolds of He atoms by multiply-charged-ion impact have been theoretically investigated using a close-coupling method at the 1.5-MeV/u incident energy. Hyperspherical wave functions are adopted to take full account of strongly correlated motion of two atomic electrons in He. For the excitation processes to the $(2l, 3l')$ manifold, the cross sections to the $^1D^e$ states show the most rapid increase as projectile charge Z_p increases, while that to the $^1P^o$ states indicate the slowest. For the $3l3l'$ excitation processes, the cross sections to the $^1D^e$ and $^1P^o$ states increase at almost the same rate. It is found that the isomorphism of the charge-density plots of the channel wave functions between the initial and final states governs collision dynamics in direct double-electron excitation processes when incident multiply charged ions strongly interact with the target He atoms.

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We have been investigating double-electron excitation processes of a He atom resulting from ion impact to understand the role of electron-electron correlation to excitation mechanisms. Until now, the processes

$$A^{Z_p+} + \mathrm{He}(1s^2) \rightarrow A^{Z_p+} + \mathrm{He}^{**}(2l2l') \quad (1)$$

and

$$B^{Z_p+} + \mathrm{He}(1s^2) \rightarrow B^{Z_p+} + \mathrm{He}^{**}(2l3l', 3l3l') \quad (2)$$

were studied [1–3]. Here A^{Z_p+} represents a proton, an antiproton, and multiply charged ions (Z_p = 2–9) with (1–10)-MeV/u impact energy, while B^{Z_p+} represents a proton and an antiproton with 1.5 MeV/u.

For proton and antiproton impact, we have found that the same excitation mechanism as that for the $2l2l'$ excitation processes operates for the $2l3l'$ ones; namely, the first-order processes dominate in the $^1P^o$ excitation process. Furthermore, a few $^1P^o$ states play an important role as an intermediate state in the second-order excitation processes to the doubly excited $^1S^e$ and $^1D^e$ states. However, in the $(3l, 3l')$ excitation, there exists a different mechanism from that in the $(2l, 2l')$ and $(2l, 3l')$ excitations; namely, for the $^1P^o$ states, the second-order process is found to be comparable with the first-order process. In these second-order processes (a ladder-climbing mechanism), both $^1P^o$ states and the singly excited $^1S^e$ ones play an important role as intermediate states [2]. This difference arises from the smaller overlap between the ground-state wave function and those of the $(3l, 3l')$ manifold.

In process (1) by multiply-charged-ion impact, the excitation processes with $\Delta v = \Delta T = \Delta A$=0 from the initial $1s1s\,^1S^e$ $\{[1(0,0)^+1\,^1S^e], v = 0\}$ state dominate for high-Z_p ions, while for small-Z_p ions, Pauli exclusion principle modifies the angular propensity rules $\Delta v = \Delta T = 0$ into those with $\Delta v = \Delta T = 1$ for optically allowed transitions [3]. The latter is consistent with the propensity rules previously obtained in the weak-coupling regime [4, 5]. Here we employ a classification scheme $[N(K,T)^A n]$ based on the set of correlation quantum numbers K, T, and A as a language to describe collision processes [6]. Further, according to this scheme, we introduce another quantum number v $(= N - K - 1)$ which can be interpreted as the bending vibrational quantum number of the flexible linear triatomic molecule (cf. Sec. II C of Ref. [1]) based on the rovibrator model [7].

In the present paper, we investigate process (2) by multiply-charged-ion (Z_p = 1–9) impact with 1.5-MeV/u impact energy to understand the excitation mechanism to the $(2l, 3l')$ and $(3l, 3l')$ manifolds and, in particular, to study whether the same mechanisms found in Refs. [1–3] operate in these excitation processes.

The same theoretical framework is employed as that used in Refs. [1–3]. Namely, the close-coupling method with the impact parameter treatment is used to describe collision processes. Furthermore, hyperspherical wave functions are adopted to take full account of strongly correlated motion of two atomic electrons in He. No charge transfer channel is included in the expansion of the total

wave function. We ignore the coupling with the continuum though recent study on the $(2s)^2$ double-electron excitation of He [8] seems to suggest the possible effect of the continuum as intermediate states.

After we test the convergence of the cross sections with respect to the increase of the numbers of the states included in the close-coupling expansion, we have calculated the cross sections with the set of the 133 states which are given in Table I in addition to the set of the 85 states employed in Ref. [2]. Column 4 of Table I gives elaborate theoretical data on the binding energies by Ho [9]. Comparison of our calculated binding energies with these values enables one to assess the quality of the wave functions employed here. We have confirmed that the set of the 61-state cross sections obtained in Ref. [3] to the $(2l, 2l')$ manifold by F^{9+} ion impact is in agreement with that of the present 133-state results within 10%.

Figures 1(a) and 1(b) show the plots of the double-electron excitation cross sections vs Z_p for processes to the $(2l, 3l')$ manifold and those to the $(3l, 3l')$ manifold at 1.5-MeV/u impact energy, respectively. From Fig. 1(a), one sees that the $(2l3l')\,^1D^e$ excitation cross sections show the most rapid increase with increase of Z_p, while the $(2s3p+3s2p)\,^1P^o$ excitation cross sections give the slowest. For the processes to the $(2l3l')^1D^e$ states, approximately, these cross sections increase proportionally to Z_p^4, while for the $(2s3p + 3s2p)\,^1P^o$ state those increase proportionally to Z_p^2 for small Z_p. It should be noted that the cross sections for first-order processes and those for second-order processes are in proportion to Z_p^2 and Z_p^4, respectively [3, 10]. Here the "order" of the process is defined with respect to the electron-projectile interaction. These results are consistent with those in Ref. [2]. Namely, we found that the second-order process dominates in the processes to the $(2l3l')\,^1D^e$ states and the first-order one does in the processes to the $(2s3p + 3s2p)\,^1P^o$ states by proton and antiproton impact.

For the processes to $(2l3l)\,^1S^e$ states, approximately, these cross sections increase proportionally to $Z_p^2 \sim Z_p^3$. These results show that the first-order process is comparable with the second-order one in these processes by proton and antiproton impact, which are consistent with the

TABLE I. Doubly excited states which are included in the 133-state calculation of the cross sections in addition to the 85 states employed in Ref. [2]. The first column gives a set of the quantum numbers for the main electronic configuration based on the independent-particle model, the second column shows a set of correlation quantum numbers $[N(K,T)^A n]$, the third column gives the values of the binding energies (in units of rydbergs) of the doubly excited states calculated from our hyperspherical wave functions, and the fourth column gives the binding energies calculated by Ho [9].

Configuration	$[N(K,T)^A n]$	Binding energy (Ry)	
		Present	Ref. [9]
$1s6s\,^1S^e$	$[1(0,0)^+6]\,^1S^e$	-4.029	
$2s5s\,^1S^e$	$[2(1,0)^+5]\,^1S^e$	-1.051	
$2s6s\,^1S^e$	$[2(1,0)^+6]\,^1S^e$	-1.034	
$2p5p\,^1S^e$	$[2(-1,0)^+5]\,^1S^e$	-1.034	
$2p6p\,^1S^e$	$[2(-1,0)^+6]\,^1S^e$	-1.024	
$3s4s\,^1S^e$	$[3(2,0)^+4]\,^1S^e$	-0.5576	-0.5623
$3p4p\,^1S^e$	$[3(0,0)^+4]\,^1S^e$	-0.5151	-0.5270
$3d4d\,^1S^e$	$[3(-2,0)^+4]\,^1S^e$	-0.4861	
$1s5p\,^1P^o$	$[1(0,0)^05]\,^1P^o$	-4.039	
$1s6p\,^1P^o$	$[1(0,0)^06]\,^1P^o$	-4.027	
$(2s5p + 5s2p)\,^1P^o$	$[2(0,1)^+5]\,^1P^o$	-1.041	
$(2s6p + 6s2p)\,^1P^o$	$[2(0,1)^+6]\,^1P^o$	-1.029	
$(2s5p - 5s2p)\,^1P^o$	$[2(1,0)^-5]\,^1P^o$	-1.052	
$2p5d\,^1P^o$	$[2(-1,0)^05]\,^1P^o$	-1.035	
$(3s4p + 4s3p)\,^1P^o$	$[3(1,1)^+4]\,^1P^o$	-0.5416	
$(3s4p - 4s3p)\,^1P^o$	$[3(2,0)^-4]\,^1P^o$	-0.5670	-0.56565
$(3p4d + 4p3d)\,^1P^o$	$[3(-1,1)^+4]\,^1P^o$	-0.4990	
$(3p4d - 4p3d)\,^1P^o$	$[3(0,0)^-4]\,^1P^o$	-0.5293	
$2p4p\,^1D^e$	$[2(1,0)^+4]\,^1D^e$	-1.062	
$2s4d\,^1D^e$	$[2(0,1)^04]\,^1D^e$	-1.058	

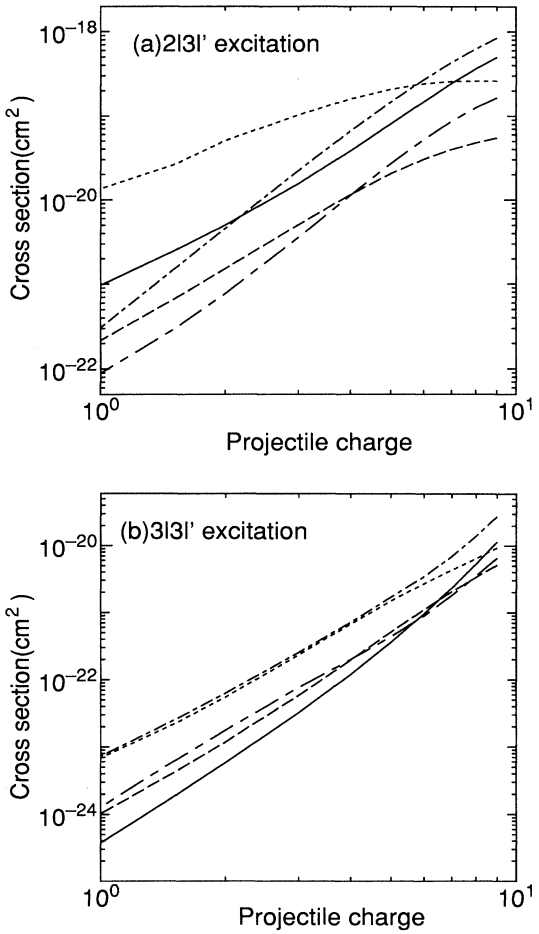

FIG. 1. Projectile-charge dependence of the double-electron excitation cross sections of He atoms: (a) The excitation processes to the $(2l, 3l')$ manifold at 1.5-MeV/u impact energy: the final states are the $2s3s\,^1S^e$ (solid line), $2p3p\,^1S^e$ (broken line), $(2s3p+3s2p)\,^1P^o$ (dotted line), $2p3p\,^1D^e$ (small chain line), and $2s3d\,^1D^e$ (large chain line) ones. (b) The excitation processes to the $(3l, 3l')$ manifold: the final states are the $3s3s\,^1S^e$ (solid line), $3p3p\,^1S^e$ (broken line), $3s3p\,^1P^o$ (dotted line), $3p3p\,^1D^e$ (small chain line), and $3s3d\,^1D^e$ (large chain line) ones.

results obtained in Ref. [2]. The mechanism of these processes by multiply-charged-ion impact also agrees with that of the processes to the $(2l, 2l')$ manifold [3].

For the processes to the $(3l, 3l')$ manifold, we find that cross sections for the processes to the $^1P^o$ states increase at almost the same rate as other processes with increase of Z_p. The cross sections to the $(3l, 3l')$ manifold increase proportionally to $Z_p^3 \sim Z_p^4$. We also see that second-order processes are comparable with or more than first-order ones in these excitation processes by proton and antiproton impact. The excitation mechanism of these processes, i.e., the relative importance of the ladder-climbing mechanism, differs from those to the $(2l, 2l')$ and $(2l, 3l')$ manifolds for the smaller-Z_p ions as discussed in Ref. [2] because of the smaller overlap between the ground-state wave function and the final $(3l, 3l')$ wave functions.

In the excitation processes to the $(2l, 3l')$ manifold, for higher Z_p, it is seen that the excitation processes to the $2p3p\ ^1D^e$ $\{[2(1,0)^+3\ ^1D^e],\ v = 0\}$ and $2s3s\ ^1S^e$ $\{[2(1,0)^+3\ ^1S^e],\ v = 0\}$ states tend to become dominant in the double-electron excitation, while for smaller Z_p, $(2s3p + 3s2p)\ ^1P^o$ $\{[2(0,1)^+3\ ^1P^o],\ v = 1\}$ excitation is most likely to take place. For the $(3l, 3l')$ manifold, it is found that the $3p3p\ ^1D^e$ $\{[3(2,0)^+3\ ^1D^e],\ v = 0\}$ and $3s3s\ ^1S^e$ $\{[3(2,0)^+3\ ^1S^e],\ v = 0\}$ excitations prevail for high-Z_p ions. However, for small-Z_p ions, processes to $(3s3p)\ ^1P^o$ $\{[3(1,1)^+3\ ^1P^o],\ v = 1\}$ and $3p3p\ ^1D^e$ $\{[3(2,0)^+3\ ^1D^e],\ v = 0\}$ are likely to occur as discussed in Ref. [2].

From these results, we find that, for high-Z_p ions, excitation processes with $\Delta v = \Delta T = \Delta A{=}0$ from the initial $1s1s\ ^1S^e$ $\{[1(0,0)^+1\ ^1S^e],\ v = 0\}$ state dominate, while for small-Z_p ions, those with $\Delta v = \Delta T{=}1$ and $\Delta A{=}0$ prevail except for the process to the $3p3p\ ^1D^e$ $\{[3(2,0)^+3\ ^1D^e],\ v = 0\}$ state. That is, the processes to the $(2l, 3l')$ and $(3l, 3l')$ manifolds have the same trend as that to the $(2l, 2l')$ manifold. The set of the propensity rules $\Delta v = \Delta T{=}0$ and $\Delta A{=}0$ is interpreted as a result of the isomorphism of the charge-density plots of the channel wave functions between the initial state wave function and the final state ones. This indicates that for high-Z_p ions, the He atoms tend to conserve their internal states as the "e–He^{2+}–e linear triatomic molecule" and to stretch their sizes or to rotate as a whole during the excitation processes. On the other hand, for small-Z_p ions, i.e., in the weak-coupling regime, as seen in the case of proton and antiproton impact, Pauli's exclusion principle modifies the isomorphism and changes the angular propensity rule $\Delta v = \Delta T{=}0$ into $\Delta v = \Delta T{=}1$. Then the He atoms tend to be "vibrational excited" and "rotational excited" along the average molecular axis according to the rovibrator model. For high-Z_p ions, i.e., the strong coupling regime, where higher-order processes prevail, the modification to a few number of the matrix elements arising from the Pauli exclusion principle is completely smeared out and the isomorphism, i.e., $\Delta v = \Delta T{=}0$ and $\Delta A{=}0$, is recovered.

In conclusion, we have theoretically investigated the double-electron excitation to the $(2l, 3l')$ and $(3l, 3l')$ manifolds of He by fast multiply-charged-ion impact using the close-coupling approach. The hyperspherical wave functions are used for the description of the electron-electron correlation. The coupling with the continuum is not included. For the processes to the $(2l, 3l')$ manifold, the cross section to the $2p3p\ ^1D^e$ state shows the most rapid increase as Z_p increases, while that to the $(2s3p + 3s2p)\ ^1P^o$ state gives the slowest. For the processes to the $(3l, 3l')$ manifold, the cross sections to the $^1D^e$ states give almost the same ratio of increase as those to the $^1P^o$ states. For both processes to the $(2l, 3l')$ and $(3l, 3l')$ manifolds, for high Z_p, excitation processes with $\Delta v = \Delta T = \Delta A{=}0$ from the initial $1s1s\ ^1S^e$ state dominate, while for small Z_p, those with $\Delta v = \Delta T = 1$ and $\Delta A{=}0$ for optically allowed transition prevail because of the modification of the propensity rules arising from the Pauli exclusion principle. For high-Z_p ions where incident bare ions strongly interact with the target He atom, the complete isomorphism is recovered. Hence we conclude that isomorphism is the key concept which governs collision dynamics in the direct excitation processes where electron-electron correlation plays a decisive role.

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