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DOUBLE EXCITATION OF HE AND H⁻ BY FAST PROTON AND ANTI-PROTON IMPACT ¹

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Theoretical investigation has been made on double excitation processes of He and H⁻ by fast proton and anti-proton impact in the MeV/u-energy region. The cross sections are calculated by use of both the close-coupling and the perturbation expansion methods, and the wave functions of target atoms are generated based on the hyperspherical coordinate method. The excitation to the $2p^2\ ^1D^o$ state of H⁻ by anti-proton impact is dominant by about three times in comparison with that by proton impact at the incident energy of 0.1 MeV/u. The spectral shape of an ejected electron from the $2s2p\ ^1P^o$ state of H⁻ at the incident energy of 1.5 MeV/u is consistent with the line profile of the H⁻ photodetachment observed by Bryant *et al.*

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1 Introduction

Recent advance of experimental technique has made it possible to reveal evidences of electron correlation effects in the course of ion-atom collisions. At CERN, Andersen *et al.* [1] made the first measurement of double ionization cross sections of He by proton (p) and anti-proton ($\bar{p}$) impact in the energy range 0.5-5.0 MeV. They found that the cross sections by $\bar{p}$ impact dominate over those by p impact by a factor of nearly two, while the associated single ionization cross sections are the same. The conventional independent particle model cannot explain this fact because the leading term of the scattering amplitude by the Born series results in null contribution. Therefore, the striking difference of the cross sections suggests the importance of correlation on simultaneous two-electron ionization processes.

This pioneering experiment highlights decisive roles of electron correlation in the entire course of high energy ion-atom collisions. A few years ago, Arcuni and Schneider [2], Pedersen and Hvelplund [3], and Giese *et al.* [4] measured a set of double excitation cross sections of He by impact of e^- , p, C^{q+} ($q=4-6$), and so on from the ground state to the lowest-lying doubly excited states in the MeV/u-energy region. Moreover, theoretical investigations on the excitation processes have been also done by Fritsch and Lin [5], and Winter [6] by solving coupled-state equations based on He wave functions generated by configuration interaction methods.

In this article, we present cross sections of double excitation processes:

$$p/\bar{p} + \text{He}(1s^2) \rightarrow p/\bar{p} + \text{He}^{**}(2l, 2l') \quad (1)$$

$$p/\bar{p} + \text{H}^-(1s^2) \rightarrow p/\bar{p} + \text{H}^{**}(2l, 2l') \quad (2)$$

in the MeV/u-energy region [7, 8]. In order to analyze details of collision dynamics and roles of correlations, the collision process is described by the close-coupling method (CC), the plane-wave Born (PWB) expansion, and the distorted-wave Born (DWB) expansion on the basis with the semi-classical impact-parameter picture. Wave functions of He and H^- are generated using the hyperspherical coordinate method. This method enables us to describe the electron correlation quite accurately. In the present calculations, we have made the two following assumptions. First, all doubly excited states of He and the $2s^2\ ^1S^e$ and $2p^2\ ^1D^e$ states of H^- , embedded in continua, are approximately expressed as discrete

states. This statement is justified because of much shorter collision times in comparison with decay life times of the associated autoionizing states. The second assumption is to neglect contributions from charge transfer channels in describing a wave function of the whole collision system. This is valid because the cross sections of charge transfer are much smaller than those of direct excitation in the energy region studied here.

Sections 2 and 3 are devoted to the results and discussion on the double excitation of He and H^- , respectively.

2 Results and discussion on He

The total wave function employed in the CC calculation is expanded in terms of a set of 21 states of He, which consists of $1s^2\ ^1S^e$, $1s2s\ ^1S^e$, $2s^2\ ^1S^e$, $2p^2\ ^1S^e$, $1s2p\ ^1P^o$, $1s3p\ ^1P^o$, $2s2p\ ^1P^o$, $23sp +\ ^1P^o$, and $2p^2\ ^1D^e$ states. For the plane-wave second-Born (PWB2) calculation, an intermediate propagating function is expanded in terms of a set of 15 states, in which both of $1s3p\ ^1P^o$ and $23sp +\ ^1P^o$ states are excluded from the set of 21 states. Table 1 shows our calculated results based on the CC and the PWB2 at the energy of 1.5 MeV/u as well as the theoretical results by Fritsch and Lin [5] and the experimental results by Giese *et al.* [4]. The PWB2 results can reproduce those by the CC qualitatively. Then, the collision dynamics of the present system can be interpreted to some extent on the basis of the PWB2 picture.

The excitation to the $2s2p\ ^1P^o$ state is most likely to take place, because the optically allowed transition determines essential aspect in collision dynamics on the occasion of high-energy ion impact. In this case, only a little difference is seen between the cross sections by p and $\bar{p}$ impact. Therefore, this means that the contributions from the first Born term are much dominant over those from the higher-order ones.

For the excitation to the $2p^2\ ^1D^e$ state, the p- and the $\bar{p}$ -cross sections are nearly the same. However, the collision dynamics is quite different from the case of the excitation to the $2s2p\ ^1P^o$ state. The effects of the first-order term is strongly suppressed because of its character of a weak quadrupole transition. Therefore, the second-order term has significant influences on the cross sections. Above all, both of the $1s2p\ ^1P^o$ and the $2s2p\ ^1P^o$ states play important roles as intermediate states propagating in the two step collisions. For the reason mentioned above, there exists only a small contribution from

interferences between the first and the second-order terms. This result leads to a small difference of cross sections by changing a sign of a projectile charge.

For the excitations to the $2s^2\ ^1S^e$ and the $2p^2\ ^1S^e$ states, the second Born term, especially the $2s2p\ ^1P^o$ state as an intermediate state, has comparable contributions to the cross sections with the first-order term. Light can be shed on the important roles of this state by detailed analyses of the impact-parameter dependences of the cross sections and the time evolution of the excitation probabilities in terms of the CC picture [7]. The presence of interference effects between the first and the second-order terms causes visible differences of the p - and $\bar{p}$ -impact on the differential cross sections and the time evolution of the transition probabilities. However, these interference effects are not clarified from the behavior of the total cross sections.

It has been found that the $2s2p\ ^1P^o$ state essentially determines the mechanism in the collision dynamics because of its strong dipole couplings. It can be understood that most of the double excitation processes begin with the simultaneous two-electron transition to this strongly correlated state caused by the first-order interaction with a projectile, and successive transitions take place from the $2s2p\ ^1P^o$ state to the final states of $2s^2\ ^1S^e$, $2p^2\ ^1S^e$, and $2p^2\ ^1D^e$. This fact indicates the importance of the electron correlation effect, because the $2s2p\ ^1P^o$ state as a propagating intermediate state cannot be described by use of theories based on the independent particle model.

Next, we mention some discrepancies between our CC results and the experimental ones by Giese *et al.* This may be ascribable to some difficulties in the procedure of extracting the experimental "total double excitation cross sections" from ejected electron spectra. The total cross sections cannot be extracted from the ejected electron spectra, because the parameters obtained from the spectra based on the Shore's formula include the interference contribution between the direct ionization part and the resonant ionization part [9].

3 Results and discussion on H^-

To calculate the excitation cross sections of H^- , two sets of 37 states and 67 states are employed as basis functions to analyze the collision dynamics. The set of 37 states consists of the discrete states $1s^2\ ^1S^e$, $2s^2\ ^1S^e$ and $2p^2\ ^1D^e$, and the shape-resonant state $2s2p\ ^1P^o$.

The $2s2p\ ^1P^\circ$ state are discretized into 10 energy-meshes for the present calculation. The set of 67 states includes the low-lying singly ionized states $1s kp\ ^1P^\circ$ discretized into 10 energy-meshes in addition to the set of 37 states. The convergences of the cross sections have been confirmed in the CC(67)-calculations. Tabel 2 indicates our calculated results based on the CC, the first- and the second-order PWB (PWB1 and PWB2), and the first- and the second-order DWB (DWB1 and DWB2) at the energy of 0.1 and 1.5 MeV/u, respectively.

First, discussion is made on the results at 1.5 MeV/u. There appears only a small difference between the cross sections of the $2s2p\ ^1P^\circ$ and the $2p^2\ ^1D^\circ$ by p and $\bar{p}$ impact as is the same with the excitations of He. Several calculations of Table 2 provide nearly the same results on the excitation to the $2s^2\ ^1S^\circ$ state except for results by the PWB2(37). This indicates that the the excitation process is caused only by the first-order interaction with a projectile and the effect of the higher-order interactions can be negligible. Such understanding of the collision dynamics is much different from that of the case of He as discussed in the preceding section. Furthermore, the comparison of the results by the PWB2(37) with those by the DWB1 and the DWB2(37) shows that a distorted potential, especially the static potential of the $1s^2\ ^1S^\circ$ state, plays an important role in the course of the collision on H^- . This may be the effect that the electron cloud of H^- can be easily polarized by an electric field arising from a projectile. In fact, the electronic state of H^- is much loosely bound in comparison with that of He.

The distorted potential also has a meaningful contribution to the excitation to the $2p^2\ ^1D^\circ$ as is the same with that to the $2s^2\ ^1S^\circ$. Moreover, the results by the DWB2(67) and the CC(67) indicate the outstanding effect of the low-lying $1s kp\ ^1P^\circ$ state on an intermediate propagation for the double collisions of a projectile. That is, the collision dynamics is mostly determined by the intermediate state of the $1s kp\ ^1P^\circ$.

At the energy of 0.1 MeV/u, the excitation to the $2s^2\ ^1S^\circ$ becomes dominant in the first-order process. This is the same situation as that at 1.5 MeV/u. As for the $2p^2\ ^1D^\circ$, the higher-order processes dominate in this excitation process, and the remarkable difference by a factor of nearly three comes out between the cross section by the p impact and that by the $\bar{p}$ impact as seen from the results of the CC(67). Especially, the low-lying $1s kp\ ^1P^\circ$ state has an essential contributions to this difference. The difference between p and $\bar{p}$

impact becomes evident in the energy below 0.5 MeV/u [8]. This is one of the evidences of a decisive role of correlation in the course of high-energy ion-atom collisions.

Finally, we discuss the excitation to the $2s2p\ ^1P^o$ state. This is the shape-resonant state characteristic of H^- . Figure 1 shows the normalized spectral line-profile of an ejected electron from this state induced by the collision by the proton impact at 0.1 to 1.5 MeV/u. This result is calculated by the CC(67). It is almost equal to the result by the PWB1 (not shown here, see [8]), and then the excitation is found to be caused by the first-order interaction with a projectile. Figure 1 also indicates the normalized values of emission spectra due to the photodetachment of H^- observed by Bryant *et al.* [10]. The experimental values are nearly the same with our calculated results at 1.5 MeV/u. This is easily understood by the fact that the optical allowed transition becomes dominant in the collision process with the incident energy of a charged-particle increasing and then the collision dynamics of both by a photon and a charged-particle impact becomes akin to each other.

As the impact energy decreases, however, the spectral shape become different from the experimental data of the photodetachment in the high-energy wing of the emission spectra. This may be due to the effect of the post collision interaction of a high-energy projectile ion with an electron [11]. To confirm it, it is necessary to calculate the spectral profiles at fixed emission angles of the electron.

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Figure Caption

Figure 1. Normalized spectral profiles of an ejected electron from the shape-resonant state $2s2p\ ^1P^\circ$ of H^- by p impact at energies of 0.1-1.5 MeV/u. The abscissa stands for the emission energy of the electron measured from the ground state energy of H^- . The solid, the long-dashed, the chain, and the short-dashed curves represent the spectra at the impact energy of 1.5, 0.5, 0.2, and 0.1 MeV/u, respectively. For comparison, experimental data of photodetachment observed by Bryant *et al.* [10] are shown. Herein, these data are normalized by the value of the peak position.

Table 1: Comparison with other experimental and theoretical cross sections (in the unit of 10^{-20}cm^2) for each double excitation process of He at impact energy of 1.5 MeV/u. The first column lists final states, the second, the third and the fourth give our CC, PWB1, and PWB2 results. The fifth column shows the experimental data by Giese, *et al*. The sixth column gives the theoretical results by Fritsch and Lin. The entries in the fifth column (b) are the experimental data by electron impact at the same velocity instead of those by the anti-proton impact.

Final States	CC	PWB1	PWB2	Giese <i>et al.</i>	Fritsch and Lin
(a) proton impact					
$2s2s^1S^e$	0.409	0.329	0.622	0.0318	0.74
$2s2p^1P^o$	7.74	8.03	8.72	0.608	3.0
$2p2p^1S^e$	0.116	0.0740	0.168		0.45
$2p2p^1D^e$	0.191	0.0168	0.164	1.84	0.48
(b) anti-proton impact					
$2s2s^1S^e$	0.314	0.329	0.538	0.0816	0.73
$2s2p^1P^o$	7.65	8.03	8.61	1.17	3.3
$2p2p^1S^e$	0.0981	0.0740	0.145		0.41
$2p2p^1D^e$	0.185	0.0168	0.174		0.27

Table 2: Calculated cross sections (in the unit of 10^{-20}cm^2) for each double excitation process of H^- at impact energy of (a) 1.5 MeV/u and (b) 0.1 MeV/u. The number in parentheses in the first column represents the number of states employed.

(a) 1.5 MeV/u

	$2s^2\ ^1S^e$		$2p^2\ ^1D^e$	
	proton	anti-proton	proton	anti-proton
PWB1	9.43	9.43	0.458	0.458
PWB2(37)	14.7	14.5	0.632	0.713
DWB1	9.35	9.41	0.456	0.458
DWB2(37)	9.31	9.20	0.495	0.575
DWB2(67)	9.40	9.31	1.29	1.57
CC(37)	9.39	9.24	0.488	0.568
CC(67)	9.62	9.49	1.26	1.43

(b) 0.1 MeV/u

	$2s^2\ ^1S^e$		$2p^2\ ^1D^e$	
	proton	anti-proton	proton	anti-proton
PWB1	141	141	6.85	6.85
CC(37)	128	137	15.9	25.9
CC(67)	118	124	24.4	79.5

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