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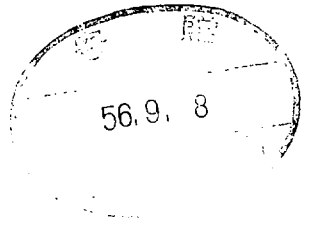

RESEARCH REPORT

NAGOYA, JAPAN

Charge Transfer in Collisions of Li^{3+} and Be^{4+} ions with Atomic Hydrogen at Low Impact Energy

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Further communication about this report is to be sent to the Research Information Center, Institute of Plasma Physics, Nagoya University, Nagoya 464, Japan.

Abstract

Total charge transfer cross sections are calculated for the collisions of Li^{3+} and Be^{4+} ions with H(1s) atoms in the low energy region (E < 25 keV/amu). The perturbed-stationary-state method in the impact parameter approximation is used with a basis set of adiabatic one-electron two-center molecular orbitals. For the Li^{3+} - H system, a reasonable agreement is found between the present calculation and the recent experiment.

1. Introduction

The charge transfer process between fully stripped ions and hydrogen atoms is of considerable interest not only as giving the basic test problems to all the charge transfer theories but also in relation to nuclear fusion research. In tokamak plasmas heated by neutral hydrogen beam injection, for instance, electron capture by highly stripped impurity ions from hydrogen atoms gives rise to serious problems such as an enhancement of radiative energy loss.

In recent years, the research at high energy region has been done extensively (Olson and Salop 1977; Golden et al. 1978; Chan and Eichler 1979; Ryufuku and Watanabe 1979; Salop and Olson 1979). A few works have been carried out, however, at lower energy regions. In the present paper the total charge transfer cross section for Li^{3+} - H and Be^{4+} - H systems are calculated at the low impact energies ($E < 25$ keV/amu). For the Li^{3+} - H system, a quantitative comparison of the result is made with the experimental data recently obtained (Seim et al. 1980). The Li^{3+} - H system may be of some significance in the future fusion reactor, in which the use of lithium blanket is planned for heat transport and tritium breeding.

A related work was carried out by Harel and Salin (1977) for the Be^{4+} - H system. Their work was primarily concerned with the population of the excited states after the charge transfer. They chose the heavier nucleus as the coordinate origin to take into account approximately

the effect of electron momentum transfer, which plays a key role in the evaluation of the excited-state population. Our approach, however, is different from that of Harel and Salin in three essential respects. First, to avoid the ambiguity caused by the electron translation factor (ETF), we deal with only the total charge transfer cross section. Second, to do that, the origin of the coordinates is placed on the proton. Finally, we use a larger basis set of the quasi-molecular orbitals. Ryufuku and Watanabe (1979) have also been studying the Li^{3+} - H and Be^{4+} - H systems using the S-matrix formulation with a basis set of traveling atomic orbitals. It is uncertain that their calculation is reliable in the low energy region, though being successful at higher energies. The theoretical results of these two groups will be compared with the present case in Section 3.

2. Formulation

The present cross section calculation is based on the standard method of perturbed stationary states (PSS) with the semiclassical impact parameter approximation (Winter and Lane 1978). We briefly summarize the method here. In the PSS method, the time dependent wave function for the collision system is expanded in terms of a basis set of adiabatic molecular orbitals. In the present case, use is made of a set of exact one-electron two-center molecular orbitals. The classical path is assumed for the heavy particle motion. In the semiclassical impact parameter

approximation, it is always difficult to determine the collision trajectory at lower energies. Recently one of the authors (Ohyama 1980) has studied the collison of He^{2+} ions with H atoms, and found that the electron transfer occurs mostly through a pseudo-crossing of the adiabatic potential energy curves of the quasi-molecule. In the present case, such a crossing occurs at rather larger internuclear distances (see Figs.1 and 2), so that the straight-line trajectory is adequate.

A set of coupled equations

$$\frac{d}{dt} C_j(t) = - \sum_j \{ M_{jk}^{rad}(b,R) + M_{jk}^{rot}(b,R) \} \times \exp\{ i \int_{-\infty}^{t} (E_j - E_k)\, dt' \}\, C_k(t), \qquad (1)$$

are solved numerically for each impact parameter b. In Eq. (1), C_j is the probability amplitude of a molecular state j, E_j is the energy eigenvalue assosiated with the state j, R is the internuclear distance and M_{jk} is the coupling matrix element between the molecular states j and k. The one-electron two-center wave functions for the relevant systems are calculated by the procedure following closely that of Bates and Carson (1956) to give the radial (M_{jk}^{rad}) and rotational (M_{jk}^{rot}) matrix elements.

When the origin of the coordinates is placed on the proton, the initial condition is automatically satisfied. Using the unitarity relation, one can write the total charge transfer probability as

$$P_{CT}(b) = 1 - \sum_k |C_k(\infty)|^2 = \sum_{k'} |C_{k'}(\infty)|^2, \qquad (2)$$

where k specifies the states for which the electron remains asymptotically on the proton and k' those corresponding to the electron capture. The quantity $C_{k'}$ does not actually give the probability amplitude for the charge transfer to the state k', because the charge-transfered wave functions must include ETF under the present choice of the origin. Nevertheless, because of the unitarity relation, the quantity $\sum_{k'} |C_{k'}(\infty)|^2$ does represent the total charge transfer probability within the limitation of the finite basis set.

The total cross section for the charge transfer is finally obtained as

$$\sigma_{CT} = 2\pi \int_0^\infty b\, db\, P_{CT}(b). \qquad (3)$$

The problem of electron momentum-transfer was fully discussed by Salin (1980). Without any ETF, some of the matrix elements in Eq.(1) show spurious long-range behavior, resulting in indefinite transition amplitudes of the corresponding states. Furthermore, these spurious effects vary depending on the place of the coordinate origin. Thus it is necessary to take into account properly the ETF to calculate the cross section for the charge transfer to each individual final state. The total charge transfer cross section, however, can be obtained without being affected by the spurious effects, if the origin is placed on the proton, as shown above. The present calculation follows this approach, which was originally suggested by Piacentini and Salin (1974).

3. Results and Discussion

Potential energy curves for the relevant adiabatic molecular states computed for the $(LiH)^{3+}$ and $(BeH)^{4+}$ systems are shown in Figs.1 and 2, respectively. Each state is labeled by a set of united-atom quantum number, (nlm). The initial state corresponding to H(1s) + Li^{3+} at infinite separation correlates to the $3d\sigma$ state, and that for H(1s) + Be^{4+} correlates to the $4f\sigma$ state.

3.1. Be^{4+} - H system

In the calculation by Harel and Salin, 3 states ($3d\sigma$, $3d\pi$ and $4f\sigma$) were taken coupled for Be^{4+} - H system. However, as shown in Fig. 2, the $4f\sigma$ curve is close to $3p\sigma$ $3p\pi$ and $3s\sigma$ curves suggesting the possibility of the significant radial and/or rotational couplings of $4f\sigma$ to the n=3 levels. Other close-lying states such as the $4f\pi$ may also have some influence on the overall charge transfer process. From an examination of the effect of the various couplings, considered here are $4f\sigma$, $4f\pi$, $3d\sigma$, $3d\pi$, $3p\sigma$ and $3p\pi$ for the Be^{4+} - H system.

The important radial and rotational coupling matrix elements are shown in Figs. 3 and 4. For comparison, the matrix elements are calculated with the coordinate origin on Be^{4+} as well as on H^{+} (solid lines for the origin on H^{+} and dashed lines for the origin on the Be^{4+} ion).

In order to look into the details of the transition mechanism, we have investigated the time dependence of the probability $P_j(b,t)$ $(=|C_j(b,t)|^2)$. Fig. 5 shows,

as an example, the time dependence of $P_j(b,t)$ at E_{impact}= 100 au and b=2 au. The electron moves from the initial state ($4f\sigma$) to other states through couplings. The amplitude of the initial state converges at infinity, but some others do not. This is due to the spurious long-range behavior of the radial matrix elements between those states (see Fig. 3), which is caused by the lack of the ETF in the present basis orbitals. It should be noted that this problem does not affect the calculation of the total charge transfer probability P_{CT}.

The resulting total charge transfer cross section is shown in Fig. 6. The calculation is made with the origin placed on the proton. No direct measurements for this process have been made so far. Our result can be compared with the theoretical investigations of this process by Harel and Salin and by Ryufuku and Watanabe.

The charge transfer cross section of Harel and Salin was obtained with the origin on the Be^{4+} ion. Their calculation gave a result for each final state. In Fig.6, our result is compared with their total charge transfer cross section, which is the simple sum of the partial cross section for $3d\sigma$ and $3d\pi$. The two sets of total charge transfer cross sections agree well with each other. This implies either of the following two situation: (1) The partial charge transfer cross section given by Harel and Salin is accurate and the states, $3d\sigma$ and $3d\pi$, are dominant in the final product, or (2) the calculation by Harel and Salin overestimates the partial cross

section. This problem will remain to be solved until the partial charge transfer cross section will be calculated with more elaborate treatment of ETF.

The unitarized distorted wave approximation (UDWA) calculation of Ryufuku and Watanabe is in poor agreement with our result at the lower impact energies. The energy dependence of their cross section is somewhat more flat than ours.

Finally, we attempt a comparison between the theoretical results for Be^{4+} - H and the charge transfer cross section measured for C^{4+} - H collision. On the comparison of the potential energy curves, there is a similar pseudo-crossing of molecular states for both the systems (Harel and Salin 1977). It is predicted that the cross section for C^{4+} - H collision should be very similar to Be^{4+} - H system. There is a good agreement between our result and the experiment.

3.2. Li^{3+} - H system

The initial state in the present case is the $3d\sigma$ state. Three sets of calculations are made starting from $3d\sigma$, $2p\sigma$ and $2p\pi$ and using progressively larger basis set. The most comprehensive calculation was based on the six states coupled: the above three plus $3p\sigma$, $3p\pi$, $3d\pi$. To assure the convergence, an eight-state calculation (with those six and $4f\sigma$, $4f\pi$) is carried out at the energies above 1 keV/amu.

As in the case of Be^{4+} - H system, our calculation

cannot give a reliable result for the final state population. The total charge transfer cross section is shown in Fig. 7. The origin of the coordinates is placed on the proton. A quantitative comparison of the result is made with the experimental data (Seim et al. 1980) recently obtained in the low energy region. Although the present calculation gives smaller cross sections at lower energies, the energy dependence is similar to the experimental result. The discrepancy in the absolute magnitude may be attributed to the inadequacy of the finite basis set.

The total charge transfer cross section was calculated by Ryufuku and Watanabe for a wide energy region. Their result is in good agreement with the experiment at the impact energy above 2 keV/amu, but below that the energy dependence of their cross section is flat. Thus the molecular-orbital approach looks more reasonable at the lower impact energy.

Acknowledgment

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Figure captions

Fig.1. Relevant adiabatic potential energy curves for Li^{3+} - H system. Each curve is labeled by a set of united-atom quantum number (nlm). At infinite separation, the $3d\sigma$ state correlates to the initial state corresponding to H(1s) and all others correlate to Li^{2+}.

Fig.2. Relevant adiabatic potential energy curves for Be^{4+} - H system. Each curve is labeled by a set of united-atom quantum number (nlm). At infinite separation, the $4f\sigma$ state correlates to the initial state corresponding to H(1s) and all others correlate to Be^{3+}.

Fig.3. Some radial coupling matrix elements for Be^{4+} - H system calculated with the origin of the coordinates on the proton (solid line) and on the Be^{4+} ion (dashed line).

(1)--- $\langle 4f\pi | \partial/\partial R | 3d\pi \rangle$, (2)--- $\langle 4f\sigma | \partial/\partial R | 3d\sigma \rangle$

The third peak of the matrix element (1) with the origin located on the Be^{4+} ion is observed at R=18 au. At larger separations it approaches zero smoothly, though not shown here because of the lack of space.

Fig.4. Some rotational coupling matrix elements for Be^{4+} - H system calculated with the origin of the coordinates on the proton (solid line) and on the Be^{4+} ion (dashed line).

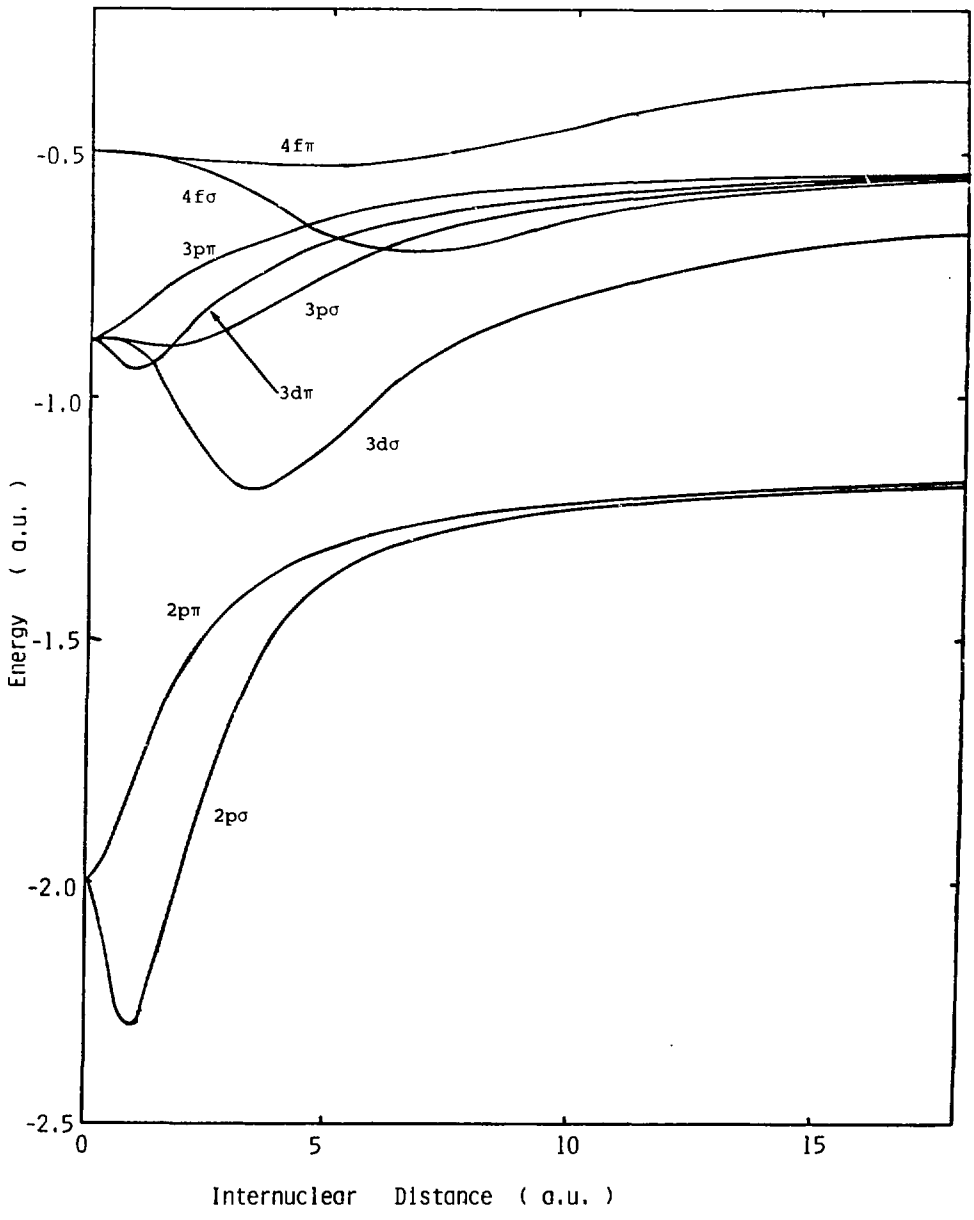
(1)--- $\langle 4f\pi | iL_y | 4f\sigma \rangle$, (2)--- $\langle 3d\pi | iL_y | 3d\sigma \rangle$

Fig.5. The time dependence of the transition probabilities $P_j(b,t)$ for the collision Be^{4+} + H, calculated at the impact parameter b=2 au and the impact energy E=100 au. The internuclear distance R indicated at the top corresponds to the time scale at the bottom.

Fig.6. Total charge transfer cross sections into all states of Be^{3+} in the collision of the Be^{4+} ion with H(1s) atom.
Theoretical results: solid line, the present calculation using six states (4fσ, 4fπ, 3dσ, 3dπ, 3pσ and 3pπ) with the origin of the coordinates on the proton; dashed line, the results of Harel and Salin (1977) using three states (4fσ, 3dσ and 3dπ) with the origin of the coordinates on the Be^{4+} ion; dot-dashed line, the results of Ryufuku and Watanabe (1979).
Experimental data (C^{4+} - H): ♦, Crandall et al (1979); ◊, Gardner et al (1980); ▲, Goffe et al (1979).

Fig.7. Total charge transfer cross sections into all states of Li^{2+} in the collision of Li^{3+} ion with H(1s) atom.
Theoretical results: solid line, the present calculation using six states (3dσ, 3dπ, 3pσ, 3pπ, 2pσ and 2pπ) below 1 keV/amu and eight states (above six plus 4fσ and 4fπ) above 1 keV/amu with the origin of the coordinates on the proton; dashed line, the results of Ryufuku and Watanabe (1979).
Experimental data: ♦, Seim et al (1980); ◊, Shah et al (1978).

Fig. 1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3pπ
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3dπ
3dσ
2pπ
2pσ
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-2.5
Energy (a.u.)
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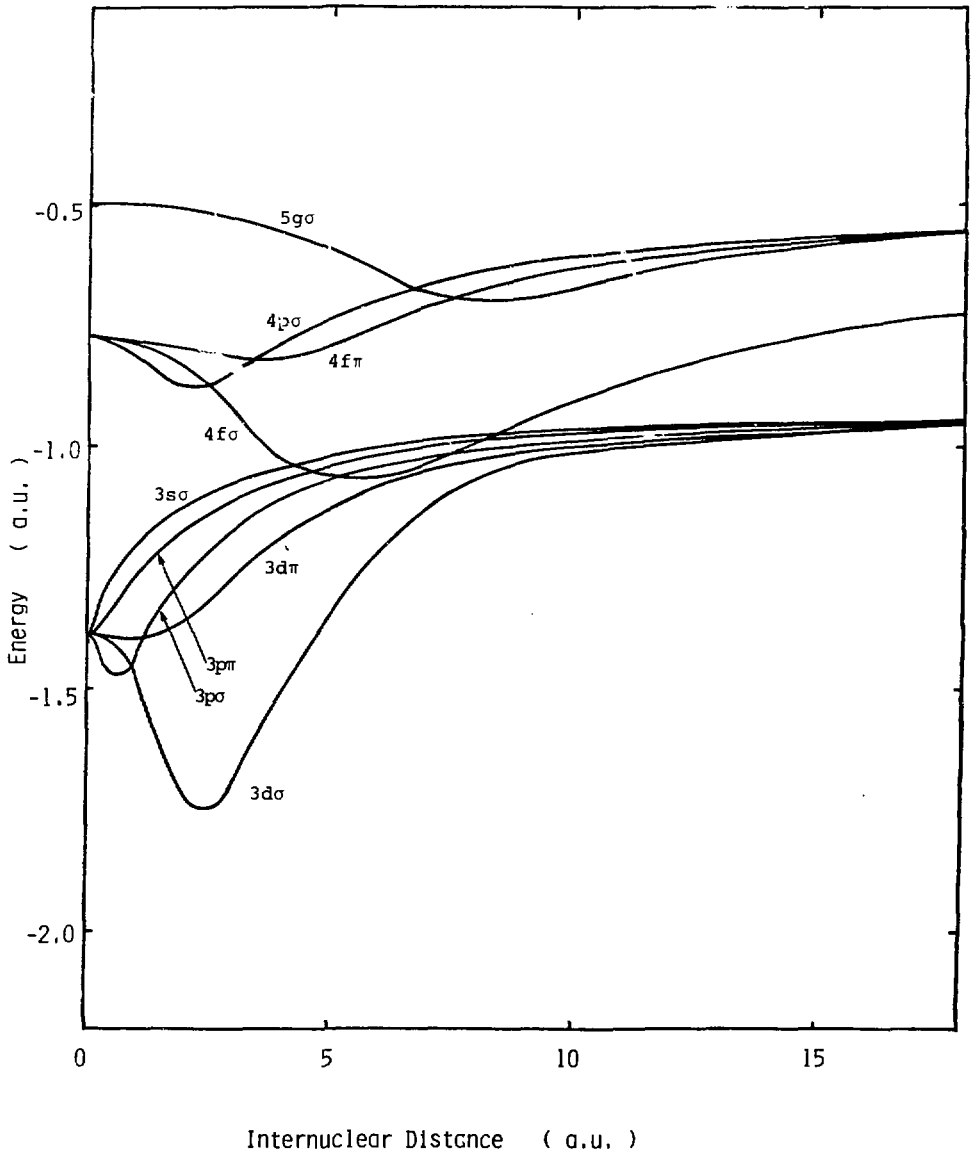
5
10
15
Internuclear Distance (a.u.)

Fig. 2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-1.0
-1.5
-2.0
Energy (a.u.)
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4pσ
4fπ
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3pσ
3dσ
0
5
10
15
Internuclear Distance (a.u.)

Fig. 3

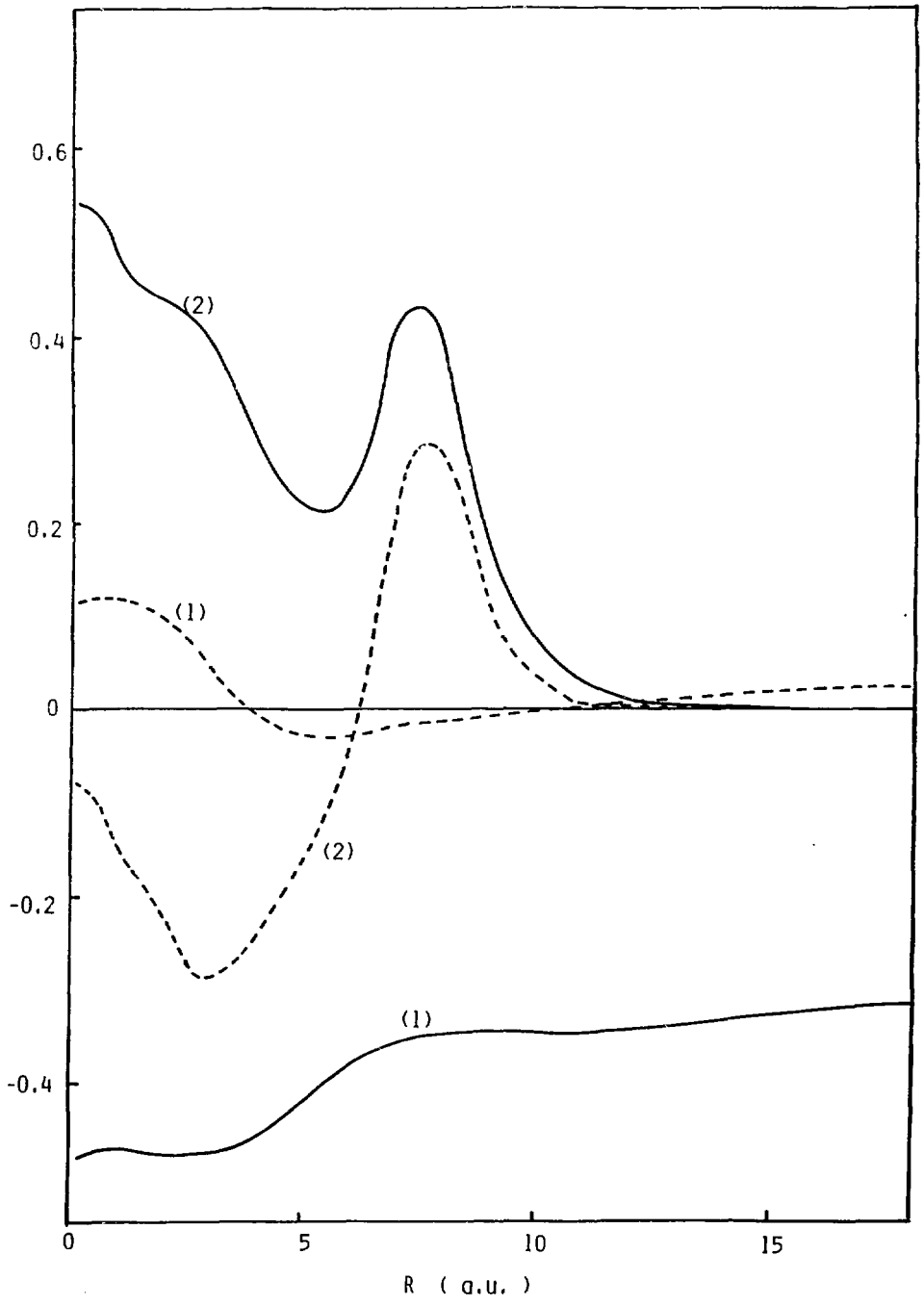
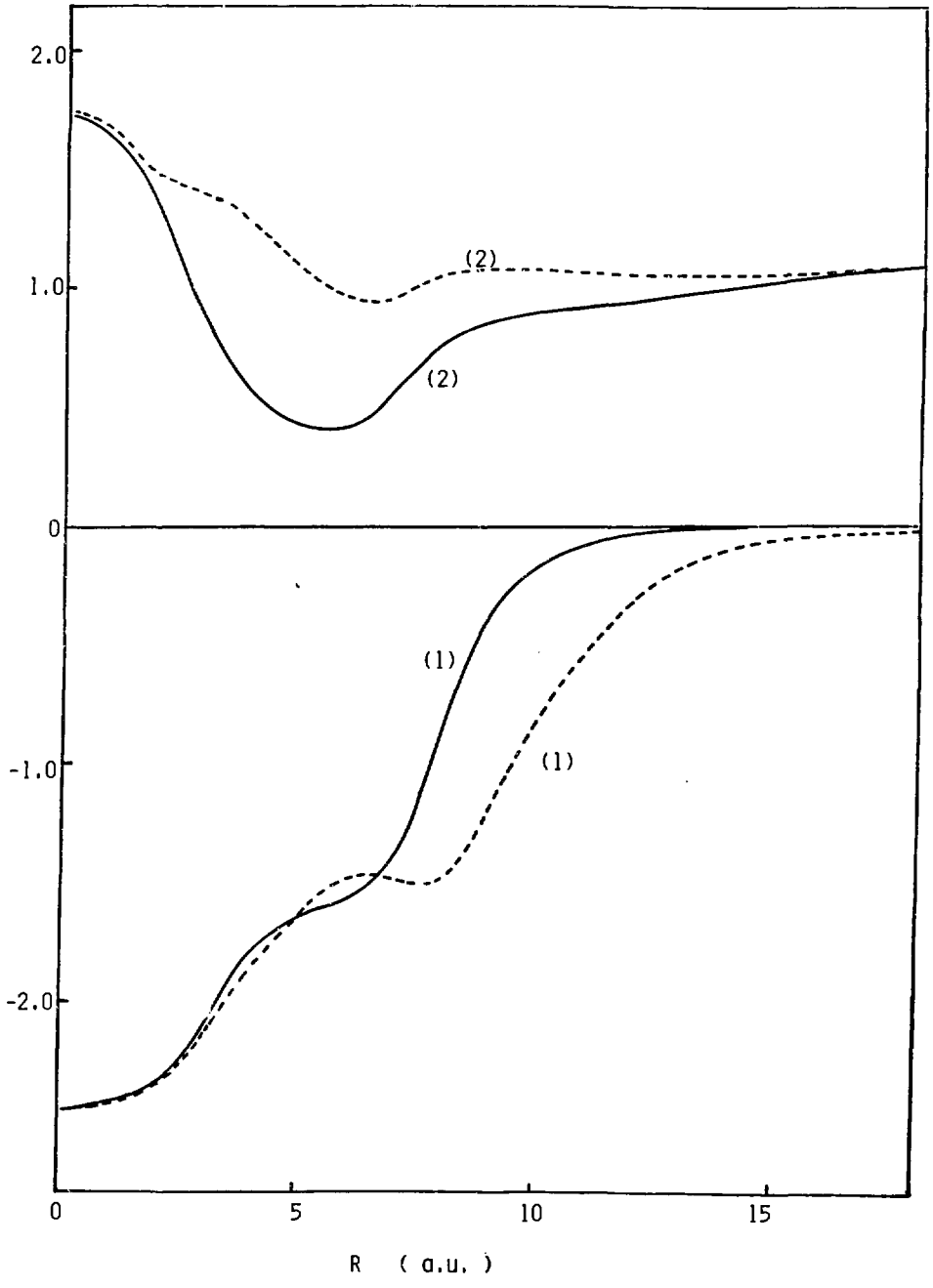
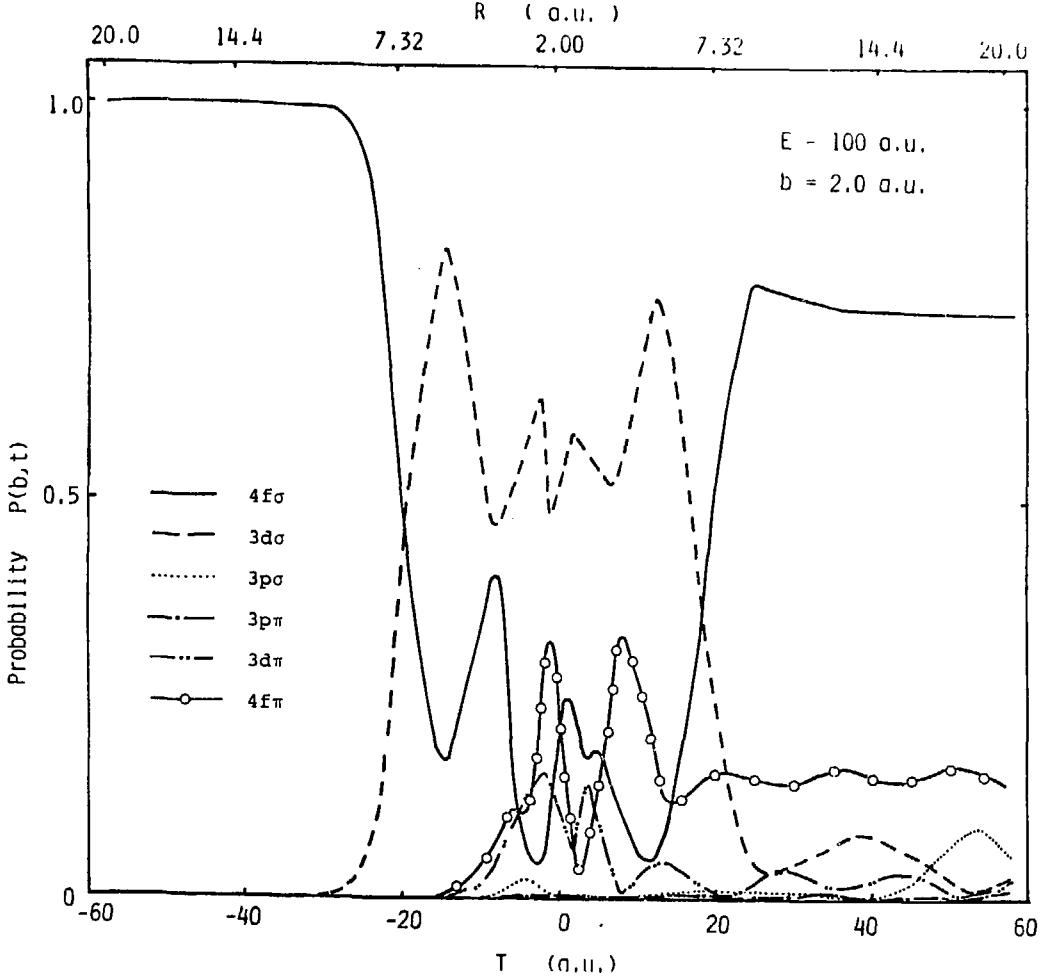


Fig. 4




R (a.u.)
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7.32
2.00
7.32
14.4
20.0
1.0
0.5
0
Probability P(b,t)
E - 100 a.u.
b = 2.0 a.u.
4fσ
3dσ
3pσ
3pπ
3dπ
4fπ
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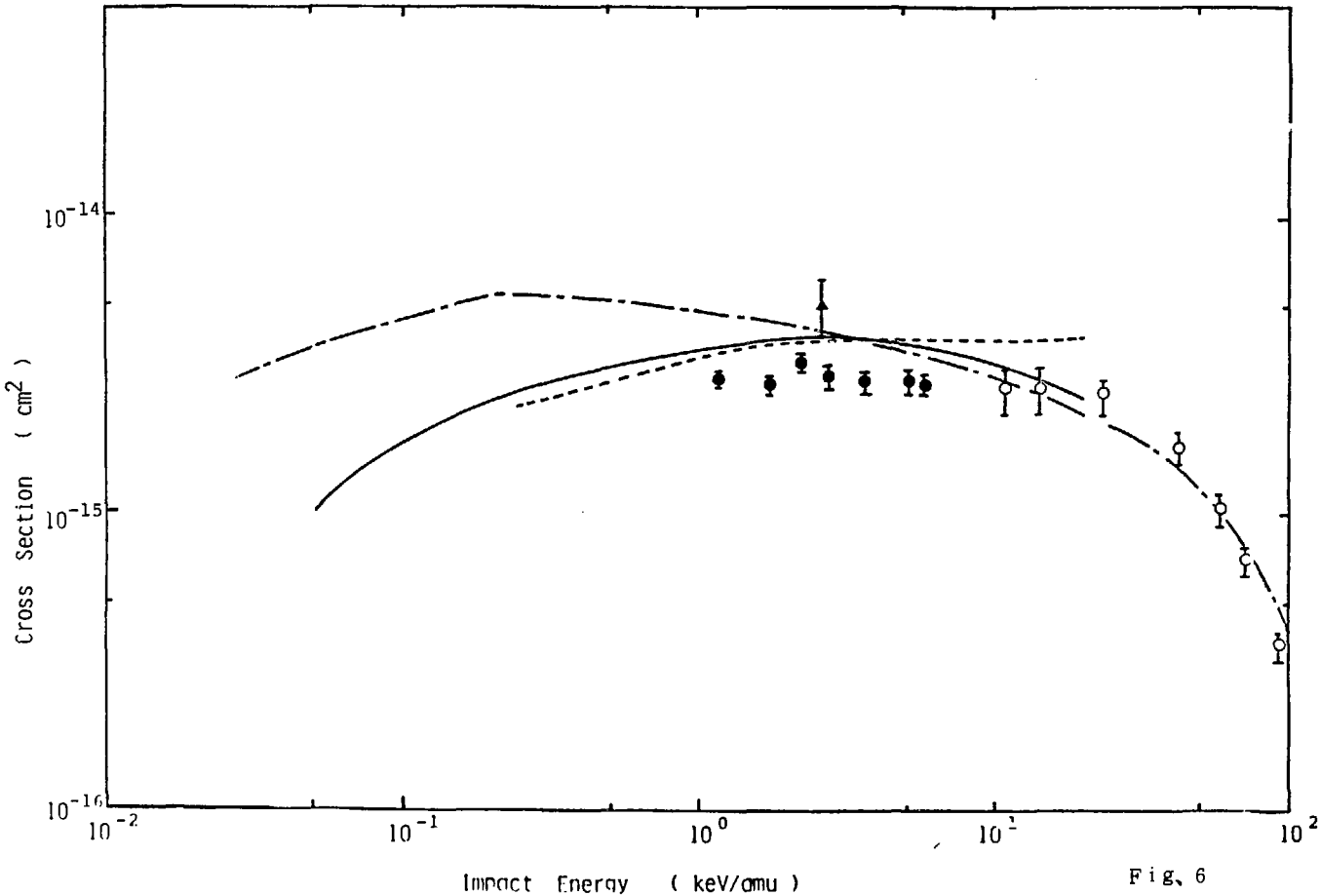
-40
-20
0
20
40
60
T (a.u.)

Fig. 5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10^{-2}
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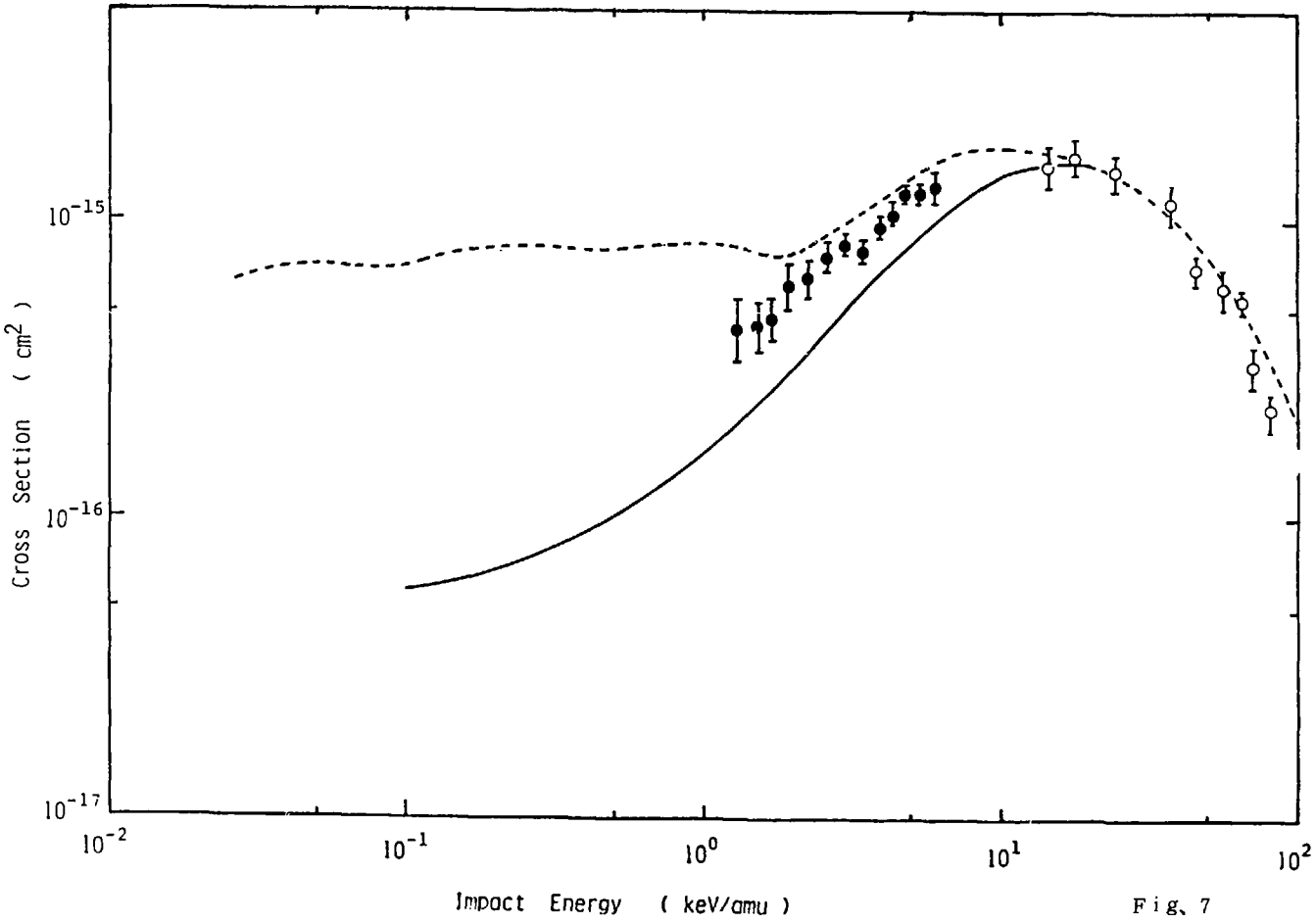
10^{1}
10^{2}
Impact Energy (keV/amu)

Fig. 6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Impact Energy (keV/amu)

Fig. 7