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Oscillatory behavior of charge transfer cross sections as a function of the charge of projectiles in low-energy collisions

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To examine experimental cross sections for charge transfer in collisions of partially stripped heavy ions with atomic hydrogen at low collision energies, unitarized-distorted-wave-approximation calculations are performed using a model in which the projectiles are replaced by bare nuclei of a given effective charge. The results show the presence of a strong oscillatory dependence of the cross sections on effective charge due to the crossings of diabatic potential curves in the low-energy region below 10 keV/amu. The considerable differences in the measured cross sections for impacts of ions of different elements (B, C, N, and O) observed by Bayfield *et al.* and Crandall *et al.* at low impact energies are attributed to this oscillatory behavior.

I. INTRODUCTION

Charge transfer processes between multicharged heavy ions and atomic hydrogen are interesting not only theoretically but also in connection with the heating of tokamak fusion plasmas by neutral-hydrogen-beam injection. Cross sections for the processes have been measured[1-8] or calculated[9-20] by many investigators. In most of the experiments, the cross sections were obtained for the impacts of partially stripped ions, while the calculations were carried out for collisions of completely stripped ions with atomic hydrogen. Therefore no direct comparisons between the experimental and theoretical results are possible, except for the impacts of Li^{3+} at energies of 15–200 keV/amu (Ref. 1), B^{5+} at 6 keV/amu (Ref. 8), and O^{8+} at 200 keV/amu (Ref. 7), for ionic charge $Z \geq 3$. For the cases of impact of ions having the same ionic charges, the comparisons show good agreement between the calculations and experiments at impact energies greater than 10 keV/amu. However, at impact energies below 10 keV/amu, the experimental cross sections are different for impacts of ions of different elements even if their ionic charges are same.

The purpose of the present work is to examine the cross sections for charge transfer in collisions of partially stripped ions of different elements with atomic hydrogen at low impact energies from a theoretical point of view. Bayfield *et al.*[6] reported the experimental charge transfer cross sections for collisions of the partially stripped ions of B, C, N, and O with atomic hydrogen at collision energies of 1–3 keV/amu. They showed that the cross sections for the ionic charges 2 and 3, respectively, are quite different in magnitude among the elements listed above, however, those for the ionic charge 4 are of almost the same magnitude. Recently, Crandall *et al.*[8] confirmed this fact, though their cross sections are smaller overall than those of Bayfield *et al.*

Critical examinations of these experimental results will be made by means of the UDWA (unitarized distorted-wave approximation) method.[18,19] The UDWA method is a unitarized formulation of the distorted-wave approximation in terms of moving atomic orbitals. It is found in the previous investigation[18,19] that the UDWA method is promising for impact energies of 2–100 keV/amu. The validity of the method at low energies will be discussed in comparison with a classical treatment.

A one-electron-model approximation will be used to treat the collision systems involving a partially stripped ion and atomic hydrogen; that is, the ion is replaced by a nucleus having such an effective charge as to yield the orbital energy of the transferred electron evaluated from spectroscopic data.[21]

In Sec. II the UDWA theory is discussed in comparison with a classical treatment, and in Sec. III the experimental cross sections are examined and discussed. Atomic units are used throughout the paper, unless otherwise stated.

II. COMPARISON BETWEEN UDWA METHOD AND CLASSICAL TREATMENT

The detailed description of the UDWA method was presented in Ref. 19. Here, we will examine the relation of the UDWA method with a classical

treatment for low-energy collisions ($E \leq 10$ keV/amu). The charge transfer cross sections at low energies are dominantly determined through the crossings of the energy levels of diabatic bases. Therefore the following classical treatment is possible.

We consider a classical model where charge transfer corresponds to the transfer of an electron having a sufficient energy to overcome the potential barrier between the projected ion and the target nucleus (proton in our case). The height of the barrier is given by those of the saddle point of the superposed Coulomb potential due to these positive ions. The potential at internuclear position is written as

$$V(x) = -Z/x - 1/(R-x), \tag{2.1}$$

where x is the distance from the projectile, Z the charge of the projectile, and R the internuclear distance. From Eq. (2.1), the maximum value of $V(x)$ for $0 < x < R$ is given by

$$V_m = -(Z^{1/2}+1)^2/R, \tag{2.2}$$

which gives the height of the potential wall. The electron is transferred if the following relations are satisfied:

$$-\tfrac{1}{2} - Z/R = -Z^2/2n^2 - 1/R, \tag{2.3}$$

$$-\tfrac{1}{2} - Z/R > -(Z^{1/2}+1)^2/R, \tag{2.4}$$

where the left-hand side of Eq. (2.3) denotes the approximate diabatic potential of the $1s$ state of the hydrogen atom perturbed by the Coulomb potential of the projectile and the right-hand side denotes that of the state of the principal quantum number n of the hydrogenlike system (projectile plus electron) perturbed by the proton. The solution R of Eq. (2.3) gives the crossing point of the two diabatic potential curves.

We can easily obtain the integer n to satisfy the conditions (2.3) and (2.4) as follows:

$$n \leq n_p, \tag{2.5}$$

with

$$n_p = [\{(2Z^{1/2}+1)/(Z+2Z^{1/2})\}^{1/2}], \tag{2.6}$$

where the squared bracket $[x]$ is the Gauss symbol to denote taking the largest integral value not exceeding x, and also the corresponding value of R:

$$R_n = \frac{2(Z-1)}{Z^2/n^2 - 1}. \tag{2.7}$$

It is clear from Eq. (2.6) that $n_p \leq Z$, and from Eq. (2.7) that $R_{n-1} < R_n$ and $R_{n-1} - R_{n-2} < R_n - R_{n-1}$ for $n \leq n_p$, that is, the crossing distance R_n becomes progressively smaller with decreasing n and the separation between two adjacent crossing points also decreases with decreasing n. From these facts we can identify n_p as the principal quantum number of the final state to be occupied most probably by the transferred electron, since probabilities of electron capture into the state of the principal quantum number n results mainly from the impact parameter ρ, being $R_{n-1} < \rho \leq R_n$.

In the UDWA calculation, the effect of the crossing of diabatic potential curves also appears at low impact energies < 10 keV/amu. For example, we can see the maxima of the distorted-wave-Born-approximation (DWBA) probability for charge transfer in $O^{8+} + H(1s)$ collisions in the vicinities of $\rho = 2.3$, 4.7, and 9.0 corresponding to the crossing points of the $O^{8+} + H(1s)$ and $O^{7+}(n=3,4,5) + H^+$ diabatic potential curves, as seen in Fig. 4 of Ref. 18. This comes from the fact that the low-energy DWBA probability results mainly when the agreement of the exponential function of Eq. (2.35) in Ref. 18 vanishes, that is,

$$\omega_n^B + u_{nn}^{BB} = \omega_0^A + u_{00}^{AA}, \tag{2.8}$$

where the right- and the left-hand sides denote the diabatic potential of the initial and final channels, respectively. Since at a large internuclear separation

$$\omega_0^A + u_{00}^{AA} \simeq -\tfrac{1}{2} - Z/R, \tag{2.9a}$$

$$\omega_n^B + u_{nn}^{BB} \simeq -Z^2/2n^2 - 1/R, \tag{2.9b}$$

then Eq. (2.8) becomes equivalent to Eq. (2.3).

Now, in the UDWA calculation we define n_p as the value of the abscissa n at which the smoothed curve representing the dependence of the partial cross section σ_n on n shows a maximum. This definition allows a nonintegral value for n. In Fig. 1, for example, the value of n_p obtained by the UDWA calculation at the impact energy of 0.1 keV/amu is shown as a function of Z by the solid line supplemented by three closed circles, compared with the classical n_p given by Eq. (2.6), which is depicted by the dotted line. Note that the quantum and classical n_p's are in good agreement with each other except in the vicinity of $Z = 2$. This shows that the most probable level n_p is basically determined by a classical Eq. (2.4).

As known from the description below Eq. (2.7), charge transfer could take place within the internuclear distance $R \leq R_p$, where

$$R_p = \frac{2(Z-1)}{Z^2/n_p^2 - 1}. \tag{2.10}$$

Then, the classical charge transfer cross section σ_{cl} can be written in terms of R_p by assuming the probability of electron transfer to be $\frac{1}{2}$.

$$\sigma_{cl} = \tfrac{1}{2}\pi R_p^2. \tag{2.11}$$

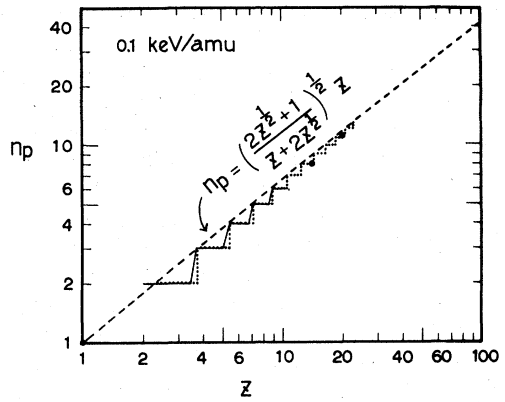

FIG. 1. Most probable principal quantum number n_p, of the final states for the charge transfer process, $X^{Z+} + H(1s) \rightarrow X^{(Z-1)+} + H$, where Z is the effective charge. The solid line and the closed circles denote the values obtained by interpolations from plots of the UDWA partial cross sections σ_n vs n at the ion impact energies of 0.1 keV/amu. The dotted line shows the results obtained by the classical treatment.

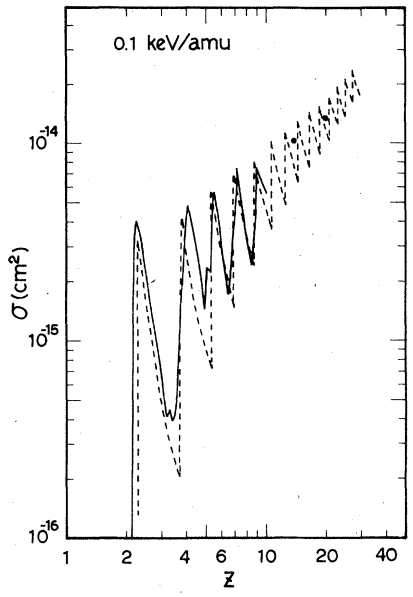

FIG. 2. Oscillatory behavior of the dependence of the charge transfer cross sections on effective charge Z. The solid line and the closed circles denote the UDWA results, at the ion impact energy of 0.1 keV/amu, and the dotted line the classical results.

Figure 2 shows the dependences of cross sections on Z obtained by the UDWA and classical treatments. The two results are much the same in magnitude and oscillatory behavior.

As seen in Fig. 2, the charge transfer cross section shows a strong oscillation as a function of Z at low collision energies. However, at intermediate energies such oscillations almost disappear, as shown in Fig. 3. Recently, Kim *et al.*[22] have observed oscillations in the charge dependence of the charge transfer cross sections for collisions of ions of Ta, W, and Au with atomic and molecular hydrogen at ion impact energies of 25–102 keV/amu, while they have not observed such oscillations for impacts of the lighter ions Si, Fe, and Mo. These oscillations found by Kim *et al.* may be attributed to an origin different from the present one, because the oscillation due to the crossing of diabatic potential curves occurs only in the low-collision-energy region. They attribute the intermediate-energy oscillations in the heavy-projectile cross sections to interference between the scattering amplitudes arising from the long-range Coulomb and short-range (screened Coulomb) forces acting on the transferred electron during the collision.

As described above, the UDWA gives much the same results as the classical treatment, which is considered to give a good estimate for the charge transfer cross section at low energies. However, the UDWA is based on the approximations in which the final-state interactions and the time-ordering operator are ignored. As described in Ref. 23, the error included in the cross sections due to these approximations can be estimated to be, at most, 50% at impact energies $E \simeq 0.3$–10 keV/amu.

III. COMPARISON WITH EXPERIMENTAL DATA AND DISCUSSION

We approximate collision of a partially stripped ion with atomic hydrogen by a model where a bare

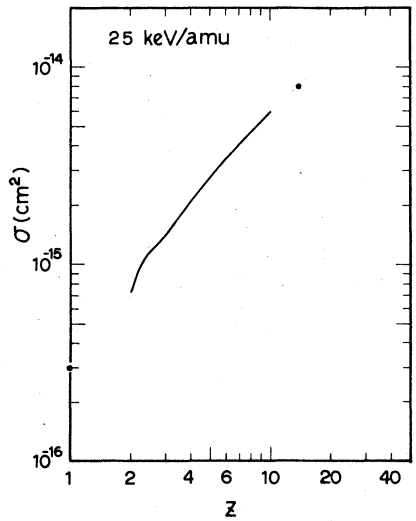

FIG. 3. Dependence of the UDWA charge transfer cross sections on effective charge Z at the ion impact energy of 25 keV/amu.

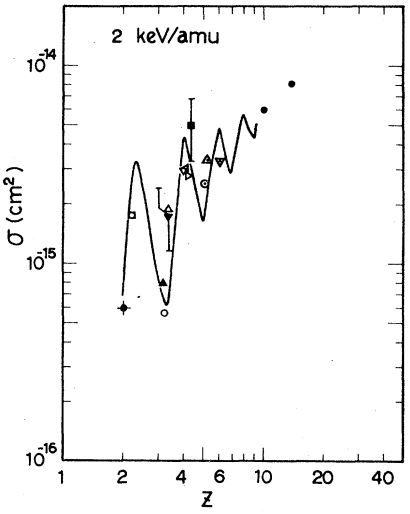

FIG. 4. Comparison between theoretical and experimental cross sections for charge transfer in collisions of completely and partially stripped ions having effective charge Z with atomic hydrogen at ion impact energy of 2 keV/amu.—and ● denote the UDWA results. Experimental data: ▲(B^{3+}), ▼ (C^{3+}), and ■ (O^{4+}) Bayfield *et al.* (Ref. 6); □ (B^{2+}), ○ (B^{3+}), △ (N^{3+}), ▽ (B^{4+}), ◁ (C^{4+}), ▷ (N^{4+}), ⊙ (N^{5+}), ▲ (O^{5+}), and ▽ (O^{6+}) Crandall *et al.* (Ref. 8); and ✦ (He^{2+}) Nutt *et al.* (Ref. 26).

nucleus having a certain effective charge collides with atomic hydrogen. The effective charge can be determined from spectroscopic energy data.[21] The effective charge Z of partially stripped ions, Z^{q+}, is determined as the average value of $Z_n = nI^{1/2}$ over dominantly occupied orbitals of the transferred electron, where n and I denote the principal quantum number and ionization energy,

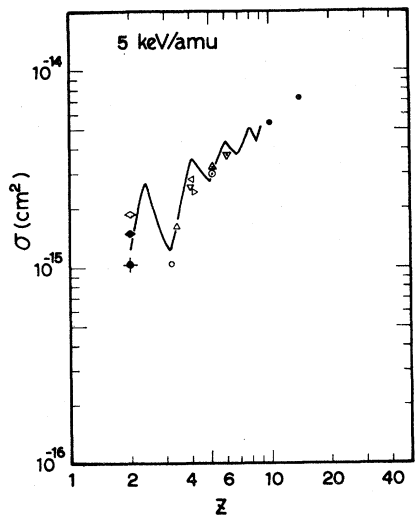

FIG. 5. Same as Fig. 4 for ion impact energy of 5 keV/amu. Additional experimental data: ◆ (He^{2+}) Fite *et al.* (Ref. 24); and ◇ (He^{2+}) Bayfield *et al.* (Ref. 25).

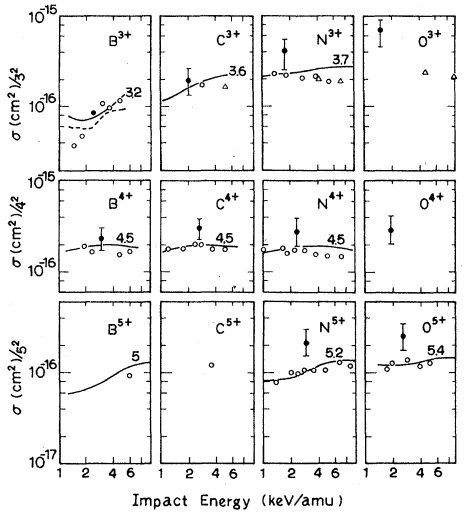

FIG. 6. Experimental and theoretical charge transfer cross sections of B^{q+}, C^{q+}, N^{q+}, and O^{q+} ions ($3 \leq q \leq 5$) at impact energies between 1 and 10 keV/amu. Experiment: △ Phaneuf *et al.* (Refs. 2 and 3); ● Bayfield *et al.* (Ref. 6); and ○ Crandall *et al.* (Ref. 8). Theory:—UDWA calculations using effective charge of which values are shown in the respective figures.

respectively, of the orbitals around X^{q+} (ground state). The effective charges calculated in this way are shown in Table I.

Comparisons between the dependence of charge transfer cross sections on the effective charge calculated in the UDWA and that obtained experimentally both at impact energies of 2 and 5 keV/amu are made in Figs. 4 and 5, respectively. The experimental results are those of Bayfield *et al.*,[6] Crandall *et al.*,[8] Fite *et al.*,[24] Bayfield and Khayrallah,[25] and Nutt *et al.*[26] The data referred to as Crandall *et al.* denote the values at 2 and 5 keV/amu which are interpolated from the cross sections measured by them at collision energies different from 2 and 5 keV/amu. In the figures, oscillatory behavior of charge transfer cross sections versus charge are clearly seen, and the theory shows good agreement with the experiments. More complete agreement between theory and experiment would be attained if the effective charges were made a little larger.

TABLE I. Effective charges evaluated from spectroscopic energy data (Ref. 21).

q	B^{q+}	C^{q+}	N^{q+}	O^{q+}
2	2.2			
3	3.2	3.4	3.4	3.6
4	4.1	4.1	4.2	4.4
5	5.0	5.0	5.1	5.2
6		6.0	6.0	6.1

Figure 6 shows experimental cross sections obtained by Phaneuf *et al.*,[2,3] Bayfield *et al.*,[6] and Crandall *et al.*,[8] and UDWA cross sections. The UDWA cross sections for effective charge $Z = 3.2$ are close to the theoretical results of Olson *et al.*[16] for $B^{3+} + H$ collisions and agree very well with experimental results at collision energies above 2 keV/amu. However, for other cases a good agreement between theory and experiment was obtained by assigning effective charge 3.6 to C^{3+}, 3.7 to N^{3+}, 4.5 to B^{4+}, C^{4+}, and N^{4+}, 5.2 to N^{5+}, and 5.4 to O^{5+}, except the data of Bayfield *et al.* for $N^{5+} + H$ and $O^{5+} + H$ collisions. These values of effective charge are a little larger than those given in Table I.

The difference between the values of effective charge determined by fitting the UDWA cross sections with the experimental ones and those estimated from the spectroscopic data for ground-state electronic configurations suggests that the projectiles can take some of the excited configurations as well. The effective charges depend on the electron configuration of the ions. The value of the effective charge shown in Table I are estimated by assuming the involved electrons to be in ground-state configurations. Crandall *et al.*[8] have confirmed that their initial ions from the low-energy ion source, the ORNL-PIG source, have the following electron orbital distributions. For Li-like ions C^{3+}, N^{4+}, and O^{5+}, they were only on $(1s^2 2s)\ ^2S$ ground state; for He-like ions C^{4+}, N^{5+}, and O^{6+}, no more than 10^{-3} of the incident ions were in metastable ^1S or ^3S excited states so that only $(1s^2)\ ^1S$ were present appreciably; for Be-like ions N^{3+}, O^{4+}, 50% of the incident ions were in $(1s^2 2s 2p)\ ^3P$ orbitals and only about 50% were in the $(1s^2 2s^2)\ ^1S$ ground state. According to this information, we can recalculate the effective charge of the N^{3+} ion, and obtain the value 3.7 which agrees with the above-described one, while for the other ions the discrepancies referred to above still remain.

The measured cross sections of Bayfield *et al.* for the impacts of N^{3+}, O^{3+}, N^{5+}, and O^{5+} are considerably larger compared with the data of Crandall *et al.*[8] and Phaneuf *et al.*[2,3] as seen in Fig. 6. According to Crandall *et al.*,[8] this disagreement comes from the difference in the techniques used to normalize the target thickness in the two sets of experiments.

In the present work, the strong oscillatory dependence of charge transfer cross section on the effective charge of projectiles was shown by means of the UDWA calculations. It is also shown that the oscillatory behavior comes from the crossings of diabatic potentials involved in the collision system under consideration and appears only in the low-collision-energy region below 10 keV/amu. Therefore it is essentially different from the oscillatory behavior observed by Kim *et al.*[22] in the intermediate-energy region. Considerable difference between the measured cross sections for charge transfer in collisions of partially stripped ions of different elements with atomic hydrogen obtained by Bayfield *et al.*[6] or Crandall *et al.*[8] at low collision energies seems to be a reflex of the low-energy oscillation due to the crossings of diabatic potentials.

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[1] M. B. Shah, T. V. Goffe, and H. B. Gilbody, J. Phys. B 11, L233 (1978).
[2] R. A. Phaneuf, F. W. Meyer, R. H. McKnight, R. E. Olson, and A. Salop, J. Phys. B 10, L425 (1977).
[3] R. A. Phaneuf, F. W. Meyer, and R. H. McKnight, Phys. Rev. A 17, 534 (1978).
[4] H. J. Kim, R. A. Phaneuf, F. W. Meyer, and P. H. Srelson, Phys. Rev. A 17, 854 (1978).
[5] L. D. Gardner, J. E. Bayfield, P. M. Koch, H. J. Kim, and P. H. Stelson, Phys. Rev. A 16, 1415 (1977).
[6] J. E. Bayfield, P. M. Koch, L. D. Gardner, I. A. Sellin, D. J. Pegg, R. S. Peterson, and D. H. Crandall, in Contributed Papers of the International Conference on Atomic Physics, edited by R. Marrus, M. H. Prior, and H. A. Shugart, Berkeley, 1976, p. 126 (unpublished); revised values in L. D. Gardner, Ph.D. thesis, Yale University, 1978 (unpublished).
[7] F. W. Meyer, R. A. Phaneuf, H. J. Kim, P. Hvelplund, and P. H. Stelson, Phys. Rev. A 19, 515 (1979).
[8] D. H. Crandall, R. A. Phaneuf, and F. W. Meyer, Phys. Rev. A 19, 504 (1979).
[9] A. Salop and R. E. Olson, Phys. Rev. A 13, 1312 (1976).
[10] R. E. Olson and A. Salop, Phys. Rev. A 14, 579 (1976).
[11] R. E. Olson and A. Salop, Phys. Rev. A 16, 531 (1977).
[12] A. Salop and R. E. Olson, Phys. Rev. A 16, 1811 (1977).
[13] C. Bottcher, J. Phys. B 10, L213 (1977).

[14]J. Vaaben and J. S. Briggs, J. Phys. B 10, L521 (1977).
[15]C. Harel and A. Salin, J. Phys. B 10, 3511 (1977).
[16]R. E. Olson, E. J. Shipsey, and J. C. Browne, J. Phys. B 11, 699 (1978).
[17]T. P. Grozdanov and R. K. Janev, Phys. Rev. A 17, 880 (1978).
[18]H. Ryufuku and T. Watanabe, Phys. Rev. A 18, 2005 (1978).
[19]H. Ryufuku and T. Watanabe, Phys. Rev. A 19, 1538 (1979).
[20]A. Salop and R. E. Olson (private communication).
[21]S. Bashkin and J. O. Stoner, Jr., *Atomic Energy Level and Grotrian Diagrams* (North-Holland, Amsterdam, 1975), Vol. I.
[22]H. J. Kim, P. Hvelplund, F. W. Meyer, R. A. Phaneuf, P. H. Stelson, and C. Bottcher, Phys. Rev. Lett. 40, 1636 (1978).
[23]H. Ryufuku and T. Watanabe, Phys. Rev. A 20, 1828 (1979).
[24]W. L. Fite, A. C. H. Smith, and R. F. Stebbings, Proc. R. Soc. A 268, 527 (1962).
[25]J. E. Bayfield and G. A. Khayrallah, Phys. Rev. A 12, 869 (1975).
[26]W. L. Nutt, R. W. McCullough, K. Brady, M. B. Shah, and H. B. Gilbody, J. Phys. B 11, 1457 (1978).