# Ionization and charge transfer in collisions of highly charged ions with helium at low velocity

Y. D. Wang,[1] C. D. Lin,[1] N. Toshima,[2] and Z. Chen[1]
[1]J.R. MacDonald Laboratory, Department of Physics, Kansas State University, Manhattan, Kansas 66506-2641
[2]Institute of Applied Physics, University of Tsukuba, Tsukuba, Ibaraki 305, Japan
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Ionization and charge transfer in slow collisions between highly charged projectiles and helium atoms are studied by the two-center atomic orbital close-coupling method within the independent electron approximation. The relative importance of single ionization to single capture is investigated. Our calculations show that ionization cross sections for $C^{6+}$, $N^{7+}$, and $O^{8+}$ projectiles increase rapidly between $v=1$ and 2 a.u. The onset is dependent on projectile charge state. At a fixed velocity, ionization cross sections decrease with increasing projectile charge. It is also found that ionization and charge transfer occur at about the same impact parameter range.

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## I. INTRODUCTION

Ionization at low velocity involving highly charged ions (HCI's) is a weak process with small transition probabilities. When multiply charged ions are used as projectiles, the ionization cross sections relative to the electron capture cross sections are expected to become smaller at decreasing velocities, and with increasing charged states of the projectiles at a fixed collision velocity. It is thus desirable to find out the relative importance of the ionization process to the dominant charge transfer process as the collision energy is varied. Unfortunately, such information is rarely available for highly charged ions as projectiles. In fact, there have been only a few measurements on ionization of one- or two-electron targets by multiply charged ions (i.e., by projectiles other than protons). Wu *et al.* [1] measured single ionization and single capture cross sections in slow collisions of $C^{6+}$, $N^{7+}$, $O^{8+}$, $Ar^{16+}$, $I^{16+}$, and $Xe^{30+}$ on helium atoms. Their measurements provided the first data for ionization of He by HCI projectiles at velocities between $v=0.2$ and 1.7 a.u. For ionization of hydrogen atoms, Shah *et al.* [2] measured ionization by $He^{2+}$ impact at energies between $v=0.6$ to 2 a.u.

On the theoretical side, the basic physical mechanism for ionization dynamics in slow collisions is still not well understood. Recently, much effort has been devoted to the study of ionization in collisions with one-electron targets. In particular, we mention the saddle point mechanism and the adiabatic electron superpromotion model [3–12]. The adiabatic superpromotion theory assumes that electrons are promoted to continuum through a series of "hidden crossings" over the potential curves, or equivalently, through a series of branch points of the multisheet potential surface in the complex plane of the internuclear distance. This theory has so far been quite successful in dealing with proton-hydrogen collisions [10,11]. Some progress has also been made in the study of ionization and charge transfer in collisions between highly charged ions with hydrogen atoms [12]. However, it is not clear how important the saddle point mechanism is for asymmetric systems where the saddle point is closer to the light target atom.

Ionization at low energies may be described also using the two-center atomic orbital expansion method. For collisions with hydrogen atoms, this was demonstrated by Shingal and Lin [13] for $He^{2+}$ impact, and, most recently, by Toshima [14] for HCI projectiles with charge states $Z=2-8$. Cross sections for ionization of H by $C^{6+}$, $N^{7+}$, and $O^{8+}$ ions obtained by Toshima from the two-center close-coupling approach are in relatively good agreement with the adiabatic superpromotion model of Janev *et al.* [12]. However, there are no experimental data available for comparison. The only data in the corresponding low-energy region are from Wu *et al.* [1] where the target is a two-electron helium atom. The "hidden crossing" model available so far cannot be applied directly to these two-electron systems since the calculations of branch points are not available at this time. We thus carried out the close-coupling calculations for the systems studied by Wu *et al.*

In this paper, we apply the two-center close-coupling method to study ionization and charge transfer in collisions with He atoms by $C^{6+}$, $N^{7+}$, and $O^{8+}$ ions at velocities between 1 and 2 a.u. Unlike the hydrogen atom target, ionization of atomic helium is much more complicated because of the presence of two electrons. Although several two-electron close-coupling methods [15–17] have been developed during the past few years, they are still not practical for ionization processes because of the prohibitive large basis set that is needed. Therefore, in this work, the independent electron approximation was employed to derive transition probabilities for the two-electron system. This paper is organized as follows. After a brief introduction of the close-coupling method, we present detailed results on ionization and capture cross sections. Comparison with the recent experiment by Wu *et al.* [1] is given. Throughout this paper, atomic units are used unless otherwise stated.

## II. METHOD

The close-coupling method has been extensively applied to a wide range of problems in atomic collisions; its success has been generally recognized and well documented [18,19]. Among the various close-coupling approaches, the semiclassical close-coupling expansion in terms of two-center atomic orbitals is frequently used in the study of atomic collision physics at not too low energies. In the intermediate energy

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region where the relative velocity of the nuclei is comparable to the average velocity of the electron, atomic orbital expansion is the most suitable approach.

The collision system under study is quite complex since both electrons can participate. In order to simplify the problem, we first treat the two-electron system as a quasi-one-electron system where the active electron experiences an effective potential due to the helium nucleus and the passive electron. A multistate close-coupling method is applied to solve the time-dependent one-electron Schrödinger equation and obtain the one-electron transition probabilities. The independent electron approximation is then used to construct probabilities for the two-electron system.

The time-dependent one-electron Schrödinger equation for the quasi-one-electron system is given by

$$\left( i\frac{\partial}{\partial t} - H \right)\Psi(\vec{r},t)=0 \tag{1}$$

with

$$H=-\frac{1}{2}\triangle_r^2+V_T(r_T)+V_P(r_P), \tag{2}$$

where $r_P$ ($r_T$) is the distance of the electron from the projectile (target). In the semiclassical impact parameter approximation, the relative motion of the heavy particles is described classically by a rectilinear trajectory with a constant velocity $v$. The time-dependent electronic wave function for the collision system is expanded in terms of atoms orbitals centered on the two heavy nuclei as

$$\Psi(\vec{r},t)=\sum_{i=1}^{N_T} a_i(t)\psi_i^T(\vec{r}_T,t)+\sum_{i=N_T+1}^{N} a_i(t)\psi_i^P(\vec{r}_P,t), \tag{3}$$

where $\psi_i^T(\vec{r}_T,t)$ and $\psi_i^P(\vec{r}_P,t)$ are the target and the projectile atomic orbitals with appropriate electron translation factors, respectively. In this work, we have employed two types of atomic orbitals. The first is based on expansion in terms of Gaussian-type orbitals (GTO's),

$$\phi_{nlm}(\vec{r})=\sum_{\nu} c_\nu^{(nl)}e^{-\alpha_\nu r^2}r^l Y_{lm}(\hat{r}). \tag{4}$$

The second is expanded in terms of Slater-type orbitals (STO's),

$$\phi_{nlm}(\vec{r})=\sum_{\nu} c_\nu^{(nl)}e^{-\alpha_\nu r}r^l Y_{lm}(\hat{r}). \tag{5}$$

In each case, the coefficients $c_\nu^{(nl)}$ are determined by diagonalizing the atomic Hamiltonian of the target and the projectile.

The effective one-electron potential for the helium atom is of the form

$$V_T(r_T)=-\frac{1}{r_T}-(1+0.4143r_T)\frac{e^{-2.499r_T}}{r_T} \tag{6}$$

for the STO basis [20], and

$$V_T(r_T)=-\frac{1}{r_T}-\frac{e^{-5.05r_T^2}}{r_T} \tag{7}$$

for the GTO basis. Both model potentials give good ground state and singly excited states energies for helium atom.

Having obtained the one-electron transition probabilities from the one-electron close-coupling calculation, we then take into account the presence of two electrons by using the independent electron approximation (IEA). Various forms of the IEA can be found in the literature and have been frequently applied to atomic collisions with two- and multielectron targets. In this work, we have employed two IEA models. They are discussed below.

*Model A*. In this model, we obtain the probabilities for one-electron transition to a state $f$ for a helium target containing two equivalent electrons as

$$P_f^A(b)=2p_{el}(\text{He},1)p_f(\text{He},2), \tag{8}$$

where $p_f$ is the one-electron probability for transition into a final state $f$, and $p_{el}$ is the one-electron elastic scattering probability. The individual one-electron probabilities are calculated from the two-center close-coupling method.

*Model B*. In this model, we treat the two electrons as nonequivalent. The first electron is described by the model potential as given above, and the second electron is identical to the electron in $He^+$. Each electron undergoes independent collisions with the projectile: the first electron has a transition probability $p_f(\text{He},1)$ to a final state $f$, and the second electron has a transition probability $p_{f'}(\text{He}^+,2)$ for transition to a final state $f'$. Thus the probability for single capture from either electron is given by

$$P_c^B(b)=p_c(\text{He},1)p_{el}(\text{He}^+,2)+p_{el}(\text{He},1)p_c(\text{He}^+,2), \tag{9}$$

and for single ionization by

$$P_i^B(b)=p_i(\text{He},1)p_{el}(\text{He}^+,2)+p_{el}(\text{He},1)p_i(\text{He}^+,2). \tag{10}$$

These models have been frequently used in the close-coupling calculations (e.g., Shingal and Lin [20]) involving two-electron transitions in helium atoms. It should be pointed out that there are no clear criteria for determining which model is superior. In general, model A may be a better description for one-electron transitions at higher energies. Model B, allowing for different binding energies for the two electrons when constructing probabilities, may be more suitable for the description of two-electron processes such as double capture and transfer ionization and at lower energies.

## III. RESULTS AND DISCUSSION

In this section we present the calculated cross section ratio between single ionization and single capture in collisions with He atoms by $C^{6+}$, $N^{7+}$, and $O^{8+}$ multiply charged ions. We test the two independent electron models and compare with the experiment of Wu *et al.* [1]. In the study of Toshima [14] on ionization of H atoms by highly charged ions, it was found that the contribution from the deep bound states of the projectile to ionization cross section cannot be

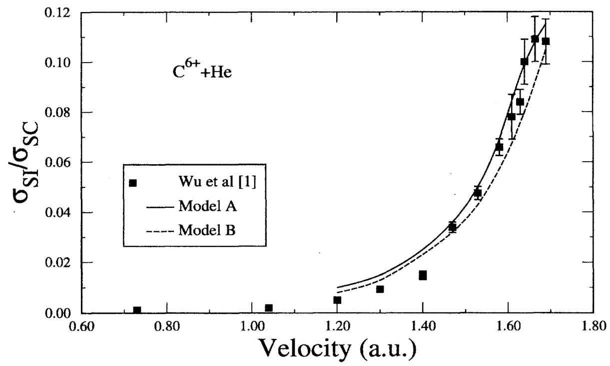


FIG. 1. The ratio of the single ionization cross section ($\sigma_{SI}$) to the single capture cross section ($\sigma_{SC}$) for He by $C^{6+}$ projectiles. Theory: solid line is from model A; dashed line is from model B (see text). Experiment: Wu *et al.* [1].

neglected. For $C^{6+}+H$, the unphysical large ionization cross section is obtained if the deep bound states of $C^{6+}$ are excluded. It is therefore necessary to include lower bound states on the projectile center when carrying out the close-coupling calculations, despite the fact that these states are not populated in the collision.

### A. $C^{6+}+He$

We first consider the dependence of the ratio between single ionization (SI) and single capture (SC) cross sections on projectile velocity. In Fig. 1, results obtained from the two independent electron models (i.e., models A and B of Sec. II) are compared with the measurement [1]. The individual one-electron probabilities required for constructing the two models were calculated by the close-coupling method. We employed a rather asymmetric basis set centered on the projectile and the target. On the $C^{6+}$ center, a fairly large STO-type basis was used, including exact hydrogenic states up to $n=5$ with maximum angular momentum $l=4$. This basis is large enough to account for electron capture into the dominant excited states ($n=3$ or 4) of the projectile. In addition, a good number of pseudostates were employed to represent the projectile continuum. The target basis on the He center includes $l=0$ and 1 states obtained from the model potential of Sec. II.

The most significant result from Fig. 1 is the apparent onset in the velocity dependence of the cross section ratio between ionization and charge transfer. Figure 1 shows that in the velocity range of 1.2–1.7 a.u., the ratio increases by a factor of 10. The two independent electron models agree with each other reasonably well. For projectile velocities larger than 1.5 a.u., it appears that model A has better agreement with the measurement and model B is slightly better at lower energies. Our calculations thus support the experimental observation of the strong apparent onset in ionization cross sections in slow collisions involving multiply charged ions.

In the experiment of Wu *et al.*, single ionization and single capture cross sections were also obtained indirectly by normalizing their SI/SC cross section ratio data to some known capture cross sections published elsewhere [1,21]. In

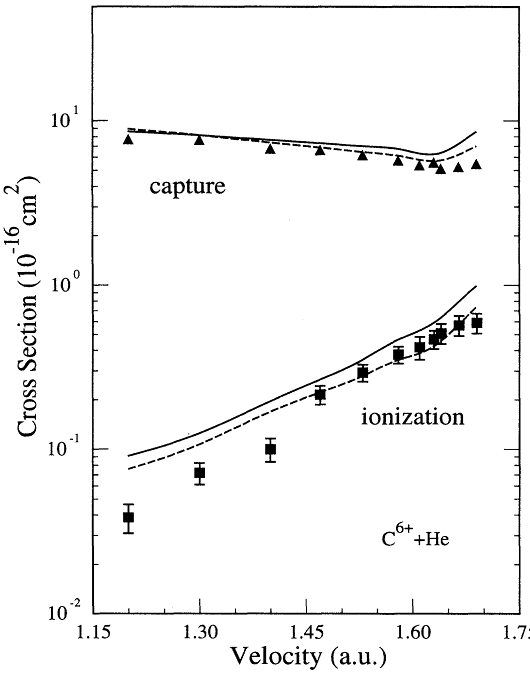


FIG. 2. The single ionization and single capture cross sections for He by $C^{6+}$ projectiles. Theory: solid line is from model A; dashed line is from model B. Experiment: Wu *et al.* [1].

Fig. 2, we compare the calculated single ionization and single capture cross sections with the experimental data [1] thus deduced. The two models give small differences in single capture, but somewhat larger differences in single ionization. Both models show the observed rapid increase in ionization cross section with increasing velocity. Between $v=1.2$ and 1.7 a.u., the capture cross section is relatively constant, whereas the ionization cross section increases by a factor of 10. In view of the normalization procedure, our calculations are in good agreement with individual electron capture and ionization cross sections.

The competition between ionization and the dominant charge transfer processes in slow collisions is a rather intriguing subject. The impact parameter dependence of the two competing processes may shed some light on the collision dynamics. It is well known that for fast collisions capture dominates at small impact parameters and ionization at large impact parameters. The situation for collisions at low velocity involving multiply charged ions is less clear. In fact our calculations show that ionization happens at an impact parameter range about the same as that for single capture. This is shown in Figs. 3(a) and 3(b), where we compare the impact parameter dependence of $bP(b)$ distributions for ionization and capture at $v=1.4$ and 1.64 a.u. respectively. In Figs. 3(a) and 3(b), only results from model A were presented. The $bP(b)$ distribution from model B is quite similar and is not included. Comparing Fig. 3(a) with Fig. 3(b), the $bP(b)$ distributions for both ionization and capture are shifted to smaller impact parameters with increasing velocity.

For the weak ionization processes to occur in the presence of the strong electron capture processes, it is interesting to examine the relative importance of target ionization and elec-

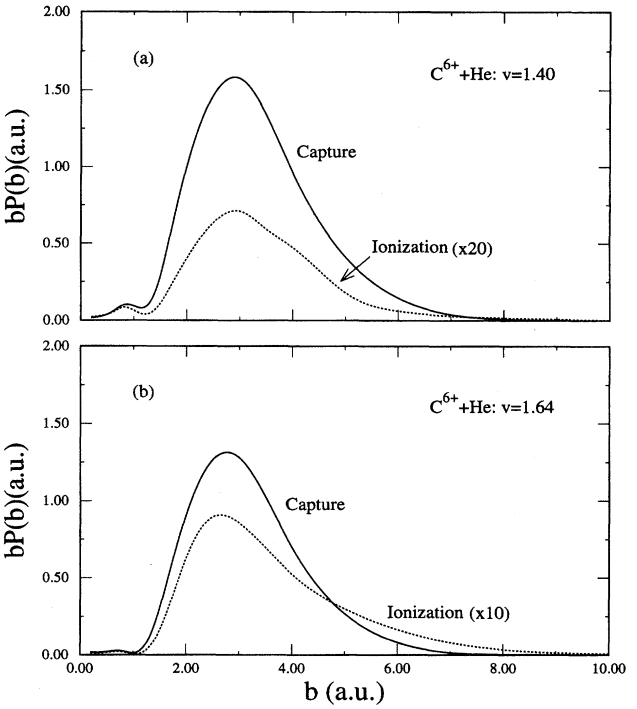


FIG. 3. The impact parameter dependence for ionization and capture in collisions between $C^{6+}$ and He atoms (a) for $v = 1.40$ a.u. and (b) for $v = 1.64$ a.u.

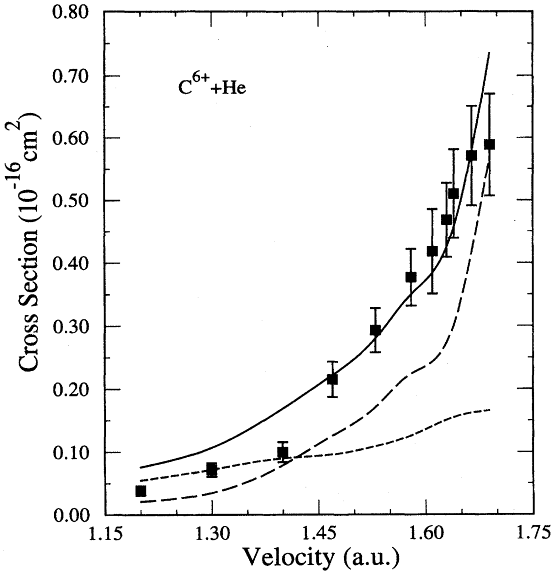


FIG. 4. Comparison of direct target ionization cross section and electron capture to the projectile continuum cross section for $C^{6+}$+He. Theory is from model B. Solid line, total single ionization cross section; short dashed line, target ionization; and long dashed line, capture to the projectile continuum. Experiment: total single ionization from Wu *et al.* [1].

tron capture to the projectile continuum. In principle, one may want to include also the so-called saddle point electrons. However, for the present system, the saddle point is very close to the target center and in our two-center basis expansion, the saddle point electrons may be grouped with the target ionization process within our model. We emphasize that the separation is relatively arbitrary, and is meaningful only within the basis set adopted. In Fig. 4 we separate the target ionization from the electron capture into the projectile continuum. The target ionization is relatively independent of collision velocity, and the rapid increase of the total ionization cross section is almost entirely due to the rapid increase in electron capture into the projectile continuum. This result is plausible and is consistent with the impact parameter dependence as shown in Fig. 3. The electron capture to the bound states is the dominant process in this velocity region, and electron capture to the projectile continuum is attributed to those continuum electrons that are moving near the projectile nucleus. As the collision velocity increases, there is a larger fraction of these electrons that does not end up in the bound states as the normal electron capture. Put another way, as the collision velocity decreases, the electrons near the projectile center tend to end up in the bound states because of the longer collision time available. This explains the rapid decrease of electron capture to the projectile continuum as the collision velocity is decreased, as shown from the calculated results in Fig. 4.

We emphasize that this conclusion is different from the result of adiabatic superpromotion models (cf. [7,9,12] for ionization of the one-electron target by multiply charged ions) where they determined that saddle point electrons are contributing to the ionization cross sections in the energy range addressed here. As discussed before, since the saddle point is close to the target center, these saddle point electrons would emerge as the target ionization in our two-center close-coupling calculations. We thus have to emphasize that the two theoretical models for ionization at low energies are different. Discrimination of these two models can be achieved in experiments where the longitudinal momenta of the ejected electrons are measured. Such measurements would give electrons with velocities centered near the collision velocity if the projectile ionization is dominant, as predicted in this calculation. Such experiments are currently underway [22].

### B. $N^{7+}$+He

As the projectile charge increases, the number of basis functions that should be included in the close-coupling expansion increases rapidly. It is therefore more practical to use the GTO-type orbitals. In this work, we employed the large basis of GTO's previously used by Toshima [14] in the study of ionization of H atoms by highly charged projectiles. Briefly, the GTO basis contains exact states up to $n=7$ on the $N^{7+}$ center. GTO orbitals are also used to obtain the target He states with the model potential, Eq. (7).

The calculated SI/SC ratio for $N^{7+}$+He is presented in Fig. 5. Individual single ionization and capture cross sections are presented in Fig. 6. The two figures also show a strong onset in the ionization cross section that is similar to that observed for $C^{6+}$. The onset seems to occur at a larger velocity for $N^{7+}$ than for $C^{6+}$. Model B agrees with the experimental ratio very well, except at $v=1.64$ a.u., where model A shows a better agreement. In regard to ionization

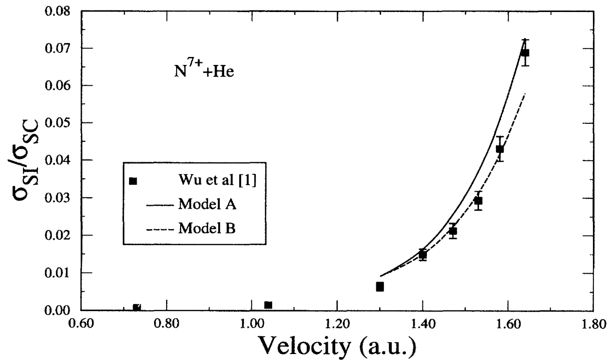


FIG. 5. Same as in Fig. 1, except for $N^{7+}$+He.

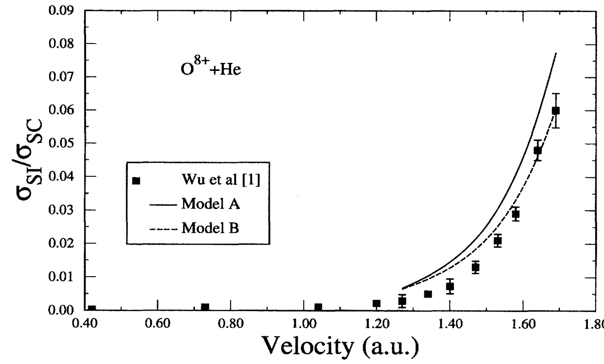


FIG. 7. Same as in Fig. 1, except for $O^{8+}$+He.

and capture cross sections, model A agrees with the experiment better than model B.

The impact parameter dependence for ionization and capture by the $N^{7+}$ projectile is quite similar to that of $C^{6+}$. Single ionization and single capture occur at about the same impact parameter range. We also found that electron capture to the projectile continuum is responsible for the strong increase in the ionization cross section.

### C. $O^{8+}$+He

For this system, we employed the large GTO basis of Toshima [14] on the $O^{8+}$ center, which includes exact states up to $n=8$. A study, similar to the previous systems, was carried out. In Figs. 7 and 8 we compare the calculated SI/SC ratio, SI and SC cross sections, with the experiment of Wu *et al.* [1]. The onset in the ionization cross section occurs at even larger velocity than that for $C^{6+}$ or $N^{7+}$. Model B gives the best overall agreement with experiment. At a fixed velocity, the ionization cross section for the $O^{8+}$ projectile is smaller than that for $C^{6+}$ and $N^{7+}$ projectiles. In Figs. 9(a) and 9(b) we show the impact parameter dependence for $bP(b)$. For this system, Wu *et al.* measured the perpendicular target recoil-ion momentum distributions at several velocities for both ionization and electron capture [1]. They found that the perpendicular recoil-ion momentum distributions for ionization and for capture have a similar shape and have the same range of perpendicular recoil-ion momentum. This observation indicates that ionization and capture occur at about the same range of impact parameters. In Fig. 10, the relative importance of the electron capture into the projectile continuum and target direct ionization is illustrated for model B.

Finally, there are some oscillations in the calculated $bP(b)$ distributions for $O^{8+}$ at low velocity (see Fig. 9).

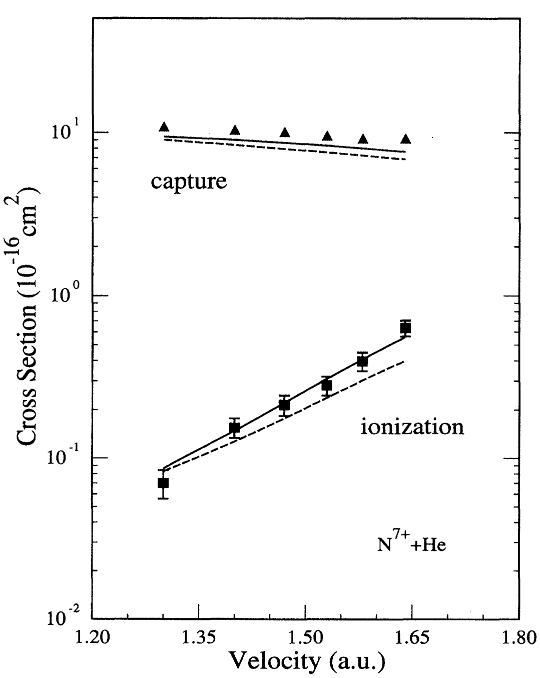


FIG. 6. Same as in Fig. 2, except for $N^{7+}$+He.

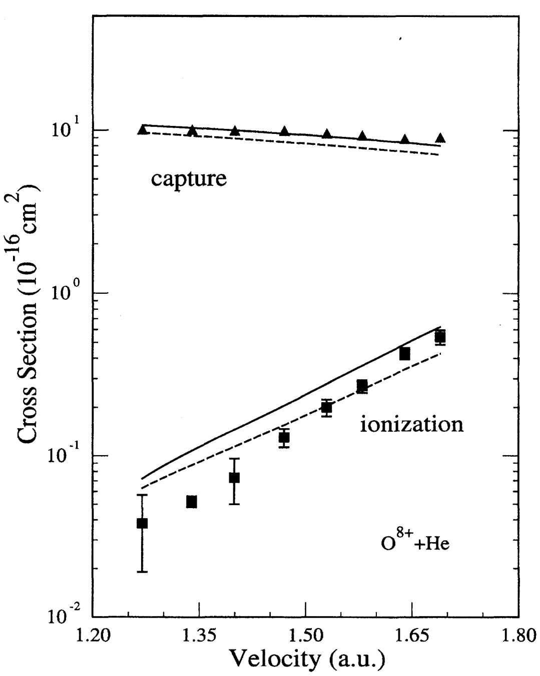


FIG. 8. Same as in Fig. 2, except for $O^{8+}$+He.

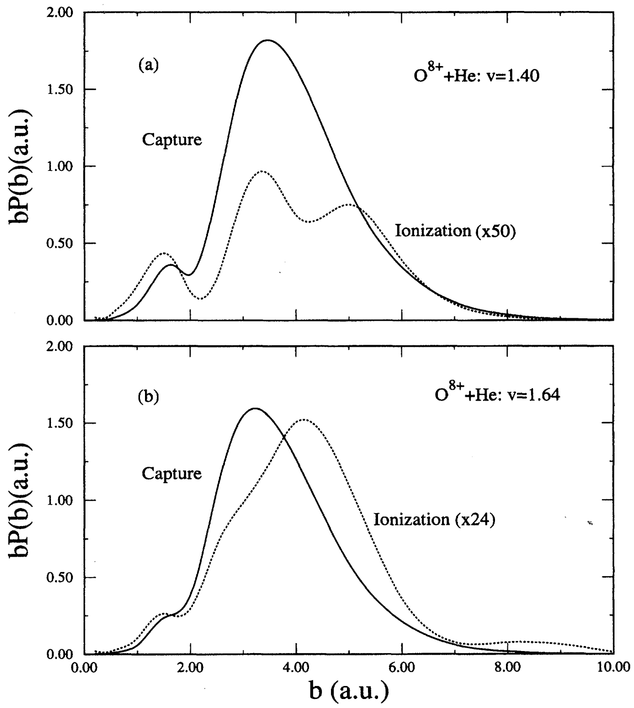


FIG. 9. Same as in Fig. 3, except for $O^{8+}$+He.

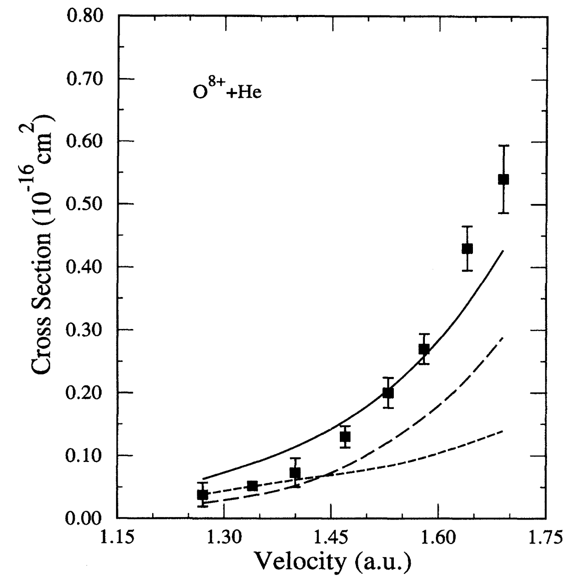


FIG. 10. Same as in Fig. 4, except for $O^{8+}$+He. Theory is from model B.

Similar oscillations can be found in the two-center atomic orbital close-coupling calculations of Toshima [14] for ionization of H by multiply charged ions. At low energies, the ionization cross sections are smaller and we may need to enlarge the basis set to achieve reliable results. Furthermore, one expects that the independent electron approximation may break down at very low energies. Because of these considerations, we did not carry out calculations below $v=1.2$ a.u.

## IV. CONCLUSIONS

In this paper we investigated single ionization and single capture in collisions between highly charged ions and atomic helium using the two-center semiclassical close-coupling method. We have confirmed the strong onset in the ionization cross section observed by Wu *et al.* [1]. At a fixed velocity, ionization aross sections decrease rapidly with decreasing projectile velocities and with increasing projectile charge states. We also showed that ionization and electron capture occur at about the same impact parameter range, which is consistent with the measurement of the perpendicular recoil momentum distributions reported by Wu *et al.* [1]. The calculation also showed that electron capture to the projectile continuum is the dominant mechanism for the strong onset in the ionization cross section. At energies below the ionization onset, target ionization is more important. This prediction can be tested in future experiments by measuring the longitudinal electron momentum distributions. Such experiments are underway [22] and the results would be able to substantiate or dispute the prediction of the ionization mechanisms discussed in this paper for collisions at low velocities involving multiply charged ions.

## ACKNOWLEDGMENTS

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