Single electron capture in collisions of N^{q+} ($q = 5, 6, 7$) ions with helium*

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Close-coupling calculations are carried out for cross sections of the single electron capture in collisions of N^{q+}(q = 5, 6, 7) ions with helium atoms in the collision velocity range from 0.3 a.u. to 1.8 a.u. The relative importances of the single ionization (SI) to the single capture (SC) are investigated for the N^{q+}(q= 5, 6, 7) projectiles, respectively. The SI/SC cross section ratio for the N^{7+} projectile obtained from our calculations is in excellent agreement with the experimental data. The ratio curves also show us distinct behaviours when the charge of the projectile is different. The partial electron capture cross sections for different projectiles indicate that the electron on the target He atom tends to be captured by the projectile into its lower orbital of the outer shell with the decreasing projectile charge.

Keywords: close-coupling method, electron capture, cross section

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1. Introduction

Electron capture in collision involving multiply charged nitrogen ions has attracted considerable attention in astrophysics, atmospheric physics and plasma physics. When a multiply charged nitrogen ion collides with a neutral target atom at a low velocity, the single electron capture is the main target charge transfer process. It is essential to explore the relative importance of the ionization to the electron capture process and the effect of q on the cross sections of the charge transfer process. Some relevant experimental and theoretical investigations have been made in the past few decades. Dijkkamp *et al.*[1] measured absolute subshell-selective single electron capture cross sections for the collisions of C^{4+}, N^{5+}, and O^{6+} with atomic and molecular hydrogen and helium at impact velocities between 0.1 a.u. and 0.5 a.u. by means of the optical spectroscopy. Harel *et al.*[2,3] developed a formalism in close-coupling calculations to deal with the two-active electrons in the collisions of N^{7+}, O^{8+}, and Ne^{8+} with He at low velocities between 0.14 a.u. and 0.6 a.u. The cross sections of ionization and single capture in the collisions of C^{6+}, N^{7+}, O^{8+}, Ar^{16+}, I^{16+}, and Xe^{30+} with the helium atom were first measured by Wu *et al.*[4,5] for velocities (v) from 0.2 a.u. to 1.7 a.u. Later, Lin *et al.*[6,7] reported the theoretical cross sections of ionization and electron capture for the slow collisions of C^{6+}, N^{7+}, and O^{8+} ions with helium atoms by using the atomic orbital close-coupling method based on an expansion in terms of the Gaussian-type orbitals. The results were in good agreement with the experimental ones obtained by Wu *et al.* Recently, Ishii *et al.*[8] reported the experimental cross sections of single- and double-electron capture by C^{q+}, N^{q+}, and O^{q+} (q = 2–6) ions from He in the energy range of (1.0–1800)q eV. So far, to our knowledge, only a few calculations have been reported for the collisions of the multiply charged N^{q+} ions with the two-electron targets in a wide velocity range, because the collisions involving the multiply charged N^{q+} ions are quite complex processes, in which many electrons can participate. It is a challenge to both experiment and theory.

In this paper, the two-centre atomic orbital close-coupling method is employed to study the single electron capture cross sections in collisions of N^{q+} ($q = 5, 6, 7$) ions with helium atoms in the velocity range from 0.3 a.u. to 1.8 a.u. For N^{5+} and N^{6+} projectiles (and also for the He target), we use the model potentials to describe the active electron in the field of the frozen inner electrons in both centres. The ratios of the single ionization (SI) cross section ($\sigma_{\rm SI}$) to the single capture (SC) cross section ($\sigma_{\rm SC}$) are explored for the N^{q+} ($q = 5, 6, 7$) projectiles respectively. The total cross sections and the main partial electron cap-

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ture cross sections are also given for the collisions of N^{q+} with the He atom.

2. Method

In our calculations, we employ the close-coupling method[9,10,11] to solve the time-dependent Schrodinger equation for the quasi-one-electron system. The Hamiltonian of the time-dependent Schrodinger equation is given by

$$H = -\frac{1}{2}\Delta_r^2 + V_{\rm T}(r_{\rm T}) + V_{\rm P}(r_{\rm P}), \tag{1}$$

where V is the effective potential, P and T refer to the projectile and the target nuclei, respectively. The time-dependent Schrodinger equation is solved by expanding the electronic wave function in terms of the atomic orbitals on the two collision centres of the collision system as

$$\Psi(\boldsymbol{r},t) = \sum_{i=1}^{N_{\rm T}} a_i(t)\psi_i^{\rm T}(\boldsymbol{r}_{\rm T},t) + \sum_{i=N_{\rm T}+1}^{N} a_i(t)\psi_i^{\rm P}(\boldsymbol{r}_{\rm P},t), \tag{2}$$

where $\psi_i^{\rm T}(\boldsymbol{r}_{\rm T},t)$ and $\psi_i^{\rm P}(\boldsymbol{r}_{\rm P},t)$ are the helium atom and the projectile bases with appropriate electron translation factors, respectively. The eigenfunctions of each centre are further expanded using the Slater-type orbitals (STO's)

$$\phi_{nlm}(\boldsymbol{r}) = \sum_{\nu} c_\nu^{(nl)}\, {\rm e}^{-\alpha_\nu r} r^l {\rm Y}_{lm}(\boldsymbol{r}), \tag{3}$$

where ${\rm Y}_{lm}(\boldsymbol{r})$ is the spherical harmonics. In each case, coefficients $c_\nu^{(nl)}$ are determined by diagonalizing the atomic Hamiltonian of the target or the projectile. The effective potential for the helium atom is of the form

$$V_{\rm T}(r_{\rm T}) = -\frac{1}{r_{\rm T}} - (1 + 0.4143 r_T)\frac{{\rm e}^{-2.499 r_{\rm T}}}{r_{\rm T}}. \tag{4}$$

For the Li-like N^{4+} ion and the He-like N^{5+} ion, the effective potential of the core formed by the inner electrons and the nucleus is

$$V_{\rm P}(r_{\rm P}) = -\frac{z_0}{r_{\rm P}} + (z_1 + z_2 r_{\rm P})\frac{{\rm e}^{-z_3 r_{\rm P}}}{r_{\rm P}}, \tag{5}$$

where $z_0 = 5$, $z_1 = -2$, $z_2 = -8.804$, and $z_3 = 8.804$ for N^{5+}; $z_0 = 6$, $z_1 = -1$, $z_2 = -4.5155$, and $z_3 = 9.031$ for N^{6+} in our work.

3. Results and discussion

In the atomic orbital close-coupling calculations, we expand the wavefunctions on two collision centres for the slow collisions of the N^{q+} ($q = 5, 6, 7$) ions with the He target atoms. The projectile basis on

Table 1. Energies of bond states for Li-like N^{4+} ($1s^2nl$) and He-like N^{5+} ($1snl$) (in units of a.u.).

n	s	p	d	f	g	h
2	−3.596[a)]	−3.236[a)]				
	−3.597[b)]	−3.231[b)]				
3	−1.520[a)]	−1.423[a)]	−1.390[a)]			
	−1.519[b)]	−1.421[b)]	−1.390[b)]			
4	−0.835[a)]	−0.796[a)]	−0.782[a)]	−0.781[a)]		
	−0.835[b)]	−0.795[b)]	−0.782[b)]	−0.781[b)]		
5	−0.528[a)]	−0.509[a)]	−0.500[a)]	−0.500[a)]	−0.500[a)]	
	−0.527[b)]	−0.507[b)]	−0.500[b)]	−0.500[b)]	−0.500[b)]	
6	−0.364[a)]	−0.349[a)]	−0.346[a)]	−0.344[a)]	−0.345[a)]	−0.345[a)]
	−0.363[b)]	−0.351[b)]	−0.347[b)]	−0.347[b)]	−0.347[b)]	−0.347[b)]
1	−20.998[a)]					
	−20.288[b)]					
2	−4.800[a)]	−4.589[a)]				
	−4.861[b)]	−4.622[b)]				
3	−2.085[a)]	−2.027[a)]	−2.002[a)]			
	−2.100[b)]	−2.035[b)]	−2.002[b)]			
4	−1.160[a)]	−1.136[a)]	−1.126[a)]	−1.125[a)]		
	−1.166[b)]	−1.140[b)]	−1.125[b)]			
5	−0.738[a)]	−0.726[a)]	−0.721[a)]	−0.720[a)]	−0.720[a)]	
	−0.741[b)]	−0.728[b)]	−0.721[b)]			
6	−0.516[a)]	−0.513[a)]	−0.500[a)]	−0.500[a)]	−0.500[a)]	−0.500[a)]
		−0.503[b)]	−0.501[b)]			

[a)] Present calculations. [b)] From Ref. [12].

the N^{q+} centre includes exact hydrogenic states up to $n = 6$ with maximum angular momentum $l = 5$. The projectile continuum is also contained by including a large number of pseudostates. In the He centre, $l = 0$, $l = 1$, and $l = 2$ states given by the effective potential shown in Eq. (4) are contained in the target basis. In Table 1, the energies of the bond states for the Li-like N^{4+} and the He-like N^{5+} ions obtained in our work by using the effective potential given in Eq. (5) are presented together with the atomic level energies cited from the NIST atomic energy database.[12] For the Li-like N^{4+} and the He-like N^{5+} ions, the active electron is supposed to move in an effective potential of the core formed by the inner electrons and the nucleus. The potential of the Li-like N^{4+} generated by the $1s^2$ electrons and the nucleus is different from that of the He-like N^{5+} generated by the 1s electron and the nucleus. The energies of the final states will be well reproduced by adjusting the parameters in the effective potential and the STO. The comparison shows that our theoretical results for those excited states are in reasonable agreement with those of the reference, because for those $1snl$ states of the He-like N^{5+} ion and $1s^2nl$ states of the Li-like N^{4+} ion, the excited nl electron is far away from the core. The discrepancy between our and the reference data for the 1s1s state in the He-like N^{5+} results from the effective potential we used, in which some of the correlations between the two equivalent 1s electrons have not been included.

Figure 1 shows the ratios of the SI cross section ($\sigma_{\rm SI}$) to the SC cross section ($\sigma_{\rm SC}$) for the collisions of N^{q+} ($q = 5, 6, 7$) with the He atom with v from 0.3 a.u. to 1.8 a.u. The ionization competes with the electron capture when the charged nitrogen ions collide with the He target atom. The three curves in Fig. 1 show us similar trends at higher velocities. For the N^{7+}+He collision, the SI/SC cross section ratio is stable for the velocity between 0.3 a.u. and 1.1 a.u. Then the ratio increases gently as the velocity increases from 1.1 a.u. to 1.4 a.u. The speedy increasing of the ratio in the above 1.4 a.u. velocity region shows us a big boost of the target direct ionization with the velocity increasing. The agreement with the experimental data of Wu *et al.*[5] is excellent in the comparable velocity region. In the mean time, the SI/SC ratio curves of the N^{5+}+He and the N^{6+}+He collisions are little different from that of N^{7+}+He due to the screening effect from the inner electrons of the N^{5+} and the N^{6+} ions to the nitrogen nuclear potential. For the N^{6+}+He and the N^{5+}+He collisions, the slight decreases of the ratio at lower velocities show that the active electron on the target He atom tends to be captured by the bound states of the projectile ions when the energy of the inner electron approaches to that of the electron on the target. At higher velocities, the SI/SC ratios of the N^{5+}+He and the N^{6+}+He collisions also increase rapidly, which means that the increasing of the target ionization is more apparent than that of the capture by N^{q+} ($q = 5, 6$) in the velocity range.

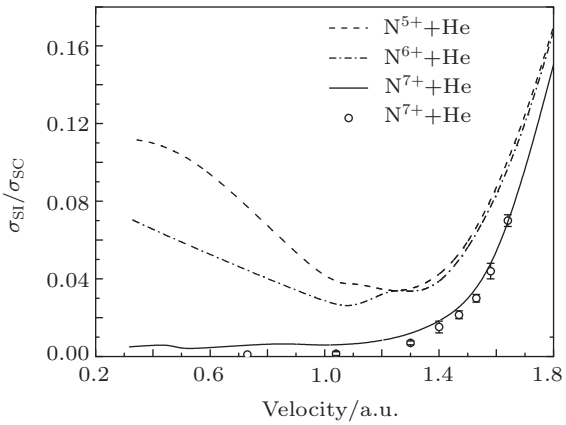


Fig. 1. Ratios of the single ionization cross section ($\sigma_{\rm SI}$) to the single capture cross section ($\sigma_{\rm SC}$) for collisions of N^{q+} ($q = 5, 6, 7$) with the He atom. The circles denote the experimental results obtained by Wu *at al.*[5]

In Fig. 2, the total single electron capture cross sections are given for the N^{q+}+He ($q = 5, 6, 7$) collisions respectively. The capture cross sections for all the three collision systems are relatively stable for v from 0.3 a.u. to 1.8 a.u. From the comparison of the three SC curves, the bare ion, N^{7+} ion, has the strongest ability to capture electrons from the target. Obviously, the screening effects of the inner electrons in the N^{5+} and the N^{6+} ions to the nitrogen nuclear potential weaken the electron capture ability of the two ions. In the velocity range from 0.3 a.u. to 0.8 a.u., the curve of N^{7+} depresses more than expected,

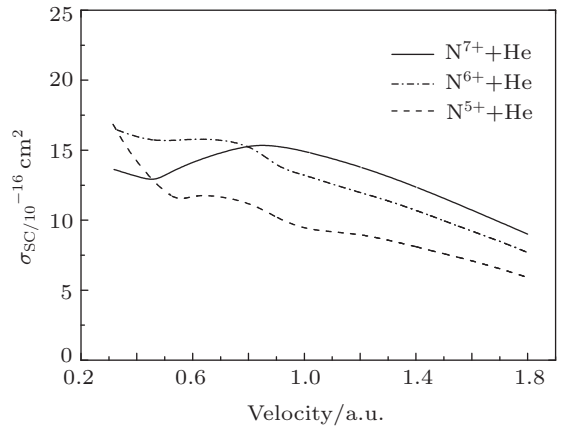


Fig. 2. Total single electron capture cross sections for N^{q+}+ He collisions ($q = 5, 6, 7$).

possibly because the projectile basis in the N^{7+} centre includes the exact hydrogenic states up to $n = 6$ with a maximum angular momentum of $l = 5$ in the calculations. A larger basis set is needed for the N^{7+} collision system to include all important contributions from higher n in the total capture cross section.

Figure 3 shows the main partial cross sections of the final states captured into by the projectile N^{q+} ($q = 5, 6, 7$) ions. An obvious tendency of being captured to higher n and l can be found in the figures when the velocity increases from 0.3 a.u. to 1.8 a.u.. From the figures, the main orbitals, into which electrons are captured by the projectiles, are those with principal quantum number $n = 3, 4$ of the N^{6+}, the N^{5+}, and the N^{4+} ions. For the N^{7+}+He collision, the rising of the 6f state curve at the higher velocity is most conspicuous in Fig. 3(a). The obvious rising tendencies are also shown by the $5l$ states of the N^{5+} and the N^{4+} ions in Figs. 3(b) and 3(c), respectively. In Fig. 3(c), the $1s^22l$ states of the N^{4+} ion also show us evident importance in the collision of N^{5+}+He, because the electron on the target He atom tends to be captured into the low orbital of the outer shell with the growth of the number of electrons in the projectile. Table 2 shows us the comparison of the partial cross sections captured to the $1s^23l$ states in the N^{5+}+He collision between the results of this work and the experimental data obtained by Dijkkampt *et al.*[1] In the comparable velocity region, our theoretical results for the partial cross sections captured to the $1s^23l$ states of the N^{4+} ions are in good agreement with the experimental ones. Table 2 also shows us that in the N^{5+}+He collision, the cross section of the $1s^23s$ state declines as the velocity increases from 0.33 a.u. to 0.54 a.u. On the other hand, the $1s^23d$ state is becoming important in the velocity region. Unfortunately, few data of the partial electron capture cross sections are available for the N^{q+}+He collisions. Our theoretical results will help us to better understand the mechanism of the excited states formed in the atomic collisions.

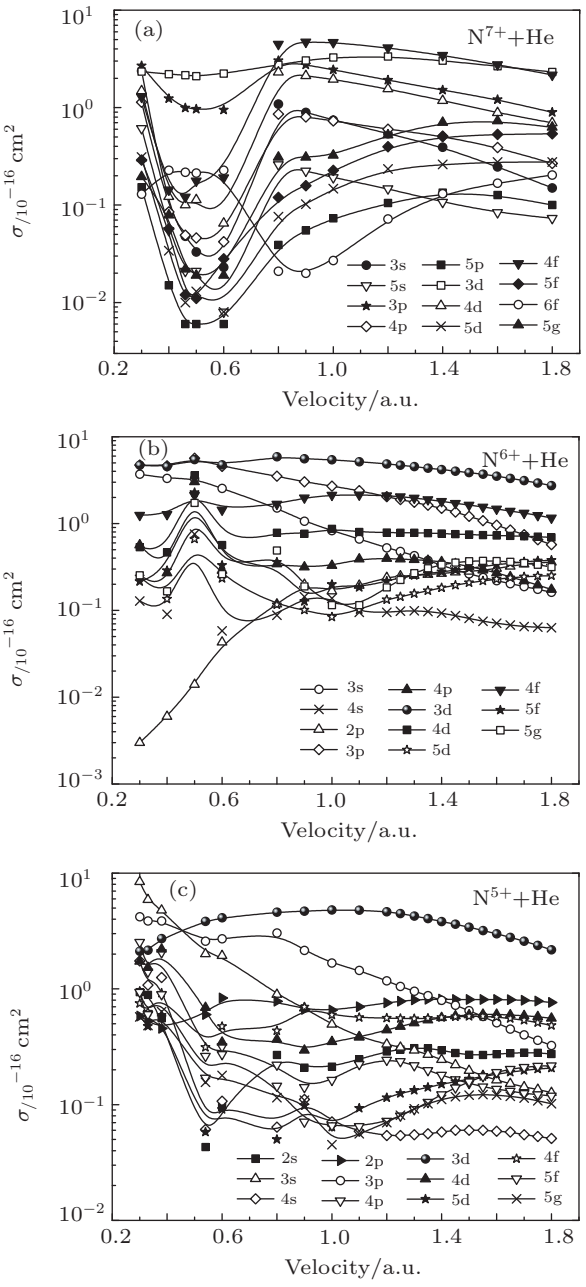


Fig. 3. Theoretical partial electron capture cross sections to nl states of N^{6+} ions, $1snl$ states of N^{5+} ions, and $1s^2nl$ states of N^{4+} ions for (a) N^{7+}+ He, (b) N^{6+}+ He, and (c) N^{5+}+ He collisions.

Table 2. Theoretical partial electron capture cross sections to $1s^23l$ states of N^{4+} ions in collision of N^{5+} with helium (in unit of 10^{-16} cm^2).

Velocity/a.u.	3s	3p	3d
0.33	5.9[a)]	3.9[a)]	2.2[a)]
	5.2[b)]	3.0[b)]	2.5[b)]
0.38	4.8[a)]	3.9[a)]	2.7[a)]
	4.6[b)]	3.1[b)]	3.0[b)]
0.46	3.1[a)]	3.2[a)]	3.8[a)]
	3.5[b)]	3.1[b)]	3.8[b)]
0.54	2.0[a)]	2.6[a)]	3.8[a)]
	2.9[b)]	3.1[b)]	4.4[b)]

[a)] Present calculations. [b)] From Ref. [1].

4. Conclusion

In this paper, we investigated the relative importance of the SI cross section to the SC cross section in the slow collisions of N^{q+} $(q = 5, 6, 7)$ with the He atom. The SI/SC ratio curves of the N^{5+}+He and the N^{6+}+He collisions show us apparent difference from that of N^{7+}+He due to the screening effect from the inner electrons of the N^{5+} and the N^{6+} ions. The difference between the N^{7+}+He and the N^{q+}+He $(q = 5, 6)$ collisions is also shown in the curves of the total SC cross sections. From our work, the main orbitals, into which electrons are captured by the projectiles, are those with principal quantum number $n = 3, 4$ of the N^{6+}, the N^{5+}, and the N^{4+} ions. However, for the different projectile ions, the electron on the target He atom is apt to be captured into the low orbital of the outer shell with the growth of the number of electrons on the projectile.

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