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Charge transfer and ionization cross-sections in collisions of singly charged lithium ions with helium and nitrogen atoms

M Al-Ajaleen^{1,2} , A Taoutioui¹ and K Tókesi^{1,3,*} 

¹ Institute for Nuclear Research (ATOMKI), Debrecen 4026, Hungary

² University of Debrecen, Doctoral School of Physics, Egyetem tér 1, 4032 Debrecen, Hungary

³ Centre for Energy Research, Budapest, Hungary

E-mail: tokesi@atomki.hu

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Abstract

We present a non-perturbative classical treatment of the charge transfer and ionization processes in collisions between singly charged lithium ions with helium and nitrogen atomic targets. Single capture and single ionization total cross sections are calculated using a three-body classical trajectory Monte Carlo (CTMC) method in which the interaction between the collision partners is described by a Garvey-type model potential. The cross sections are evaluated for collision energies between 20 keV and 100 MeV. In particular, we found excellent agreement between our results and the available experimental data for the case of the single capture of He(1s) by Li⁺ ions. In addition, our CTMC results are in a reasonable agreement with the experimental results for collision energies higher than 200 keV for single capture of N(2p) atoms by Li⁺. Furthermore, we present single ionization cross sections for both collision systems.

Keywords: CTMC method, single capture, single ionization, total cross section, Garvey-type model potential

(Some figures may appear in colour only in the online journal)

1. Introduction

Inelastic electron processes in ion–atom collisions play a crucial role in several fields, such as particle beam therapy, which currently uses mainly protons and carbon ion beams [1, 2] and diagnostics and/or modeling of the nuclear fusion plasma in tokamak reactors. In particular, neutral high-energy beams of

hydrogen isotopes and/or helium are injected into the vacuum vessel of the tokamak reactor to heat the fusion plasma and to diagnose it as well [3, 4]. Nitrogen seeding is used for cooling purposes of the edge plasma in tokamak reactors [5]. According to a number of fusion experiments, using the liquid lithium allows the protection of the plasma facing components and improvement of the magnetic fusion plasma performance [6–8]. Due to its high reactivity, lithium can readily ionize and form lithium ions, which may interact with neutral atoms at the plasma edge, like helium, nitrogen and others. Therefore, modeling and controlling the edge plasma facing the blanket and the divertor of the tokamak reactor rely on accurate cross sections of possible induced processes. In particular, in this work we are interested in presenting accurate total cross

* Author to whom any correspondence should be addressed.



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sections for single-electron processes, mainly single-electron capture of projectile bound states and single-ionization of the target in collisions between singly charged lithium ions with helium and nitrogen atomic targets.

In ion–atom collisions involving a single electron, many classical, semi-classical and quantum mechanical theoretical approaches have been developed to calculate the cross sections of possible electron processes (see [9–12] and references therein). Regarding the collisions involving two or more active electrons, the non-perturbative semi-classical or quantum treatments are difficult to apply and few works are available in this context [13, 14]. In order to study the electron transfer in ion–atom collisions in the mid to high impact energy range, several theories have been used, such as the continuum distorted wave (CDW) method [15–17] and the approximations based on it. For instance, the eikonal initial state approximation [18], the boundary-corrected continuum intermediate state approximation and the Born distorted wave model [19]. Other theories have also been used, such as the well-known classical trajectory Monte Carlo (CTMC) method [20, 21], the two-center basis generator method [22] and the four-body boundary-corrected continuum intermediate state (BCCIS-4B) approximation [23, 24].

The single electron capture from molecular targets of biological interest (e.g. DNA/RNA nucleobases) with fast bare ions has been investigated by Belkić using the full CDW method, in which the molecular cross sections are computed within the independent atom model combined with the Bragg additivity rule [25] from atomic cross sections. When considering collisions between ions and multi-electron targets, the problem can be reduced to a three-body problem in which the atomic cross section of the interested process is evaluated within the independent electron model [26]. In evaluating the single capture cross section from several atomic targets (e.g. C, N, O, Ne) by protons, Belkić found that the contribution to single capture from core electrons is not negligible for high-impact energies [25].

Our present work is devoted to a classical treatment of the most relevant inelastic electron processes in $\text{Li}^+ - \text{He}(1s)$ and $\text{Li}^+ - \text{N}(2p)$ collision systems. For the sake of simplicity, the considered collision systems are treated as three-body problems. Helium and nitrogen atomic targets are described within the single active electron (SAE) approximation using a Garvey-type distance-dependent model potential where only the ground-state outermost electron is involved in the collision dynamics as an active electron, while the other bound electrons are considered inactive [27, 28]. The scattering problem of the three-body system is solved within the framework of the CTMC method [9, 20].

In this work, we present our CTMC total cross sections for single-electron charge transfer and single-electron ionization in $\text{Li}^+ - \text{He}(1s)$ and $\text{Li}^+ - \text{N}(2p)$ collision systems from intermediate to high impact energies. The present CTMC results are compared with the existing experimental data.

The paper is organized as follows. In section 2, we review the CTMC method in the framework of non-coulombic interactions between the colliding partners. In section 3, we present

and discuss our results. Finally, in section 4, we provide the concluding remarks and a future outlook.

Atomic units (a.u.) are used throughout this paper unless otherwise specified.

2. Theoretical model

The CTMC model in ion–atom collisions is a computer scattering experiment based on the numerical solution of the equations of motion by sampling randomly the initial conditions of the colliding partners. Here, our three-body problem consists of the singly charged projectile ion (P), the target nucleus (T) and its initially bounded outermost electron (e) (see figure 1). Thus, the total Hamiltonian of the three-body collision system reads,

$$H = T + V(s, x, r) \quad (1)$$

where the total kinetic energy T is simply given by

$$T = \frac{p_p^2}{2m_p} + \frac{p_T^2}{2m_T} + \frac{p_e^2}{2m_e}. \quad (2)$$

The associated total potential energy can be written as

$$V = V_{PT}(s) + V_{Te}(r) + V_{Pe}(x), \quad (3)$$

where V_{PT} , V_{Te} and V_{Pe} are the potentials resulting from the interactions between the projectile ion and the target core, between the target core and the active target electron and between the projectile ion and the active target electron, respectively. The interaction between the colliding partners is modelled by a Garvey type model potential [27, 28] of the form

$$V(\zeta) = q \frac{Q(\zeta)}{\zeta}, \quad (4)$$

where q is a test charge and $\zeta = r, s, x$ is the separation distance between the nucleus and the charge test q . The function $Q(\zeta)$ is a distance dependent nuclear charge given by

$$Q(\zeta) = Z - (N - 1)(1 - \Omega(\zeta)), \quad (5)$$

where Z being the atomic number, N being the total number of electrons in the atom or ion and the function $\Omega(\zeta)$ is the screening potential given by the following expression

$$\Omega(\zeta) = \left[(\eta/\xi)(e^{\xi\zeta} - 1) + 1 \right]^{-1}. \quad (6)$$

The potential parameters ξ and η can be obtained in such a way that they minimize the energy for a given atom or ion. We note that this type of potential has further advantages, because it has the correct asymptotic form for both small and large values of ζ which is stated in the equations (7a) and (7b) below,

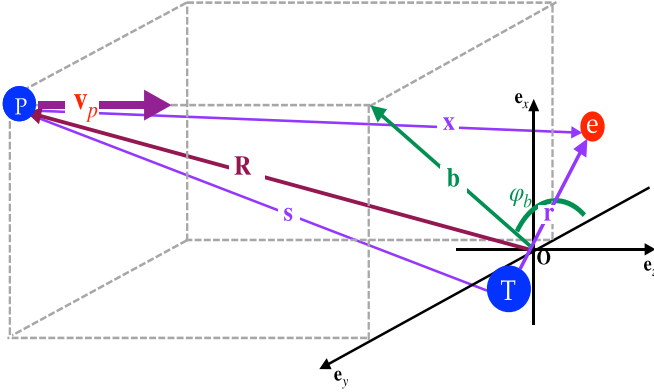


Figure 1. Schematic illustration of the relative position vectors $\vec{r} = \vec{r}_e - \vec{r}_T$, $\vec{s} = \vec{r}_P - \vec{r}_T$ and $\vec{x} = \vec{r}_e - \vec{r}_P$. The vector $\vec{R}$ refers to the position of the projectile with respect to the center-of-mass of the target system (O), $\vec{v}_p$ is its corresponding velocity and b being the impact parameter.

$$\lim_{\zeta \rightarrow 0} Q(\zeta) = Z \quad (7a)$$

$$\lim_{\zeta \rightarrow \infty} Q(\zeta) = Z - (N - 1). \quad (7b)$$

We use this potential form to mimic the distance dependent charge of the dressed projectile. The parameters η and ξ for the projectile (P) and target (T) are given by

$$\eta_P = \eta_P^{(0)} + \eta_P^{(1)}(Z_P - N_P - 1), \quad (8a)$$

$$\xi_P = \xi_P^{(0)} + \xi_P^{(1)}(Z_P - N_P - 1), \quad (8b)$$

$$\eta_T = \eta_T^{(0)} + \eta_T^{(1)}(Z_T - N_T), \quad (8c)$$

$$\xi_T = \xi_T^{(0)} + \xi_T^{(1)}(Z_T - N_T), \quad (8d)$$

where the parameters $\eta_X^{(0)}$, $\eta_X^{(1)}$, $\xi_X^{(0)}$, and $\xi_X^{(1)}$ ($X = T$ or P) are tabulated by Garvey *et al* [27].

The total potential energy V in our three-body system can then be written as

$$V(s, r, x) = \frac{Q_P(s)Q_T(s)}{s} + \frac{Q_T(r)q_e}{r} + \frac{Q_P(x)q_e}{x}, \quad (9)$$

where q_e is the charge of electron and the functions Q_T and Q_P are the distance dependent nuclear charges given by equation (5).

The equations of motion are derived from Hamilton's equations, which are solved numerically by using a Runge–Kutta method with adaptive step size. This latter step is carried out after the determination of the initial positions and momenta of all particles.

The initial position of the projectile ion is defined by its initial separation distance to the center-of-mass of the target system R_0 and the impact parameter b (see figure 1) which is sampled randomly in the interval $[0, b_{\max}]$. With respect to

the initial momentum vector of the projectile ion, which is supposed to be initially moving along the z -direction, it is defined by the impact velocity v_p of the projectile ion with respect to the target centre-of-mass. When the active target electron initially bound to the target nucleus is moving in a non-coulombic potential, its initial position and momentum vector are determined using the procedure first introduced by Reinhold and Falcón [26].

The equations of motion are solved for a large number of a set of initial conditions until a reasonable statistical error (SE) is obtained (in our calculations the $SE < 4\%$). The total cross sections can then be evaluated using the following approximate formula

$$\sigma_\tau(E) = \frac{2\pi b_{\max}}{N_{\text{tot}}} \sum_{i=1}^{N_\tau} b_i, \quad (10)$$

where N_{tot} is the total number trajectories calculated for impact parameters less than $b_{\max}$ and N_τ and b_i is the number of trajectories and the actual impact parameter satisfying the studied electron process (electron capture and ionization). The associated SE is then given by

$$\Delta\sigma_\tau = \sigma_\tau \left(\frac{N_{\text{tot}} - N_\tau}{N_{\text{tot}}N_\tau} \right). \quad (11)$$

We note that as we use the independent-electron model evaluate the total cross sections [25, 26] for the case of a helium target, the single capture and single ionization cross sections computed by equation (10) has to be multiplied by two which is the number of electrons in the K-shell. In the case of nitrogen targets, the computed cross sections have to be multiplied by the number of equivalent electrons in the sub-shell 2p, i.e. with three.

3. Results and discussion

3.1. Single-electron capture

The total cross sections of the electron capture from He(1s) and N(2p) by lithium ion Li^+ are presented and discussed for a wide range of projectile impact energies, which cover the area of interest for both fusion plasma and interstellar space research.

In figures 2 and 3, we present the probability of the electron capture from He(1s) and N(2p) by Li^+ , respectively as a function of the impact parameter for different projectile impact energies. By using a fitting of our results, we found that the probabilities follow almost a Gaussian law for all projectile impact energies. The analysis of the probabilities is a necessary step to determine the appropriate maximum impact parameter $b_{\max}$ of the studied electron process at a defined impact velocity. We note that the total cross sections can be calculated by using the approximate expression of equation (10). Alternatively, the evaluation of the total cross section (TCS) can also be done also by integrating a Gaussian fit multiplied by 2π .

Before we show our total cross section results, we would like to note an interesting feature of the classical and semi-classical treatments of the collision problem (which are good

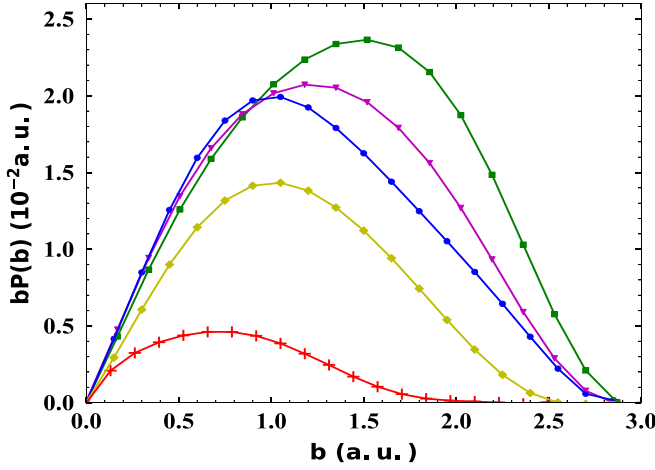


Figure 2. Probability, $bP(b)$, of the electron capture from He(1s) by Li^+ as a function of the impact parameter b at different projectile impact energies. Green squares: 10 keV, magenta triangles: 50 keV, blue circles: 100 keV, yellow diamonds: 400 keV and red plus: 1000 keV. The dashed curves represent the fit of our results.

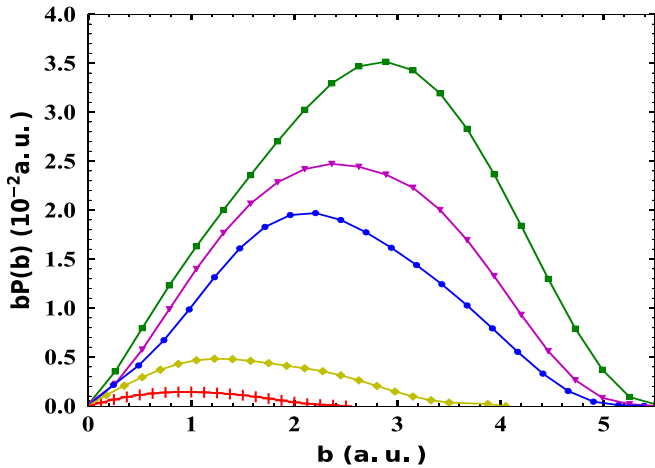


Figure 3. Same as figure (2) but for electron capture from N(2p) by Li^+ .

approximations in the intermediate to high collision energies), namely that the effect of the interaction between the target and projectile nuclei (internuclear potential) does not significantly affect the electron dynamics and thus the total cross sections [29, 30]. For example, in semi-classical atomic orbitals at close coupling the nucleus–nucleus interaction can be eliminated by a simple phase transformation [30]. Along this line we have checked the effect of the internuclear potential on the single capture process in our simulations by computing the cross sections with and without the nuclear potential. Our results are summarized in tables 1 and 2. As can be seen from the tables, according to our expectation, no significant contribution of the internuclear potential was found.

Figure 4 shows the single-electron capture total cross section as a function of the projectile impact energy in $\text{Li}^+ - \text{He}(1s)$ collision system. Our results are compared with experimental data, and with theoretical data by Samanta *et al* [23] who used a BCCIS-4B approximation. In general, the

Table 1. The electron capture total cross sections for $\text{Li}^+ + \text{He}(1s)$ with (σ_c^{on}) and without (σ_c^{off}) internuclear potential and their ratio.

$\text{Li}^+ + \text{He}(1s)$			
E (keV)	σ_c^{on} (cm^2)	σ_c^{off} (cm^2)	Ratio
10	4.10×10^{-17}	3.98×10^{-17}	1.03
100	5.68×10^{-17}	5.70×10^{-17}	0.99
1000	1.23×10^{-17}	1.23×10^{-17}	1.00

Table 2. Same as table 1 but for $\text{Li}^+ + \text{N}(2p)$.

$\text{Li}^+ + \text{N}(2p)$			
E (keV)	σ_c^{on} (cm^2)	σ_c^{off} (cm^2)	Ratio
10	2.46×10^{-16}	2.50×10^{-16}	0.98
100	2.97×10^{-16}	3.01×10^{-16}	0.98
1000	8.11×10^{-18}	8.24×10^{-18}	0.98

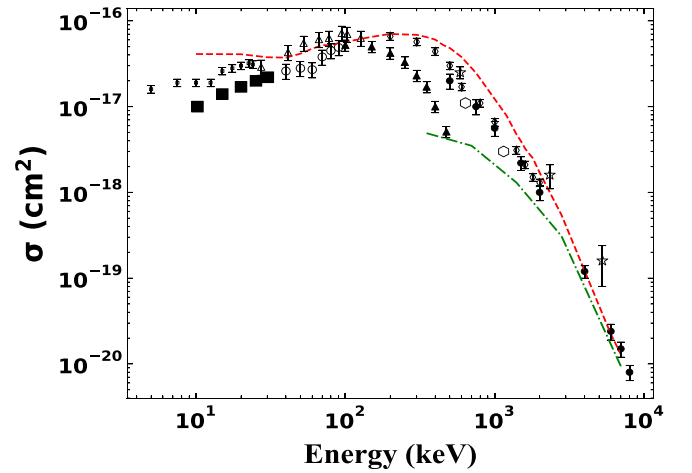


Figure 4. Total cross sections of the single-electron capture from He(1s) by Li^+ as a function of the projectile impact energy. Present CTMC results of the model potential: red dashed line; BCCIS-4B results of Samanta *et al* [23]: dash-dotted line; experiments: Woitke *et al* [31]: $\bullet$, Allison *et al* [32]: $\blacktriangle$, Dmitriev *et al* [33]: $\star$, Pivovarov *et al* [34]: $\triangle$, Nikolaev *et al* [35]: $\diamond$, Pivovarov *et al* [36]: $\diamond$, Ogurtsov *et al* [37]: $\blacksquare$, Hvelplund [38]: $\circ$ and Van Eck *et al* [39]: $\square$.

present CTMC results are in good agreement with the experimental data in the investigated impact energy range. We note that the experimental data of Allison *et al* [32] are lower than those of Pivovarov *et al* [36] between 200 keV and 500 keV. The theoretical results of Samanta *et al* and our CTMC results are in very good agreement with the experimental data at projectile impact energies higher than 5 MeV. However, the BCCIS-4B model of Samanta *et al* strongly underestimate the electron capture cross sections for impact energies lower than 5 MeV.

Figure 5 shows our CTMC results for the electron capture in $\text{Li}^+ - \text{N}$ collisions as a function of the projectile impact energy compared to the experimental data. In order to compare our CTMC results with the existing experimental data on collisions between Li^+ and nitrogen ground states, we have performed calculations of the electron capture from the N(1s),

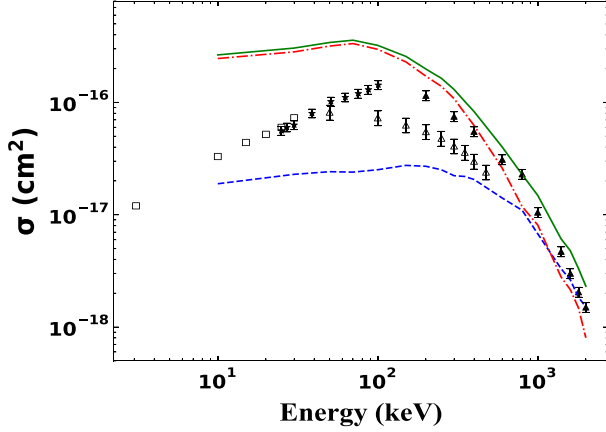


Figure 5. Total cross sections of the single-electron capture from the nitrogen ground state by Li^+ as a function of the projectile impact energy. Present CTMC results: blue dashed curve, capture from N(2s); capture from N(2s), red dot-dashed curve; solid green curve, sum of cross sections from N(2s) and N(2p) (the capture from N(1s) is not included because it is negligible in the considered range of projectile impact energies). Experiments: Pivovar *et al* [36]: $\blacktriangle$, Allison *et al* [32]: $\triangle$, Ogurtsov *et al* [37]: $\square$ and Lockwood [40]: $\star$.

Table 3. Total cross section of electron capture from N(1s), N(2s) and N(2p) by Li^+ .

E (keV)	σ_c^{1s} (cm ²)	σ_c^{2s} (cm ²)	σ_c^{2p} (cm ²)
600	4.4470×10^{-21}	1.4093×10^{-17}	2.5991×10^{-17}
1000	3.9026×10^{-20}	6.7748×10^{-18}	8.1135×10^{-18}
1400	2.4266×10^{-20}	3.3120×10^{-18}	2.7918×10^{-18}
1600	2.4318×10^{-20}	2.6264×10^{-18}	2.1513×10^{-18}
1800	2.9212×10^{-20}	1.8373×10^{-18}	1.4759×10^{-18}
2000	3.6426×10^{-20}	1.5117×10^{-18}	8.0249×10^{-19}

N(2s), and N(2p) states. The calculated cross sections for several impact energies are shown in table 3. We found that the cross sections from N(1s) are negligibly small compared to the contributions from the N(2s) and N(2p) shells. We have not included the N(1s) shell contributions in our CTMC data. The present CTMC cross sections are simply the sum of the electron capture from the N(2s) and N(2p) weighted by the number of electrons in each state. According to our CTMC calculations, the main contribution to the electron capture comes from the outermost electrons in the nitrogen target (i.e. N(2p)) for impact energies below 800 keV. However, for impact energies higher than 800 keV, the contribution of the electron capture from the N(2s) becomes important and cannot be neglected.

The present CTMC results are in a good agreement with the experimental data of Pivovar *et al* [36] for impact energies higher than 200 keV. We note that the experimental data of Allison *et al* underestimates the electron transfer cross sections for impact energies higher than 100 keV [32]. For energies lower than 200 keV, our CTMC results for electron capture overestimate the existing experimental data of Ogurtsov *et al* [37] and Lockwood [40]. Based on the available experimental data, it is worth mentioning that the electron capture cross sections from the nitrogen ground state by Li^+ decreases at

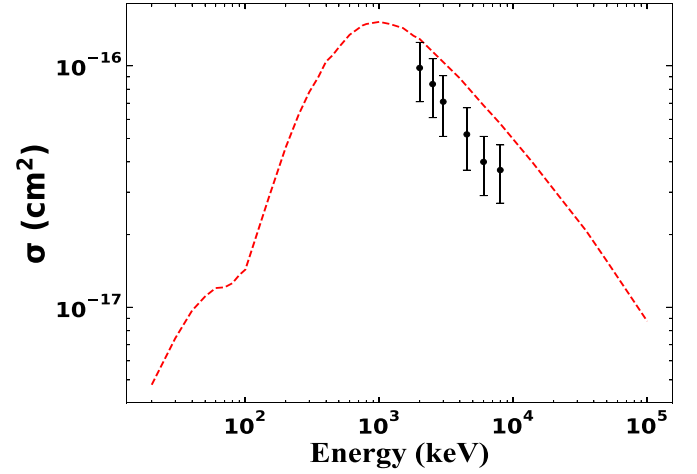


Figure 6. Total cross sections of the single-electron ionization from He(1s) by Li^+ as a function of the projectile impact energy. Present CTMC results of the model potential: red dashed line; experiments: Woitke *et al* [31]: $\bullet$.

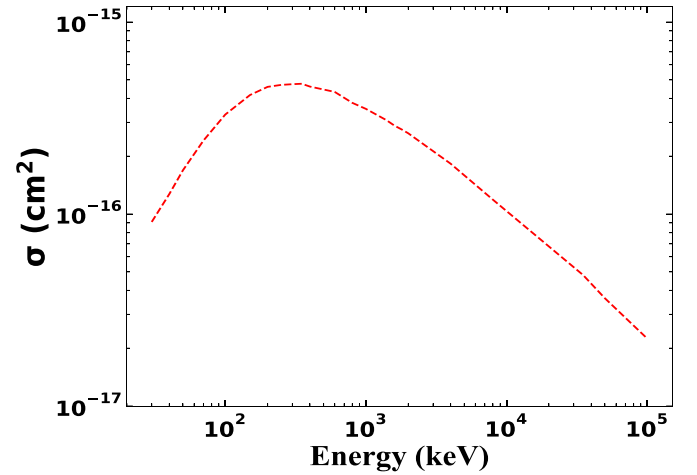


Figure 7. Total cross sections of the single-electron ionization from N(2p) by Li^+ as a function of the projectile impact energy. Present CTMC results of the model potential: red dashed line.

high and low projectile impact energies. The highest cross sections are around 100 keV energies.

3.2. Single ionization

In the following, we present and discuss only our CTMC results for the total single ionization cross sections. In figures 6 and 7, we present the single ionization cross section as a function of the projectile impact energy in Li^+ –He(1s) and Li^+ –N(2p) collision systems. At first glance, we notice the presence of a bump at low impact energies for the ionization cross section of helium by Li^+ (see figure 6). According to the work of Schultz *et al*, the origin of this bump is attributed to the oscillation of the target's electron between the projectile ion and the target nucleus before it gets ionized [41]. However, we do not see a bump in the Li^+ –N(2p) system (see figure 7).

For $\text{Li}^+ - \text{He}(1s)$ system, only Woitke *et al* [31] has previous ionization results in the energy range between 2000 and 8000 keV. Our CTMC results are slightly larger than the experimental data of Woitke *et al* [31]. By comparing the ionization cross-section of the current two systems, we see that the ionization cross-sections in $\text{Li}^+ - \text{N}(2p)$ are higher at the corresponding impact energies (see figures 6 and 7) than those obtained in the $\text{Li}^+ - \text{He}(1s)$ collision system. This can be attributed to the fact that the $\text{N}(2p)$ active electron has a lower binding energy than that of the $\text{He}(1s)$ target.

4. Conclusion

We have presented three-body CTMC calculations for Li^+ ions on helium and nitrogen atomic targets. The collision problem has been treated within the SAE approximation where the total cross sections of the charge exchange and ionization processes were presented and discussed for a wide range of impact projectile energies. Our CTMC results for the capture process show good agreement with the existing results in the high projectile impact velocity range for both systems. In the low-impact velocity range, in the case of nitrogen targets, our CTMC results slightly overestimate the total cross-sections of the capture process compared with the experimental data. However, the total capture cross section in the case of the helium target follows the trend of the experimental data even at low impact velocities. In addition, we presented and discussed the total ionization cross-sections of helium and nitrogen atomic targets with singly charged lithium ions.

Our future plan is to use the current model potential to test other collision systems, extend our study to calculate the differential ionization cross sections and perform calculations on the state selective charge exchange cross sections.

Data availability statement

The data cannot be made publicly available upon publication because they contain sensitive personal information. The data that support the findings of this study are available upon reasonable request from the authors.

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ORCID iDs

M Al-Ajaleen  <https://orcid.org/0000-0002-3019-0883>

K Tőkési  <https://orcid.org/0000-0001-8772-8472>

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