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SINGLE-ELECTRON CAPTURE IN COLLISIONS OF POSITIVELY CHARGED MUONS WITH HYDROGEN AND HELIUM ATOMS

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Abstract. *The prior form of the three-body boundary-corrected first Born (CB1-3B) method is used to calculate the state-selective total cross sections for single-electron capture into 1s, 2s and 2p final states of a fast muon projectiles from a ground-state hydrogen and helium targets at energies 10 keV to 1 MeV. For helium target, the frozen-core approximation and the independent particles model were used. The state-summed total cross sections for electron capture into all final states of the muonium systems (μ^+, e) are obtained by applying the Oppenheimer (n^{-3}) scaling law. Unfortunately, there are no available experimental data, so our theoretical results were compared to the CDW-3B theoretical results.*

Key words: *muon-atom collisions, electron capture, muonium system*

1. INTRODUCTION

Single-electron capture, as one of the most significant charge-exchange processes in fast ion-atoms, ion-molecules and atom-atoms collisions is very important not only in physics such as astrophysics, plasma physics but also in medicine such as hadron therapy. Because of all of these, the single-electron capture has been the subject of intensive experimental and theoretical research for many years (Mančev and Milojević, 2010; Mančev et al., 2012; Mančev et al., 2013; Milojević, 2014; Mančev et al., 2015; Milojević et al., 2017; Milojević et al., 2020). Muonium formation in collisions of positive mesons with hydrogen and helium atoms has been subject of many investigations, see for example (Moussa and Abdel-Monem, 1967; Belkić and Janev, 1973; Janev and Belkić, 1972; Sakimoto, 2015; Kulhar, 2006; Kulhar, 2004). The earliest study of this process was by

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Moussa and Abdel-Monem (Moussa and Abdel-Monem, 1967), who used the first Born approximation for incident muon energies below 6 keV. Also, the single-electron capture in collisions of positive muons with hydrogen atoms in the energy range from 0.4 to 5 keV was investigated by Janev and Belkić (Janev and Belkić, 1972) using the adiabatical methods for near-resonant atomic reactions. About muon physics can be found in (Huges and Wu, 1975; Scheck, 1978).

In the present work we report our theoretical investigation of the single-electron capture process in the typical $Z_P - (Z_T, e)$ collision at intermediate and high incident energies, by employing the prior version of the three-body boundary-corrected first Born approximation (CB1-3B). Generally speaking, all collision theories can be classified into two groups: perturbation and non-perturbation theories. Furthermore, perturbation theories can be divided into first and second-order theories. The second-order theories take into account the electronic Coulomb continuum intermediate states in one (entrance or exit) channel or in both channels, while the first-order theories do not include the electronic continuum intermediate states. The CB1-3B approximation is the first-order three-body perturbation method which satisfies the correct boundary conditions in both collision channels, according to the principles of quantum scattering theory (Belkić, 2004). The correct Coulomb boundary conditions are equivalent to the concept of asymptotic convergence (Belkić et al., 1979; Belkić, 2004; Belkić, 2008; Belkić et al., 2008). The CB1-3B method in both (prior and post) forms was first developed in the work (Belkić and Taylor, 1987). Atomic units will be used throughout unless otherwise stated.

2. Theory

We examine single-electron capture in collisions fast heavy nucleus P of mass M_P and charge Z_P (projectile) with hydrogen and helium atoms (target) consisting of a one electron e and two electrons e_1 and e_2 bound to the nucleus T of mass M_T and charge Z_T, respectively:

$$Z_P + (Z_T, e)_{1s} \rightarrow (Z_P, e)_{nlm} + Z_T, \tag{1}$$

$$Z_P + (Z_T, e)_{1s} \rightarrow (Z_P, e)_{nl} + Z_T, \tag{2}$$

$$Z_P + (Z_T, e)_{1s} \rightarrow (Z_P, e)_{\Sigma} + Z_T, \tag{3}$$

$$Z_P + (Z_T, e_1, e_2)_{1s^2} \rightarrow (Z_P, e_1)_{nlm} + (Z_T, e_2)_{1s}\ , \tag{4}$$

$$Z_P + (Z_T, e_1, e_2)_{1s^2} \rightarrow (Z_P, e_1)_{nl} + (Z_T, e_2)_{1s}\ , \tag{5}$$

$$Z_P + (Z_T, e_1, e_2)_{1s^2} \rightarrow (Z_P, e_1)_{\Sigma} + (Z_T, e_2)_{1s}\ , \tag{6}$$

or equivalent:

$$\mu^+ + {}^1\mathrm{H}(1s) \rightarrow \mu(nlm) + {}^1\mathrm{H}^+, \tag{7}$$

$$\mu^+ + {}^1\mathrm{H}(1s) \rightarrow \mu(nl) + {}^1\mathrm{H}^+, \tag{8}$$

$$\mu^+ + {}^1\mathrm{H}(1s) \rightarrow \mu(\Sigma) + {}^1\mathrm{H}^+, \tag{9}$$

$$\mu^+ + {}^4\mathrm{He}(1s^2) \rightarrow \mu(nlm) + {}^4\mathrm{He}^+(1\mathrm{s}), \tag{10}$$

$$\mu^{+} + {}^{4}\mathrm{He}(1s^{2}) \rightarrow \mu(nl) + {}^{4}\mathrm{He}^{+}(1\mathrm{s}), \tag{11}$$

$$\mu^{+} + {}^{4}\mathrm{He}(1s^{2}) \rightarrow \mu(\Sigma) + {}^{4}\mathrm{He}^{+}(1\mathrm{s}), \tag{12}$$

where nlm is the usual set of the three quantum numbers of hydrogen-like atomic systems, while symbol Σ denotes the capture into all final states of the projectile. The symbol μ (Mu) denotes the muonium (μ^{+}, e) system, $\mu = (\mu^{+}, e)$. The $1s$ and $1s^{2}$ denote the ground state of the one- and two-electron atoms, respectively. Let $\vec{s}$ ($\vec{x}$) be the position vector of the electron e relative to the nuclear charge of the projectile μ^{+} (target H^{+}), while $\vec{s}_1$ and $\vec{s}_2$ ($\vec{x}_1$ and $\vec{x}_2$) be the position vectors of the first and second electron (e_1 and e_2) relative to the nuclear charge of the projectile μ^{+} (target He^{2+}), respectively. Further, let $\vec{R}$ be the position vector of the projectile P with respect to target nucleus T.

In the case of a helium target the frozen-core approximation and the independent particles model were used. Additionally, non-relativistic quantum scattering theory has been used. The non-relativistic quantum scattering theory does not count the spin effects and in this spin-independent formalism the two target electrons can considered as distinguishable from each other. In the frozen-core approximation the non-captured (passive) electron e_2 is assumed to occupy the same orbital before and after capture of the active electron e_1, while in the independent particles model the passive electron is included only through a shielding of the original nuclear charge of the target. Based on these assumptions we can write $\mathrm{Z_T^{eff}} = \mathrm{Z_T} - 5/16 = 1.6875$ instead $\mathrm{Z_T} = 2$, where 5/16 is the Slater screening constant charge which is obtained minimizing the expectation value of the total two-electron Hamiltonian of a heliumlike atomic system. We could have also chosen the opposite, to have electron e_1 passive and electron e_2 active. The probability of capturing electron e_1 with e_2 participating in the screening of the target nucleus is equal to the probability of capturing electron e_2 with e_1 participating in the screening. For this reason, we multiplied the calculated state-selective total cross sections for capturing electron e_1 while electron e_2 remains in the target by 2.

Therefore, in three-body formalism, the original four-body processes (4), (6), (10) and (12) are reduced to three-body counterpart:

$$\mathrm{Z_P} + \left(\mathrm{Z_T^{eff}}, e\right)_{1\mathrm{s}} \rightarrow (\mathrm{Z_P}, e)_{nlm} + \mathrm{Z_T^{eff}}, \tag{13}$$

$$\mathrm{Z_P} + \left(\mathrm{Z_T^{eff}}, e\right)_{1\mathrm{s}} \rightarrow (\mathrm{Z_P}, e)_{\Sigma} + \mathrm{Z_T^{eff}}. \tag{14}$$

The prior state-selective transition amplitude for processes (7) in the CB1-3B approximation read as (Belkić and Taylor, 1987):

$$T_{nlm}^{\mathrm{Z_T}=1}(\vec{\eta}) = \int\int \mathrm{d}\vec{s}\mathrm{d}\vec{R}\, \varphi_{nlm}^{*}(\vec{s}) \left(\frac{1}{R} - \frac{1}{s}\right) \varphi_{100}^{\mathrm{Z_T}=1}(\vec{x}) e^{i\vec{\beta}_1\cdot\vec{R} - i\vec{v}\cdot\vec{s}}, \tag{15}$$

while for processes (10):

$$T_{nlm}^{Z_T^{\mathrm{eff}}=1.6875}(\vec{\eta}) = \int\int \mathrm{d}\vec{s}\mathrm{d}\vec{R}\, \varphi_{nlm}^{*}(\vec{s}) \left(\frac{1}{R} - \frac{1}{s}\right) \cdot \varphi_{100}^{\mathrm{Z_T^{eff}}=1.6875}(\vec{x}) e^{i\vec{\beta}_2\cdot\vec{R} - i\vec{v}\cdot\vec{s}} \left(vR + \vec{v}\cdot\vec{R}\right)^{-i\frac{0.6875}{v}}, \tag{16}$$

where v is the velocity of the projectile along the z- axis. Here the $\vec{\beta}_1 = -\vec{\eta} - (v/2 + (1/[2n^2]-0.5)/v)\hat{\vec{v}}$ and $\vec{\beta}_2 = -\vec{\eta} - (v/2 + (1/[2n^2] - 1.423828125)/v)\hat{\vec{v}}$ are the linear momentum transfers, while transverse momentum transfer is given by $\vec{\eta} = (\eta \cos \phi_\eta, \eta \sin \phi_\eta, 0)$ with the property $\vec{\eta} \cdot \vec{v} = 0$. In writing the equations (15) and (16), we used the eikonal hypothesis, according to which scattering dominates at small angles, which is valid when the masses of the projectile and target are much greater than the mass of the electron. In our case, this fulfilled because the masses of muon, hydrogen nucleus (proton) and helium nucleus (alpha particle) are 206.7, 1836.12 and 7344.48 times greater than the mass of the electron, respectively. The functions $\varphi_{nlm}(\vec{s})$, $\varphi_{100}^{Z_T=1}(\vec{x})$ and $\varphi_{100}^{Z_T^{eff}=1.6875}(\vec{x})$ represent the bound state wave functions of the hydrogen-like atomic systems $(Z_P, e)_{nlm}$, $(Z_T, e)_{1s}$ and $(Z_T^{eff}, e)_{1s}$, respectively. The six-dimensional integrals (15) and (16) are reduced to a two dimensional over real variables. The state-selective total cross sections for processes (7) and (10) are given by:

$$Q_{nlm}^{Z_T=1,\, Z_T^{eff}=1.6875}(\pi a_0^2) = \frac{1}{2\pi^2 v^2}\int_0^\infty d\eta\eta\, |T_{nlm}^{Z_T=1,\, Z_T^{eff}=1.6875}(\vec{\eta})|^2. \quad (17)$$

Numerical calculations of the three dimensional integral (17) are performed by means of the Gauss-Legendre (GL) quadratures. The number of integration points NGL was taken to be such that all the computed cross sections converge to at least two decimal places. A substitution $\eta = \sqrt{2(1+z)/(1-z)}$, where $z \in [-1,1]$, was introduced for numerical integration with respect to η. This change of variable is important, since it concentrates integration points near the forward cone, which provides the main contribution to the total cross sections.

The state-selective total cross sections for single-electron capture into the given shell n, summed over the orbital $l \in [0, n-1]$ and magnetic $m \in [-l, l]$ quantum numbers, are:

$$Q_n^{Z_T=1,\, Z_T^{eff}=1.6875} = \sum_{l=0}^{n-1} Q_{nl}^{Z_T=1,\, Z_T^{eff}=1.6875}, \quad (18)$$

$$Q_{nl}^{Z_T=1,\, Z_T^{eff}=1.6875} = \sum_{m=-l}^{l} Q_{nlm}^{Z_T=1,\, Z_T^{eff}=1.6875}. \quad (19)$$

The state-summed total cross sections for electron capture into all the final states (μ^+, e) systems are obtained by applying the Oppenheimer (n^{-3}) scaling law (Oppenheimer, 1928) via:

$$Q_\Sigma^{Z_T=1,\, Z_T^{eff}=1.6875} = Q_1^{Z_T=1,\, Z_T^{eff}=1.6875} + 1.616 Q_2^{Z_T=1,\, Z_T^{eff}=1.6875}. \quad (20)$$

3. Results and Discussions

Muonium can simply be regarded as an isotope of hydrogen and hence muonium formation in gases can generally be understood in terms of well-established concepts of charge-exchange in proton-atoms collisions. In this section, state-selective and state-summed total cross sections for electron capture by fast muon from H and He targets, calculated by using the prior form of CB1-3B approximations, are presented in the energy region from 10 keV to 1 MeV. The obtained results are presented in Figure 1 and Figure 2, as well as in Table 1 and Table 2. These results are compared with the CDW-3B predictions obtained following Belkić and Janev (Belkić and Janev, 1973).

Figure 1 is devoted to the case of hydrogen target. It can be seen that both CB1-3B and CDW-3B methods give the similar results. In the case of capture into $1s$, $2s$ as well as Q_Σ the CB1-3B results slightly overestimates CDW-3B results in the whole considered impact energies. The curves representing them are nearly parallel to each other. Different situation is for capture in $2p$ state where at higher impact energies (above 240 keV) CB1-3B underestimates the CDW-3B method. The main contribution to the state-summed total cross section comes from the transition to the ground state.

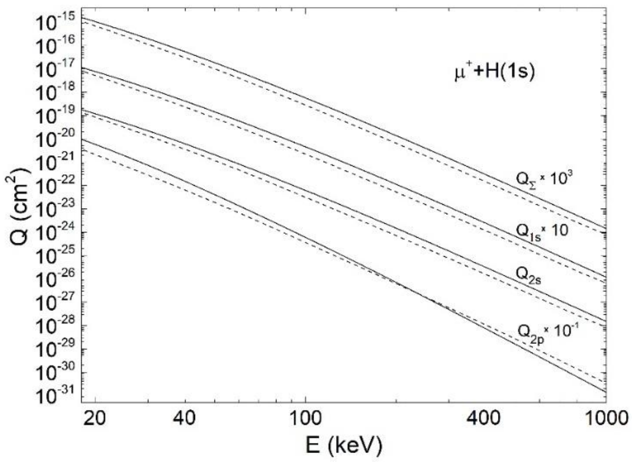

Fig. 1 State-selective Q_{1s}, Q_{2s}, Q_{2p} and state-summed Q_Σ total cross sections (in cm^2) as a function of impact energies E (keV) for single-electron capture by muon from H(1s), as per processes (8) and (9). Theoretical results: full line – CB1-3B (present results) and dashed line – CDW-3B (Belkić and Janev, 1973).

Figure 2 shows the total cross sections Q_{1s}, Q_{2s}, Q_{2p} and Q_Σ as a function of the collision energy E for the single-electron capture into $1s$, $2s$, $2p$ and all final states, respectively, from helium targets. Here it can also be seen that the transition to the $1s$ state has a dominant contribution to the state-summed total cross section Q_Σ. The energy dependence is overall similar for the electron capture from hydrogen atoms. The results of the capture into $1s$ and $2p$ states obtained within the CB1-3B approximation overestimates CDW-3B results over the entire range considered. In the case of Q_{2s} and $Q_{\Sigma,}$ the CB1-3B curves exceed the CDW-3B curves at energies of 35 keV and 25 keV, respectively. However, at lower energies, the behavior is reversed, meaning that the CDW-3B curves become higher than the CB1-3B curves.

Experimentally, the investigation of this type of mesonic atom is difficult and they have not been studied. There are no corresponding experimental values for the two reactions to confirm our theory.

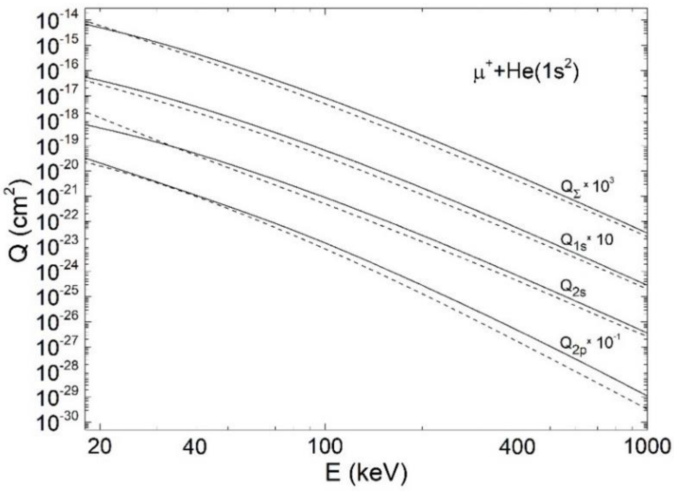

Fig. 2 State-selective Q_{1s}, Q_{2s}, Q_{2p} and state-summed Q_Σ total cross sections (in cm^2) as a function of impact energies E (keV) for single-electron capture by muon from He(1s^2), as per processes (11) and (12). Theoretical results: full line - CB1-3B (present results) and dashed line - CDW-3B (Belkić and Janev, 1973).

It should be noted that there are different muonic systems and collisional processes are possible such as a muonic hydrogen (p, μ^-), a muon-antimuon pair (μ^+, μ^-) or atomic collision processes of a negative muon and a Mu atom, i.e., $\mu^- + (\mu^+, e^-) \rightarrow (\mu^+, \mu^-) + e^-$. While no experimental plan has been arranged thus far to utilize muon exchange in atomic collisions of a positive muon and a muonic hydrogen atom, i.e., $\mu^+ + (p, \mu^-) \rightarrow (\mu^+, \mu^-) + p$, this reaction may be also expected to be an efficient means of producing the (μ^+, μ^-) atoms (Sakimoto, 2015). These collisional processes can also be evaluated by means of CB1-3B as well as CDW-3B methods.

However, how is the mass of the muon 206.7 times heavier than the mass of electron, i.e. $M_\mu = \frac{1}{8.88} M_p$ (M_p is the mass of the proton), the (μ^+, μ^-) atomic system has a deep ground ($1s$) state energy of -1.41 keV, and a very small Bohr radius of mere 512 fm. Due to this compactness, the (μ^+, μ^-) atom has not yet been observed experimentally.

Table 1 State-selective and state-summed total cross sections (in cm^2) for processes (7)-(9) as a function of impact energy E(keV) of μ^+ projectiles for single-electron capture from H(1*s*) into the final bound states of muonium (μ^+, *e*) systems (Mu) with *nlm*. The row labeled by *nlm* refers to the state-selective cross sections Q_{nlm} and Q_{nl}. The column denoted by Σ represents the cross-sections Q_Σ, summed over all the final bound states of the (μ^+, *e*) (*nlm*) atom by using Eq. (20). Notation *X* [Z] implies *X* times 10^Z.

E(keV)	*nlm*					
	100	200	210	211	21	Σ
10	9.40[-18]	1.49[-18]	1.02[-18]	1.62[-19]	1.35[-18]	1.40[-17]
20	8.44[-19]	1.31[-19]	4.98[-20]	7.48[-21]	6.48[-20]	1.16[-18]
40	4.46[-20]	6.53[-21]	1.27[-21]	1.76[-22]	1.62[-21]	5.78[-20]
100	4.84[-22]	6.57[-23]	5.09[-24]	6.42[-25]	6.37[-24]	6.00[-22]
200	1.15[-23]	1.51[-24]	5.79[-26]	6.93[-27]	7.17[-26]	1.41[-23]
300	1.19[-24]	1.54[-25]	3.92[-27]	4.59[-28]	4.84[-27]	1.45[-24]
400	2.33[-25]	2.98[-26]	5.68[-28]	6.55[-29]	6.99[-28]	2.82[-25]
600	2.27[-26]	2.89[-27]	3.64[-29]	4.12[-30]	4.47[-29]	2.74[-26]
800	4.28[-27]	5.43[-28]	5.12[-30]	5.73[-31]	6.26[-30]	5.17[-27]
1000	1.16[-27]	1.48[-28]	1.11[-30]	1.23[-31]	1.36[-30]	1.41[-27]

Table 2 State-selective and state-summed total cross sections (in cm^2) for processes (10)-(12) as a function of impact energy E(keV) of μ^+ projectiles for single-electron capture from He(1s^2) into the final bound states of muonium (μ^+, *e*) systems (Mu) with *nlm*. The row labeled by *nlm* refers to the state-selective cross sections Q_{nlm} and Q_{nl}. The column denoted by Σ represents the cross-sections Q_Σ, summed over all the final bound states of the (μ^+, *e*)(*nlm*) atom by using Eq. (20). Notation *X* [Z] implies *X* times 10^Z.

E(keV)	*nlm*					
	100	200	210	211	21	Σ
10	2.60[-17]	2.95[-18]	1.03[-18]	1.20[-19]	1.27[-18]	3.28[-17]
20	4.46[-18]	5.85[-19]	1.45[-19]	2.10[-20]	1.88[-19]	5.70[-18]
40	4.06[-19]	5.52[-20]	8.63[-21]	1.26[-21]	1.12[-20]	5.13[-19]
100	7.30[-21]	9.72[-22]	6.99[-23]	9.49[-24]	8.89[-23]	9.01[-21]
200	2.19[-22]	2.85[-23]	1.06[-24]	1.36[-25]	1.34[-24]	2.67[-22]
300	2.49[-23]	3.20[-24]	8.05[-26]	9.96[-27]	1.01[-25]	3.02[-23]
400	5.11[-24]	6.53[-25]	1.24[-26]	1.50[-27]	1.54[-26]	6.19[-24]
600	5.26[-25]	6.67[-26]	8.43[-28]	9.98[-29]	1.04[-27]	6.35[-25]
800	1.02[-25]	1.29[-26]	1.22[-28]	1.43[-29]	1.51[-28]	1.23[-25]
1000	2.83[-26]	3.58[-27]	2.71[-29]	3.12[-30]	3.33[-29]	3.42[-26]

Muonium formation state-selective and state-summed total cross section results can be also obtained from proton-hydrogen (helium) charge-exchange state-selective and state-summed total cross section results, using energy (velocity) scaling.

4. CONCLUSION

Single-electron capture (muonium formation) in collisions between positive muon with atomics hydrogen and helium is investigated by using the prior version of the three-body boundary-corrected first Born (CB1-3B) approximation. Total cross sections for electron capture into 1*s*, 2*s*, 2*p* states as well as for capture into all the final states of atomic muonium $\mu(\Sigma)$ have been calculated. Unfortunately, there are no available experimental data to compare our theoretical results. Therefore, our CB1-3B results were compared to the CDW-3B theoretical results. It was observed that the obtained CB1-3B curves for Q_{1s}, Q_{2s}, Q_{2p}, and Q_{Σ} have a similar shape, almost parallel to the CDW-3B curves.

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JEDNOSTRUKI ELEKTRONSKI ZAHVAT U SUDARIMA POZITIVNO NAELEKTRISANIH MIONA SA VODONIKOVIM I HELIJUMOVIM ATOMIMA

Prior forma tročestične granično korektne prve Bornove aproksimacije je iskorišćena za izračunavanje parcijalnih totalnih efikasnih preseka za jednostruki elektronski zahvat u 1s, 2s i 2p finalna stanja mionskog projektila iz osnovnog stanja vodonične i helijumske mete na energijama od 10 keV do 1 MeV. U slučaju helijumske mete iskorišćena je aproksimacija smrznutog jezgra i model nezavisnih čestica. Sumirani totalni efikasni preseci za zahvat elektrona u ma koje stanje mionskog sistema (μ^+, e) su dobijeni primenom Openhajmerovog (n^{-3}) zakona skaliranja. Nažalost, nema dostupnih eksperimentalnih rezultata, tako da smo naše teorijske rezultate poredili sa CDW-3B teorijskim rezultatima.

Ključne reči: *mion-atomski sudari, elektronski zahvat, mionski sistemi*