SINGLE ELECTRON CAPTURE IN $p - \mathrm{Li}^+$ COLLISIONS

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Abstract. We report theoretical state-selective and total single-capture cross sections for $p-\mathrm{Li}^+$ collisions by using the four-body boundary-corrected first Born (CB1-4B) approximation for impact energies between 50 and 1500 keV. The calculated results are found to be in good agreement with experimental findings.

1. INTRODUCTION

Charge exchange process in fast heavy particle collisions with atomic and molecular targets is very important in various branches of physics such as astrophysics and plasma physics. The data of these collisions processes are in great need in plasma diagnostics for fusion research. This work is focused on the theoretical investigation of single electron capture in the $p-\mathrm{Li}^+$ collisions by using the four-body boundary-corrected first Born (CB1-4B) approximation. The CB1-4B method is a fully quantum mechanical four-body formalism, since it explicitly considers each individual particle and all the interactions among them in the collision under investigation. This method strictly preserves the correct Coulomb boundary conditions in both collisional channels [1, 2]. In the CB1-4B model, the proper connection between the long-range Coulomb distortion effects and the accompanying perturbation potentials is accomplished according to the well-established principles of scattering theory [2]. As evidenced in abundant applications, imposing the correct Coulomb boundary conditions in the entrance and exit channels is of crucial importance, particularly for ion-atom(ion) collisions [3, 4].

In the present work the CB1-4B approximation is applied to calculate state-selective and total cross section for single electron capture in $p - \mathrm{Li}^+$ collisions. Atomic units will be used throughout unless otherwise stated.

2. THEORY AND RESULTS

We consider single electron capture in collisions of a proton with a lithium ion:

$$p + \mathrm{Li}^{+}(1s^2) \longrightarrow \mathrm{H}(nlm) + \mathrm{Li}^{2+}(1s)\,, \tag{1}$$

where nlm is the usual set of three hydrogen quantum numbers. Let $\vec{s}_1$ 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 proton (target nucleus), respectively. Further, let $\vec{R}$ be the position vector of target nucleus with respect to projectile.

The prior form of the transition amplitude for process (1) in the CB1-4B approximation reads as [5]:

$$\begin{aligned} T_{if}(\vec{\eta}) \;=& \int\int\int \mathrm{d}\vec{x}_1 \mathrm{d}\vec{x}_2 \mathrm{d}\vec{R} \varphi^{*}_{nlm}(\vec{s}_1)\varphi^{*}_{\mathrm{T}}(\vec{x}_2) \left(\frac{2}{R} - \frac{1}{s_1} - \frac{1}{s_2}\right) \\ & \times \varphi_i(\vec{x}_1,\vec{x}_2)\, \mathrm{e}^{-i\vec{\alpha}\cdot\vec{R} - i\vec{v}\cdot\vec{x}_1} (vR - \vec{v}\cdot\vec{R})^{-i\xi}\,, \end{aligned} \tag{2}$$

where $\xi = -1/v$ while $\vec{v}$ is the incident velocity vector. The momentum transfer $\vec{\alpha}$ is defined by: $\vec{\alpha} = \vec{\eta} - (v/2 - \Delta E/v)\hat{\vec{v}}$, where $\Delta E = E_i - E_f$ with E_i being the binding energy of the two-electron target and $E_f = -1/(2n^2) - 3^2/2$. The transverse component of the change in the relative linear momentum of a heavy particle is denoted by $\vec{\eta} = (\eta\cos\phi_\eta, \eta\sin\phi_\eta, 0)$ and has the property $\vec{\eta}\cdot\vec{v} = 0$. The function $\varphi_i(\vec{x}_1,\vec{x}_2)$ denotes the two-electron ground state wave function of the $\mathrm{Li}^{+}(1s^2)$ ion. The functions $\varphi_{nlm}(\vec{s}_1)$ and $\varphi_{\mathrm{T}}(\vec{x}_2)$ in Eq. (2) represent the bound state wave functions of the hydrogen-like atomic systems $\mathrm{H}(nlm)$ and $\mathrm{Li}^{2+}(1s)$ respectively.

As shown in Ref. [5], the original nine-dimensional integral for transition amplitude from Eq. (2) can be reduced to a two-dimensional integral over real variables from 0 to 1, whereas for computations of the total cross sections, three-dimensional quadratures are needed. An extensive analytical study of the post version of the transition amplitude for electron capture into the arbitrary nlm final states of the projectile was carried out in Ref. [6]. The post form of the transition amplitude was derived in terms of five-dimensional real integrals for numerical computations.

In the present work, we have used the two parameter wave-function of Silverman *et al.* [7] for the ground state of lithium ion: $\varphi_i(\vec{x}_1,\vec{x}_2) = (N/\pi)(\mathrm{e}^{-\alpha_1 x_1 - \alpha_2 x_2} + \mathrm{e}^{-\alpha_2 x_1 - \alpha_1 x_2})$, where $N^{-2} = 2[(\alpha_1\alpha_2)^{-3} + (\alpha_1/2 + \alpha_2/2)^{-6}]$ with $\alpha_1 = 3.294909$, $\alpha_2 = 2.078981$ and $E_i = -7.248748$. The total cross section is given by: $Q_{if}(\pi a_0^2) = \frac{1}{2\pi^2 v^2}\int\limits_0^\infty \mathrm{d}\eta\eta|T_{if}|^2$. The total cross sections for capture into any states for reaction (1), can be obtained by means of following formulae according to the Oppenheimer $(n)^{-3}$ scaling law: $Q_{\mathrm{tot}} \simeq Q_1 + Q_2 + Q_3 + 2.56124 Q_4$.

The results of our computations of the state-selective and the total cross sections for reaction (1) in prior form are summarized in Table

at impact energies 50-1500 keV. The cross sections are obtained by means of the two-parameter wave function of Silverman *et al.* [7] for the ground state of the Li^+ target. The results from Table 1 indicate that $Q_{ns} > Q_{np}$, $Q_{np} > Q_{nd}$ and $Q_{nd} > Q_{nf}$ at all the considered energies. All numerical integrations are performed by means of the Gauss-Legendre quadrature. The numbers of the Gauss-Legendre quadrature points are varied until convergence to two decimal places has been attained for state-selective and total cross sections.

In Figure 1. we compare our theoretical results for prior total cross sections for $p - Li^+$ collisions with the available experimental data. The full line shows the results obtained by means of the two-parameter wave function of Silverman *et al.* [7], whereas dashed line represents the cross sections obtained by using uncorrelated one-parameter Hylleraas wave function.

	Energy (keV)				
Final state nl	50	70	100	150	200
$1s$	2.57[-17]	1.78[-17]	1.12[-17]	5.57[-18]	2.99[-18]
$2s$	2.20[-18]	1.66[-18]	1.14[-18]	6.29[-19]	3.57[-19]
$2p$	1.27[-18]	7.32[-19]	3.81[-19]	1.63[-19]	7.96[-20]
$3s$	6.08[-19]	4.63[-19]	3.25[-19]	1.83[-19]	1.05[-19]
$3p$	4.09[-19]	2.42[-19]	1.28[-19]	5.53[-20]	2.73[-20]
$3d$	1.43[-20]	8.16[-21]	3.83[-21]	1.43[-21]	6.43[-22]
$4s$	2.50[-19]	1.92[-19]	1.35[-19]	7.65[-20]	4.40[-20]
$4p$	1.77[-19]	1.05[-19]	5.59[-20]	2.43[-20]	1.21[-20]
$4d$	8.26[-21]	4.77[-21]	2.25[-21]	8.43[-22]	3.82[-22]
$4f$	7.51[-23]	4.38[-23]	1.92[-23]	6.30[-24]	2.66[-24]
Q_{tot}	3.13[-17]	2.17[-17]	1.37[-17]	6.86[-18]	3.70[-18]

	Energy (keV)				
Final state nl	300	500	700	1000	1500
$1s$	1.03[-18]	1.99[-19]	5.72[-20]	1.33[-20]	2.19[-21]
$2s$	1.29[-19]	2.57[-20]	7.40[-21]	1.73[-21]	2.83[-22]
$2p$	2.35[-20]	3.43[-21]	7.77[-22]	1.36[-22]	1.55[-23]
$3s$	3.82[-20]	7.65[-21]	2.21[-21]	5.15[-22]	8.43[-23]
$3p$	8.15[-21]	1.20[-21]	2.73[-22]	4.78[-23]	5.47[-24]
$3d$	1.68[-22]	1.97[-23]	3.67[-24]	5.04[-25]	4.19[-26]
$4s$	1.61[-20]	3.23[-21]	9.34[-22]	2.18[-22]	3.59[-23]
$4p$	3.61[-21]	5.34[-22]	1.22[-22]	2.13[-23]	2.43[-24]
$4d$	1.00[-22]	1.18[-23]	2.20[-24]	3.02[-25]	2.52[-26]
$4f$	6.33[-25]	6.09[-26]	9.44[-27]	1.02[-27]	6.27[-29]
Q_{tot}	1.28[-18]	2.47[-19]	7.06[-20]	1.63[-20]	2.68[-21]

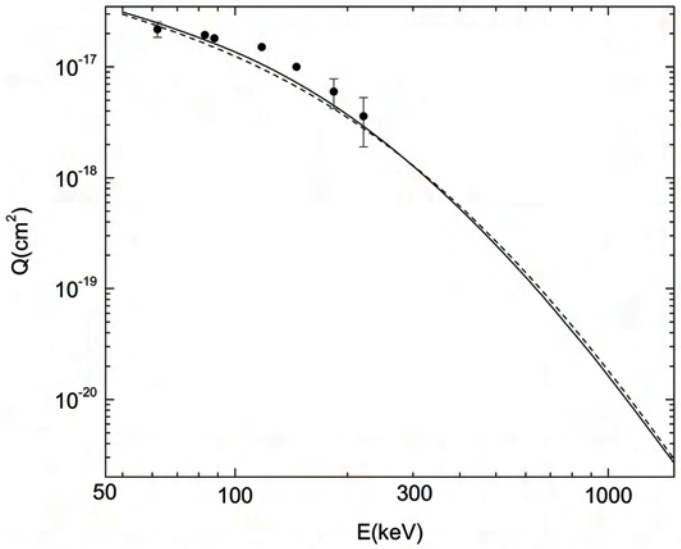

Figure 1. Total cross section for reaction (1). Full line: the CB1-4B results with Silverman *et al.* [7] function, dashed line: CB1-4B results with Hylleraas wave function. Experimental data: • Sewell *et al.* [8]

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REFERENCES

[1] Dž. Belkić, R. Gayet and A. Salin, Phys. Rep. **56**, 279 (1979); D. Dollard, J. Math. Phys. **5**, 729 (1964).

[2] Dž. Belkić, *Principles of Quantum Scattering Theory* (Institute of Physics, Bristol, 2004).

[3] Dž. Belkić, *Quantum Theory of High-Energy Ion-Atom Collisions* (Taylor & Francis, London 2008).

[4] Dž. Belkić, I. Mančev and J. Hanssen, Rev. Mod. Phys. **80**, 249 (2008).

[5] I. Mančev, N. Milojević and Dž. Belkić, Phys. Rev. A **86**, 022704 (2012).

[6] I. Mančev, N. Milojević and Dž. Belkić, Phys. Rev. A **88**, 052706 (2013).

[7] J.N. Silverman, O. Platas, F.A. Matsen, J. Chem. Phys. **32**, 1402 (1960).

[8] E.C. Sewell, G.C. Angel, K.F. Dunn and H.B. Gilbody, J. Phys. B: At. Mol. Phys. **13**, 2269 (1980).