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POST-PRIOR DISCREPANCY IN THE CB1-4B METHOD FOR SINGLE-ELECTRON CAPTURE IN FAST Li^{3+} + He COLLISIONS

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Abstract. Post-prior discrepancy in the four-body boundary-corrected first Born approximation (CB1-4B) is investigated. For this purpose, the state-selective Q_{nlm} and state-summed Q_{nl}, Q_n and Q_Σ total cross sections for single-electron capture at intermediate and high impact energies in Li^{3+} + He collisions in post form of the CB1-4B approximation have been calculated. For state-summed total cross sections Q_Σ, the theoretically obtained results were compared with available measurements, and excellent agreement was observed. Examining the post-prior discrepancy is essential to determine whether the same physical assumptions are included in the prior and post forms of the CB1-4B approximations.

1. INTRODUCTION

The systematic study of collision processes is one of the main sources of information about the structure of matter (atoms and molecules) as well as the interactions between the particles that make up these systems. On the other hand, charge-exchange collision processes are very important in assessing the energy loss of ions (e.g. protons and carbon nuclei) passing through tissue in the process of ion therapy for tumor tissue (Belkić 2010, Belkić 2013a, Belkić 2013b). Also, single-electron capture in collisions of fast projectiles with atomic and ionic targets, as one of the most extensively studied charge-exchange processes (Mančev et al. 2012, Mančev et al. 2013a, Mančev et al. 2013b, Milojević 2014, Milojević et al. 2017), is crucial for describing astrophysical phenomena (Heng et al. 2008), processes of neutralization and charging of plasma constituents (Thomas 2012), as well as in thermonuclear research (Marchuk 2014). Because of all these, single-electron capture remains a subject of significant theoretical investigation today (Milojević et al. 2020, Milojević et al. 2023).

In this paper, single-electron capture in collisions of fast lithium nuclei with helium atoms in the ground state is theoretically investigated. A four-body boundary-corrected first Born (CB1- 4B) approximation in both prior and post forms is used. For this collision system, the results in the prior form of the CB1-4B approximation have already been calculated in previous work (Mančev et al. 2012), while in the post form of the CB1-4B approximation, the results for capture into the excited states of the projectile Li^{2+} in the exit channel are presented here for the first time.

Atomic units will be used throughout unless otherwise stated.

2. THEORY

The considered single-electron capture is schematically represented as:

$$\mathrm{Li}^{3+} + \mathrm{He}(1s^2) \longrightarrow \mathrm{Li}^{2+}(nlm) + \mathrm{He}^{+}(1s), \tag{1}$$

$$\mathrm{Li}^{3+} + \mathrm{He}(1s^2) \longrightarrow \mathrm{Li}^{2+}(\Sigma) + \mathrm{He}^{+}(1s), \tag{2}$$

where nlm is the usual set of three quantum numbers of hydrogenlike atomic systems Li^{2+}, while the symbol Σ denotes the capture into all final states of the projectile Li^{2+} in the exit channel. The parentheses symbolize the bound states.

The prior form of the state-selective transition amplitude for process (1) in the CB1-4B approximation read as (Mančev et al. 2012):

$$T_{nlm}^{\mathrm{CB1-4B-}}(\vec{\eta}) = 3\iiint \mathrm{d}\vec{x}_1\mathrm{d}\vec{x}_2\mathrm{d}\vec{R}\,\varphi_{nlm}^{*}(\vec{s}_1)\varphi_{100}^{*}(\vec{x}_2)(2/R-1/s_1-1/s_2)\varphi_i(\vec{x}_1,\vec{x}_2) \times \mathrm{e}^{-i\vec{\alpha}\cdot\vec{R}-i\vec{v}\cdot\vec{x}_1}(vR+\vec{v}\cdot\vec{R})^{2i/v} \equiv T_{nlm}^{-}(\vec{\eta}), \tag{3}$$

while in the post form of the state-selective transition amplitude is given by (Mančev et al. 2013):

$$T_{nlm}^{\mathrm{CB1-4B+}}(\vec{\eta}) = \iiint \mathrm{d}\vec{x}_1\mathrm{d}\vec{x}_2\mathrm{d}\vec{R}\,\varphi_{nlm}^{*}(\vec{s}_1)\varphi_{100}^{*}(\vec{x}_2)\Big[3(1/R-1/s_2) + 1/R-2/x_1+1/r_{12}\Big]\varphi_i(\vec{x}_1,\vec{x}_2)\mathrm{e}^{-i\vec{\alpha}\cdot\vec{R}-i\vec{v}\cdot\vec{x}_1}(vR+\vec{v}\cdot\vec{R})^{2i/v} \equiv T_{nlm}^{+}(\eta), \tag{4}$$

where $\vec{v} = v\hat{z}$ is the velocity of the projectile along the $z-$ axis, with the unit vector $\hat{z}$, which is determined by the velocity of the projectile before the collision. In processes (1) and (2), two electrons are also involved, denoted as e_1 and e_2, which are bound to the helium atom in the entrance channel. Quantities $\vec{s}_1$ and $\vec{s}_2$ ($\vec{x}_1$ and $\vec{x}_2$) represent the position vectors of the first and second electrons (e_1 and e_2) relative to the Li^{3+} (alpha particles, He^{2+}), respectively. The relative position of lithium Li^{3+} with respect to He^{2+} denoted as $\vec{R}$. The vector of the distance between the two electrons e_1 and e_2 is denoted by $\vec{r}_{12} = \vec{x}_1 - \vec{x}_2 = \vec{s}_1 - \vec{s}_2$, and we have $r_{12} = |\vec{r}_{12}|$. Here the $\vec{\alpha} = \vec{\eta} - (v/2 - (E_i + 9/[2n^2] + 2)/v)\hat{\vec{v}}$ is the momentum transfer, while transferse momentum transfer is given by $\vec{\eta} = (\eta\cos\phi_\eta, \eta\sin\phi_\eta, 0)$ with the property $\vec{\eta}\cdot\vec{v} = 0$. The functions $\varphi_{nlm}(\vec{s}_1)$ and $\varphi_{100}(\vec{x}_2)$ represent the bound state wave functions of the hydrogenlike atomic systems Li^{2+} and He^{+} in exit channel, respectively. The helium atom in the entrance channel is in the ground state $1s^2$ ($^1S_0$), so we used the symmetric two-parameter wave function of Silverman et al. (Silverman et al. 1960), which corresponds to the singlet (antisymmetric) spin state: $\varphi_{\mathrm{i}}(\vec{x}_1,\vec{x}_2) = N(\mathrm{e}^{-\alpha_1 x_1-\alpha_2 x_2} + \mathrm{e}^{-\alpha_2 x_1-\alpha_1 x_2})$, with variational parameters $\alpha_1 = 2.183171$ and $\alpha_2 = 1.18853$ where binding energy is $E_i = -2.8756614$. The normalization constant is $N = [(\alpha_1\alpha_2)^{-3} + (\alpha_1/2+\alpha_2/2)^{-6}]^{-1/2}/(\pi\sqrt{2})$.

The state-selective and state-summed total cross sections in the prior and post form CB1-4B approximation are given by:

$$Q_{nlm}^{\pm}(\pi a_0^2) = \frac{1}{2\pi^2 v^2}\int_0^\infty d\eta\eta|T_{nlm}^{\pm}(\vec{\eta})|^2,\;\; Q_{nl}^{\pm} = \sum_{m=-l}^{+l} Q_{nlm}^{\pm},\;\; Q_{n}^{\pm} = \sum_{l=0}^{n-1} Q_{nl}^{\pm}. \tag{5}$$

Numerical calculations of the integrals (5) (five-dimensional in the case of post form, and three-dimensional in the case of prior form) are performed by means of the Gauss-Legendre (GL) and Gauss-Mehler (GM) quadratures. The numbers of integration

points, $N_{\rm GL}$ and $N_{\rm GM}$, were $N_{\rm GL} \leq 96$ and $N_{\rm GM} = 20$. Namely, since the singlet spin state is in the entrance channel, the singlet spin state must also be in the exit channel because the perturbation is not spin-dependent. It follows that the total wave function in the configuration space must be symmetric in the exit channel:

$$\chi_f = N_1[\varphi^*_{nlm}(\vec{s}_1)\varphi^*_{100}(\vec{x}_2)\mathrm{e}^{-i\vec{\alpha}\cdot\vec{R}-i\vec{v}\cdot\vec{s}_1} + \varphi^*_{nlm}(\vec{s}_2)\varphi^*_{100}(\vec{x}_1)\mathrm{e}^{-i\vec{\alpha}\cdot\vec{R}-i\vec{v}\cdot\vec{x}_2}]/\sqrt{2} \qquad (6)$$

The transition amplitudes (3) and (4) are the same for both terms. Due to the non-triviality of calculating the generalized expression for the normalization constant N_1, we can approximately assume it to be equal to 1. To account for this, the total cross sections $Q^{\pm}_{nlm}(\pi a_0^2)$ needs to be multiplied by 2. The previous consideration is entirely equivalent to the consideration in the spin-independent formalism where electrons e_1 and e_2 are distinguishable, and where the multiplication by two arises from the fact that the probability of capturing electron e_1 while electron e_2 remains in the target is the same as the probability of capturing electron e_2 while electron e_1 remains in the target. State-summed total cross sections for electron capture into all the final states are obtained by applying the Oppenheimer (n^{-3}) scaling law (Oppenheimer 1928, Belkić et al. 1987) via:

$$Q_{\Sigma}^{\rm CB1-4B\pm} = Q_1^{\rm CB1-4B\pm} + Q_2^{\rm CB1-4B\pm} + 2.081 Q_3^{\rm CB1-4B\pm}. \qquad (7)$$

3. RESULTS AND DISCUSSION

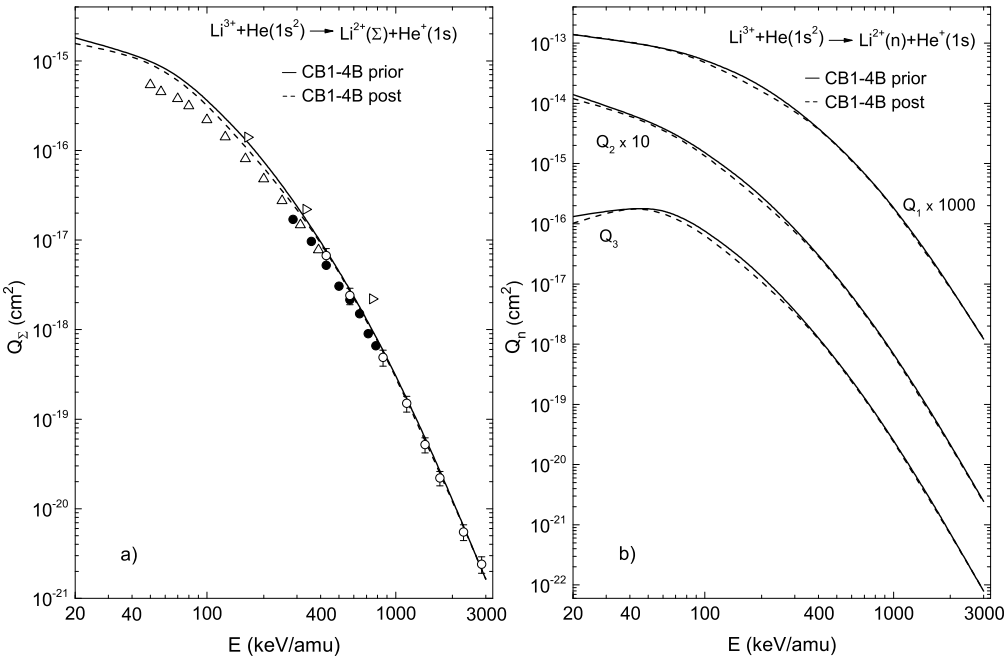

Figure 1: Panel a): Experimental data: △ (Shah and Gilbody 1985), ○ (Woitke et al. 1998), ▷ (Nikolaev et al. 1961), ● (Sant'Anna et al. 2009).

For the study of single-electron capture (1) and (2), numerical results have been obtained in post form for the total cross sections Q_1, Q_2, Q_3 and Q_Σ in the energy

range from 20 keV/amu to 3000 keV/amu. These results, together with those from the prior form (Mančev et al. 2015), are presented in Figure 1, Q_Σ in panel (a) alongside available experimental data, and Q_1, Q_2, Q_3 in panel (b). As can be seen, the experimental data are well matched except for the measurements by Nikolaev et al. (Nikolaev et al. 1961), which exceed the others in the energy range of 164-752 keV. Both forms show excellent agreement with the measurements at energies above 300 keV/amu, while at lower energies better agreement is achieved in the post form, except for one measurement (Nikolaev et al. 1961) at an energy of 164 keV/amu, which is better described by the prior form. Additionally, the panels indicate that the post-prior discrepancy is almost negligible at higher energies.

4. CONCLUSIONS

The post-prior discrepancy in the CB1-4B approximation for the process of single-electron capture in fast collisions of lithium nuclei with helium atoms has been investigated. It has been shown that this discrepancy is small, almost negligible at high energies for the obtained state-summed cross sections. This means that the physical assumptions in the post and prior forms of the CB1-4B approximation are included in the same way (as we know, the exact transition amplitudes in the prior and post forms are equal on the energy shell). Additionally, the calculated stated-summed total cross sections Q_Σ are in excellent agreement with the experimental data at energies above 160 keV/amu.

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