**Publ. Astron. Obs. Belgrade No. 102 (2022), 41 - 44** *Contributed Paper*

# SINGLE-ELECTRON CAPTURE FROM He BY FAST ALPHA PARTICLES

NENAD MILOJEVIĆ, DANILO DELIBAŠIĆ and IVAN MANČEV

*Department of Physics, Faculty of Sciences and Mathematics, University of Niš, P.O. Box 224, 18000 Niš, Serbia*
*E–mail nenad.milojevic@pmf.edu.rs*

**Abstract.** Single-electron capture cross sections in collisions between fast alpha particles and helium atoms are investigated by means of the prior form of the three- and the prior and post form of the four-body boundary-corrected first Born approximation (CB1-3B and CB1-4B, respectively). The dielectronic interaction $1/r_{12} \equiv 1/|\mathbf{r}_1 - \mathbf{r}_2|$ explicitly appears in the complete perturbation potential $V^+$ of the post four-body transition probability amplitude $T_{nlm}^{4B+}$. An illustrative computation is performed involving state-selective and state-summed total cross sections at intermediate and high impact energies. The obtained theoretical state-summed total cross sections are in excellent agreement with the available experimental data.

## 1. INTRODUCTION

Single-electron capture from one- and multielectron targets, as one of the charge-exchange processes, is very important in a number of applications in astrophysics (Heng et al. 2008), plasma physics (Thomas 2012), thermonuclear fusion research (Marchuk 2014) and medical ion therapy of tumors (Belkić 2021a, Belkić 2021b). Electron capture from He by ionized impurities in plasma gives a unique method for measuring the concentration of impurity nuclei (Joachain et al. 1981).

The present work is a theoretical investigation of single-electron capture from helium atoms in the ground state $\mathrm{He}(1s^2)$ colliding with alpha particles $\mathrm{He}^{2+}$. We studied this pure four-body problem by using three high energy first order theories, the prior form of the three-body boundary-corrected first Born (CB1-3B) approximation and the prior and the post form of the four-body boundary-corrected first Born (CB1-4B) approximation. These methods preserve the correct boundary conditions in both entrance and exit collisional channels according to the principles of quantum scattering theory, where it is known that the boundary conditions (Dollard 1964, Belkić 2004, Belkić 2009) are of essential importance for atomic collisions whenever the aggregates are charged in the asymptotic channels. The CB1-3B method in both forms was first developed in the work (Belkić et al. 1979), while the CB1-4B, also in both forms, was formulated and applied in the works (Mančev et al. 2012, Mančev et al. 2013) Atomic units will be used throughout unless otherwise stated.

## 2. THEORY

We are considering the following symmetric collisions:

$$Z_{\rm P} + (Z_{\rm T}, e_1, e_2)_{1s^2} \rightarrow (Z_{\rm P}, e_1)_{nlm} + (Z_{\rm T}, e_2)_{1s}\,, \tag{1}$$

$$Z_{\rm P} + (Z_{\rm T}, e_1, e_2)_{1s^2} \rightarrow (Z_{\rm P}, e_1)_{\Sigma} + (Z_{\rm T}, e_2)_{1s}, \tag{2}$$

where $Z_{\rm P} = 2$ and $Z_{\rm T} = 2$ are the charges of the bare projectile P and target nucleus T, $nlm$ is the usual set of three quantum numbers of hydrogenlike atomic systems while the symbol $\Sigma$ denotes the capture into all final states of the projectile. The parentheses symbolize the bound states. 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 nuclear charge of the projectile $Z_{\rm P}$ (target $Z_{\rm T}$), respectively. Further, let $\vec{R}$ be the position vector of $Z_{\rm P}$ with respect to $Z_{\rm T}$. The CB1-3B method, as a purely three-body theory, is not instantly usable for the four-particle process (1). For this reason we used the frozen-core approximation in which the non-captured, passive electron ($e_2$) is assumed to occupy the same orbital before and after capture of the active electron ($e_1$). We also applied independent particles model in which the passive electron $e_2$ is turned on only through a shielding the original nuclear charge $Z_{\rm T}$. Based on these assumptions we can write $Z_{\rm T}^{\rm eff} = Z_{\rm T} - 5/16$ instead $Z_{\rm T}$, where 5/16 is the Slater screening constant charge. Now, in three-body formalism, the original processes (1) and (2) are reduced to one-electron counterpart:

$$Z_{\rm P} + (Z_{\rm T}^{\rm eff}, e)_{1s} \rightarrow (Z_{\rm P}, e)_{nlm} + Z_{\rm T}^{\rm eff},\; Z_{\rm P} + (Z_{\rm T}^{\rm eff}, e)_{1s} \rightarrow (Z_{\rm P}, e)_{\Sigma} + Z_{\rm T}^{\rm eff}. \tag{3}$$

The prior and post form of the state-selective transition amplitude for process (1) in the CB1-4B approximation read as (Mančev et al. 2012, Mančev et al. 2013):

$$T_{nlm}^{4B\pm}(\vec{\eta}) = \iiint {\rm d}\vec{x}_1 {\rm d}\vec{x}_2 {\rm d}\vec{R} \varphi_{nlm}^{*}(\vec{s}_1)\varphi_{100}^{*}(\vec{x}_2) V^{\pm} \varphi_i(\vec{x}_1, \vec{x}_2) {\rm e}^{-i\vec{\alpha}\cdot\vec{R} - i\vec{v}\cdot\vec{x}_1} (vR + \vec{v}\cdot\vec{R})^{i\xi}\,, \tag{4}$$

$$V^{-} = Z_{\rm P}\left(\frac{2}{R} - \frac{1}{s_1} - \frac{1}{s_2}\right),\; V^{+} = Z_{\rm P}\left(\frac{1}{R} - \frac{1}{s_2}\right) + (Z_{\rm T} - 1)\left(\frac{1}{R} - \frac{1}{x_1}\right) + \frac{1}{r_{12}} - \frac{1}{x_1}. \tag{5}$$

On the other hand, the prior form of the state-selective transition amplitude for process (3) in the CB1-3B approximation can be written as (Belkić et al. 1987):

$$T_{nlm}^{3B-}(\vec{\eta}) = Z_{\rm P} \iint {\rm d}\vec{s} {\rm d}\vec{R} \varphi_{nlm}^{*}(\vec{s}) \left(\frac{1}{R} - \frac{1}{s}\right) \varphi_{100}(\vec{x}) {\rm e}^{i\vec{\beta}\cdot\vec{R} - i\vec{v}\cdot\vec{s}} (vR + \vec{v}\cdot\vec{R})^{i\frac{Z_{\rm P} - Z_{\rm T}^{\rm eff}}{v}}\,, \tag{6}$$

where $\xi = (Z_{\rm P} - Z_{\rm T} + 1)/v$ and $v$ is the velocity of the projectile along the $z-$ axis. 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 $\vec{\alpha} = \vec{\eta} - (v/2 - (E_i + Z_{\rm P}^2/[2n^2] + Z_{\rm T}^2/2)/v)\hat{\vec{v}}$ and $\vec{\beta} = -\vec{\eta} - (v/2 + (Z_{\rm P}^2/[2n^2] - (Z_{\rm T}^{\rm eff})^2/2)/v)\hat{\vec{v}}$ are the momentum transfers, 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 position vectors of the electron relative to the $Z_{\rm T}^{\rm eff}$ and $Z_{\rm P}$ are denoted by $\vec{x}$ and $\vec{s}$, respectively. The functions $\varphi_{nlm}(\vec{s}_1)$, $\varphi_{100}(\vec{x}_2)$, $\varphi_{nlm}(\vec{s})$ and $\varphi_{100}(\vec{x})$ represent the bound state wave functions of the hydrogen-like atomic systems $(Z_{\rm P}, e_1)_{nlm}$, $(Z_{\rm T}, e_2)_{1s}$, $(Z_{\rm P}, e)_{nlm}$ and $(Z_{\rm T}^{\rm eff}, e)_{1s}$, respectively. The superscripts $-$ and $+$ denote the prior and the post form, respectively. We shall use the two-parameter wave function of Silverman et al. (Silverman et al. 1960) for the ground state of the He($1s^2$):

$\varphi_{\rm i}(\vec{x}_1,\vec{x}_2) = N(\mathrm{e}^{-\alpha_1 x_1-\alpha_2 x_2}+\mathrm{e}^{-\alpha_2 x_1-\alpha_1 x_2})$, with $\alpha_1 = 2.183171$ and $\alpha_2 = 1.18853$ and $E_i = -2.8756614$, where $N$ is the normalization constant.

The nine-dimensional integral for transition amplitude (4) can be analytically reduced to a two- and four-dimensional integral over real variables in prior and post form, respectively. In the three-body case, six-dimensional integral (6) is reduced to a two dimensional over real variables. Finally, the state-selective total cross sections in the CB1-4B and CB1-3B methods are given by:

$$Q_{nlm}^{4B\pm,3B-}(\pi a_0^2)=\frac{1}{2\pi^2 v^2}\int_0^\infty d\eta\eta|T_{nlm}^{4B\pm,3B-}(\vec{\eta})|^2,\;\; Q_n^{4B\pm,3B-}=\sum_{l=0}^{n-1}\sum_{m=-l}^{+l} Q_{nlm}^{4B\pm,3B-}. \quad (7)$$

Numerical calculations of the integral (7) are performed by means of the Gauss-Legendre (GL) and Gauss-Mehler (GM) quadratures. The numbers $N_{GL}$ and $N_{GM}$ of integration points were $N_{GL} \leq 112$ and $N_{GM} \leq 20$. 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) via:

$$Q_\Sigma^{4B-,3B-} = Q_1^{4B-,3B-} + Q_2^{4B-,3B-} + Q_3^{4B-,3B-} + 2.561 Q_4^{4B-,3B-}, \quad (8)$$

$$Q_\Sigma^{4B+} = Q_1^{4B+} + Q_2^{4B+} + 2.081 Q_3^{4B+}. \quad (9)$$

## 3. RESULTS AND DISCUSSION

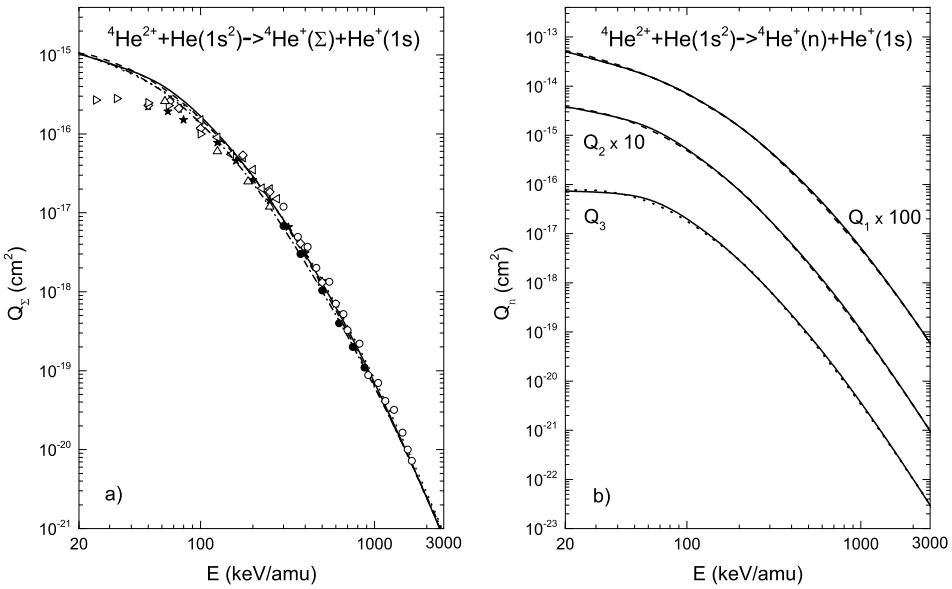


Figure 1: Panel a): State-summed total cross sections as a function of the laboratory incident energy. Present results: the full curve - CB1-4B prior, the dashed curve - CB1-4B post and the dotted curve - CB1-3B prior approximations. The dash-dotted curve represents theoretical results in the CB1 model within the RHF model (Belkić 1989). Experimental data: ○ (Hvelplund et al. 1976), △ (Mergel et al. 1995), ◇ (DuBois 1987), ▷ (Alessi et al. 2011), ◁ (Pivovar et al. 1962), ⋆ (Shah et al. 1985), • (de Castro Faria et al. 1988). Panel b): State-selective total cross sections as a function of the laboratory incident energy. Present results: the full curve - CB1-4B prior and the dashed curve - CB1-4B post approximations.

Total cross sections for the $^4He^{2+} + He(1s^2) \rightarrow {}^4He^+ + He^+(1s)$ reaction in the energy range 20 to 3000 keV/amu are plotted in Figure 1. It can be seen from panel a) that the all theoretical results (four curves) for capture into all the final states systematically exhibit excellent agreement with experimental results and each other, except that the theoretical curve (Belkić 1989) slightly underestimates presented curves, at all energies above 100 keV/amu. At energies below that value our results overestimate experimental data, which is not unexpected because these are high-energy approximations. Post-prior discrepancy is very small and only noticeable at energies below 35 keV/amu, which can be seen in panel b), where the results of the capture into $n = 1\,(Q_1 \equiv Q_1^{4B\pm})$ , $n = 2\,(Q_2 \equiv Q_2^{4B\pm})$ and $n = 3\,(Q_3 \equiv Q_3^{4B\pm})$ states are shown.

## 4. CONCLUSIONS

We have investigated the process of single-electron capture in collisions of alpha particles with helium atoms by means the prior and the post form of the CB1-4B approximations as well as the prior form of the CB1-3B method. It is found that the methods are in excellent agreement with the available measurements at energies above 100 keV/amu. The difference between the results for the prior and post cross sections is very small. This is an excellent property of the CB1-4B approximation, since the same physical assumptions are involved in the prior and post forms of this theory.

**Acknowledgements** Authors thank the Ministry of Education, Science and Technological Development of the Republic of Serbia for support under Contract No. 451-03-68/2022-14/200124.

## References

Alessi, M., Otranto, S., Focke, P. : 2011, *Phys. Rev. A* **83**, 014701.
Belkić, Dž. : 2004, *Principles of Quantum Scattering Theory*, Institute of Physics, Bristol.
Belkić, Dž. : 2008, *Quantum theory of High-Energy Ion-Atom Collisions*, London: Taylor & Francis.
Belkić, Dž. : 2021a, *Z. Med. Phys.*, **31**, 122.
Belkić, Dž. : 2021b, *Adv. Quantum Chem.*, **84**, 267.
Belkić, Dž., Gayet, R., Salin, A. : 1979 *Phys. Rep.* **56**, 279.
Belkić, Dž., Taylor, H. S. : 1987 *Phys. Rev. A* **35**, 1991.
Belkić, Dž. : 1989, *Phys. Scr.* **40**, 610.
Dollard, D. : 1964, *J. Math. Phys.*, **5**, 729.
DuBois, R. D. : 1987, *Phys. Rev. A* **36**, 2585.
de Castro Faria, N. V., Freire, Jr. F. L., de Pinho, A. G. : 1988, *Phys. Rev. A* **37**, 280.
Heng, K., Sunyaev, R. A. : 2008, *Astronomy & Astrophysics*, **481**, 117.
Hvelplund, P., Heinemeier, J., Horsdal-Pedersen, E., Simpson., F. R. : 1976, *J. Phys.B* **9**, 491.
Joachain, C. J., Post, D. E. : 1981, *Atomic and Molecular Processes in Controlled Thermonuclear Fusion*, New York: Plenum.
Marchuk, O. : 2014, *Phys. Scr.*, **89**, 114010.
Mančev I., Milojević N., Belkić Dž. : 2012, *Phys. Rev. A* **86**, 022704.
Mančev I., Milojević N., Belkić Dž. : 2013, *Phys. Rev. A* **88**, 052706.
Mergel, V., et al. : 1995, *Phys. Rev. Lett.* **74**, 2200.
Oppenheimer, J. R. : 1928, *Phys. Rev.* **31**, 349.
Pivovar, L. I., Tabuev, V. M., Novikov, M. T. : 1962, *JETP* **14**, 20.
Silverman, J. N., Platas, O., Matsen, F. A. : 1960, *J. Chem. Phys.* **32**, 1402.
Shah, M. B., Gilbody, H. B. : 1985, *J. Phys. B* **18**, 899.
Thomas, D. M., : 2012, *Phys. Plasmas* **19**, 056118.