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Single electron transfer in He⁺-He⁺ collision and production of helium atom

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Abstract. The four body Born distorted wave (BDW-4B) approximation with correct boundary condition is used for single electron transfer in He⁺-He⁺ collision. The post and prior total cross sections are obtained in the energy range 10–1000 keV/amu and the post-prior discrepancy is estimated. The sensitivity of the results with respect to the choice of the final helium-like ground state wave function is evaluated through two different wave functions. The importance of the dynamic electron correlations is tested as a function of impact energy. Additional experimental data at higher impact energies is needed for a better assessment of the validity of the present theory.

1 Introduction

A great deal of attention since the early years of quantum mechanics has been paid to the high energy collisions [\[1](#page-5-0)[–3](#page-5-1)]. One reason for this large amount of attention is the significant importance of high-energy collisions across interdisciplinary fields, which are extended from astrophysics to medicine [\[4](#page-5-2)[–8\]](#page-5-3). Among all types of collision charge exchange and ionization attract more consideration. Firstly most of the theoretical methods which used to describe ion-atom collisions were three body ones and frequently, for the processes with more than three particles, the independent particle model (IPM) was employed. As the experiments became more and accurate, new theoretical methods such as different four-body methods were developed with the primary purpose of better understanding of double electron transfer in the ion-atom collisional processes [\[9](#page-5-4)[–11](#page-5-5)].

In four-body theories, two electrons and two nuclei participate. These processes included: (a) collisions of bare ion as a projectile with helium-like atomic system as a target; (b) collisions between two hydrogen-like atomic systems. Various four-body theories have been proposed up to now, for describing one and two-electron transitions. Among them, there are theories which satisfy correct boundary conditions both in the entrance and exit channels. The concept of correct boundary condition is not just the correct asymptotic behavior of the scattering wave functions at asymptotic states furthermore, these wave functions must be in full accordance with associated perturbation potentials $[4-7,12]$ $[4-7,12]$ $[4-7,12]$ $[4-7,12]$. Some of these methods with

correct boundary conditions are as follows: the four-body corrected first Born approximation (CB1-4B) [\[13](#page-5-8)[–16\]](#page-5-9), the four-body continuum distorted wave (CDW-4B) [\[17](#page-5-10)[–21](#page-5-11)], the four-body boundary corrected continuum intermediate states (BCIS-4B) [\[22](#page-5-12)[–25](#page-5-13)], the four-body Born distorted wave (BDW-4B) [\[26](#page-5-14)[–32](#page-5-15)] and the Coulomb-Born distorted wave approximation (CBDW-4B) [\[33](#page-5-16)].

In this work, the BDW-4B method is used. This method is one kind of the distorted wave theories. In 1966 Dodd and Greider [\[34](#page-5-17)] showed that the kernel of the general distorted wave integral equation, in the case of rearrangement collisions, suffers from the disconnected diagrams which leads to troublesome divergence. These dangerous diagrams come from the freely propagating particles which do not interact with the other particles. To eliminate these disconnected diagrams Dodd and Greider offered a method [\[35](#page-6-0)] in which, under the mass condition, the obtained integral equation can be made connected via the introduction of the virtual intermediate channel and by suitable choice of channel potentials. Dodd and Greider integral equation can also be written for four-body collisions [\[7](#page-5-6)[,36](#page-6-1)]. BDW-4B method is a consistent first-order perturbation term of the Dodd-Greider integral equations.

In present work, we are interested to employ the BDW-4B approximation for the collision of two hydrogen-like atoms. This approximation is a hybrid type method with asymmetric treatment of the entrance and exit channel. In fact, the perturbation potentials which appear in the transition amplitudes of the CDW-4B and BDW-4B methods are completely the same. In contrary with the CDW-4B method which takes full account of the electronic Coulomb continuum intermediate states in both channels, the BDW-4B method applies these states only in one

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channel depending on whether the post or prior version of the transition amplitude is used. On the other hand, in the other channel, instead of the full Coulomb wave function, it's asymptotic logarithmic phase factor for the relative motion of heavy nuclei is placed, just like CB1-4B method.

The BDW-4B method was introduced for the first time by Belkić $[27]$ $[27]$ for double electron capture in fast ionatom collisions. Then Mančev and co-workers (Mergel, Schmidt and Belkić) $[28-31]$ $[28-31]$ used this method to describe single electron exchange in the collisions of bare ions with helium-like atoms. Transfer-ionization in the protonhelium collisions has been also successfully described by this method [\[32](#page-5-15)]. Recently the post version of the BDW-4B approximation [\[37\]](#page-6-3) is used to describe the collision of H, He^{\ddagger} , Li^{2+} , B^{4+} , $\text{C}^{\ddagger+}$ with hydrogen atoms and in the reference [\[38](#page-6-4)] the post and prior version of this method for He+-H and H-H collisions are compared and their discrepancy is estimated with two different helium-like wave functions. Single electron capture from one and multi-electron target atoms by hydrogen-like projectiles has been already studied by Mančev via the CB1-4B [\[39](#page-6-5)[–41\]](#page-6-6) and CDW-4B methods [\[41](#page-6-6)[,42](#page-6-7)].

In this work, the BDW-4B method is employed for He⁺-He⁺ collisions. This collision has been previously studied by the CB1-4B and CDW-4B approximations [\[39](#page-6-5)[,41](#page-6-6)] but no computation has been reported so far within the BDW-4B method. In the second part of the present paper the post and prior versions of the BDW-4B is formulated for He⁺-He⁺ collision. In the third part, the obtained numerical results are discussed and the contribution of the electron-electron interaction which is appeared in the initial perturbation potential of the prior form of the matrix element is evaluated.

2 Theory

In the framework of nonrelativistic spin-independent quantum mechanics, a four-body process is considered here in which one hydrogen-like system as a projectile captures one electron from another hydrogen-like system, i.e.

$$
(Z_P, e_1)_{1s} + (Z_T, e_2)_{1s} \to (Z_P, e_1, e_2)_{1s^2} + Z_T. \tag{1}
$$

Here a nuclear charge of the projectile (target) is denoted by $Z_P(Z_T)$. The position vector of Z_T with the mass of M_P with respect to Z_P with the mass of M_T is indicated by \vec{R} . Let, $\vec{s}_k(\vec{x}_k)$ be the relative vector of the kth electrons with respect to $Z_P(Z_T)$. Further $\vec{r}_{12} = |\vec{s}_1 - \vec{s}_2|$ $|\vec{x}_1 - \vec{x}_2|$ is the vector of distance between the two active electrons. The center of mass of (Z_P, e_1) with respect to the center of mass of (Z_T, e_2) in the entrance channel is denoted by \vec{r}_i and Similarly, in the exit channel \vec{r}_f is the position vector of Z_T with respect to the center of mass of (Z_P, e_1, e_2) .

The prior and post form of the transition amplitudes in the BDW-4B model are given by

$$
T_{if}^{-} = \langle \phi_f^{c} | U_i | \chi_i^{+} \rangle \quad T_{if}^{+} = \langle \chi_f^{-} | U_f^{\dagger} | \phi_i^{c} \rangle, \tag{2}
$$

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respectively. Here $U_{i,f}$ and $\chi_{i,f}^{\pm}$ are the perturbation potentials and the distorted waves respectively which are the same as those come from the CDW-4B approximation. The wave functions $\phi_{i,f}^c$ are plane waves with logarithmic phase distortion at large separation distance. The mentioned potentials and wave functions are obtained in [\[37](#page-6-3)[,38\]](#page-6-4) in details. It should be mentioned that using the correct boundary condition for the BDW-4B model causes the distorted waves χ_i^+, χ_f^- , be in full accordance with the corresponding channel perturbation potentials U_i , U_f , respectively. Therefore we have

$$
U_i = Z_T \left(\frac{1}{R} - \frac{1}{x_1} \right) + \left(\frac{1}{r_{12}} - \frac{1}{s_2} \right) - \vec{\nabla}_{x_2} \ln \varphi_T(\vec{x}_2) \cdot \vec{\nabla}_{s_2}
$$
\n(3)

$$
U_f = Z_T \left(\frac{1}{R} - \frac{1}{x_1}\right) - \vec{\nabla}_{s_2} \ln \varphi_f(\vec{s}_1, \vec{s}_2) \cdot \vec{\nabla}_{x_2}
$$
(4)

$$
\chi_i^+ = N^+(\nu_P)N^+(\nu)e^{i\vec{k}_i \cdot \vec{r}_i}\varphi_P(\vec{s}_1)\varphi_T(\vec{x}_2)
$$

× ${}_1F_1(i\nu_P, 1, ivs_2 + i\vec{v} \cdot \vec{s}_2)$
× ${}_1F_1(-i\nu, 1, ik_ir_f + i\vec{k}_i \cdot \vec{r}_f)$ (5)

$$
\chi_f^- = N^-(\nu_T)N^-(\nu)e^{-i\vec{k}_f \cdot \vec{r}_f} \varphi_f(\vec{s}_1, \vec{s}_2)
$$

$$
\times {}_1F_1(-i\nu_T, 1, -i\nu x_2 - i\vec{v} \cdot \vec{x}_2)
$$

$$
\times {}_1F_1(i\nu, 1, -i k_f r_i - i\vec{k}_f \cdot \vec{r}_i)
$$
 (6)

$$
\phi_i^c = N^+(\nu_i)\varphi_P(\vec{s}_1)\varphi_T(\vec{x}_2)e^{i\vec{k}_i \cdot \vec{r}_i}
$$

× ${}_1F_1(-i\nu_i, 1, ik_ir_f + i\vec{k}_i \cdot \vec{r}_f)$ (7)

$$
\phi_f^c = N^-(\nu_f)\varphi_f(\vec{s}_1, \vec{s}_2)e^{-i\vec{k}_f \cdot \vec{r}_f}
$$

$$
\times {}_1F_1(i\nu_f, 1, -ik_f r_i + i\vec{k}_f \cdot \vec{r}_i), \qquad (8)
$$

with

$$
\nu_P = (Z_T - 1)/\nu, N^+(\nu_P) = \Gamma(1 - i\nu_P)e^{\pi\nu_P/2},
$$

\n
$$
\nu = Z_T(Z_P - 1)/\nu, N^{\pm}(\nu) = \Gamma(1 \pm i\nu)e^{-\pi\nu/2},
$$

\n
$$
\nu_T = Z_T/\nu, N^-(\nu_T) = \Gamma(1 + i\nu_T)e^{\pi\nu_T/2},
$$

\n
$$
\nu_i = (Z_P - 1)(Z_T - 1)/\nu, N^+(\nu_i) = \Gamma(1 + i\nu_i)e^{-\pi\nu_i/2},
$$

\n
$$
\nu_f = Z_T(Z_P - 2)/\nu
$$

and

$$
N^-(\nu_f) = e^{-\pi \nu_f/2} \Gamma(1 - i\nu_f).
$$

Here $_1F_1(a, b, c)$ is the symbol of the conventional confluent hypergeometric function. The bound-state wave functions of the initial atomic systems (Z_P, e_1) and (Z_T, e_2) are denoted by $\varphi_P(\vec{s}_1)$ and $\varphi_T(\vec{x}_2)$ respectively and $\varphi_f(\vec{s}_1, \vec{s}_2)$ is the bound-state wave function of the newly formed helium-like atomic system. The quantities \vec{k}_i and \vec{k}_f represent the initial and final wave vectors respectively and v is the incident velocity chosen along the Z-axis. By inserting (3) – (8) in (2) , the prior and post transition amplitude take the following forms

$$
T_{if}^{-} = N^{+}(\nu_{P}) \iiint d\vec{s_{1}} d\vec{x_{2}} d\vec{R} e^{i(\vec{k}_{i} \cdot \vec{r}_{i} + \vec{k}_{f} \cdot \vec{r}_{f})}
$$

\n
$$
\times \varphi_{f}^{*}(\vec{s_{1}}, \vec{s_{2}}) \Re^{-} \left\{ [V(R, x_{1}) + V(r_{12}, s_{2})] \varphi_{P}(\vec{s_{1}}) \varphi_{T}(\vec{x_{2}}) {_{1}F_{1}}(i\nu_{P}, 1, i\nu s_{2} + i\vec{v} \cdot \vec{s_{2}}) - \vec{\nabla}_{x_{2}} \varphi_{T}(\vec{x_{2}}) \cdot \vec{\nabla}_{s_{2}1} F_{1}(i\nu_{P}, 1, i\nu s_{2} + i\vec{v} \cdot \vec{s_{2}}) \varphi_{P}(\vec{s_{1}}) \right\}
$$

\n
$$
T_{if}^{+} = N^{-^{*}}(\nu_{T}) \iiint d\vec{s_{1}} d\vec{s_{2}} d\vec{R} e^{i(\vec{k}_{i} \cdot \vec{r}_{i} + \vec{k}_{f} \cdot \vec{r}_{f})}
$$

\n
$$
\times \varphi_{P}(\vec{s_{1}}) \varphi_{T}(\vec{x_{2}}) \Re^{+}
$$

\n
$$
\times \left[V(R, x_{1}) \varphi_{f}^{*}(\vec{s_{1}}, \vec{s_{2}}) {_{1}F_{1}}(i\nu_{T}, 1, i\nu x_{2} + i\vec{v} \cdot \vec{x_{2}}) - \vec{\nabla}_{s_{2}} \varphi_{f}^{*}(\vec{s_{1}}, \vec{s_{2}}) \cdot \vec{\nabla}_{x_{2}1} F_{1}(i\nu_{T}, 1, i\nu x_{2} + i\vec{v} \cdot \vec{x_{2}}) \right]
$$

\n(10)

where the terms

$$
V(R, x_1) = Z_T \left(\frac{1}{R} - \frac{1}{x_1}\right), \quad V(r_{12}, s_2) = \left(\frac{1}{r_{12}} - \frac{1}{s_2}\right)
$$

are short range potentials, since they are the difference between the finite terms $1/x_1$, $1/s_2$ and their asymptotic tails $1/R$, $1/r_{12}$, respectively. The $\vec{\nabla} \cdot \vec{\nabla}$ terms in [\(9\)](#page-2-0) and [\(10\)](#page-2-1) are the non-local potentials which show that the two centers Z_p and Z_T simultaneously act on the active electron e_2 via bound states $\varphi_{i.f}$ and continuum states $_1F_1$. Using the eikonal mass limit $\vec{R} \simeq -\vec{r}_f \simeq \vec{r}_i \ (M_{P,T} \gg 1),$ the functions \Re^{\mp} are reduced to

$$
\mathcal{R}^{-} = N^{+}(\nu)(N^{-}(\nu_{f}))^{*} {}_{1}F_{1} \left(-i\nu, 1, ik_{i}r_{f} + i\vec{k}_{i} \cdot \vec{r}_{f}\right)
$$

\n
$$
\times {}_{1}F_{1} \left(-i\nu_{f}, 1, ik_{f}r_{i} + i\vec{k}_{f} \cdot \vec{r}_{i}\right)
$$

\n
$$
\simeq \mu_{i}^{i\nu}\mu_{f}^{i\nu_{f}}(\rho v)^{2i\nu} \left(\nu R + \vec{v} \cdot \vec{R}\right)^{i\xi^{-}}
$$
, $\xi^{-} = -\frac{Z_{T}}{\nu}$
\n
$$
\mathcal{R}^{+} = N^{+}(\nu_{i})N^{-*}(\nu) {}_{1}F_{1} \left(-i\nu_{i}, 1, ik_{i}r_{f} + i\vec{k}_{i} \cdot \vec{r}_{f}\right)
$$

\n
$$
\times {}_{1}F_{1} \left(-i\nu, 1, ik_{f}r_{i} + i\vec{k}_{f} \cdot \vec{r}_{i}\right)
$$

\n
$$
\simeq \mu_{i}^{i\nu_{i}}\mu_{f}^{i\nu}(\rho v)^{2i\nu_{i}} \left(\nu R + \vec{v} \cdot \vec{R}\right)^{i\xi^{+}}
$$
, $\xi^{+} = \frac{Z_{p} - 1}{\nu}$
\n(12)

where an unimportant phase factors $(\mu_i^{i\nu} \mu_f^{i\nu_f} v^{2i\nu})$ and $\mu_i^{i\nu_i} \mu_f^{i\nu} v^{2i\,\nu_i}$) of unit moduli can be dropped. Furthermore $\vec{\rho}$ is the projection of \vec{R} onto XOY plane, i.e. $\vec{\rho} \cdot \vec{Z} = 0$. It should be stated that in spite of the existence of vector \vec{R} which is the inter-nuclear distance, in the eikonal logarithmic phase factors (11) and (12) , the only dependence of the transition amplitude to the inter-nuclear repulsive potential $V_{PT} = Z_{PT}/R$ is through the factor $\rho^{2iZ_PZ_T/v}$. The factor $\rho^{2iZ_PZ_T/v}$ as a part of factors

 $\rho^{2i\nu} = \rho^{2iZ_T(Z_P-1)/\nu}$ and $\rho^{2i\nu_i} = \rho^{2i(Z_P-1)(Z_T-1)/\nu}$ has no effect on the total cross sections. Thus the eikonal total cross section is independent of inter-nuclear repulsive potential. The factors $\rho^{2i \nu}$ and $\rho^{2i \nu_i}$ are important only for differential cross sections but do not contribute to the total cross sections. Using the eikonal mass limit which is associated with the scattering in also the forward direction for heavy particles, we have

$$
\vec{k}_i \cdot \vec{r}_i + \vec{k}_f \cdot \vec{r}_f = -\vec{\alpha} \cdot \vec{R} - \vec{v} \cdot \vec{x}_2
$$

$$
= \vec{\beta} \cdot \vec{R} - \vec{v} \cdot \vec{s}_2
$$

$$
= \vec{\alpha} \cdot \vec{s}_2 + \vec{\beta} \cdot \vec{x}_2 \tag{13}
$$

where $\vec{\alpha}$ and $\vec{\beta}$ are momentum transfers and defined by

$$
\vec{\alpha} = \vec{\eta} - \left(\frac{v}{2} - \frac{\varepsilon_i - \varepsilon_f}{v}\right)\hat{v}, \ \vec{\beta} = -\vec{\eta} - \left(\frac{v}{2} + \frac{\varepsilon_i - \varepsilon_f}{v}\right)\hat{v},
$$

$$
\vec{\alpha} + \vec{\beta} = -\vec{v}
$$
(14)

and $\varepsilon_{i,f}$ are the initial and final bound-states energies respectively. $\vec{\eta} = (\eta \cos \phi_{\eta}, \eta \sin \phi_{\eta}, 0)$ is the transverse component of the change in the relative momentum of a heavy particle i.e. $\vec{\eta} \cdot \vec{v} = 0$.

Finally the transition amplitudes can be expressed as

$$
T_{if}^{-BDW-4B} = N^+(\nu_P) \iiint d\vec{s_1} d\vec{x_2} d\vec{R} e^{i\vec{\beta} \cdot \vec{R} - i\vec{v} \cdot \vec{s_2}
$$

$$
\times \left(vR + \vec{v} \cdot \vec{R}\right)^{i\xi^-} \varphi_f^*(\vec{s_1}, \vec{s_2})
$$

$$
\times \left\{ [V(R, x_1) + V(r_{12}, s_2)]
$$

$$
\times {}_1F_1(i\nu_P, 1, i\nu s_2 + i\vec{v} \cdot \vec{s_2})\varphi_P(\vec{s_1})\varphi_T(\vec{x_2})
$$

$$
- \vec{\nabla}_{s_2}\varphi_T(\vec{x_2}) \cdot \vec{\nabla}_{s_2}
$$

$$
\times {}_1F_1(i\nu_P, 1, i\nu s_2 + i\vec{v} \cdot \vec{s_2})\varphi_P(\vec{s_1}) \right\}. (15)
$$

$$
T_{if}^{+BDW-4B} = N^{-*}(\nu_T) \iiint d\vec{s_1} d\vec{s_2} d\vec{R} e^{i\vec{\beta} \cdot \vec{R} - i\vec{v} \cdot \vec{s_2}
$$

$$
JJJ
$$

\n
$$
\times \left(vR + \vec{v} \cdot \vec{R}\right)^{i\xi^+} \varphi_P(\vec{s}_1)\varphi_T(\vec{x}_2)
$$

\n
$$
\times \left[V(R, x_1)\varphi_f^*(\vec{s}_1, \vec{s}_2)\right]
$$

\n
$$
\times {}_1F_1(i\nu_T, 1, ivx_2 + i\vec{v} \cdot \vec{x}_2)
$$

\n
$$
- \vec{\nabla}_{s_2}\varphi_f^*(\vec{s}_1, \vec{s}_2) \cdot \vec{\nabla}_{x_2}
$$

\n
$$
\times {}_1F_1(i\nu_T, 1, ivx_2 + i\vec{v} \cdot \vec{x}_2).
$$
 (16)

where $\xi^- = -Z_T/v$ and $\xi^+ = (Z_P - 1)/v$.

The analytical calculations of the prior and post form of the transition amplitude are completely performed in [\[37](#page-6-3)[,38](#page-6-4)]. After analytical calculations the prior and post versions are obtained in terms of five and two dimensional numerical integrals respectively. It should be mentioned that the calculation of the prior form is more difficult than the post one, especially from the numerical point of view, because of the existence of electron-electron interaction.

Fig. 1. Total cross sections in collision of two $He⁺$ ions as a function of a laboratory incident energy. The solid line represents the results of the prior form of the BDW-4B approximation. The dashed curve refers to the total cross sections of the prior form of the CDW-4B approximation [\[41](#page-6-6)]. The dotted curve represents the cross sections obtained without the term $V(r_{12}, s_2)$. The final state of He atom is described by means of the wave function of Silverman et al. [\[44](#page-6-8)]. Experimental data: Peart et al. [\[45\]](#page-6-9), \triangle Melchert et al. [\[46](#page-6-10)], \bigcirc Murphy et al. [\[47\]](#page-6-11).

The prior and post cross sections in the present method are given by the following formula

$$
Q_{if}^{\mp}(\pi a_0^2) = \frac{1}{2\pi^2 v^2} \int_0^{\infty} d\eta \eta \left| T_{if}^{\mp}(\eta) \right|^2.
$$
 (17)

3 The results of numerical computations

Presently, the total post and prior cross sections are computed for the following charge-exchange reaction

$$
{}^{4}\text{He}^{+}(1s) + {}^{4}\text{He}^{+}(1s) \rightarrow {}^{4}\text{He}(1s^{2}) + {}^{4}\text{He}^{2+}.
$$
 (18)

The computations are carried out only for capture into the final ground state $(1s^2)$. Two different final wave function are used here to assess the sensitivity of the total cross sections to the choice of the helium-like bound state wave functions. The employed wave functions are the uncorrelated one-parameter Hylleraas wave func-tion [\[43\]](#page-6-12), $\varphi_f(\vec{s_1}, \vec{s_2}) = (\vec{b}^3/\pi) e^{-b(s_1+s_2)}$ with $b = Z_p$ – 5/16 and the two-parameter wave function of Silverman et al. [\[44\]](#page-6-8) with the radial static correlations, $\varphi_f(\vec{s}_1, \vec{s}_2) =$ $(N/\pi)(e^{-\alpha_1 s_1 - \alpha_2 s_2} + e^{-\alpha_2 s_1 - \alpha_1 s_2})$ where

$$
N^{-2} = 2 [(\alpha_1 \alpha_2)^{-3} + (\alpha_1/2 + \alpha_2/2)^{-6}].
$$

The post and prior total cross sections results are presented in Table [1](#page-4-0) as well as Figures [1](#page-3-0)[–3.](#page-3-1) In Figure [1](#page-3-0) our results with the prior version of BDW-4B (solid line) are plotted and compared with the results of the prior version of CDW-4B [\[41\]](#page-6-6) (dashed line) and available experimental data $[45-47]$ $[45-47]$ in the energy range 10–1000 keV/amu. To estimate the contribution of the correlation term $V(r_{12}, s_2)$,

 100

 $Q(cm²)$

1E-18

 $1E-19$

 $1E-20$

 10

E(keV/amu) Fig. 2. Total cross sections in collisions of two He⁺ ions as a function of the laboratory incident energy. The solid line represents the results of the post form of BDW-4B theory. The dashed line shows the prior version results. The dotted line displays the results of the post form of CB1-4B approximation [\[41\]](#page-6-6). The dashed-dot-dot line refers to the results of the post version of the CDW-4B approximation [\[38\]](#page-6-4). The twoparameter wave function of Silverman et al. [\[44\]](#page-6-8) is used in all cases for the He atom. Experimental data: \blacksquare Peart et al. [\[45\]](#page-6-9), \triangle Melchert et al. [\[46\]](#page-6-10), \bigcirc Murphy et al. [\[47](#page-6-11)].

Fig. 3. Total cross sections (in cm²) as a function of incident energy E (keV/amu), for reaction 4 He⁺(1*s*)+ 4 He⁺(1*s*) → 4 He(1*s*²)+ 4 He²⁺*.* Upper (Lower) pair of curves: solid line represents the results of the prior (post) form of the BDW-4B approximation with the wave function of Silverman et al. [\[44\]](#page-6-8); dashed line shows the prior (post) version of the BDW-4B approximation with the wave function of Hylleraas [\[43](#page-6-12)]. The values of the lower curves should be multiplied by 10.

our results without this term (dotted line) are also presented in this figure. As mentioned before this correlation term is a short range potential thus omitting it from the perturbation potential U_i do not destroy the correct boundary condition. All the displayed results are obtained via the wave function of Silverman et al. [\[44\]](#page-6-8). It is clear from this figure that the present results are closer to the experiments than the CDW-4B results but all three curves overestimate the experiments especially at lower impact

1000

Table 1. Total cross sections (in cm²) as a function of incident energy E (keV/amu), for reaction ⁴He⁺(1s) + ⁴He⁺(1s) → ⁴He²⁺. The quantities $Q_{Sil}^{\pm}(Q_{Hyl}^{\pm})$ represent the results of the post and prio from the two-parameter Silverman et al. [\[44](#page-6-8)] (one-parameter Hylleraas [\[43](#page-6-12)]) wave function respectively. The prior cross sections computed without the term $V(r_{12}, s_2)$ are displayed by symbol $Q_{Si}^{1-}(Q_{Hyl}^{1-})$. The number in the square brackets indicates the powers of 10.

E	Q_{Si}^+	Q^-_{Sil}	Q_{Si}^{1-}	Q_{Hyl}^+	Q^-_{Hyl}	Q_{Hyl}^{1-}
10	$1.35 - 16$	$1.50[-15]$	$1.45\overline{[-15]}$	$1.59[-16]$	$2.04 - 15$	$1.44[-15]$
20	$1.31[-16]$	$6.36[-16]$	$5.09[-16]$	$1.58[-16]$	$8.88[-16]$	$5.19[-16]$
30	$1.38[-16]$	$3.19[-16]$	$2.54[-16]$	$1.65[-16]$	$4.83[-16]$	$2.64[-16]$
40	$1.41[-16]$	$1.89[-16]$	$1.48[-16]$	$1.68[-16]$	$2.98[-16]$	$1.56[-16]$
50	$1.19[-16]$	$1.24[-16]$	$9.45[-17]$	$1.41[-16]$	$1.99[-16]$	$1.01[-16]$
60	$9.60[-17]$	$8.66[-17]$	$6.39[-17]$	$1.13[-16]$	$1.41[-16]$	$6.92[-17]$
70	$7.67[-17]$	$6.33[-17]$	$4.51[-17]$	$9.03[-17]$	$1.04[-16]$	$4.94[-17]$
80	$6.15[-17]$	$4.77[-17]$	$3.29[-17]$	$7.22[-17]$	$7.90[-17]$	$3.64[-17]$
90	$4.96[-17]$	$3.70[-17]$	$2.47[-17]$	$5.82[-17]$	$6.14[-17]$	$2.75[-17]$
100	$4.03[-17]$	$2.92[-17]$	$1.89[-17]$	$4.71[-17]$	$4.85[-17]$	$2.12[-17]$
150	$1.57[-17]$	$1.10[-17]$	$6.22[-18]$	$1.81[-17]$	$1.81[-17]$	$7.11[-18]$
200	$7.01[-18]$	$5.12[-18]$	$2.60[-18]$	$8.03[-18]$	$8.20[-18]$	$2.98[-18]$
300	$1.91[-18]$	$1.54[-18]$	$6.67[-19]$	$2.14[-18]$	$2.33[-18]$	$7.65[-19]$
400	$6.78[-19]$	$5.97[-19]$	$2.32[-19]$	$7.44[-19]$	$8.60[-19]$	$2.63[-19]$
500	$2.87[-19]$	$2.70[-19]$	$9.74[-20]$	$3.08[-19]$	$3.74[-19]$	$1.09[-19]$
600	$1.37[-19]$	$1.37[-19]$	$4.64[-20]$	$1.45[-19]$	$1.83[-19]$	$5.13[-20]$
700	$7.20[-20]$	$7.55[-20]$	$2.43[-20]$	$7.44[-20]$	$9.72[-20]$	$2.65[-20]$
800	$4.04[-20]$	$4.35[-20]$	$1.36[-20]$	$4.11[-20]$	$5.53[-20]$	$1.47[-20]$
1000	$1.49[-20]$	$1.65[-20]$	$5.05[-21]$	$1.47[-20]$	$2.09[-20]$	$5.36[-21]$

energies. We neglect the contribution of the helium excited states in our computations and a part of this underestimation might be due to it. Unfortunately the measurements for this reaction are limited up to $E_{lab} = 114.5 \text{ keV/amu}$ and there is no experimental data at higher energies where the BDW-4B and CDW-4B are expected to have better agreement with the experiments. At higher energies the present results and the CDW-4B results are so close together. The present results without the correlation term (dotted line) lies under the prior curve at all energy range and the difference between this two curves increase at higher energies. It shows the contribution of this term is augmented as the energy increased. The same behavior has been seen in previous works [\[14](#page-5-21)[,38](#page-6-4)[,42](#page-6-7)[,48\]](#page-6-13).

The obtained results of the post version of the BDW-4B (solid line) approximation with Silverman et al. [\[44](#page-6-8)] wave function are compared with the prior results (dashed line) in Figure [2.](#page-3-2) The energy range is from 10 to 1000 keV/amu. For comparison the results of the post version of CB1-4B [\[41\]](#page-6-6) (dotted line) and CDW-4B [\[41](#page-6-6)] (dashed dot dot) methods are also presented in this figure. A comparison with the available experimental data is also made. As can be seen from this figure at lower energies the post form of the BDW-4B cross sections are smaller than the other cross sections and are closer to the experiments. All the depicted curves overestimate the available experiments. It should be mentioned that the BDW-4B, CDW-4B and CB1-4B methods are high energy approximations and better agreement with the experiments is expected at higher energies. The relative difference between

the post (line curve) and prior form (dashed curve) of the BDW-4B cross sections is significant at lower impact energies but as the energy increases this discrepancy decreases and the two curves converge at higher impact energies. At lower energies the plotted curves do not predict the same behavior for cross section but as the energy increases the curves become so close together.

The numerical results obtained by the wave function of Hylleraas [\[43](#page-6-12)] are close to the results of Silverman et al. wave function [\[44\]](#page-6-8) and to avoid clutter are not shown in Figures [1](#page-3-0) and [2.](#page-3-2) However they are available in Figure [3](#page-3-1) and Table [1.](#page-4-0) The post and prior cross sections obtained by means of the wave function of Silverman et al. are denoted by Q_{Sil}^{\pm} in Table [1](#page-4-0) respectively. The quantities Q_{Hyl}^{\pm} displayed the post and prior cross sections obtained by Helleraas wave function. Comparisons between the columns related to the post and prior cross sections show that in the case of Hylleraas wave function the discrepancy between the cross sections is significant at lower energy but it decreases at higher energies. For example the relative post-prior discrepancy expressed via δ_{Hyl} = $|Q_{Hyl}^- - Q_{Hyl}^+|/Q_{Hyl}^-$ is 92.2%, 17.6% and 29.7% at impact energies 10 keV/amu, 500 keV/amu and 1000 kev/amu respectively. Similar behavior of the cross sections was seen in the case of Silverman et al. wave function in Figure [2.](#page-3-2) and the quantity $\delta_{Sil} = |Q_{Sil} - Q_{Sil}^+|/Q_{Sil}^-$ is 91%, 6.3% and 9.7% at the same energies. The level of approximation which is made in determination of the helium-like wave function has an influence on the post- prior discrepancy.

It should be mentioned that there is no exact wave function for helium-like atoms. The columns labeled by the symbols Q_{Sil}^{1-} Q_{Sil}^{1-} Q_{Sil}^{1-} and Q_{Hyl}^{1-} in Table 1 are computed by ignoring the term $V(r_{12}, s_2)$ in the prior form. As can be seen from Table [1](#page-4-0) the contribution of this term is nonnegligible especially at higher impact energies. For example in the case of Silverman et al. wave function the quantity $\gamma = |Q_{Sil}^- - Q_{Sil}^{1-}|/Q_{Sil}^-$ which expressed the relative contribution of the correlation term is 3.3%, 63.9% and 71.4% at impact energies 10, 500 and 1000 keV/amu respectively. For Hylleraas wave function at the same energies following values of $\gamma = |Q_{Hyl}^- - Q_{Hyl}^{1-}|/Q_{Hyl}^-$ is obtained: 4.16%, 70.9% and 74.4%. previous works for single electron capture in other collisional systems show the same deduction [\[14](#page-5-21)[,38](#page-6-4)[,42\]](#page-6-7).

Finally in Figure [3](#page-3-1) we compare the total post and prior cross section obtained via two different wave function. Upper pair of curves show the results of the prior form of the cross sections obtained with two-parameter wave function of Silverman et al. [\[44\]](#page-6-8) (solid line) and one-parameter wave function of Hylleraas [\[43](#page-6-12)] (dash line). The solid line in the lower curves is the results of the post form with Silverman wave function and the dashed curve is the post cross sections with Hylleraas wave function. The values of the lower curves should be multiplied by 10. It is obvious from this figure that the results of the total cross sections, with theses two wave functions, for both forms are so close together and the sensitivity of the cross sections to the choice of the final bound state wave function is weak especially for the post form. The same conclusion was seen in our previous work $[38]$ for the collision of $He⁺$ and H with Hydrogen atom.

Previous works with BDW-4B approximation [\[26](#page-5-14)[–32](#page-5-15)[,38\]](#page-6-4) for single and two electron capture collisional processes show that this method give systematically good agreement with different experimental data at higher energies. Therefore we could say that the present theoretical results could also be reliable for He⁺-He⁺ collision. However to assess the validity of this theory for the mentioned collision new measurements are required.

4 Conclusions

This paper used the four-body born distorted wave method for the collision of two $He⁺$ ions. The BDW-4B method is an intermediate method between the CDW-4B and CB1-4B methods and satisfies the correct boundary conditions in both entrance and exit channels. Theoretical data for the post and prior cross sections is obtained here at intermediate and high energies and is compared with the CDW-4B and CB1-4B methods and available experimental data. Present calculations show that the postprior discrepancy is significant at lower impact energies for He⁺-He⁺ reaction but it decreases at higher energies. Neglecting the dynamic electron correlation term, which is explicitly included in the corresponding perturbation of the prior form, shows that the contribution of this term is not negligible especially at higher energies. The assessment of the sensitivity of the total cross sections to the choice of the final helium-like wave function with two different wave functions, shows that the dependency of the total cross sections upon the bound state wave function is weak in both versions especially in post one. To estimate the validity of present theoretical results for the mentioned reaction, additional experimental data at higher energies is desired.

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