INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS B: ATOMIC, MOLECULAR AND OPTICAL PHYSICS

J. Phys. B: At. Mol. Opt. Phys. **36** (2003) 93–104 PII: S0953-4075(03)52424-5

# Single charge exchange in fast collisions of alpha particles with helium

**Ivan Mančev**

Department of Physics, Faculty of Sciences and Mathematics, University of Niš, PO Box 224, 18000 Niš, Yugoslavia
and
Institut für Kernphysik, Universität Frankfurt, Auger-Euler-Strasse 6, 60486 Frankfurt am Main, Germany

Received 6 August 2002, in final form 1 November 2002
Published 20 December 2002
Online at stacks.iop.org/JPhysB/36/93

**Abstract**

A new second-order theory termed the Born distorted wave (BDW) approximation is introduced within the framework of the four-body scattering theory and applied to single charge exchange in fast symmetric collisions between alpha particles and helium. The present formulation allows us to isolate the role of intermediate electron continuum states. At the intermediate projectile energies, the present BDW approximation represents a substantial improvement over the continuum distorted-wave four-body formulation, thus illustrating a remarkable sensitivity of second-order theories for single charge exchange to the treatment of electronic ionization continua. Numerical results for the total cross sections show a good agreement with the available experimental data.

## 1. Introduction

The theoretical investigation of single electron capture from two- or multi-electron targets is a difficult task and, in practice, applications of many-body collision theory involve laborious calculations. The calculations are usually simplified by approximating a many-electron collision system by a model one-active electron system. According to this model, there is only one active electron whereas the others provide an effective potential where the active electron evolves, while non-captured electron(s) are considered as being passive. The net result of such a 'frozen core' approximation is a reduction of the many-particle problem to a three-body problem. Such models have been developed for single charge exchange in fast collisions between bare projectiles and helium atoms (see for example [1–13]). These models often differ in their description of the active electron. A substantially different approach to the problem of high-energy single electron capture from helium-like atoms or ions by completely stripped projectiles at intermediate and high incident energies has recently been introduced by Belkić *et al* [14]. They went beyond the model of one active electron and devised the boundary-corrected four-body version of the continuum distorted-wave (CDW-4B) theory.

0953-4075/03/010093+12$30.00  

Such extension of Cheshire's [15] three-body CDW theory to the four-body problem has been successfully applied to studies of single capture in various processes [14, 16, 17]. It should be emphasized that the CDW-4B model enables one to study the role of electronic correlation effects. In a very recent review Belkić [18] studied various mechanisms which can produce the Thomas peak in the differential cross sections. The double elastic collision of the electron $e_1$ which first scatters on the projectile ($Z_P$), and then on $e_2$, before it finally becomes bound to the projectile nucleus, leads to the maximum in the differential cross section. The first quantitative evidence of the Thomas peak due to such a $Z_P - e_1 - e_2$ mechanism in single capture from $He(e_1, e_2)$ by protons has been provided by the CDW-4B theory [18]. The charge exchange process in ion–atom collisions has been studied over a very wide region of energy, ranging from thermal to extreme relativistic energies. These collisions shall presently be examined at intermediate and high non-relativistic impact energies. However, the role of single capture and ionization events is exchanged in this energy region. Namely, it is well known that ionization dominates over charge exchange at high energies, whereas at intermediate and lower energies, electron capture becomes the dominant process over ionization. Therefore, to properly describe electron transfer to a final bound state, in the limit of high energies, electronic continuum intermediate states must be included. This is fully accomplished in the CDW-4B theory, through the introduction of the on-shell electronic Coulomb waves centred at $Z_P$ and $(Z_T - 1)$. At lower energies, however, charge exchange dominates over ionization. This time, electronic continuum states represent a drawback, since they over-account for the intermediate ionization paths of the reaction. As a result, the CDW-4B method yields unphysically large cross sections at lower energies. Hence, an overemphasis of these continuum states invalidates the CDW method for single charge exchange in comparison with experimental data at lower impact energies. Thus, we should expect that a neglect of the electronic intermediate ionization states in one channel would yield considerably smaller cross sections, especially at low energies, and formulation of such a theory is the aim of this work.

In this paper, we propose a new second-order distorted wave theory, termed the Born distorted wave (BDW) method for single charge exchange treated within the pure four-body quantum-mechanical formalism. It is a hybrid-type model which exactly coincides with the CDW-4B theory in one channel and with the four-body corrected first Born (CB1-4B) approximation in the other channel. The CB1-4B theory has already been developed for double charge exchange [19, 20] as well as single electron capture [21, 22]. The BDW method preserves the correct boundary conditions in both scattering channels, since both the CDW-4B and CB1-4B approximations do so. Such four-body one-channel distorted-wave approaches have already been developed for double electron capture [23–25].

Atomic units will be used throughout unless otherwise stated.

## 2. Theory

A four-body collision is considered in which a bare projectile ion $P$ captures one electron from a target consisting of two active electrons $e_{1,2}$, and a target ion $T$. Let the position vectors of electrons $e_{1,2}$ relative to $P$ and $T$ be respectively denoted by $\vec{s}_{1,2}$ and $\vec{x}_{1,2}$. The inter-electron distance $r_{12}$ is given by $r_{12} = |\vec{s}_1 - \vec{s}_2| = |\vec{x}_1 - \vec{x}_2|$. Let further the position vector of $P$ relative to $T$ be denoted by $\vec{R}$. In the entrance channel, it is convenient to use the set of the Jacobi coordinate vectors $\{\vec{x}_1, \vec{x}_2, \vec{r}_i\}$ where $\vec{r}_i$ is the relative vector of $P$ with respect to the centre of mass of the helium-like target. In the exit channel, the positions of the constituents of the studied system are represented by the set of vectors $\{\vec{s}_1, \vec{x}_2, \vec{r}_f\}$, with $\vec{r}_f$ being the relative vector of the centre of mass of $(T, e_2)$ with respect to the centre of mass of the newly formed hydrogen-like atomic system $(P, e_1)$.

The exact prior $T_{if}$ transition amplitude in the distorted wave theory (see for example [18]) for a charge exchanging process is

$$T_{if} = \langle \Psi_f^- | U_i | \chi_i^+ \rangle, \tag{2.1}$$

where

$$|\Psi_f^-\rangle = (1 + G^- U_f)|\chi_f^-\rangle, \qquad \text{and} \qquad U_{i,f} = V_{i,f} - W_{i,f}. \tag{2.2}$$

Here, $V_{i,f}$ are the perturbation potentials in the entrance and exit channel

$$V_i = \frac{Z_P Z_T}{R} - \frac{Z_P}{s_1} - \frac{Z_P}{s_2}, \qquad V_f = \frac{Z_P Z_T}{R} - \frac{Z_P}{s_2} - \frac{Z_T}{x_1} + \frac{1}{r_{12}}. \tag{2.3}$$

The projectile and target nuclear charges in equation (2.3) are denoted by $Z_P$ and $Z_T$. Distorting potential operators $W_{i,f}$ can be selected in the additive form $W_{i,f} = w_{i,f} + W_{i,f}^d$, where $w_{i,f}$ are certain short-range distorting potentials, while $W_{i,f}^d$ are long-range distortion Coulomb potentials which come from residual interactions between the two scattering particles, i.e.

$$V_i \longrightarrow W_i^d = \frac{Z_P(Z_T - 2)}{R}, \qquad V_f \longrightarrow W_f^d = \frac{(Z_P - 1)(Z_T - 1)}{R}, \qquad (r_{i,f} \to \infty).$$

Here, the limits also involve the eikonal mass approximation ($M_{P,T} \gg 1$) by neglecting all the terms of the order of or larger than $\sup\{1/\mu_i, 1/\mu_f\}$. Quantities $\mu_i$ and $\mu_f$ are the reduced masses of the two aggregates in the entrance and exit channel: $\mu_i = M_P(M_T + 2)/M, \mu_f = (M_P + 1)(M_T + 1)/M, M = M_P + M_T + 2$, with $M_P(M_T)$ being the mass of the $P(T)$ nucleus. The quantity $H$ denotes the full Hamiltonian, whereas the total energy of the system is given by $E = k_i^2/(2\mu_i) + \varepsilon_i = k_f^2/(2\mu_f) + \varepsilon_f$, where $\vec{k}_i$ and $\vec{k}_f$ are the initial and final wavevectors and $\varepsilon_i$ and $\varepsilon_f$ are the initial and final bound-state energies. Further $G^-$ in equation (2.2) represents the full Green operator $G^- = 1/(E - H - \mathrm{i}\epsilon)$ satisfying the incoming-wave boundary condition, where $\epsilon$ is an infinitesimally small positive number. The distorted wave $\chi_i^+$ from equation (2.1) is introduced through

$$|\chi_i^+\rangle = \Omega_i^+ |\Phi_i^+\rangle \equiv (1 + G_i^+ w_i)|\Phi_i^+\rangle$$

where $\Omega_i^+$ is the Møller wave operator and $G_i^+ = 1/(E - H_i - W_i + \mathrm{i}\epsilon)$. Operator $H_i$ represents the channel Hamiltonian defined by $H_i = H - V_i$. The asymptotic channel state $|\Phi_i^+\rangle$ is given by

$$\Phi_i^+ = \varphi_i(\vec{x}_1, \vec{x}_2) \exp[\mathrm{i}\vec{k}_i \cdot \vec{r}_i + \mathrm{i}\nu_i \ln(k_i r_i - \vec{k}_i \cdot \vec{r}_i)],$$

where $\varphi_i(\vec{x}_1, \vec{x}_2)$ is the initial bound-state wavefunction, whereas $\nu_i = Z_P(Z_T - 2)/v$ with $v$ being the incident velocity. Of course, the function $\Phi_i^+$ is the solution of $(E - H_i - W_i^d)\Phi_i^+ = 0$. The choice of the perturbation potential operator $U_i$ as

$$U_i = Z_P\left(\frac{1}{R} - \frac{1}{s_2}\right) - \sum_{k=1}^{2} \vec{\nabla}_{x_k} \ln \varphi_i \cdot \vec{\nabla}_{x_k}$$

together with the eikonal approximation $\vec{R} \simeq -\vec{r}_f (M_{P,T} \gg 1)$, provides the final solution of the equation $(E - H_i - W_i)\chi_i^+ = 0$ as follows:

$$\chi_i^+ = N^+(\nu_P)\mathcal{N}^+(\nu)\mathrm{e}^{\mathrm{i}\vec{k}_i \cdot \vec{r}_i} \varphi_i(\vec{x}_1, \vec{x}_2)\, {}_1F_1(\mathrm{i}\nu_P, 1, \mathrm{i}\nu s_1 + \mathrm{i}\vec{v} \cdot \vec{s}_1)\, {}_1F_1(-\mathrm{i}\nu, 1, \mathrm{i}k_i r_i - \mathrm{i}\vec{k}_i \cdot \vec{r}_i),$$

with

$$\nu_P = \frac{Z_P}{v}, \qquad \nu = \frac{Z_P(Z_T - 1)}{v}, \qquad N^+(\nu_P) = \Gamma(1 - \mathrm{i}\nu_P)\mathrm{e}^{\pi\nu_P/2},$$
$$\mathcal{N}^+(\nu) = \Gamma(1 + \mathrm{i}\nu)\mathrm{e}^{-\pi\nu/2},$$

where the symbol ${}_1F_1(a,b,c)$ stands for the confluent hypergeometric function. It is now readily verified that the distorted wave $\chi_i^+$ satisfies the proper boundary condition $\chi_i^+ \to \Phi_i^+$ when $r_i \to \infty$.

Next we shall determine the wavefunction in the exit channel. First, in this work we shall discard the total Green operator $G^-$ in equation (2.2) so that $|\Psi_f^-\rangle \simeq |\chi_f^-\rangle$. The choice of $W_f$ in the form $W_f = (Z_P-1)(Z_T-1)/r_f$ implies that, within the eikonal limit, the distorted wave $|\chi_f^-\rangle$ reads as

$$\chi_f^- = \mathcal{N}^+(\nu_f)\varphi_P(\vec{s}_1)\varphi_T(\vec{x}_2)\mathrm{e}^{-\mathrm{i}\vec{k}_f\cdot\vec{r}_f}\,{}_1F_1(\mathrm{i}\nu_f,1,-\mathrm{i}k_fr_i-\mathrm{i}\vec{k}_f\cdot\vec{r}_i),$$

where $\nu_f = (Z_P-1)(Z_T-1)/v$. The bound-state wavefunctions of the atomic systems $(Z_P,\mathrm{e}_1)$ and $(Z_T,\mathrm{e}_2)$ are denoted by $\varphi_P(\vec{s}_1)$ and $\varphi_T(\vec{x}_2)$, respectively. The distorted wave $\chi_f^-$ possesses the proper asymptotic behaviour in accordance with

$$\chi_f^- \longrightarrow \Phi_f^- = \varphi_P(\vec{s}_1)\varphi_T(\vec{x}_2)\exp[-\mathrm{i}\vec{k}_f\cdot\vec{r}_f-\mathrm{i}\nu_f\ln(k_fr_f-\vec{k}_f\cdot\vec{r}_f)], \qquad (r_f\to\infty).$$

This fully determines the BDW approximation for single charge exchange. This is a hybrid-type theory, because the quantities $W_i$ and $\chi_i^+$ are the same as in the CDW-4B model, whereas $W_f$ and $\chi_f^-$ coincide with the CB1-4B approach. The CB1-4B approximation as a first-order model ignores altogether the electronic continuum intermediate states by selecting the distorting potential in the form $W_f = W_f^d$.

The transition amplitude (2.1) in the BDW approximation takes the following form:

$$\begin{aligned}T_{if} = N^+(\nu_P)\iiint \mathrm{d}\vec{x}_1\,\mathrm{d}\vec{x}_2\,\mathrm{d}\vec{R}\,\mathrm{e}^{\mathrm{i}\vec{k}_i\cdot\vec{r}_i+\mathrm{i}\vec{k}_f\cdot\vec{r}_f}\varphi_P^*(\vec{s}_1)\varphi_T^*(\vec{x}_2)\mathcal{L}(R)\\ \times[V(R,s_2)\varphi_i(\vec{x}_1,\vec{x}_2)\,{}_1F_1(\mathrm{i}\nu_P,1,\mathrm{i}vs_1+\mathrm{i}\vec{v}\cdot\vec{s}_1)\\ -\vec{\nabla}_{x_1}\varphi_i(\vec{x}_1,\vec{x}_2)\cdot\vec{\nabla}_{s_1}\,{}_1F_1(\mathrm{i}\nu_P,1,\mathrm{i}vs_1+\mathrm{i}\vec{v}\cdot\vec{s}_1)]\end{aligned}$$

with

$$V(R,s_2) = Z_P\left(\frac{1}{R}-\frac{1}{s_2}\right),$$

where the product

$$\mathcal{L}(R) = \mathcal{N}^{+*}(\nu_f)\mathcal{N}^+(\nu)\,{}_1F_1(-\mathrm{i}\nu_f,1,\mathrm{i}k_fr_i+\mathrm{i}\vec{k}_f\cdot\vec{r}_i)\,{}_1F_1(-\mathrm{i}\nu,1,\mathrm{i}k_ir_i-\mathrm{i}\vec{k}_i\cdot\vec{r}_i)$$

can be reduced to its consistent eikonal form

$$\mathcal{L}(R) \simeq \rho^{2\mathrm{i}Z_P(Z_T-1)/v}(vR+\vec{v}\cdot\vec{R})^{-\mathrm{i}\xi}, \qquad \xi = (Z_T-1)/v,$$

where the unimportant phase factors of the unit moduli are dropped. Here $\vec{\rho}$ is a component of the vector of the internuclear distance perpendicular to the $Z$-axis ($\vec{R} = \vec{\rho}+\vec{Z}$). The factor $\rho^{2\mathrm{i}Z_P(Z_T-1)/v}$ does not contribute to the total cross section. In addition to this simplification of $\mathcal{L}(R)$, we shall use the eikonal hypothesis, since the small-angle limit implies

$$\vec{k}_i\cdot\vec{r}_i+\vec{k}_f\cdot\vec{r}_f = \vec{\alpha}\cdot\vec{s}_1+\vec{\beta}\cdot\vec{x}_1 = -\vec{\alpha}\cdot\vec{R}-\vec{v}\cdot\vec{x}_1,$$

with $\vec{\alpha} = \vec{\eta}-v^-\hat{\vec{v}}$, $\vec{\beta} = -\vec{\eta}-v^+\hat{\vec{v}}$, $v^\pm = v/2\pm(\varepsilon_i-\varepsilon_f)/v$, where $\vec{\eta} = (\eta\cos\phi_\eta,\eta\sin\phi_\eta,0)$ is the transversal two-dimensional component of the momentum transfer. Hence, the final working expression for the transition amplitude is

$$\begin{aligned}T_{if}(\vec{\eta}) = N^+(\nu_P)\iiint \mathrm{d}\vec{x}_1\,\mathrm{d}\vec{x}_2\,\mathrm{d}\vec{R}\,\mathrm{e}^{\mathrm{i}\vec{\alpha}\cdot\vec{s}_1+\mathrm{i}\vec{\beta}\cdot\vec{x}_1}(vR+\vec{v}\cdot\vec{R})^{-\mathrm{i}\xi}\varphi_P^*(\vec{s}_1)\varphi_T^*(\vec{x}_2)\\ \times[V(R,s_2)\varphi_i(\vec{x}_1,\vec{x}_2)\,{}_1F_1(\mathrm{i}\nu_P,1,\mathrm{i}vs_1+\mathrm{i}\vec{v}\cdot\vec{s}_1)\\ -\vec{\nabla}_{x_1}\varphi_i(\vec{x}_1,\vec{x}_2)\cdot\vec{\nabla}_{s_1}\,{}_1F_1(\mathrm{i}\nu_P,1,\mathrm{i}vs_1+\mathrm{i}\vec{v}\cdot\vec{s}_1)].\end{aligned}$$

The method of the analytical calculation outlined in the appendix provides the matrix elements $T_{if}(\vec{\eta})$ in terms of *two*-dimensional real quadratures over the real variables $\tau$ and $t$ both ranging from 0 to 1. In the computation of the total cross sections $Q_{if}$, we can analytically perform the integration over $\phi_\eta$, since the matrix elements $T_{if}(\vec{\eta})$ do not depend upon the azimuthal angle $\phi_\eta$, i.e. $T_{if}(\vec{\eta}) = T_{if}(\eta)$, and this yields

$$Q_{if}(\pi a_0^2) = \frac{1}{2\pi^2 v^2}\int_0^\infty \mathrm{d}\eta\, \eta |T_{if}(\eta)|^2.$$

We shall employ a change of variable which concentrates the integration points near the forward cone [11]: $\eta = \sqrt{2(1+u)/(1-u)}$ where $u \in [-1, +1]$. All the three integrations over $\tau$, $t$ and $u$ are numerically carried out by means of the standard Gauss–Legendre method.

## 3. Results and discussion

As an illustration of the proposed four-body BDW approximation, the total cross sections are computed for the following single charge exchange:

$$^4\mathrm{He}^{2+} + {}^4\mathrm{He}(1s^2) \longrightarrow {}^4\mathrm{He}^+(\Sigma) + {}^4\mathrm{He}^+(1s). \tag{3.1}$$

The explicit computations are carried out only for capture to the ground 1s state. The symbol $\Sigma$ in $\mathrm{He}^+(\Sigma)$ means that the obtained results are multiplied additionally by a factor of 1.202 in order to include a contribution from all the excited states according to the $n^{-3}$ Oppenheimer scaling law [26]. Namely, the total cross sections are obtained via $Q_{tot} \simeq Q_{1s,1s}\sum_{n=1}^{\infty} n^{-3} = 1.202 Q_{1s,1s}$. The results of the computations of the total cross sections at impact energies ranging from 100 keV to 10 MeV are summarized in table 1 and figure 1. The present BDW results are compared with the corresponding CDW-4B findings from [16]. We emphasize again that the distorting potential $U_i$ is the same in the CDW-4B and BDW theories. Both methods satisfy the correct boundary conditions in the entrance and exit channels. However, unlike the CDW-4B approach, the second-order BDW method takes full account of the Coulomb continuum intermediate state of the captured electron *only* in the entrance channel. Hence, by comparing these two theories, we would learn about the relative importance of the intermediate ionization electron continua. As can be seen from figure 1, the BDW method provides similar cross sections as the CDW-4B theory at higher impact energies, but at lower energies the BDW results are much smaller than the corresponding results of the CDW-4B model. This illustrates a remarkable sensitivity of second-order theories for single charge exchange to the effect of the electronic ionization continua. A comparison between the present results and a number of experimental data on the total cross sections is also displayed in figure 1. The BDW method is found to be in good agreement with the majority of measurements throughout the energy range of overlap. The total cross sections measured by Hvelplund *et al* [32] overestimate our theoretical results. It should be noted that there is a difference between the proposed four-body BDW method and other one-channel distorted wave approaches such as the continuum distorted wave-eikonal initial state (CDW-EIS) and the continuum distorted wave-eikonal final state (CDW-EFS) [7, 34–36].

For this purpose, we shall perform a short comparative study of these two types of models.

(i) According to the CDW-EIS and the CDW-EFS approximations [7], the single electron capture reaction from a two-electron target is reduced to a one-electron process. The initial state of the active electron has been described by the Roothan–Hartree–Fock $5z$ function [7]. Hence, the CDW-EIS and CDW-EFS are three-body models, whereas the BDW method deals with two active electrons and, therefore, preserves the four-body nature of the problem.

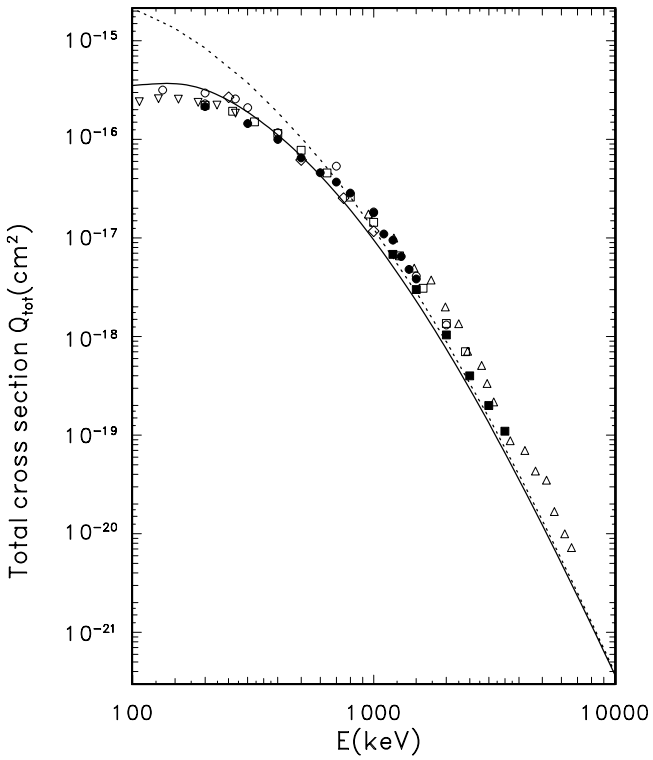


**Figure 1.** The total cross sections $Q_{tot}$ (cm$^2$) as a function of the laboratory incident energy $E$ (keV) for the reaction $^4He^{2+} + {}^4He(1s^2) \longrightarrow {}^4He^+(\Sigma) + {}^4He^+(1s)$. The symbol $\Sigma$ in $He^+(\Sigma)$ means that the obtained results are multiplied by 1.202 in order to include the influence of all the excited states. The full curve represents the cross sections $Q_{tot}$ of the present BDW approximation. The dashed curve refers to the theoretical CDW-4B results of Mančev [16]. Experimental data: ○, DuBois [27]; ▽, Shah *et al* [28]; ◇, Mergel *et al* [29]; ●, Shah and Gilbody [30]; □, Pivovar *et al* [31]; △, Hvelplund *et al* [32]; ■, de Castro Faria *et al* [33].

**Table 1.** Total cross sections (in cm$^2$) as a function of the incident energy $E$ (keV) for the single charge exchange reaction $^4He^{2+} + {}^4He(1s^2) \longrightarrow {}^4He^+(\Sigma) + {}^4He^+(1s)$. The symbol $\Sigma$ in $He^+(\Sigma)$ means that the obtained results are multiplied by 1.202 in order to include the influence of all the excited states. The displayed results are obtained by means of the BDW approximation using the one-parameter Hylleraas wavefunction for the initial helium bound state. The numbers in brackets denote the powers of ten by which the numbers are to be multiplied.

| $E$ (keV) | $Q_{tot}$ (cm$^2$) | $E$ (keV) | $Q_{tot}$ (cm$^2$) |
|---|---|---|---|
| 100 | 3.52(−16) | 1000 | 9.48(−18) |
| 150 | 3.67(−16) | 1500 | 2.28(−18) |
| 200 | 3.17(−16) | 2000 | 7.40(−19) |
| 300 | 1.88(−16) | 3000 | 1.32(−19) |
| 400 | 1.11(−16) | 4000 | 3.53(−20) |
| 500 | 6.76(−17) | 5000 | 1.22(−20) |
| 600 | 4.29(−17) | 6000 | 4.98(−21) |
| 700 | 2.82(−17) | 7000 | 2.30(−21) |
| 800 | 1.91(−17) | 8000 | 1.17(−21) |
| 900 | 1.33(−17) | 10000 | 3.67(−22) |

(ii) Within the framework of the three-body CDW approximation (CDW-3B) the distorted wavefunctions for the considered process are given by

$$\chi_i^{CDW-3B} = N^+(\nu_P)\mathrm{e}^{\mathrm{i}\vec{k}_i\cdot\vec{r}_i}\varphi_i(\vec{x}_1)\,{}_1F_1(\mathrm{i}\nu_P, 1, \mathrm{i}vs_1 + \mathrm{i}\vec{v}\cdot\vec{s}_1),$$
$$\chi_f^{CDW-3B} = N^-(\nu_T)\varphi_P(\vec{s}_1)\mathrm{e}^{-\mathrm{i}\vec{k}_f\cdot\vec{r}_f}\,{}_1F_1(-\mathrm{i}\nu_T, 1, -\mathrm{i}vx_1 - \mathrm{i}\vec{v}\cdot\vec{x}_1),$$

where $\nu_T = (Z_T - 1)/v$, $N^-(\nu_T) = \Gamma(1+\mathrm{i}\nu_T)\mathrm{e}^{\pi\nu_T/2}$. In the CDW-EIS approximation the distorted wavefunction in the entrance channel $\chi_i^{CDW-3B}$ is replaced by the corresponding eikonal phase, i.e.

$$\chi_i^{CDW-EIS} = \mathrm{e}^{\mathrm{i}\vec{k}_i\cdot\vec{r}_i - \mathrm{i}\nu_P\ln(vs_1+\vec{v}\cdot\vec{s}_1)}\varphi_i(\vec{x}_1),$$

whereas in the exit channel $\chi_f^{CDW-3B}$ is used. For the CDW-EFS model the distorted function in the exit channel is approximated by the eikonal phase

$$\chi_f^{CDW-EFS} = \mathrm{e}^{-\mathrm{i}\vec{k}_f\cdot\vec{r}_f + \mathrm{i}\nu_T\ln(vx_1+\vec{v}\cdot\vec{x}_1)}\varphi_f(\vec{s}_1),$$

while the wavefunction in the entrance channel is chosen as in the CDW-3B model. Hence, the continuum intermediate states are approached by their asymptotic representation (i.e. Coulomb phases) in one of the channels. According to the BDW model in the final state the following approximation is used:

$$F_f = \mathcal{N}^+(\nu_f)\mathrm{e}^{-\mathrm{i}\vec{k}_f\cdot\vec{r}_f}\,{}_1F_1(\mathrm{i}\nu_f, 1, -\mathrm{i}k_f r_f + \mathrm{i}\vec{k}_f\cdot\vec{r}_f)$$
$$\simeq \exp[-\mathrm{i}\vec{k}_f\cdot\vec{r}_f - \mathrm{i}\nu_f\ln(k_f r_f - \vec{k}_f\cdot\vec{r}_f)] \simeq \mathrm{e}^{-\mathrm{i}\vec{k}_f\cdot\vec{r}_f}(vR + \vec{v}\cdot\vec{R})^{-\mathrm{i}\nu_f},$$

where the factor $F_f$ originates from the long-range Coulomb repulsion between the screened positively charged nuclei $(Z_P - 1)$ and $(Z_T - 1)$ in the exit channel. It should also be noted that an eikonal phase is a good approximation of the continuum factor only when the third argument of the confluent hypergeometric function involved is sufficiently large.

The high-energy behaviour of the BDW cross section for 1s— $n_f l_f$ capture is $Q_{if} \sim v^{-11-2l_f}$. Thus, for capture into excited states with $l_f > 0$, at very high energies, the BDW approximation does not give the correct $v^{-11}$ behaviour. Nevertheless, this deficiency at asymptotic energies is not usually of crucial importance in the intermediate- and high-energy region, where the Thomas double-scattering mechanism does not contribute significantly. A similar problem with the velocity dependence has been found in the case of the other one-channel distorted models, such as the target continuum distorted-wave approximation [8, 37, 38] and the CDW-EIS and CDW-EFS [7, 35]. The deficiencies of the various models in reproducing the correct high-energy behaviour of the charge exchange cross section has recently been discussed in the review paper of Belkić [18].

## 4. Conclusions

We have examined the problem of single electron capture from a helium-like atomic system by a bare projectile at intermediate and high impact energies. A new four-body one-channel distorted-wave theory termed the BDW method is introduced.

The BDW theory is presently applied to the case of single charge exchange in symmetric collisions between $\alpha$ particles and helium at impact energies from 100 keV to 10 MeV. By comparing the BDW and CDW-4B results we have studied the role of the intermediate ionization continua. The BDW and CDW-4B total cross sections are very close to each other at higher impact energies. However, the BDW theory is adequate also at the lower edge of

intermediate energies, at which the CDW-4B model considerably overestimates the available experimental data. The CDW-4B approximation incorporates two Coulomb waves for the captured electron in both the entrance and exit channel. However, such an over-account on the role played by the double electronic ionization continua could potentially be responsible for the inadequacy of the CDW-4B model at intermediate energies.

## Acknowledgments

Thanks are due to Professors Dževad Belkić and Horst Schmidt-Böcking for helpful discussions and a critical review of the manuscript. The author gratefully acknowledges the financial support from the Deutscher Akademischer Austausch Dienst (DAAD) and from the Ministry of Science and Technology of Republic of Serbia through project no 1470.

## Appendix

The initial bound state of the target is described by the uncorrelated one-parameter wavefunction for a helium-like atomic system

$$\varphi_i(\vec{x}_1,\vec{x}_2)=\varphi_b(\vec{x}_1)\varphi_b(\vec{x}_2),\qquad \varphi_b(\vec{r})=N_b\mathrm{e}^{-br},\qquad N_b=\sqrt{b^3/\pi},$$

where $b$ is the effective charge $b=Z_T-\sigma$, with parameter $\sigma$ being the inner Slater screening ($\sigma=5/16=0.3125$). Employing the well-known integral representation for the confluent hypergeometric function [39]:

$${}_1F_1(\mathrm{i}\nu_P,1,\mathrm{i}vs_1+\mathrm{i}\vec{v}\cdot\vec{s}_1)=\frac{1}{\Gamma(\mathrm{i}\nu_P)\Gamma(1-\mathrm{i}\nu_P)}\int_0^1\mathrm{d}\tau\, g(\tau)\mathrm{e}^{\mathrm{i}(vs_1+\vec{v}\cdot\vec{s}_1)\tau},$$

with $g(\tau)=\tau^{\mathrm{i}\nu_P-1}(1-\tau)^{-\mathrm{i}\nu_P}$, the expression for $T_{if}$ can be written in the form:

$$T_{if}=T_{if}^{(1)}-T_{if}^{(2)},\tag{A.1}$$

where

$$T_{if}^{(1)}=M^+\int_0^1\mathrm{d}\tau\, g(\tau)[\mathcal{S}(\tau)+\mathcal{R}(\tau)],\qquad T_{if}^{(2)}=M^+\int_0^1\mathrm{d}\tau\, g(\tau)\mathcal{D}(\tau),$$

with

$$\mathcal{S}(\tau)=\int\mathrm{d}\vec{R}\,\mathrm{e}^{-\mathrm{i}\vec{\alpha}\cdot\vec{R}}(vR+\vec{v}\cdot\vec{R})^{-\mathrm{i}\xi}\mathcal{F}_s(\vec{R}),$$

$$\mathcal{R}(\tau)=\int\mathrm{d}\vec{R}\,\mathrm{e}^{-\mathrm{i}\vec{v}\cdot\vec{x}_1}(vR+\vec{v}\cdot\vec{R})^{-\mathrm{i}\xi}\mathcal{F}_R(\vec{R}),$$

$$\mathcal{D}(\tau)=\int\mathrm{d}\vec{R}\,\mathrm{e}^{-\mathrm{i}\vec{\alpha}\cdot\vec{R}}(vR+\vec{v}\cdot\vec{R})^{-\mathrm{i}\xi}\mathcal{T}(\vec{R}),$$

$$\mathcal{F}_s=-Z_P\mathcal{F}_1(\vec{R})\mathcal{F}_2(\vec{R}),\qquad \mathcal{F}_R=\frac{Z_P}{R}\mathcal{F}_1(\vec{R})\mathcal{F}_3,$$

$$\mathcal{T}=\mathcal{T}_1(\vec{R})\mathcal{F}_3,\qquad M^+=\frac{N^+(\nu_P)}{\Gamma(\mathrm{i}\nu_P)\Gamma(1-\mathrm{i}\nu_P)},$$

$$\mathcal{T}_1(\vec{R})=\int\mathrm{d}\vec{x}_1\,\mathrm{e}^{-\mathrm{i}\vec{v}\cdot\vec{x}_1}\varphi_P^*(\vec{s}_1)\vec{\nabla}_{s_1}\Omega(\vec{s}_1)\cdot\vec{\nabla}_{x_1}\varphi_b(\vec{x}_1),$$

$$\Omega(\vec{s}_1)=\exp[\mathrm{i}(vs_1+\vec{v}\cdot\vec{s}_1)\tau],$$

$$\mathcal{F}_1(\vec{R})=\int\mathrm{d}\vec{x}_1\,\mathrm{e}^{-\mathrm{i}\vec{v}\cdot\vec{x}_1}\varphi_P^*(\vec{s}_1)\Omega(\vec{s}_1)\varphi_b(\vec{x}_1),$$

$$\mathcal{F}_2(\vec{R}) = \int \mathrm{d}\vec{x}_2\, \varphi_T^*(\vec{x}_2)\frac{1}{s_2}\varphi_b(\vec{x}_2),$$
$$\mathcal{F}_3 = \int \mathrm{d}\vec{x}_2\, \varphi_T^*(\vec{x}_2)\varphi_b(\vec{x}_2) = \frac{8\pi N_T N_b}{\zeta^3},$$
$$N_K = \sqrt{Z_K^3/\pi}, \qquad \zeta = Z_K + b, \qquad (K = P, T).$$

Integral $\mathcal{T}_1(\vec{R})$ has been calculated in [20, 24] with the result

$$\mathcal{T}_1(\vec{R}) = 2\pi b\omega\tau N_P N_b \mathrm{e}^{\mathrm{i}\vec{\alpha}\cdot\vec{R}} \int_0^1 \mathrm{d}t\, \frac{t(1-t)}{\Delta_1^5}\, \mathrm{e}^{-\mathrm{i}\vec{Q}\cdot\vec{R}-\Delta_1 R}$$
$$\times [a_1 R^2 - b_1 R - c_1 - d_1(1+\Delta_1 R)\hat{\vec{v}}\cdot\vec{R}],$$

where

$$\vec{Q} = (\vec{\alpha} + \tau\vec{v})t - \vec{\beta}(1-t), \qquad \Delta_1^2 = v_1^2 t(1-t) + \lambda_1^2 t + b^2(1-t),$$
$$a_1 = (\Delta_1^2 + \gamma\delta)\Delta_1^2, \qquad b_1 = 3(\Delta_1^2 - \gamma\delta)\Delta_1,$$
$$c_1 = 3(\Delta_1^2 - \gamma\delta), \qquad d_1 = (\gamma+\delta)\Delta_1^2,$$
$$\gamma = \omega t\tau', \qquad \delta = \lambda_1 - \gamma', \qquad \omega = \mathrm{i}v, \qquad \vec{v}_1 = (1-\tau)\vec{v},$$
$$\gamma' = \omega t'\tau', \qquad t' = 1-t, \qquad \tau' = 1-\tau, \qquad \lambda_1 = Z_P - \omega\tau.$$

The three-dimensional integral $\mathcal{F}_1(\vec{R})$ can be reduced to the one-dimensional real quadrature following a procedure similar to [23, 25], so that we finally obtain

$$\mathcal{F}_1(\vec{R}) = 2\pi N_P N_b \lambda_1 b \mathrm{e}^{\mathrm{i}\vec{\alpha}\cdot\vec{R}} \int_0^1 \mathrm{d}t\, \frac{t(1-t)}{\Delta_1^5}\, \mathrm{e}^{-\mathrm{i}\vec{Q}\cdot\vec{R}-\Delta_1 R}(3 + 3\Delta_1 R + \Delta_1^2 R^2).$$

Further, integral $\mathcal{F}_2(\vec{R})$ can be solved analytically as follows. Employing the Fourier transform

$$\frac{1}{s_2} = \frac{1}{2\pi^2}\int \frac{\mathrm{d}\vec{q}}{q^2}\, \mathrm{e}^{-\mathrm{i}\vec{q}\cdot(\vec{x}_2-\vec{R})}$$

we have

$$\mathcal{F}_2(\vec{R}) = \frac{N_T N_b}{2\pi^2}\int \frac{\mathrm{d}\vec{q}}{q^2}\, \mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{R}} \int \mathrm{d}\vec{x}_2\, \mathrm{e}^{-\mathrm{i}\vec{q}\cdot\vec{x}_2 - \zeta x_2} = \frac{4\zeta N_T N_b}{\pi}\int \mathrm{d}\vec{q}\, \frac{\mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{R}}}{q^2(q^2+\zeta^2)^2}.$$

Using the Feynman parametrization integral

$$\frac{1}{AB^2} = 2\int_0^1 \frac{\mathrm{d}t\,(1-t)}{[At + B(1-t)]^3},$$

we derive the result

$$\int \mathrm{d}\vec{q}\, \frac{\mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{R}}}{q^2(q^2+\zeta^2)^2} = 2\int_0^1 \mathrm{d}t\,(1-t)\int \mathrm{d}\vec{q}\, \frac{\mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{R}}}{(q^2+\Delta^2)^3} = \frac{\pi^2}{2\zeta^3}\int_0^1 \frac{\mathrm{d}t}{\sqrt{1-t}}(1+\Delta R)\mathrm{e}^{-\Delta R},$$

where $\Delta = \zeta\sqrt{1-t}$ and

$$\mathcal{F}_2(\vec{R}) = \frac{2\pi N_T N_b}{\zeta^2}\int_0^1 \frac{\mathrm{d}t}{\sqrt{1-t}}(1+\Delta R)\mathrm{e}^{-\Delta R} = \frac{4\pi N_T N_b}{\zeta^3}\left[\frac{2}{R} - \zeta\mathrm{e}^{-\zeta R}\left(1 + \frac{2}{\zeta R}\right)\right].$$

Utilizing the above results for the quoted integrals, we can express the quantities $T_{if}^{(1)}$ and $T_{if}^{(2)}$ as

$$T_{if}^{(1)} = M^+ 8\pi^2 N_T N_P N_b^2 \frac{Z_P b}{\zeta^3}\int_0^1 \mathrm{d}\tau\, \lambda_1 g(\tau)\int_0^1 \mathrm{d}t\, \frac{t(1-t)}{\Delta_1^5}$$
$$\times [6I_0^{(2)} + 3(\zeta + 2\Delta_1)I_1^{(2)} + \Delta_1(3\zeta + 2\Delta_1)I_2^{(2)} + \zeta\Delta_1^2 I_3^{(2)}], \qquad \text{(A.2)}$$

$$T_{if}^{(2)} = M^{+}16\pi^{2}N_{T}N_{P}N_{b}^{2}\omega\frac{b}{\zeta^{3}}\int_{0}^{1}\mathrm{d}\tau\,\tau g(\tau)\int_{0}^{1}\mathrm{d}t\,\frac{t(1-t)}{\Delta_{1}^{5}}$$
$$\times\,[a_{1}I_{3}^{(1)} - b_{1}I_{2}^{(1)} - c_{1}I_{1}^{(1)} + \frac{d_{1}}{\omega}(I_{1}' + \Delta_{1}I_{2}')], \tag{A.3}$$

where

$$I_{n}^{(j)} = \int \mathrm{d}\vec{R}\,\mathrm{e}^{-\mathrm{i}\vec{Q}\cdot\vec{R}-\Delta_{j}R}R^{n-1}(vR+\vec{v}\cdot\vec{R})^{-\mathrm{i}\xi}, \qquad I_{n}' = \vec{v}\cdot\vec{\nabla}_{\vec{Q}}I_{n}^{(1)}, \qquad (j=1,2),$$

$$\Delta_{j} = \begin{cases} \Delta_{1}, & j=1 \\ \Delta_{1}+\zeta, & j=2. \end{cases}$$

The final results of the necessary integrals are given by [23, 25]

$$I_{0}^{(j)} = 4\pi\Gamma(1-\mathrm{i}\xi)\mathcal{P}_{j},$$
$$I_{1}^{(j)} = 8\pi\Gamma(1-\mathrm{i}\xi)\frac{A_{j}\mathcal{P}_{j}}{\Delta_{j}}(1+\mathrm{i}\xi C_{j}),$$
$$I_{2}^{(j)} = -8\pi\Gamma(1-\mathrm{i}\xi)\frac{A_{j}\mathcal{P}_{j}}{\Delta_{j}^{2}}(1-4A_{j}-\mathrm{i}\xi B_{\alpha}^{(j)}),$$
$$I_{3}^{(j)} = -16\pi\Gamma(1-\mathrm{i}\xi)\frac{A_{j}^{2}\mathcal{P}_{j}}{\Delta_{j}^{3}}[6(1-2A_{j})-\mathrm{i}\xi B_{\beta}^{(j)}],$$
$$I_{1}' = -16\pi\Gamma(1-\mathrm{i}\xi)\frac{A_{1}^{2}\mathcal{P}_{1}}{\Delta_{1}^{3}}(A_{\alpha}-\mathrm{i}\xi B_{\gamma}),$$
$$I_{2}' = 16\pi\Gamma(1-\mathrm{i}\xi)\frac{A_{1}^{2}\mathcal{P}_{1}}{\Delta_{1}^{4}}(A_{\beta}-\mathrm{i}\xi B_{\delta}),$$

where

$$A_{j} = \frac{\Delta_{j}^{2}}{Q^{2}+\Delta_{j}^{2}}, \qquad B_{j} = 2\frac{v\Delta_{j}-\mathrm{i}\vec{Q}\cdot\vec{v}}{Q^{2}+\Delta_{j}^{2}}, \qquad C_{j} = \frac{v}{B_{j}\Delta_{j}}-1, \qquad \mathcal{P}_{j} = \frac{B_{j}^{-\mathrm{i}\xi}}{Q^{2}+\Delta_{j}^{2}},$$
$$B_{\alpha}^{(j)} = 1+2A_{j}C_{j}[4+(1+\mathrm{i}\xi)C_{j}],$$
$$B_{\beta}^{(j)} = 2A_{j}C_{j}[18+9(1+\mathrm{i}\xi)C_{j}+(1+\mathrm{i}\xi)(2+\mathrm{i}\xi)C_{j}^{2}]+3[2-(1-\mathrm{i}\xi)C_{j}],$$
$$A_{\alpha} = \{2-\mathrm{i}\xi[2-(1-\mathrm{i}\xi)C_{1}]\}(\vec{v}\cdot\vec{Q}),$$
$$B_{\gamma} = (1+C_{1})\Delta_{1}\omega[2+(1+\mathrm{i}\xi)C_{1}],$$
$$A_{\beta} = \{2(1-6A_{1})-\mathrm{i}\xi[2A_{1}C_{\alpha}+(3-\mathrm{i}\xi)]\}(\vec{v}\cdot\vec{Q}),$$
$$C_{\alpha} = (1-\mathrm{i}\xi)C_{1}[6+(1+\mathrm{i}\xi)C_{1}]-6,$$
$$B_{\delta} = (1+C_{1})\Delta_{1}\omega[1-\mathrm{i}\xi-2A_{1}D_{\alpha}],$$
$$D_{\alpha} = (1+\mathrm{i}\xi)C_{1}[6+(2+\mathrm{i}\xi)C_{1}]+6.$$

Inserting the results for the integrals $I_{n}^{(j)}$ and $I_{n}'$ into equations (A.2) and (A.3), we arrive at the following expression for the transition amplitude $T_{if}$:

$$T_{if} = N\int_{0}^{1}\mathrm{d}\tau\,g(\tau)\int_{0}^{1}\mathrm{d}t\,\frac{t(1-t)}{\Delta_{1}^{5}}(\mathcal{A}+\mathrm{i}\xi\mathcal{B}), \tag{A.4}$$

with

$$N = 64\pi\Gamma(1-\mathrm{i}\xi)M^{+}(Z_{P}Z_{T})^{3/2}b^{4}/\zeta^{3},$$
$$\mathcal{A} = Z_{P}\lambda_{1}\mathcal{P}_{2}\mathcal{A}' - 2\omega\tau\mathcal{P}_{1}A_{1}D\mathcal{A}''/\Delta_{1},$$

$$\mathcal{B} = Z_P\lambda_1\mathcal{P}_2\mathcal{B}' - 2\omega\tau\mathcal{P}_1 A_1\mathcal{B}''/\Delta_1,$$

$$\mathcal{A}' = 3 + 3(\zeta + 2\Delta_1)\frac{A_2}{\Delta_2} - \frac{\Delta_1 A_2}{\Delta_2^2}(3\zeta + 2\Delta_1)(1 - 4A_2) - 12\frac{\Delta_1^2 A_2^2}{\Delta_2^3}\zeta(1 - 2A_2),$$

$$\mathcal{B}' = 3(\zeta + 2\Delta_1)A_2 C_2/\Delta_2 + \frac{\Delta_1 A_2}{\Delta_2^2}(3\zeta + 2\Delta_1)B_\alpha^{(2)} + 2\frac{A_2^2\Delta_1^2}{\Delta_2^3}\zeta B_\beta^{(2)},$$

$$\mathcal{A}'' = -12a_1\frac{A_1}{\Delta_1^2}(1 - 2A_1) + \frac{b_1}{\Delta_1}(1 - 4A_1) - c_1 - 2\frac{d_1}{\omega}\frac{A_1}{\Delta_1^2}(A_\alpha - A_\beta),$$

$$\mathcal{B}'' = 2a_1\frac{A_1}{\Delta_1^2}B_\beta^{(1)} - \frac{b_1}{\Delta_1}B_\alpha^{(1)} - c_1 C_1 + 2\frac{d_1}{\omega}\frac{A_1}{\Delta_1^2}(B_\gamma - B_\delta).$$

The function $g(\tau) = \tau^{\mathrm{i}\nu_P - 1}(1 - \tau)^{-\mathrm{i}\nu_P}$ in equation (A.4) possesses integrable branch-point singularities at $\tau = 0$ and 1. The standard Cauchy regularization of the whole integrand in equation (A.4) is accomplished before applying the universal Gauss–Legendre numerical quadratures.

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