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Quasi–four-body treatment of charge transfer in the collision of protons with atomic helium: I. Thomas related mechanisms*

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Abstract. The scattering of a completely bare ion by atoms larger than hydrogen is at least a four-body interaction, and the charge transfer channel involves a two-step process. Amongst the two-step interactions of the high-velocity single charge transfer in an anion-atom collision, there is one whose amplitude demonstrates a peak in the angular distribution of the cross sections. This peak, the so-called Thomas peak, was predicted by Thomas in a two-step interaction, classically, which could also be described through three-body quantum mechanical models. This work discusses a four-body quantum treatment of the charge transfer in ion-atom collisions, where two-step interactions illustrating a Thomas peak are emphasized. In addition, the Pauli exclusion principle is taken into account for the initial and final states as well as the operators. It will be demonstrated that there is a momentum condition for each two-step interaction to occur in a single charge transfer channel, where new classical interactions lead to the Thomas mechanism.

1 Introduction

The single charge transfer has been extensively studied and reported in the literature [1–13] for the case of a three-body interaction. There are also studies on the single charge transfer based on a four-body interaction under the CDW [14–17] DWB [18–20], B1B, and B2B [3,21–23] approximations or formalisms. A three- or four-body treatment is the perfect choice when hydrogen or helium are the target, respectively. When targets are more complex than helium, however, a model has to be devised to make use of a three-, four-, or few-body formalism.

Faddeev developed an expansion by rearranging the Born expansion [24,25], benefiting from the advantage that each term explains an individual interaction. Faddeev's work led to the Faddeev-Watson-Lovelace (FWL) formalism, which is a quantum treatment for describing different channels in atomic and nuclear scattering problems. The FWL formalism is applied to describe different channels in the collision of ions with atomic targets, where long-range Coulomb forces are present. The problems described under the FWL formalism are three-body, or adapted for a three-body description of scattering channels like charge transfer [26], ionization [27], and excitation [28]. However, the FWL formalism has also been applied to describe four-body problems [29–34]. The method is powerful enough to be applied to few-body problems, with the expense of increased number of terms to be dealt with as expected.

We have developed a method implementing the three-body FWL formalism and its expansion toward a four-body scattering process defined by Sloan [34], to calculate the single electron transfer in the collision of protons by helium atoms as

$$P + (T + e_1 + e_2) \rightarrow (P + e_P) + (T + e_T), \tag{1}$$

where P stands for the proton as the projectile and $(T + e_1 + e_2)$ denotes helium as the target. Note that we have named the two electrons after the collision e_P, and e_T as they are indistinguishable. The original form of the FWL transition operators from an initial channel α to a final channel β is [35]

$$U^{-}_{\beta\alpha} = V_{PC} + T_{Pe_T,PC} + T_{Te_P,PC} + T_{e_Pe_T,PC} + T_{PT,PC} + T_{Pe_T,PT} + T_{Te_P,PT} + T_{e_Pe_T,PT} + T_{PT,PT}, \tag{2}$$

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where C, V_{PC}, and $T_{f,i}$ stand for the initial electronic cloud of the target, the interaction potential between the projectile and the electronic cloud, and the elements of four-body transition operator between initial interacting particles i to a final interacting particles f, respectively. We call this method the quasi–four-particle FWL formalism, as in the initial channel a three-body system composed of the projectile, the target's nucleus, and the electronic cloud is assumed, while the final channel is described by a four-body (four-particle) system.

The two-step interaction mechanism for a high-velocity charge transfer in an ion-atom collision has been studied rigorously [36–40]. In a three-body Faddeev formalism, the Thomas peak is the signature of the two-step interactions. Thomas [37] originally explained the charge transfer process as a double-scattering mechanism, classically. He stated that the projectile heads toward the target's nucleus after colliding with the target's electron and ejecting it from the target at 0.47 mrad angle with respect to the projectile [37]. The projectile then scatters off the target's nucleus in parallel with and at the same speed as the ejected electron while the two form a bound atom or ion. In practice, a peak at the scattering angle of 0.47 mrad is observed in the differential cross sections for charge transfer between a projectile and a target. Here, we intend to revisit the Thomas peak as a two-step interaction within a four-body Faddeev formalism.

In this study, we will show that in a four-body treatment of electron capture, different two-step interactions lead to a peak at the scattering angle 0.47 mrad, the same scattering angle as the Thomas peak. In addition, we will extend our earlier works [26,35,41,42], where it is important to apply the Pauli exclusion principle to the operators and wave functions, as we are dealing with two electrons. The Pauli exclusion principle applied to operators is important as we are dealing with the transition matrix operators. This paper is the continuation of our recent work, which we shall call the First Order Paper [35]. As we are only calculating some of the second-order terms in the charge transfer collision, it is not possible to calculate the corresponding cross sections to compare with experimental data. Besides, it is not possible to measure the partial amplitudes. Understanding the physics of some of the partial amplitudes is the main goal of this paper. Previous works in the literature (as examples see [41,43]) assume an active electron for targets having more than one electron and solve the charge transfer collision in a three-body formalism. The present work differs from those, in the sense that all electrons are active and the electronic cloud is taken into account.

The theoretical background is shortly discussed in the next section, while the kinematics of the various interactions is pointed out in sect. 3. In sect. 4, the FWL amplitude leading to the Thomas-like mechanisms of charge transfer is simplified for a practical calculation in sect. 5. Finally, the concluding remarks are made in sect. 6.

2 Theoretical background

In this section, we define the main structure of the present model and apply the Pauli exclusion principle to the operators, where electrons are involved. Therefore, the interaction potential between the projectile and the electronic cloud for a single electron transfer, two-body transition operators, and the elements of a four-body transition operator are

$$V_{PC} = \frac{1}{2}(V_{Pe_1} + V_{Pe_2}), \tag{3}$$

$$t_{PC} = \frac{1}{2}(t_{Pe_1} + t_{Pe_2}) \tag{4}$$

and

$$T_{j,PC} = \frac{1}{2}(T_{j,Pe_1} + T_{j,Pe_2}), \tag{5}$$

respectively, where j in $T_{j,PC}$ denotes a pair of particles, and the Pauli exclusion principle is taken into account.

The two-particle transition matrices play an essential role in describing the interaction channel [44–47], as they provide all the information on the two-particle interacting systems. In order to calculate the charge transfer cross sections, one needs a functional form of the transition matrix elements, for which there are different forms of near-shell and off-shell transition matrix elements available in the literature [41,43,48–56].

The general off-shell form of the transition matrix elements is derived by Nutt and Schwinger [48,54] as

$$t_{ij}\left(\vec{k},\vec{k}';E\right) = \frac{4\pi Z}{|\vec{k}'-\vec{k}|^2}\left\{1 - \frac{4i\nu}{e^{2\pi\nu}-1}\oint_{c_0}\frac{t^{-i\nu}}{\varepsilon(1-t)^2-4t}\mathrm{d}t\right\}, \tag{6}$$

where i and j are the interacting particles and ν $(= -Z_1Z_2\mu/p)$ is the Somerfield parameter for $p = \sqrt{2\mu E}$ and

$$\varepsilon = \frac{\left(p^2-k^2\right)\left(p^2-k'^2\right)}{p^2|\vec{k}'-\vec{k}|^2}; \quad k \neq p \neq k' \neq k. \tag{7}$$

Different methods have been devised in the literature to calculate the integral in eq. (6) [57–59].

There is an exact form for the off-shell Coulomb T-matrix in terms of hypergeometric functions as [53]

$$t_{ij}\left(\vec{k},\vec{k}';E\right)=\frac{4\pi Z_1Z_2}{|\vec{k}'-\vec{k}|^2}\left\{1+1/\sqrt{1+\varepsilon}\left[{}_2F_1(1,-i\nu,1-i\nu;g_-)-{}_2F_1(1,-i\nu,1-i\nu;g_+)\right]\right\}, \tag{8}$$

where

$$g_\pm=\frac{(1+\varepsilon)^{1/2}\mp 1}{(1+\varepsilon)^{1/2}\pm 1} \tag{9}$$

and ε is defined by eq. (7). This form of the exact off-shell Coulomb T-matrix is used to calculate the data of partial amplitudes, which are discussed in this article. Additionally, several approximate off-shell Coulomb T-matrix forms were calculated by Alston [56], Chen [53], and using the Padé approximation [42].

Chen [53] introduced a two-body transition matrix for two interacting particles:

$$t_{ij}\left(\vec{k},\vec{k}';E\right)=\frac{4\pi Z_1Z_2}{|\vec{k}'-\vec{k}|^2}\left\{|\Gamma(1-i\nu)|^2\,\mathrm{e}^{-\pi\nu}\left[\frac{\varepsilon}{4}\right]^{-i\nu}\right\}. \tag{10}$$

In addition, a relatively simple and efficient method, the Haar multi-resolution analysis, was implemented to calculate the transition matrix element for single charge transfer in proton-hydrogen collisions [42]. According to Haar multi-resolution analysis, the two-body transition matrix can be written as

$$t_{ij}\left(\vec{k},\vec{k}';E\right)\approx\frac{4\pi Z_1Z_2}{|\vec{k}'-\vec{k}|^2}\left\{1-4i\nu\left(2^{-m}\right)\left[\sum_{n=0}^{2^m-1}\frac{[2^{-m}(n+\frac{1}{2})]^{-i\nu}}{\varepsilon(1-2^{-m}(n+\frac{1}{2}))^2-4(2^{-m}(n+\frac{1}{2}))}\right]\right\}, \tag{11}$$

where summation contains 2^m terms in subspace V_m. If m is chosen adequately large, the approximation converges to the exact value of transition matrix.

We calculated the transition elements and their corresponding amplitudes by the adaptive Monte Carlo method employing the exact form of eq. (8), the approximated form derived by Chen (eq. (10)) and the Haar multi-resolution forms. The calculated transition element differs slightly. Therefore, we devised the Haar multi-resolution approximation in V_2, as it was the most efficient one in this report.

3 Definition of coordinates and conservation laws

At first, as the quasi–four-particle interaction is assumed, we needed to introduce five sets of Jacobi coordinate vectors with three vectors for each set that define the positions of the constituents of the interacting system, similar to the three Jacobi coordinate vectors employed by Alston [43]. These Jacobi coordinates were introduced in our previous work, the First Order Paper [35]. If the kinetic energy operator related to a Jacobi coordinate set depends only on the square of the momentum operators and no mass polarization term appear in it, the chosen Jacobi coordinate set is proper for this kind of calculations [60,61].

Defining $\vec{K}_i$ and $\vec{K}_{f_j}$ (with the j being the number assigned to the transferred electron) as initial and final wave vectors of the heavy particles in the center of mass frame, respectively, the total energy operator of the system is

$$E=\frac{1}{2\nu_i}K_i^2+\varepsilon_i=\frac{1}{2\nu_f}{K_{f_j}}^2+\varepsilon_f, \tag{12}$$

where ε_i and ε_f are the initial and final bound-state energies, respectively. It should be noted that the initial (final) heavy-particle velocities are defined in terms of the initial (final) wave vectors as $\vec{V}_i=\vec{K}_i/\nu_i$ ($\vec{V}_f=\vec{K}_{f_j}/\nu_f$) while ν_i and ν_f are the reduced masses of the initial and final particles, respectively.

The target ion and projectile momentum transfers experienced during the collision are defined as

$$\vec{T}=-\vec{K}_{f_j}+\gamma'\vec{K}_i \tag{13}$$

and

$$\vec{J}=\alpha'\vec{K}_{f_j}-\vec{K}_i, \tag{14}$$

respectively, where $\gamma'=(M_T+m)/(M_T+2m)$ and $\alpha'=M_P/(M_P+m)$ are the mass ratios and they are approximately equal to 1.

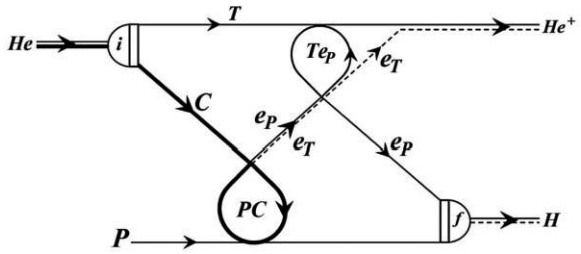

Fig. 1. The mechanism for the term $T_{Te_P,PC}$.

It must be added that the mass ratios m/M_T, m/M_P or $m/(M_P + M_T)$ are negligible with respect 1 and should be utilized at the last stage of simplifications of formulae to avoid an expanded error in the final results. Making use of this approximation, the momentum and energy conservation in the process takes the following form:

$$\vec{T} + \vec{J} + \vec{V} = \vec{0} \tag{15}$$

and

$$T^2 - 2\varepsilon_i = J^2 - 2\varepsilon_f, \tag{16}$$

respectively, where for a direct collision, one concludes $\vec{V}_i = \vec{V}_f = \vec{V}$.

The partial amplitude for each term of a four-body FWL expansion is written as

$$A = \langle \psi_f | \, T_{j,i} \, | \psi_i \rangle \,, \tag{17}$$

where the bra, $\langle \psi_f |$, and the ket, $| \psi_i \rangle$, are the final and initial asymptotic states, respectively, and $T_{j,i}$ as an element of the four-body transition operator.

The initial and final asymptotic states in momentum space are, respectively,

$$\psi_i = (2\pi)^6 \varphi_i \left(\vec{k}_{1i}, \vec{k}_{2i} \right) \delta \left(\vec{K} - \vec{K}_i \right) \tag{18}$$

and

$$\psi_f = \frac{1}{\sqrt{N}} \left(\psi_{f_1} \pm \psi_{f_2} \right) = \frac{1}{\sqrt{N}} \left(1 \pm P_{12} \right) \psi_{f_1} = \frac{(2\pi)^6}{\sqrt{N}} \varphi_f \left(\vec{k}_{1P}, \vec{k}_{2T} \right) \delta \left(\vec{K} - \vec{K}_{f_1} \right), \tag{19}$$

where φ_i and $\varphi_f = (1 \pm P_{12}) \varphi_{f_1}$ are the initial and final bound state wave functions. The notation $\varphi_{He}(\vec{k}_{1i}, \vec{k}_{2i})$ is used as the wave function of the helium atom prior to collision for φ_i and $\varphi_{He^+}(\vec{k}_{2T}) \varphi_H(\vec{k}_{1P})$ for φ_{f_1} after the collision. P_{12} in eq. (19) is the exchange operator for electrons 1 and 2. The positive (+) and negative (−) signs in eq. (19) stand for the final singlet and triplet state wave functions, respectively, while the target is initially in the singlet ground state as defined by eq. (18). The delta function in eq. (18) describes the free particle with the center of mass, while the delta function in eq. (19) describes the relative motion of two atoms after the collision.

4 Mechanisms and developments of the Thomas related amplitude terms

4.1 Term $T_{Te_P,PC}$

The third term in the prior form of the FWL transition operator, eq. (2), indicates an interaction leading to the charge transfer in the collision of a bare ion projectile (proton) with helium (the two-electron system). This charge transfer interaction has both a classical [37,53] and a quantum interpretation. When the incident projectile interacts with the target electronic cloud and creates two separate electronic clouds (electrons), one of these electrons collides with the target's nuclei and scatters in the same direction and at the same speed as the scattered projectile to form a bound hydrogen atom. This mechanism is shown in fig. 1. A similar mechanism in three-body formalism, originally described by Thomas [37], shows a peak in the angular distribution of the charge transfer amplitude at the same angle as predicted classically, now called the Thomas peak. As described by eqs. (4) and (5) and applying the Pauli exclusion principle to the four-body transition matrix, $T_{Te_P,PC}$, this term takes the following form:

$$T_{Te_P,PC} = \frac{1}{2} \left(t_{Te_P} G_0 t_{Pe_T} + t_{Te_P} G_0 t_{Pe_P} \right), \tag{20}$$

in terms of the two-body transition operators where G_0 is the free-particle Green's operator.

Applying the Pauli exclusion principle to the initial and final wave functions, the transition amplitude for the charge transfer operator, $T_{Te_P,PC}$, is

$$A_{TP} = \frac{1}{2\sqrt{N}} \langle \psi_{f_1} \pm \psi_{f_2} | \, t_{Te_1} G_0 t_{Pe_1} + t_{Te_1} G_0 t_{Pe_2} \, | \psi_i \rangle \,, \tag{21}$$

where the positive (+) and negative (−) signs stand for the singlet and triplet final states, respectively. This amplitude consists of four different terms. It is noteworthy that the final triplet state is possible only if the corresponding transition amplitude is non-zero. This triplet state is for the two electrons, one being in final atomic hydrogen and the other in helium ion. This triplet state is non-zero for a short time interval during the collision. It should be cited that specific momentum conditions are derived from each non-zero integral. These conditions are specific to each integral and are able to determine interacting particles of partial amplitudes. These momentum conditions are derived and explained in the next section.

At this point, we introduce these four integrals and their simplified form in the momentum space:

$$\begin{aligned} I_{10} &= \langle \psi_{f_1} | \, t_{Te_1} G_0 t_{Pe_1} \, | \psi_i \rangle \\ &= (2\pi)^{-3} \int \mathrm{d}\vec{k}_{1i} \mathrm{d}\vec{k}_{2i} \mathrm{d}\vec{k}_{1P} \Phi^*_{He^+} \left(\vec{k}_{2i} \right) \Phi^*_H \left(\vec{k}_{1P} \right) \left\langle \vec{k}_{1P} + \vec{V} \right| t_{Te_1} \left| \vec{k}_{1P} + \vec{k}_{1i} - \vec{J} \right\rangle G_0(E_{Pe_1}) \\ &\quad \left\langle \vec{k}_{1i} + \vec{k}_{1P} + \vec{T} \right| t_{Pe_1} \left| \vec{k}_{1i} - \vec{V} \right\rangle \Phi_{He} \left(\vec{k}_{1i}, \vec{k}_{2i} \right), \end{aligned} \tag{22}$$

$$\begin{aligned} I_{11} &= \langle \psi_{f_1} | \, t_{Te_1} G_0 t_{Pe_2} \, | \psi_i \rangle \\ &= (2\pi)^{-3} \int \mathrm{d}\vec{k}_{1i} \mathrm{d}\vec{k}_{2i} \mathrm{d}\vec{k}_{1P} \Phi^*_{He^+} \left(\vec{k}_{2i} + \vec{k}_{1P} - \vec{J} \right) \Phi^*_H \left(\vec{k}_{1P} \right) \left\langle \vec{k}_{1P} + \vec{V} \right| t_{Te_1} \left| \vec{k}_{1i} \right\rangle G_0 \left(E_{Pe_2} \right) \\ &\quad \left\langle \vec{k}_{2i} + \vec{k}_{1P} + \vec{T} \right| t_{Pe_2} \left| \vec{k}_{2i} - \vec{V} \right\rangle \Phi_{He} \left(\vec{k}_{1i}, \vec{k}_{2i} \right), \end{aligned} \tag{23}$$

$$\begin{aligned} I_{12} &= \langle \psi_{f_2} | \, t_{Te_1} G_0 t_{Pe_1} \, | \psi_i \rangle \\ &= (2\pi)^{-3} \int \mathrm{d}\vec{k}_{1i} \mathrm{d}\vec{k}_{1T} \mathrm{d}\vec{k}_{2P} \Phi^*_{He^+} \left(\vec{k}_{1T} \right) \Phi^*_H \left(\vec{k}_{2P} \right) \left\langle \vec{k}_{1T} \right| t_{Te_1} \left| \vec{k}_{1i} + \vec{k}_{2P} - \vec{J} \right\rangle G_0 \left(E_{Pe_1} \right) \\ &\quad \left\langle \vec{k}_{1i} + \vec{k}_{2P} + \vec{T} \right| t_{Pe_1} \left| \vec{k}_{1i} - \vec{V} \right\rangle \Phi_{He} \left(\vec{k}_{1i}, \vec{k}_{2P} + \vec{V} \right) \end{aligned} \tag{24}$$

and

$$\begin{aligned} I_{13} &= \langle \psi_{f_2} | \, t_{Te_1} G_0 t_{Pe_2} \, | \psi_i \rangle \\ &= (2\pi)^{-3} \int \mathrm{d}\vec{k}_{1i} \mathrm{d}\vec{k}_{1T} \mathrm{d}\vec{k}_{2P} \Phi^*_{He^+} \left(\vec{k}_{1T} \right) \Phi^*_H \left(\vec{k}_{2P} \right) \left\langle \vec{k}_{1T} \right| t_{Te_1} \left| \vec{k}_{1i} \right\rangle G_0 \left(E_{Pe_2} \right) \left\langle \vec{k}_{2P} \right| t_{Pe_2} \left| \vec{J} \right\rangle \Phi_{He} \left(\vec{k}_{1i}, -\vec{T} \right), \end{aligned} \tag{25}$$

where

$$A_{TP} = \frac{1}{2\sqrt{N}} \left(I_{10} + I_{11} \pm I_{12} \pm I_{13} \right). \tag{26}$$

Again the positive (+) and negative (−) signs stand for the singlet and triplet final states, respectively.

In addition, the free Green's operator, which appears in each integral, has two equivalent forms that depend on the scattering energies. However, the free Green's functions in the sub-amplitude terms take one of the two forms, respectively, as follows:

$$\begin{cases} G_0(E_{Pe_1}) = \left(E_{Pe_1} - \left| \vec{k}_{1i} + \vec{k}_{1P} + \vec{T} \right|^2 \Big/ 2 + i\eta \right)^{-1} \\ G_0(E_{Te_1}) = \left(E_{Te_1} - \left| \vec{k}_{1P} + \vec{k}_{1i} - \vec{J} \right|^2 \Big/ 2 + i\eta \right)^{-1} \end{cases}, \tag{27}$$

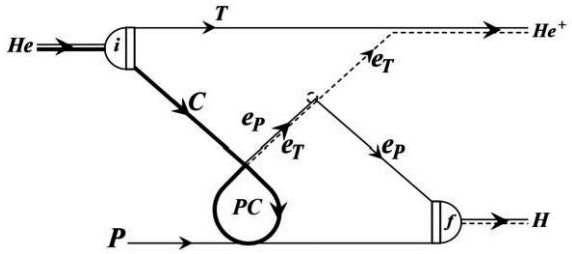

Fig. 2. The mechanism of term $T_{e_P e_T,PC}$.

$$\begin{cases} G_0(E_{Pe_2}) = \left(E_{Pe_2} - \left|\vec{k}_{2i} + \vec{k}_{1P} + \vec{T}\right|^2 \Big/ 2 + i\eta\right)^{-1} \\ G_0(E_{Te_1}) = \left(E_{Te_1} - \left|\vec{k}_{1i}\right|^2 \Big/ 2 + i\eta\right)^{-1} \end{cases}, \tag{28}$$

$$\begin{cases} G_0(E_{Pe_1}) = \left(E_{Pe_1} - \left|\vec{k}_{1i} + \vec{k}_{2P} + T\right|^2 \Big/ 2 + i\eta\right)^{-1} \\ G_0(E_{Te_1}) = \left(E_{Te_1} - \left|\vec{k}_{1i} + \vec{k}_{2P} - \vec{J}\right|^2 \Big/ 2 + i\eta\right)^{-1} \end{cases}, \tag{29}$$

and

$$\begin{cases} G_0(E_{Pe_2}) = \left(E_{Pe_2} - \left|\vec{k}_{2P}\right|^2 \Big/ 2 + i\eta\right)^{-1} \\ G_0(E_{Te_1}) = \left(E_{Te_1} - \left|\vec{k}_{1i}\right|^2 \Big/ 2 + i\eta\right)^{-1} \end{cases}. \tag{30}$$

By definition, the scattering energy is the total energy minus the out-of-interaction particle energies. We used the expansion coefficients of wave plane phase between any two Jacobi coordinate to calculate the corresponding scattering energies in the same manner as was done for three-body interactions [41,56]. The scattering energies like E_{Pe_2} or E_{ee} are unique in a four-body formalism as compared with a three-body formalism. The scattering energies present in the free Green's functions (27) to (30) are approximately as

$$E_{Pe_1} \cong \frac{1}{2}V^2 - \vec{k}_{1i} \cdot \vec{V} - \frac{1}{2}k_{2i}^2 + \varepsilon_i, \tag{31}$$

$$E_{Pe_2} \cong \frac{1}{2}V^2 - \vec{k}_{2i} \cdot \vec{V} - \frac{1}{2}k_{1i}^2 + \varepsilon_i \tag{32}$$

and

$$\begin{cases} E_{Te_1} \cong \frac{1}{2}V^2 + \vec{k}_{1P} \cdot \vec{V} - \frac{1}{2}k_{2T}^2 + \varepsilon_f \\ E_{Te_1} \cong \varepsilon_f - \frac{k_{2P}^2}{2\mu_{Pe}} \end{cases}. \tag{33}$$

The scattering energies given here are used in the calculation of partial amplitudes and finally the differential cross section. However, there are other forms of the scattering energies that are used for the calculation of different sub-amplitudes. Specifically, the top form of E_{Te_1} in eq. (33) is used for calculating I_{10} and I_{11} while the second form of E_{Te_1} is used in calculating the sub-amplitudes I_{12} and I_{13}.

4.2 Term $\mathsf{T_{e_P e_T,PC}}$

The electron-electron interaction leads to the Thomas peak (let us not call it a Thomas mechanism), due to the transfer of an electron to the projectile after that projectile interacts with the target electronic cloud. Because of this interaction, described by $T_{e_P e_T,PC}$, the incident projectile consequently forms an atom (atomic hydrogen in this case) with the ejected electron, as shown by fig. 2.

Applying the Pauli exclusion principle (5) to the operator $T_{e_Pe_T,PC}$, expanding $T_{e_Pe_T,PC}$ in terms of the two-particle transition operators and substituting the initial and the final states in transition amplitude definition by eq. (17), we will get the transition amplitude as

$$A^e_{TP} = \frac{1}{\sqrt{N}} \langle \psi_{f_1} | t_{e_1e_2} G_0 t_{Pe_1} + t_{e_1e_2} G_0 t_{Pe_2} | \psi_i \rangle, \tag{34}$$

for a final singlet state while it is zero for a final triplet state. It has to be noted that the final triplet state is forbidden in this electron-electron mechanism.

We will write A^e_{TP}, in short, as

$$A^e_{TP} = \frac{1}{\sqrt{N}} \left(I_{14} + I_{15} \right), \tag{35}$$

where I_{14} and I_{15} are equal to $\langle \psi_{f_1} | t_{e_1e_2} G_0 t_{Pe_1} | \psi_i \rangle$ and $\langle \psi_{f_1} | t_{e_1e_2} G_0 t_{Pe_2} | \psi_i \rangle$, respectively. We simplify the integral I_{14}, as

$$\begin{aligned} I_{14} = (2\pi)^{-3} \int \mathrm{d}\vec{k}_{1P} \mathrm{d}\vec{k}_{1i} \mathrm{d}\vec{k}_{2i} \Phi^*_{He^+}(\vec{q}_1) \Phi^*_H \left(\vec{k}_{1P} \right) \left\langle \frac{1}{2} \left(\vec{q}_2^{+} + \vec{T} - \vec{V} \right) \right| t_{e_1e_2} \left| \frac{1}{2} \left(\vec{q}_2^{-} + \vec{J} \right) \right\rangle G^+_0(E_{Pe_1}) \\ \left\langle \vec{k}_{1i} + \vec{k}_{1P} + \vec{T} \right| t_{Pe_1} \left| \vec{k}_{1i} - \vec{V} \right\rangle \Phi_i \left(\vec{k}_{1i}, \vec{k}_{2i} \right), \end{aligned} \tag{36}$$

where $\vec{q}_1 = \vec{k}_{1i} + \vec{k}_{2i} + \vec{T}$ and $\vec{q}_2^{\pm} = \vec{k}_{2i} - \vec{k}_{1P} \pm \vec{k}_{1i}$. The two forms of momentum-space Green's function are

$$\begin{cases} G_0(E_{Pe_1}) = \left(E_{Pe_1} - \frac{1}{2} \left| \vec{k}_{1i} + \vec{k}_{1P} + \vec{T} \right|^2 + i\eta \right)^{-1} \\ G_0(E_{e_1e_2}) = \left(E_{e_1e_2} - \frac{1}{4} \left| \vec{q}_2^{-} + \vec{J} \right|^2 + i\eta \right)^{-1} \end{cases}. \tag{37}$$

In the same way, we simplify the integral I_{15} as

$$\begin{aligned} I_{15} = (2\pi)^{-3} \int \mathrm{d}\vec{k}_{1P} \mathrm{d}\vec{k}_{1i} \mathrm{d}\vec{k}_{2i} \Phi^*_{He^+}(\vec{q}_1) \Phi^*_H \left(\vec{k}_{1P} \right) \left\langle \frac{1}{2} \left(\vec{q}_2^{+} + \vec{T} - \vec{V} \right) \right| t_{e_1e_2} \left| \frac{1}{2} \left(\vec{q}_3 - \vec{J} \right) \right\rangle G^+_0(E_{Pe_2}) \\ \langle \vec{q}_4 | \, t_{Pe_2} \left| \vec{k}_{2i} - \vec{V} \right\rangle \Phi_i \left(\vec{k}_{1i}, \vec{k}_{2i} \right), \end{aligned} \tag{38}$$

where $\vec{q}_3 = \vec{k}_{2i} + \vec{k}_{1P} - \vec{k}_{1i}$ and $\vec{q}_4 = \vec{k}_{2i} + \vec{k}_{1P} + \vec{T}$, where the two forms of momentum-space Green's function are

$$\begin{cases} G_0(E_{Pe_2}) = \left(E_{Pe_2} - \left| \vec{k}_{2i} + \vec{k}_{1P} + \vec{T} \right|^2 \Big/ 2 + i\eta \right)^{-1} \\ G_0(E_{e_1e_2}) = \left(E_{e_1e_2} - \frac{1}{4} \left| \vec{k}_{1i} - \vec{k}_{2i} - \vec{k}_{1P} + \vec{J} \right|^2 + i\eta \right)^{-1} \end{cases}. \tag{39}$$

Here, the momentum vectors $\vec{q}s$ are defined simply to make eqs. (36) and (38) shorter. The scattering energy $E_{e_1e_2}$ simplifies as

$$E_{e_1e_2} \cong \varepsilon_f + \frac{1}{4} \left[V^2 + 2 \left(\vec{k}_{1P} - \vec{k}_{2T} \right) \cdot \vec{V} - \left(\vec{k}_{1P} + \vec{k}_{2T} \right)^2 \right] \tag{40}$$

and the scattering energies E_{Pe_1} and E_{Pe_2} are introduced by eqs. (31) and (32), respectively. Calculation of I_{14} and I_{15} introduces momentum conditions, which are discussed in the next section. In the present work, the Green's functions $G_0(E_{Pe_1})$ and $G_0(E_{Pe_2})$ are used to calculate I_{14} and I_{15}, respectively.

Here, the initial bound state wave function φ_i, which describes the ground state of a helium atom, is considered as the product of two hydrogenic wave functions by $Z_e = 1.7$ as an effective charge of the nucleus. It has the form

$$\begin{aligned} \varphi_i(\vec{p}_1, \vec{p}_2) &= \varphi_{100}(\vec{p}_1, Z_e) \varphi_{100}(\vec{p}_2, Z_e) \\ &= \frac{11.092}{(2.84766 + {p_1}^2)^2 (2.84766 + {p_2}^2)^2}. \end{aligned} \tag{41}$$

The wave function φ_{f_1} is the product of hydrogenic wave functions for helium ion with $Z_{He} = 2$ and hydrogen atom with $Z_H = 1$. Hence, the final bound state wave function is

$$\begin{aligned} \varphi_f(\vec{p}_1, \vec{p}_2) &= \frac{1}{\sqrt{2}} \left(\varphi_{100}(\vec{p}_2, Z_{He}) \varphi_{100}(\vec{p}_1, Z) \pm \varphi_{100}(\vec{p}_1, Z_{He}) \varphi_H(\vec{p}_2, Z) \right) \\ &= \frac{32}{\pi^2} \left(\frac{1}{(1 + {p_1}^2)^2 (4 + {p_2}^2)^2} \pm \frac{1}{(1 + {p_2}^2)^2 (4 + {p_1}^2)^2} \right). \end{aligned} \tag{42}$$

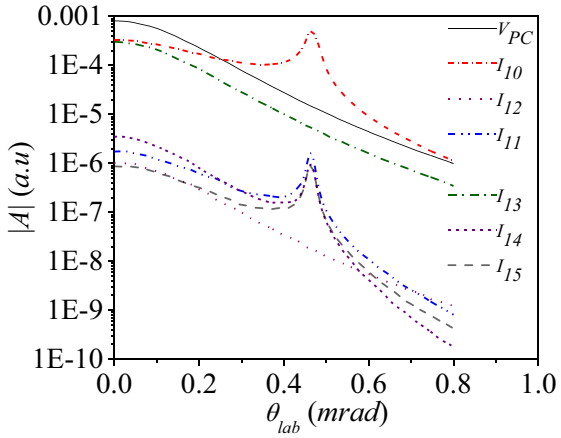

Fig. 3. Plots of the sub-amplitudes related to the second-order terms $\langle\psi_f|t_{Te_1}G_0t_{PC}|\psi_i\rangle$ and $\langle\psi_f|t_{e_1e_2}G_0t_{PC}|\psi_i\rangle$, for charge transfer as a function of scattering angle, which leads to a Thomas peak.

The energy of projectile in the laboratory frame is chosen to be 7.42 MeV in our calculations.

We integrated our integrands using the adaptive Monte Carlo method, which is the best method for taking high dimension integrals and takes care of the singularities. During calculations to achieve the final form of the integrand in I_{10} to I_{15}, we use the common simplifications in the works of Alston [43] and Ghanbari-Adivi and Bolorizadeh [41].

5 Discussion

5.1 Angular distributions of the partial amplitude norms

The major amplitude in the charge transfer channel is the first-order electronic amplitude, namely the projectile-electronic cloud interaction V_{PC}, which is equal to the first Born amplitude discussed in our First Order Paper [35], which can be seen in fig. 3. All terms, leading to a Thomas mechanism or showing a peak at the same scattering angle, in the charge transfer collision of protons with helium, include the interaction of the projectile with the electronic cloud. The physics behind these sub-amplitudes is important since all of them show a peak at the same location as the Thomas mechanism predicts. Other terms and the second-order terms not discussed here could add up to be (partially) constructive or (partially) destructive with the first-order electronic amplitude. We discuss the physics of the calculated partial amplitudes and sub-amplitudes, next.

a) The sub-amplitudes I_{10}, I_{11}, I_{12}, and I_{13} describe the interaction of the target's nucleus with the ejected electron after the scattering of the projectile with the electronic cloud, $t_{Te_1}G_0t_{PC}$; however, not all of them result in a peak at the same scattering angle as the Thomas mechanism in the angular distribution of the amplitude. In particular:

1) The sub-amplitude $I_{10} = \langle\psi_{f_1}|t_{Te_1}G_0t_{Pe_1}|\psi_i\rangle$, which represents a three-body interaction and the Thomas mechanism, results in a Thomas peak. Even though the initial and final wave functions include the second electron, this electron is passive in I_{10} and is absent in the interaction operator $t_{Te_1}G_0t_{Pe_1}$. In calculating the sub-amplitude I_{10}, the appearing delta functions result in a momentum condition; hence, the momentum transferred to the electron remained with the target, $\Delta\vec{k}_2 = \vec{k}_{2T} - \vec{k}_{2i}$, is equal to $-[m/(M_T+m)]\vec{T}$, which is approximately equal to zero since $m/(M_T+m)$ is very small. This is the momentum change required in changing the state of the second electron from the ground state of the helium atom to the ground state of the helium ion. This condition clarifies that the second electron plays a minor role in this interaction, and the target momentum transfer during the collision, $[M_T/(M_T+m)]\vec{T}$, is approximately equal to $\vec{T}$. The wave functions, which are used in a three-body treatment, do not even include the second electron, while here, in a four-body treatment, it is not the case. However, the Thomas peak is observed at 0.47 mrad degrees as expected and as is shown in fig. 3.
2) A peak at the same location as the Thomas peak is present in the sub-amplitude $I_{11} = \langle\psi_{f_1}|t_{Te_1}G_0t_{Pe_2}|\psi_i\rangle$, which is specific to this four-body treatment, as is shown in fig. 3. This sub-amplitude describes the charge transfer while all four particles are involved. The probability of charge transfer occurrence by this term is small and has a minor effect on the total amplitude and the final cross sections, which provide experimental evidence for it. It has to be noted that the delta function dictates a momentum condition, $\Delta\vec{k}_2 = \vec{k}_{2T} - \vec{k}_{2i} = \vec{k}_{1P} - \vec{J}$, for the electron remaining with the target during the interaction. A Thomas peak is observed at 0.47 mrad degree as expected.
3) Based on the interaction operator, the sub-amplitudes $I_{12} = \langle\psi_{f_2}|t_{Te_1}G_0t_{Pe_1}|\psi_i\rangle$ and I_{10} are similar. However, a peak at 0.47 mrad or any other angle calculated does not appear for the amplitude I_{12}, as is shown in fig. 3. This sub-amplitude is present due to the Pauli exclusion principle, where the electrons are indistinguishable.

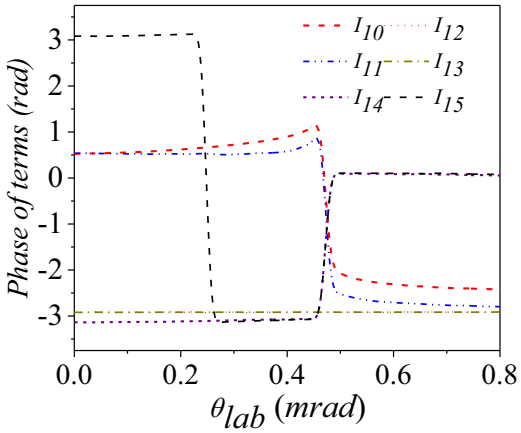

Fig. 4. Phase of the sub-amplitudes discussed and calculated in this study; the matrix for V_{PC} has a negative value with π phase.

As is shown in fig. 3, the sub-amplitude I_{12} has a very small contribution to the total amplitude as well as the calculated cross sections for the charge transfer. In calculating I_{12}, the delta function dictates the relation $\Delta\vec{k}_2 = \vec{k}_{2P} - \vec{k}_{2i} = -\vec{V}$, demonstrating that the charge transfer occurs, while the momentum transfer to the second electron is equal to the projectile velocity, $\vec{V}$, but in the opposite direction. Although it is not possible to describe this interaction classically, the interaction occurs with a small probability and therefore one could technically neglect this sub-amplitude.

4) The interaction described by the sub-amplitude $I_{13} = \langle\psi_{f_2}|t_{Te_1}G_0t_{Pe_2}|\psi_i\rangle$ is similar to that for I_{11} in terms of the interaction operator and is similar to I_{12} in terms of the final wave function. The probability of charge transfer from the initial channel to the final channel f_2, which is introduced by this sub-amplitude, is relatively high and affects the charge transfer cross sections. However, this sub-amplitude does not produce a peak at the location of Thomas peak. The delta function condition is now $\vec{k}_{2i} = -\vec{T}$, which demonstrates that the initial momentum of the second electron, the electron transferred to the projectile, should be as large as that for the target nucleus momentum transfer but in the opposite direction.

The partial amplitude $\langle\psi_f|t_{e_1e_2}G_0t_{PC}|\psi_i\rangle$ consists of the sub-amplitudes I_{14} and I_{15}. Here, the second electron replaces the target nucleus in the amplitude $\langle\psi_f|t_{Te_1}G_0t_{PC}|\psi_i\rangle$. Hence, the electron-electron interaction replaces the electron-nucleus interaction in the second step. This term does not appear in any three-body treatment, as only one active electron is assumed there.

As mentioned earlier, the partial amplitude $\langle\psi_f|t_{e_1e_2}G_0t_{PC}|\psi_i\rangle$ is zero for the triplet final state; nonetheless, the final singlet state for it is not zero. The momentum condition derived in the integration for this interaction proves that the momentum transfer to the second electron is $\Delta\vec{k}_2 = \vec{k}_{2T} - \vec{k}_{2i} = \vec{k}_{1i} + \vec{T}$. As is shown in fig. 3, a peak is observed at 0.47 mrad for both sub-amplitudes of this partial amplitude. Further relevant results from this study include:

1) The interaction and form of the sub-amplitude I_{14} are similar to those of I_{10} if the target nucleus replaces the second electron. However, I_{14} is smaller than I_{10} by two orders of magnitude; hence, the probability of an electron-electron collision is much less than the probability of an electron-target nucleus collision. Nevertheless, around the Thomas peak, this term affects the charge transfer cross sections somehow.
2) Similarly, the interaction and form of sub-amplitude I_{15} are similar to those for I_{11}. In this case, the sub-amplitude I_{11} is slightly larger in magnitude as compared with I_{15} (fig. 3). Again, this difference indicates that the interaction of the electron-target nucleus, leading to charge transfer, is more probable than the interaction of electron-electron collisions. It is also expected that the magnitude of both sub-amplitudes, I_{11} and I_{15}, are small because they contain interactions between the projectile and the second electron, which results in the transfer of the first electron to the projectile. This interaction, despite showing a Thomas equivalent mechanism, has no counterpart in a three-body formalism.

5.2 Angular distribution of the partial amplitude phases

The first-order electronic term in the Faddeev series is a negative real number and, thus, it has a phase of π. It is notable that by phase difference, we mean the phase difference between the specific sub-amplitude in question and the first-order electronic amplitude. The phases of all the sub-amplitudes derived here are shown in fig. 4. In the following, we discuss the effect of those sub-amplitudes on the first-order electronic amplitude in the charge transfer interaction between the proton and the helium atom.

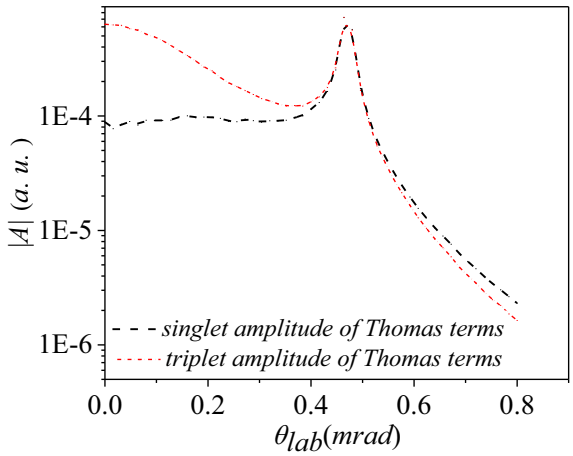

Fig. 5. Singlet and triplet amplitudes of Thomas terms *versus* scattering angles.

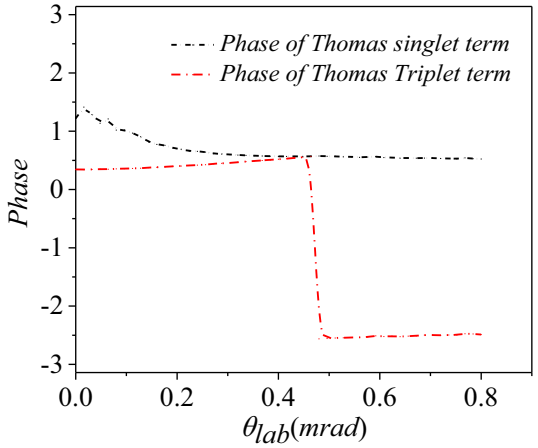

Fig. 6. Phase of singlet and triplet amplitudes for Thomas terms plotted *versus* scattering angles.

The first-order electronic amplitude and the sub-amplitudes I_{12} and I_{13} show an almost similar angular dependence and therefore add up constructively, although I_{13} and I_{12} are by a factor of 3 and 10^3 smaller in magnitude, respectively. Thus, I_{12} has a minute effect on the total amplitude for charge transfer.

I_{10} is the second-order sub-amplitude showing a strong Thomas peak (fig. 3), where it adds to the first-order electronic amplitude almost destructively below the Thomas peak and then constructively above this peak (fig. 4). The three sub-amplitudes I_{11}, I_{14}, and I_{15}, which physically arise from different mechanisms, show a peak exactly at the same location as the Thomas peak in the sub-amplitude I_{10} but are by two orders of magnitude smaller than I_{10}, as is shown in fig. 3. The sub-amplitudes I_{14} and I_{15} contribute to the total amplitude constructively for the singlet final state; however, they both are almost destructive when added with the sub-amplitude I_{11}, as is shown in fig. 4. Sub-amplitude I_{11} adds to the first-order electronic amplitude almost destructively below the Thomas peak, and almost constructively for the case of scattering angles above the Thomas peak (fig. 4). When the three sub-amplitudes I_{11}, I_{14}, and I_{15} are added, they affect the total amplitude with the values of about 3% (1%) for the final singlet (triplet) state.

To form a triplet state, I_{11} adds to I_{10} constructively, although I_{11} is by a factor of 100 smaller in magnitude than I_{10}, I_{12}, and I_{13}, which turn from being constructive to destructive when going from scattering angles below to above the Thomas peak (fig. 4).

In fig. 5, the singlet and triplet amplitudes for the Thomas related peaks are shown. The singlet amplitude is smaller by a factor of ten than the triplet amplitude, while the two converge at the Thomas scattering angle, 0.47 mrad. The two are approximately equal in magnitude above the Thomas angle. In fig. 6, the phase of the singlet and the triplet Thomas related amplitudes are plotted as a function of scattering angle. As is known, the phase of the first-order electronic amplitude is $-\pi$, hence in the range 0–0.47 mrad of scattering angle both singlet and triplet terms have a destructive effect on the first-order electronic amplitude. However, in the range 0.47–0.8 the triplet amplitude adds constructively to the first-order electronic amplitude, while the singlet one keeps its destructive effect on this term.

6 Concluding remarks

In this paper, the electronic cloud concept was used to study the interaction of protons and atomic helium, specifically for Thomas-related partial amplitudes in a charge transfer collision. The physics involved in a four-body treatment of the charge transfer interaction was mainly discussed. In this model, both electrons of the helium atom are assumed to be active. The four-body FWL formalism was applied up to the second order, where the Thomas mechanism is observed by the term $t_{Te_1}G_0t_{Pe_1}$. In the present four-body FWL formalism, the terms $t_{Te_1}G_0t_{Pe_2}$, $t_{e_1e_2}G_0t_{Pe_2}$ and $t_{e_1e_2}G_0t_{Pe_1}$ are found in addition to the $t_{Te_1}G_0t_{Pe_1}$, where they show a peak at the same angle as the Thomas peak in the partial amplitude. The sub-amplitude I_{12} and I_{13} do not show a peak at the Thomas angle; however, all the sub-amplitudes, as well as I_{12} and I_{13}, change their constructive/destructive effect on the first-order term at the Thomas angle. The four terms discussed here result in different momentum conditions, which are different from the momentum condition for the Thomas mechanism. It has to be noted that the two electrons, one being bound in the atomic hydrogen (formed atom) and the other one being bound in the helium ion (ion being left), form a singlet or triplet state that both contribute to the charge transfer process. The final triplet state leads to very small amplitudes as compared with the singlet state.

The quasi–four-body model presented here could be applied to single or double ionization, excitation, charge transfer, or a combination of these effects. The method could also be applied to larger atoms, as well.

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