Electron correlations in single-electron capture from helium by fast protons and α particles

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Single-electron capture from heliumlike atomic systems by bare projectiles is investigated by means of the four-body boundary-corrected first Born approximation (CB1-4B). The effect of the dynamic electron correlation is explicitly taken into account through the complete perturbation potential. The quantum-mechanical post and prior transition amplitudes for single charge exchange encompassing symmetric and/or asymmetric collisions are derived in terms of two-dimensional real integrals in the case of the prior form and five-dimensional quadratures for the post form. An illustrative computation is performed for single-electron capture from helium by protons and α particles at intermediate and high impact energies. The role of dynamic correlations is examined as a function of increased projectile energy. The validity and utility of the proposed CB1-4B method is critically assessed in comparison with the existing experimental data for total cross sections, and excellent agreement is obtained.

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I. INTRODUCTION

For atomic processes in which two (or more) active electrons are involved in high-energy ion-atom collisions, one must address the question of the influence of electronic correlations on the magnitude of the process. The study of interelectronic correlation has played a central role in atomic collision physics for a long time (see, e.g., [1]). The helium atom has, to a large extent, been a benchmark system of such studies. It should be noted that the concept of correlation arises in many different contexts. Correlation may be defined mathematically as a deviation from the product of a single particle term, for example, $\Psi(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_n)-\Psi_1(\vec{r}_1)\Psi_2(\vec{r}_2),\ldots,\Psi_n(\vec{r}_n)$. Thus, correlation may be understood as a deviation from an independent-particle model and is a useful concept in the study of many-body problems. However, the situation becomes significantly more difficult if many-electron systems are considered. In that case, the many-body time-dependent Schrödinger equation (TDSE) is not solvable in a closed form for more than two mutually interacting particles even if the underlying forces are precisely known. Accordingly, mean-field models, usually based on time-dependent Hartree Fock (TDHF) or time-dependent density functional theory have been developed and implemented (see, e.g., [2–4]). From a practical point of view, this implies that the many-electron dynamics are described in terms of single-particle equations with a single-particle Hamiltonian which contains a mean-field potential that account for the electron-electron interaction. For the investigation of electron capture processes, the TDSE can be solved by using the two-center (TC) extension of the basis generator method (BGM) [5,6]. Essentially, the BGM is a nonperturbative coupled-channel method that includes basis states which structurally adapt to the dynamics of the collision problem [7]. A good agreement between experimental and TC-BGM results [6] based on the independent electron model (IEM) and the one-active-electron model for the p-He collisions may indicate that electron correlation effects give relatively small corrections to the investigated processes. Moreover, Zapukhlyak *et al.* [6] suggested that the appearance of a peak structure in the double ratio of transfer excitation to single transfer versus double excitation to single excitation at 0.5 mrad is not connected with electron-electron correlations. The TC-BGM based on the IEM used by Zapukhlyak and Kirchner [8] has also been applied very recently to electron-transfer processes in p-He and α-He collisions at intermediate impact energies. Their results [8] demonstrate that the IEM, which neglects electron-correlation effects, provides an adequate framework for describing a number of one- and two-electron processes in these systems. A breakthrough in allowing for dynamic correlation was achieved in the works of Reading and Ford [9,10]. The role of electron correlation during a high-energy ion-atom collision was also investigated in Refs. [11–13] by means of the frozen-correlation approximation (FCA), which exactly includes correlation in the initial and final states but freezes correlation during the collision. Despite the fact that FCA neglects dynamic correlation, the cross sections for double excitation and double ionization of He by protons and antiprotons provided by the FCA are in good agreement with experimental data. In spite of this success, a complete neglect of dynamic correlation may lead to an unphysical behavior of the transition probability at large impact parameters [14]. On the other hand, a proper four-body treatment of the Z_P-$(Z_T,e_1,e_2)_i$ collision should be a more natural starting point, because it offers various possibilities to adequately incorporate both dynamic and static correlations. Dynamic or scattering correlation is that which occurs during the collision. The dynamic correlations as one of the causes of the transition from the initial to the final state of the whole four-body system would be included by selecting the appropriate forms of the four-body perturbation potentials. Static correlation originates from the Coulomb interaction between the two electrons in the heliumlike atomic system before the collision takes place. An adequate description of the static correlations for heliumlike atomic systems must explicitly include the two electronic coordinates $\vec{r}_{1,2}$ and directly or indirectly the interelectronic distance $r_{12}=|\vec{r}_1-\vec{r}_2|$. When this is accomplished, the resulting correlated theory diverges in a clear manner from the standard Hartree-Fock method.

The status of the first-order theories for electron capture was considerably changed when Belkić *et al.* [15] in 1979 focused much attention on the correct boundary conditions,

recognizing the first Born approximation (CB1) to be a first-order term of a divergent-free perturbation expansion. The boundary condition problem requires that both initial- and final-state wave functions exhibit the correct asymptotic behaviors at the infinite internuclear separation R. This is equivalent to the asymptotic convergence problem [16], which consists of showing the existence of Møller wave matrices $\Omega^{(\pm)}$ [17]. The fundamental work of Belkić *et al.* [15] initialized a number of computations (see for example [18–26]) which were carried out by means of a three-body CB1 with correct boundary conditions (CB1-3B). These computations resolved the longstanding dilemma about the alleged "general" inadequacy of the first-order theories for charge exchange. By preserving the correct boundary conditions, the first-order theories emerge as quite accurate for the prediction of total cross sections. However, in collisions involving two or more electrons, three-body methods (such as CB1-3B) treat the noncaptured electrons as being passive in the sense that their interactions with the active electron do not contribute to the capture process. In the case of single-electron transfer from two or more electron atoms by a bare projectile, the active electron is often described by the Roothaan-Hartree-Fock orbital [20–26]. Thus, pure four-body problems, such as charge exchange in p-He or α-He collisions, are reduced to three-body problems for which the CB1-3B model completely neglects dynamic (i.e., collisional) correlations.

In principle, a generalization of a three-body collision theory to a four-body or many-body collision system can be done in essentially a straightforward manner. However, in practice, applications of a four-body collision theory involve laborious calculations even in a first-order model. The present work is aimed at investigating single-electron capture from heliumlike atomic systems by bare projectiles as well as the role of dynamic electronic correlations in such collisions using the four-body version of the boundary-corrected first Born (CB1-4B) approximation. Different quantum-mechanical four-body methods for various inelastic high-energy ion-atom collisions (single and double charge exchange, simultaneous transfer and ionization, simultaneous transfer and excitation, electron detachment, etc.) have recently been extensively discussed in the review paper of Belkić *et al.* [27] and the book of Belkić [28]. High-energy single-electron capture from one- and multielectron atoms by *hydrogenlike* projectiles has been examined by Mančev [29,30], who introduced the CB1-4B approximation. However, in these articles [29,30] only the version that does not contain $1/r_{12}$ was used. Such a model cannot yield any information about the significance of the role of the dynamic interelectron interaction.

Although interest in four-body methods has been considerably revived [27,28], no computations have thus far been reported on $Z_P - (Z_T, e_1, e_2)_i$ charge exchange by the means of CB1-4B approximation. We shall focus on the role of the interelectron (e_1-e_2) potential $V_{12} = 1/r_{12}$ from a dynamic point of view. To achieve this goal within the CB1-4B method, one ought to employ the post formalism with the appropriate full perturbation V_f in the exit channel. A contribution from $V_{12} = 1/r_{12}$ to single capture in the p-He and α-He collisions has not been previously assessed with the help of the first-order model. The second aim of this work is to assess the usefulness of the CB1-4B method at intermediate and high impact energies. This plan will be achieved by comparisons between theoretical and experimental data. The third goal is to assess the post-prior discrepancy.

Atomic units will be used throughout unless otherwise stated.

II. THEORY

We examine single-electron capture in the following typical single charge exchange in fast collisions of completely stripped projectiles with heliumlike targets:

$$Z_P + (Z_T, e_1, e_2)_i \longrightarrow (Z_P, e_1)_{f_1} + (Z_T, e_2)_{f_2}, \qquad (1)$$

where Z_K is the charge of the Kth nucleus and $j(=i, f_1, f_2)$ is the collective label for the set of usual quantum numbers. The parentheses $(\cdots)$ symbolize the bound states. Let $\vec{s}_1$ and $\vec{s}_2$ ($\vec{x}_1$ and $\vec{x}_2$) be position vectors of the first and second electrons (e_1 and e_2, respectively) relative to the nuclear charge of the projectile Z_P (target Z_T). Further, let us denote by $\vec{R}$ the position vector of Z_T with respect to Z_P. The vector of the distance between the two active electrons (e_1 and e_2) is denoted by $\vec{r}_{12} = \vec{x}_1 - \vec{x}_2 = \vec{s}_1 - \vec{s}_2$. In the entrance channel, it is convenient to introduce $\vec{r}_i$ as the relative vector of Z_P with respect to the center of mass of $(Z_T, e_1, e_2)_i$. Symmetrically, in the exit channel, let $\vec{r}_f$ be the position vector of the center of mass of $(Z_P, e_1)_{f_1}$ relative to $(Z_T, e_2)_{f_2}$.

It is convenient to express the kinetic-energy operator H_0 via the set of the independent Jacobian coordinates $\{\vec{x}_1, \vec{x}_2, \vec{r}_i\}$ or $\{\vec{r}_f, \vec{s}_1, \vec{x}_2\}$: $H_0 = -\nabla^2_{r_i}/(2\mu_i) - \nabla^2_{x_1}/(2b) - \nabla^2_{x_2}/(2b) - \vec{\nabla}_{x_1} \cdot \vec{\nabla}_{x_2}/M_T = -\nabla^2_{r_f}/(2\mu_f) - \nabla^2_{s_1}/(2a) - \nabla^2_{x_2}/(2b)$, where $\mu_i = M_P(M_T + 2)/(M_P + M_T + 2)$, $\mu_f = (M_T + 1)(M_P + 1)/(M_P + M_T + 2)$, $a = M_P/(M_P + 1)$, $b = M_T/(M_T + 1)$, and M_P and M_T are the masses of the projectile and target, respectively. The term $\vec{\nabla}_{x_1} \cdot \vec{\nabla}_{x_2}/M_T$ can be neglected for heavy particles because $M_T \gg 1$. The full Hamiltonian of the system under study, in the center-of-mass frame for the whole system, is given by $H = H_0 + V$, where V represents the total interaction potential operator $V = Z_P Z_T/R - Z_P/s_1 - Z_P/s_2 - Z_T/x_1 - Z_T/x_2 + 1/r_{12}$. As usual for rearranging collisions, the complete Hamiltonian can further be split into the following form: $H = H_i + V_i$. Here, H_i and V_i are the channel Hamiltonian and the perturbation potential in the entrance channel: $H_i = H_0 + V_T \equiv H_0 - Z_T/x_1 - Z_T/x_2 + 1/r_{12}$, $V_i = Z_P Z_T/R - Z_P/s_1 - Z_P/s_2$. The unperturbed channel state Φ_i is defined by $(H_i - E_i)\Phi_i = 0$, with $\Phi_i = \varphi_i(\vec{x}_1, \vec{x}_2)e^{i\vec{k}_i \cdot \vec{r}_i}$. Function $\varphi_i(\vec{x}_1, \vec{x}_2)$ represents the two-electron bound-state wave function of the atomic system $(Z_T; e_1, e_2)_i$, whereas $\vec{k}_i$ is the initial wave vector and E_i is the binding energy of the two-electron target. The initial state Φ_i is distorted even at infinity, due to the presence of the asymptotic Coulomb repulsive potential, $V_i^\infty = Z_P(Z_T - 2)/R$, between the projectile and the screened target nucleus. Bearing in mind the long-range nature of the Coulomb interaction, the Hamiltonian H can be decomposed according to $H = H_i^c + V_i^c$, with

$$H_i^c = -\frac{1}{2\mu_i}\nabla^2_{r_i} + \frac{Z_P(Z_T - 2)}{r_i} - \frac{1}{2b}\nabla^2_{x_1} - \frac{1}{2b}\nabla^2_{x_2} - \frac{Z_T}{x_1} - \frac{Z_T}{x_2} + \frac{1}{r_{12}}, \qquad (2)$$

$$V_i^c = \frac{Z_P Z_T}{R} - \frac{Z_P(Z_T-2)}{r_i} - \frac{Z_P}{s_1} - \frac{Z_P}{s_2} \simeq \frac{2Z_P}{R} - \frac{Z_P}{s_1} - \frac{Z_P}{s_2}, \tag{3}$$

where we neglect the terms of the order of $1/M_T$, which implies $r_i \simeq R$. Potential V_i^c exhibits a short-range behavior when $R \to \infty$. It should be noted that the perturbation V_i^c depends *only* on the interaction between electrons and a projectile. The term Z_P/R in Eq. (3), despite its form, is not related to the internuclear potential, but originates solely from the electron-projectile interaction. The asymptotic tail of the potential $-Z_P/s_1$ is $-Z_P/R$, since $s_1 \to R$ as $R \to \infty$. This can be seen by using the Taylor expansion for $Z_P/s_1 = Z_P/|\vec{R} - \vec{x}_1|$ around R. A small value of the x_1 coordinate in the entrance channel justifies such a development. The same statement also holds true for the potential $-Z_P/s_2$. With the Hamiltonian H_i^c the eigenproblem in the entrance channel reads as $(H_i^c - E_i)\Phi_i^c = 0$. The solution of the eigenproblem for Φ_i^c is given by $\Phi_i^c = \varphi_i(\vec{x}_1, \vec{x}_2) e^{i\vec{k}_i\cdot\vec{r}_i} \mathcal{N}^+(\nu_i)\, {}_1F_1(-i\nu_i, 1, ik_i r_i - i\vec{k}_i\cdot\vec{r}_i)$, where $\mathcal{N}^+(\nu_i) = e^{-\pi\nu_i/2}\Gamma(1+i\nu_i)$ and $\nu_i = Z_P(Z_T-2)/v$. The symbol ${}_1F_1(a,b,z)$ stands for the confluent hypergeometric function, whereas v is the incident velocity. The Coulomb wave function Φ_i^c has the asymptotic form

$$\Phi_i^c(r_i \to \infty) \equiv \Phi_i^+ = \varphi_i(\vec{x}_1, \vec{x}_2) \times \exp[i\vec{k}_i\cdot\vec{r}_i + i\nu_i \ln(vR - \vec{v}\cdot\vec{R})]. \tag{4}$$

In the exit channel we can write $H = H_f + V_f$, where the channel Hamiltonian H_f and perturbation V_f are respectively defined by $H_f = H_0 + V_{PT} \equiv H_0 - Z_P/s_1 - Z_T/x_2$ and $V_f = Z_P Z_T/R - Z_T/x_1 - Z_P/s_2 + 1/r_{12}$. Solving the eigenvalue equation, $(H_f - E_f)\Phi_f = 0$, we obtain the unperturbed state Φ_f in the exit channel as $\Phi_f = \varphi_P(\vec{s}_1)\varphi_T(\vec{x}_2) e^{-i\vec{k}_f\cdot\vec{r}_f}$, where $\varphi_P(\vec{s}_1)$ and $\varphi_T(\vec{x}_2)$ are single-electron hydrogenlike wave functions in the exit channel. Furthermore, $\vec{k}_f$ is the final wave vector and $E_f = -Z_P^2/2 - Z_T^2/2$. The distortion of the unperturbed state Φ_f is caused by the potential $V_f^\infty = (Z_T-1)(Z_P-1)/R$, which represents the asymptotic form of the perturbation V_f. In this case, the constituent two terms of the separable Hamiltonian $H = H_f^c + V_f^c$ are defined as

$$H_f^c = -\frac{1}{2\mu_f}\nabla_{r_f}^2 + \frac{(Z_T-1)(Z_P-1)}{r_f} - \frac{1}{2a}\nabla_{s_1}^2 - \frac{1}{2b}\nabla_{x_2}^2 - \frac{Z_P}{s_1} - \frac{Z_T}{x_2}, \tag{5}$$

$$V_f^c = \frac{Z_P Z_T}{R} - \frac{(Z_T-1)(Z_P-1)}{r_f} - \frac{Z_P}{s_2} - \frac{Z_T}{x_1} + \frac{1}{r_{12}}. \tag{6}$$

Using $r_f \simeq R$, we obtain the following approximate expression:

$$V_f^c \simeq Z_P\left(\frac{1}{R} - \frac{1}{s_2}\right) + (Z_T-1)\left(\frac{1}{R} - \frac{1}{x_1}\right) + \left(\frac{1}{r_{12}} - \frac{1}{x_1}\right). \tag{7}$$

With this, the solution of the eigenvalue equation $H_f^c\Phi_f^c = E_f\Phi_f^c$ is given by $\Phi_f^c = \varphi_P(\vec{s}_1)\varphi_T(\vec{x}_2) e^{-i\vec{k}_f\cdot\vec{r}_f}\mathcal{N}^-(\nu_f)\, {}_1F_1(i\nu_f, 1, -ik_f r_f + i\vec{k}_f\cdot\vec{r}_f)$, where $\mathcal{N}^-(\nu_f) = e^{-\pi\nu_f/2}\Gamma(1 - i\nu_f)$ and $\nu_f = (Z_T-1)(Z_P-1)/v$. The asymptotic form of Φ_f^c as $r_f \to \infty$ reads as

$$\Phi_f^c(r_f \to \infty) \equiv \Phi_f^- = \varphi_P(\vec{s}_1)\varphi_T(\vec{x}_2) \times \exp[-i\vec{k}_f\cdot\vec{r}_f - i\nu_f \ln(vR + \vec{v}\cdot\vec{R})]. \tag{8}$$

The prior and post forms of the transition amplitudes in the CB1 approximation with the asymptotically correct boundary conditions (CB1-4B) for process (1) can be written as

$$T_{if}^- = \langle\Phi_f^-|V_i^c|\Phi_i^+\rangle, \qquad T_{if}^+ = \langle\Phi_f^-|V_f^c|\Phi_i^+\rangle. \tag{9}$$

In the present CB1-4B model, the proper connection between the long-range Coulomb distortion effects and the accompanying perturbation potentials are established according to the principles of scattering theory [17]. It must be emphasized that imposing the proper Coulomb boundary conditions in the entrance and exit channels is of crucial importance for ion-atom collisions [28]. Experience has shown that if this requirement is disregarded, serious problems may arise, such as divergence of the scattering operator S, as well as of the other related quantities. Thus, such models are generally inadequate for describing experimental findings [28]. In the CB1-4B approximation, the scattering state vectors are given by the product of the unperturbed channel states and the logarithmic distortion phase factors due to the Coulomb long-range remainders of the perturbation potentials. Invoking the eikonal approximation, the product of these logarithmic Coulomb factors can be reduced to the single term

$$\exp[i\nu_i \ln(vR - \vec{v}\cdot\vec{R}) + i\nu_f \ln(vR + \vec{v}\cdot\vec{R})] = \begin{cases}(\rho v)^{2i\nu_i}(vR + \vec{v}\cdot\vec{R})^{i\xi}\\ (\rho v)^{2i\nu_f}(vR - \vec{v}\cdot\vec{R})^{-i\xi},\end{cases} \tag{10}$$

where $\xi = (Z_P - Z_T + 1)/v$ and $\vec{\rho}$ is the projection of vector $\vec{R}$ onto the x-y plane ($\vec{\rho} = \vec{R} - \vec{Z}$, $\vec{\rho}\cdot\vec{Z} = 0$). The multiplying term $(\rho v)^{2i\nu_i}$ or $(\rho v)^{2i\nu_f}$ does not contribute to the total cross section and can be dropped from the transition amplitudes. Therefore, the single Coulomb phase such as $(vR + \vec{v}\cdot\vec{R})^{i\xi}$ or $(vR - \vec{v}\cdot\vec{R})^{-i\xi}$ needs to be retained in the calculation. In addition to this simplification, we shall also use the eikonal hypothesis, since the small-angle limit applies to heavy particles, so that

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

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

$$\vec{\beta} = -\vec{\eta} - \beta_z\hat{\vec{v}}, \quad \vec{\alpha} = \vec{\eta} - \alpha_z\hat{\vec{v}}, \quad \vec{\alpha} + \vec{\beta} = -\vec{v},$$
$$\alpha_z = v/2 - \Delta E/v, \quad \beta_z = v/2 + \Delta E/v,$$

with $\Delta E = E_i - E_f$. The transverse component of the change in the relative linear momentum of a heavy particle is denoted by $\vec{\eta} = (\eta\cos\phi_\eta, \eta\sin\phi_\eta, 0)$, $(\vec{\eta}\cdot\vec{v} = 0)$. We have used the general factorized form for the bound state of the heliumlike atom (or ion) $(Z_T, e_1, e_2)_{1s^2}$,

$$\varphi_i(\vec{x}_1, \vec{x}_2) = \sum_{k,l}\varphi_{\alpha k}(\vec{x}_1)\varphi_{\alpha l}(\vec{x}_2), \tag{11}$$

where $\varphi_{\alpha j}(\vec{r}) = N_{\alpha_j}\exp(-\alpha_j r)$, $N_{\alpha_j} = a_j\sqrt{N}$, $(j = k, l)$, and N is the normalization constant. The values of the

summation indices k and l, as well as the variationally determined parameters α_j and a_j, depend upon a concrete choice of the wave function. Hence, we are led to the following forms for $T_{if}^{\pm} = \sum_{k,l} N_{kl} \mathcal{T}_{k,l}^{\pm}$, where

$$\mathcal{T}_{k,l}^{-} = Z_P\big[2J_R^{(k,l)} - J_{s_1}^{(k,l)} - J_{s_2}^{(k,l)}\big], \tag{12}$$

$$\begin{aligned}\mathcal{T}_{k,l}^{+} = \big\{&Z_P\big[J_R^{(k,l)} - J_{s_2}^{(k,l)}\big] + (Z_T - 1)\big[J_R^{(k,l)} - J_{x_1}^{(k,l)}\big] \\ &+ \big[J_{r_{12}}^{(k,l)} - J_{x_1}^{(k,l)}\big]\big\},\end{aligned} \tag{13}$$

with

$$\begin{aligned}J_\omega^{(k,l)} &= \int d\vec{R} e^{-i\vec{\alpha}\cdot\vec{R}} (vR + \vec{v}\cdot\vec{R})^{i\xi} W_\omega^{(k,l)}(\vec{R}), \\ &(\omega = R, x_1, s_1, s_2, r_{12}),\end{aligned} \tag{14}$$

$$W_R^{(k,l)} = \frac{1}{R}\mathcal{B}_k\mathcal{A}_l, \quad W_{s_1}^{(k,l)} = \mathcal{C}_k\mathcal{A}_l, \quad W_{s_2}^{(k,l)} = \mathcal{B}_k\mathcal{D}_l, \tag{15}$$

$$W_{x_1}^{(k,l)} = \mathcal{L}_k\mathcal{A}_l, \quad W_{r_{12}}^{(k,l)} = \frac{1}{2\pi^2}\int \frac{d\vec{\tau}}{\tau^2}\mathcal{B}_{k,\tau}\mathcal{A}_{l,\tau}, \tag{16}$$

$$\begin{aligned}\mathcal{A}_l &= \int d\vec{x}_2 e^{-(Z_T+\alpha_l)x_2} = \frac{8\pi}{(Z_T+\alpha_l)^3}, \\ \mathcal{A}_{l,\tau} &= \int d\vec{x}_2 e^{i\vec{\tau}\cdot\vec{x}_2 - (Z_T+\alpha_l)x_2} = \frac{8\pi(Z_T+\alpha_l)}{[\tau^2 + (Z_T+\alpha_l)^2]^2},\end{aligned} \tag{17}$$

$$\begin{aligned}\mathcal{B}_k &= \int d\vec{x}_1 e^{-i\vec{v}\cdot\vec{x}_1 - \alpha_k x_1} e^{-Z_P s_1} = \frac{8Z_P\alpha_k}{\pi} e^{i\vec{\alpha}\cdot\vec{R}} \\ &\times \int d\vec{q} \frac{e^{-i\vec{q}\cdot\vec{R}}}{(|\vec{q}-\vec{\alpha}|^2 + Z_P^2)^2(|\vec{q}+\vec{\beta}|^2 + \alpha_k^2)^2},\end{aligned} \tag{18}$$

$$\begin{aligned}\mathcal{C}_k &= \int d\vec{x}_1 e^{-i\vec{v}\cdot\vec{x}_1 - \alpha_k x_1} \frac{e^{-Z_P s_1}}{s_1} = \frac{4\alpha_k}{\pi} e^{i\vec{\alpha}\cdot\vec{R}} \\ &\times \int d\vec{q} \frac{e^{-i\vec{q}\cdot\vec{R}}}{\big(|\vec{q}-\vec{\alpha}|^2 + Z_P^2\big)\big(|\vec{q}+\vec{\beta}|^2 + \alpha_k^2\big)^2},\end{aligned} \tag{19}$$

$$\begin{aligned}\mathcal{D}_l &= \int d\vec{x}_2 e^{-(Z_T+\alpha_l)x_2} \frac{1}{s_2} \\ &= \frac{4(Z_T+\alpha_l)}{\pi}\int d\vec{q} \frac{e^{i\vec{q}\cdot\vec{R}}}{q^2[q^2 + (Z_T+\alpha_l)^2]^2},\end{aligned} \tag{20}$$

$$\begin{aligned}\mathcal{L}_k &= \int d\vec{x}_1 \frac{e^{-i\vec{v}\cdot\vec{x}_1 - \alpha_k x_1}}{x_1} e^{-Z_P s_1} = \frac{4Z_P}{\pi} e^{i\vec{\alpha}\cdot\vec{R}} \\ &\times \int d\vec{q} \frac{e^{-i\vec{q}\cdot\vec{R}}}{\big(|\vec{q}-\vec{\alpha}|^2 + Z_P^2\big)^2\big(|\vec{q}+\vec{\beta}|^2 + \alpha_k^2\big)},\end{aligned} \tag{21}$$

$$\begin{aligned}\mathcal{B}_{k,\tau} &= \int d\vec{x}_1 e^{-i(\vec{\tau}+\vec{v})\cdot\vec{x}_1 - \alpha_k x_1} e^{-Z_P s_1} = \frac{8Z_P\alpha_k}{\pi} e^{i\vec{\alpha}\cdot\vec{R}} \\ &\times \int d\vec{q} \frac{e^{-i\vec{q}\cdot\vec{R}}}{\big(|\vec{q}-\vec{\alpha}|^2 + Z_P^2\big)^2\big(|\vec{q}+\vec{\beta}_1|^2 + \alpha_k^2\big)^2},\end{aligned} \tag{22}$$

where $\vec{\beta}_1 = \vec{\beta} - \vec{\tau}$ and $N_{k,l} = (Z_P Z_T)^{3/2} N_{\alpha_k} N_{\alpha_l}/\pi$. Employing the Feynman parametrization integral,

$$\frac{1}{A^n B^m} = \frac{(n+m-1)!}{(n-1)!(m-1)!}\int_0^1 dt \frac{t^{n-1}(1-t)^{m-1}}{[At + B(1-t)]^{n+m}}, \tag{23}$$

and with the help of the results

$$\int d\vec{q} \frac{e^{i\vec{q}\cdot\vec{R}}}{(|\vec{q}-\vec{p}\,|^2 + \lambda^2)^3} = \frac{\pi^2}{4\lambda^3}(1+\lambda R)e^{i\vec{p}\cdot\vec{R} - \lambda R}, \tag{24}$$

$$\int d\vec{q} \frac{e^{i\vec{q}\cdot\vec{R}}}{(|\vec{q}-\vec{p}\,|^2 + \lambda^2)^4} = \frac{\pi^2}{24\lambda^5}(3 + 3\lambda R + \lambda^2 R^2)e^{i\vec{p}\cdot\vec{R} - \lambda R}, \tag{25}$$

we can perform the integration over $\vec{q}$ in Eqs. (18)–(22) with the following results for the quantities $J_\omega^{(k,l)}$:

$$\begin{aligned}J_{s_2}^{(k,l)} &= 4\pi^2 Z_P\alpha_k(Z_T+\alpha_l)\int_0^1\int_0^1 \frac{dt_1 dt_2 t_2(1-t_1)(1-t_2)}{\Delta_1^3\Delta_2^5} \\ &\times \big[3I_{1,\Delta}^{(\vec{Q}_2)} + 3\Delta I_{2,\Delta}^{(\vec{Q}_2)} + \Delta_2(3\Delta_1 + \Delta_2)I_{3,\Delta}^{(\vec{Q}_2)} \\ &+ \Delta_1\Delta_2^2 I_{4,\Delta}^{(\vec{Q}_2)}\big],\end{aligned} \tag{26}$$

$$\begin{aligned}J_R^{(k,l)} &= 16\pi^2 Z_P \frac{\alpha_k}{(Z_T+\alpha_l)^3}\int_0^1 \frac{dt_2 t_2(1-t_2)}{\Delta_2^5} \\ &\times \big[3I_{0,\Delta_2}^{(\vec{Q}_2)} + 3\Delta_2 I_{1,\Delta_2}^{(\vec{Q}_2)} + \Delta_2^2 I_{2,\Delta_2}^{(\vec{Q}_2)}\big],\end{aligned} \tag{27}$$

$$J_{s_1}^{(k,l)} = 16\pi^2 \frac{\alpha_k}{(Z_T+\alpha_l)^3}\int_0^1 \frac{dt_2(1-t_2)}{\Delta_2^3}\big[I_{1,\Delta_2}^{(\vec{Q}_2)} + \Delta_2 I_{2,\Delta_2}^{(\vec{Q}_2)}\big], \tag{28}$$

$$\begin{aligned}J_{r_{12}}^{(k,l)} &= 8Z_P(Z_T+\alpha_l)\int_0^1 dt_2 t_2(1-t_2) \\ &\times \int \frac{d\vec{\tau}}{\tau^2[\tau^2 + (Z_T+\alpha_l)^2]^2} \\ &\times \frac{1}{\Delta_\tau^5}\big[3I_{1,\Delta_\tau}^{(\vec{Q}_\tau)} + 3\Delta_\tau I_{2,\Delta_\tau}^{(\vec{Q}_\tau)} + \Delta_\tau^2 I_{3,\Delta_\tau}^{(\vec{Q}_\tau)}\big],\end{aligned} \tag{29}$$

$$J_{x_1}^{(k,l)} = \frac{16\pi^2 Z_P}{(Z_T+\alpha_l)^3}\int_0^1 \frac{dt_2 t_2}{\Delta_2^3}\big[I_{1,\Delta_2}^{(\vec{Q}_2)} + \Delta_2 I_{2,\Delta_2}^{(\vec{Q}_2)}\big], \tag{30}$$

where

$$\begin{aligned}I_{n,\lambda}^{(\vec{p})} &= \int d\vec{R} R^{n-1} e^{-i\vec{p}\cdot\vec{R} - \lambda R}(vR + \vec{v}\cdot\vec{R})^{i\xi}, \\ &(\lambda = \Delta_2, \Delta_\tau, \Delta), \quad (\vec{p} = \vec{Q}_2, \vec{Q}_\tau).\end{aligned} \tag{31}$$

The quantities used in Eqs. (26)–(30) are defined as

$$\begin{aligned}\Delta_1 &= (Z_T+\alpha_l)\sqrt{1-t_1}, \\ \Delta_2^2 &= v^2 t_2(1-t_2) + Z_P^2 t_2 + \alpha_k^2(1-t_2), \\ \Delta_\tau^2 &= |\vec{v}+\vec{\tau}|^2 t_2(1-t_2) + Z_P^2 t_2 + \alpha_k^2(1-t_2),\end{aligned} \tag{32}$$

$$\vec{Q}_2 = \vec{\alpha}t_2 - \vec{\beta}(1-t_2), \tag{33}$$

$$\vec{Q}_\tau = \vec{\alpha}t_2 - (\vec{\beta} - \vec{\tau})(1-t_2), \quad \Delta = \Delta_1 + \Delta_2. \tag{34}$$

Integrals $I_{n,\lambda}^{(\vec{p})}$, $(n = 0, 1, 2, 3, 4)$ can be calculated analytically, and the results are given in the Appendix. In this manner, we arrive at the final results for the prior and post transition amplitudes:

$$\begin{aligned}T_{k,l}^{-} = \sum_{k,l}\mathcal{N}_{k,l}\int_0^1 dt_2(1-t_2)\Big[&2Z_P t_2\mathcal{H}_R - \mathcal{H}_{s_1} \\ &- \frac{Z_P t_2(Z_T+\alpha_l)^4}{2}\int_0^1 dt_1(1-t_1)\mathcal{H}_{s_2}\Big],\end{aligned} \tag{35}$$

$$T_{k,l}^{+} = \sum_{k,l} \mathcal{N}_{k,l} \int_0^1 dt_2 t_2 \Big\{ Z_P(1-t_2) \times \Big[\mathcal{H}_R - \frac{(Z_T+\alpha_l)^4}{2} \int_0^1 dt_1 (1-t_1)\mathcal{H}_{s_2} \Big] + (Z_T-1)\Big[(1-t_2)\mathcal{H}_R - \frac{2}{\alpha_k}\mathcal{H}_{x_1} \Big] + \Big[\frac{(Z_T+\alpha_l)^4}{\pi^2}(1-t_2)\mathcal{H}_{12} - \frac{2}{\alpha_k}\mathcal{H}_{x_1} \Big] \Big\}, \quad (36)$$

$$\mathcal{H}_{12} = \int_0^\infty \frac{d\tau}{[\tau^2 + (Z_T+\alpha_l)^2]^2} \int_0^\pi d\theta_\tau \sin\theta_\tau \int_0^{2\pi} d\phi_\tau h_{12} \quad (37)$$

$$h_{12} = \frac{D_{\Delta_\tau}^{(\vec{Q}_\tau)} \mathcal{F}_{\Delta_\tau}^{(\vec{Q}_\tau)}}{\Delta_\tau^5} \big\{ 3\big[1 - i\xi C_{\Delta_\tau}^{(\vec{Q}_\tau)}\big] - 3\Delta_\tau \mathcal{F}_{\Delta_\tau}^{(\vec{Q}_\tau)} - 2\Delta_\tau D_{\Delta_\tau}^{(\vec{Q}_\tau)} \big[A_{\beta,\Delta_\tau}^{(\vec{Q}_\tau)} + \imath\xi B_{\beta,\Delta_\tau}^{(\vec{Q}_\tau)} \big] \big\}, \quad (38)$$

$$\mathcal{H}_{s_2} = \frac{D_{\Delta}^{(\vec{Q}_2)} \mathcal{F}_{\Delta}^{(\vec{Q}_2)}}{\Delta_1^3 \Delta_2^5} (\gamma - i\xi\delta), \qquad \mathcal{N}_{k,l} = 64 Z_P^{5/2} Z_T^{3/2} \pi^2 \Gamma(1+i\xi) \frac{\alpha_k N_{\alpha_k} N_{\alpha_l}}{(Z_T+\alpha_l)^3}, \quad (39)$$

$$\mathcal{H}_{x_1} = \frac{D_{\Delta_2}^{(\vec{Q}_2)} \mathcal{F}_{\Delta_2}^{(\vec{Q}_2)}}{\Delta_2^3} \big[1 - i\xi C_{\Delta_2}^{(\vec{Q}_2)} - \Delta_2 \mathcal{F}_{\Delta_2}^{(\vec{Q}_2)} \big], \quad (40)$$

$$\mathcal{H}_R = \frac{\mathcal{F}_{\Delta_2}^{(\vec{Q}_2)}}{\Delta_2^5} \big\{ 3 + 6\Delta_2 D_{\Delta_2}^{(\vec{Q}_2)} \big[1 - i\xi C_{\Delta_2}^{(\vec{Q}_2)} \big] - 2\Delta_2^2 D_{\Delta_2}^{(\vec{Q}_2)} \mathcal{F}_{\Delta_2}^{(\vec{Q}_2)} \big\}, \quad (41)$$

$$\mathcal{H}_{s_1} = \frac{2 D_{\Delta_2}^{(\vec{Q}_2)} \mathcal{F}_{\Delta_2}^{(\vec{Q}_2)}}{\Delta_2^3} \big[1 - i\xi C_{\Delta_2}^{(\vec{Q}_2)} - \Delta_2 \mathcal{F}_{\Delta_2}^{(\vec{Q}_2)} \big], \quad (42)$$

$$\gamma = 3\big[1 - A_{\alpha,\Delta}^{(\vec{Q}_2)}\big] - 2\frac{D_{\Delta}^{(\vec{Q}_2)}}{\Delta} \Delta_2(3\Delta_1 + \Delta_2) A_{\beta,\Delta}^{(\vec{Q}_2)} + 2\frac{D_{\Delta}^{(\vec{Q}_2)}}{\Delta^2} \Delta_1 \Delta_2^2 A_{\gamma,\Delta}^{(\vec{Q}_2)}, \quad (43)$$

$$\delta = 3\big[C_{\Delta}^{(\vec{Q}_2)} + B_{\alpha,\Delta}^{(\vec{Q}_2)}\big] + 2\frac{D_{\Delta}^{(\vec{Q}_2)}}{\Delta} \Delta_2(3\Delta_1 + \Delta_2) B_{\beta,\Delta}^{(\vec{Q}_2)} + 2\frac{D_{\Delta}^{(\vec{Q}_2)}}{\Delta^2} \Delta_1 \Delta_2^2 B_{\gamma,\Delta}^{(\vec{Q}_2)}. \quad (44)$$

This completes the calculation of the matrix elements T_{if}^{-} in terms of the two-dimensional integrals over real variables t_1 and t_2, both ranging from 0 to 1. On the other hand, T_{if}^{+} is obtained in terms of the five-dimensional integrals, since the term $1/r_{12}$ in V_f from Eq. (7) requires an additional three-dimensional integral over $\tau \in [0,\infty]$, $\theta_\tau \in [0,\pi]$, $\phi_\tau \in [0, 2\pi]$.

III. THE RESULTS OF NUMERICAL COMPUTATIONS

The post and prior total cross sections in the CB1-4B method are given by

$$Q_{if}^{\pm}(\pi a_0^2) = \frac{1}{2\pi^2 v^2} \int_0^\infty d\eta \eta |T_{if}^{\pm}|^2. \quad (45)$$

The integration over η is performed by means of the Gauss-Legendre routine, after performing the change of variable [24] $\eta = \sqrt{2(1+z)/(1-z)}$, $z \in [-1,+1]$ with the purpose of concentrating the integration points near the forward cone, where the total cross section peaks. The Gauss-Legendre quadrature is also used for the remaining numerical integration over $t_1, t_2, \tau, \theta_\tau, \phi_\tau$ after the appropriate change of variables: $t_{1,2} = (u_{1,2}+1)/2$, $\tau = (1+x)/(1-x)$, $\cos\theta_\tau = \zeta$, $\phi_\tau = \pi(y+1)$, where $u_{1,2}, x, \zeta, y \in [-1,+1]$. The presented algorithm is general, in the sense that it can be applied to both heteronuclear and homonuclear single charge exchange of the type (1).

Numerical computations of the total cross sections are presently carried out for the following charge-exchange reactions:

$$p + \mathrm{He} \longrightarrow \mathrm{H} + \mathrm{He}^+, \quad (46)$$

$$\alpha + \mathrm{He} \longrightarrow \mathrm{He}^+ + \mathrm{He}^+. \quad (47)$$

The explicit computations of the total cross sections are performed only for the final ground states $f_1 = 1s$ and $f_2 = 1s$. The obtained results are multiplied additionally by a factor of 1.202 in order to include a contribution from the excited states according to the n^{-3} Oppenheimer scaling law.

First, we shall consider the asymmetric reaction (46). The results of the computations of the post and prior total cross sections at impact energies 20–20 000 keV are summarized in Table I as well as Figs. 1 and 2. The columns in Table I headed by the symbols Q_{if}^{-} and Q_{if}^{+} represent the prior and post cross sections, respectively. The total cross sections obtained by means of the uncorrelated one-parameter Hylleraas wave function [31], $\varphi_i(\vec{x}_1, \vec{x}_2) = (\alpha^3/\pi) e^{-\alpha(x_1+x_2)}$ with $\alpha = Z_T - 5/16$ are labeled "Hyll." in Table I, whereas the results obtained by using the configuration interaction (CI) wave function $(1s1s')$ of Ref. [32] with the radial static correlations $\varphi_i(\vec{x}_1, \vec{x}_2) = (N/\pi)(e^{-\alpha_1 x_1 - \alpha_2 x_2} + e^{-\alpha_2 x_1 - \alpha_1 x_2})$ are labeled "Silv.," where $N^{-2} = 2[(\alpha_1\alpha_2)^{-3} + (\alpha_1/2 + \alpha_2/2)^{-6}]$. The total cross sections obtained with these wave functions are close to each other, as can be seen from Table I. The prior form does not contain the term $1/r_{12}$, which explicitly accounts for the dynamical correlations. As a result, the prior amplitude, and therefore the prior cross sections, are more sensitive to the accuracy of the initial state than the corresponding results from the post form. This is verified in Table I by comparing the values of the Q_{if}^{+} and Q_{if}^{-} computed with the Hylleraas and the Silverman *et al.* [32] wave functions. The relative difference of the post cross sections between these wave functions does not exceed 10%, whereas in the prior form it can be up to 36%.

The prior and post CB1-4B cross sections obtained with the complete perturbations according to Eqs. (9), (3), and (7) are plotted in Fig. 1. Despite the obvious discrepancy between V_i and V_f from Eqs. (3) and (7), computations show that the post-prior discrepancy is relatively small, as can be seen from Fig. 1 and Table I. This is a good property of the method, since the same physical assumptions are involved in the prior and post forms. The post results are larger than the prior ones. In Fig. 1, we also compare our theoretical results for prior (solid curve) and post (dashed curve) cross sections for p-He collision together with a number of experimental data. The cross sections of the CB1-4B approximation are

TABLE I. Total cross sections (in cm^2) as a function of the impact energy E (keV) for electron capture $p + He \longrightarrow H + He^+$. The displayed theoretical results are obtained by means of the CB1-4B method using the one-parameter Hylleraas wave function (labeled "Hyll.") and the two-parameter Silverman *et al.* orbital [32] (labeled "Silv.") for the initial bound state of helium. The quantities $Q_{if}^{\pm}$ represent the cross sections in the post (+) and prior (−) forms, respectively, obtained with the complete perturbation potentials, whereas Q_1^+ refers to the cross sections computed without the term $V_{\rm corr} = 1/r_{12} - 1/x_1$ in Eq. (7). The numbers in the square brackets denote the powers of 10.

E (keV)	Q_{if}^- Hyll.	Q_{if}^+ Hyll.	Q_1^+ Hyll.	Q_{if}^- Silv.	Q_{if}^+ Silv.	Q_1^+ Silv.
20	4.22[−16]	6.22[−16]	4.75[−16]	5.06[−16]	5.67[−16]	4.52[−16]
30	2.44[−16]	3.70[−16]	2.62[−16]	2.95[−16]	3.37[−16]	2.45[−16]
40	1.56[−16]	2.40[−16]	1.61[−16]	1.85[−16]	2.21[−16]	1.49[−16]
50	1.07[−16]	1.65[−16]	1.05[−16]	1.22[−16]	1.53[−16]	9.74[−17]
70	5.61[−17]	8.57[−17]	5.08[−17]	5.98[−17]	8.07[−17]	4.69[−17]
80	4.23[−17]	6.41[−17]	3.69[−17]	4.37[−17]	6.06[−17]	3.41[−17]
100	2.53[−17]	3.79[−17]	2.07[−17]	2.48[−17]	3.60[−17]	1.91[−17]
150	8.73[−18]	1.26[−17]	6.25[−18]	7.80[−18]	1.20[−17]	5.80[−18]
200	3.65[−18]	5.11[−18]	2.37[−18]	3.11[−18]	4.84[−18]	2.22[−18]
300	8.93[−19]	1.21[−18]	5.08[−19]	7.41[−19]	1.13[−18]	4.85[−19]
400	2.90[−19]	3.87[−19]	1.52[−19]	2.43[−19]	3.61[−19]	1.48[−19]
500	1.13[−19]	1.50[−19]	5.58[−20]	9.67[−20]	1.39[−19]	5.52[−20]
700	2.46[−20]	3.27[−20]	1.12[−20]	2.21[−20]	3.04[−20]	1.14[−20]
800	1.30[−20]	1.74[−20]	5.78[−21]	1.20[−20]	1.62[−20]	5.95[−21]
1000	4.34[−21]	5.86[−21]	1.84[−21]	4.15[−21]	5.47[−21]	1.93[−21]
1500	5.35[−22]	7.44[−22]	2.12[−22]	5.51[−22]	7.00[−22]	2.27[−22]
2000	1.14[−22]	1.63[−22]	4.32[−23]	1.23[−22]	1.54[−22]	4.71[−23]
3000	1.22[−23]	1.80[−23]	4.34[−24]	1.40[−23]	1.72[−23]	4.80[−24]
4000	2.42[−24]	3.64[−24]	8.28[−25]	2.87[−24]	3.52[−24]	9.19[−25]
5000	6.80[−25]	1.04[−24]	2.27[−25]	8.28[−25]	1.01[−24]	2.52[−25]
7000	9.91[−26]	1.53[−25]	3.18[−26]	1.24[−25]	1.50[−25]	3.53[−26]
8000	4.59[−26]	7.13[−26]	1.45[−26]	5.80[−26]	7.02[−26]	1.61[−26]
10 000	1.26[−26]	1.97[−26]	3.92[−27]	1.62[−26]	1.95[−26]	4.35[−27]
15 000	1.20[−27]	1.88[−27]	3.61[−28]	1.56[−27]	1.87[−27]	3.99[−28]
20 000	2.23[−28]	3.50[−28]	6.64[−29]	2.93[−28]	3.51[−28]	7.30[−29]

seen to be in very good agreement with all the measurements at very wide (three orders of magnitude) impact energies. In addition to computations by means of one- and two-parameter wave functions, we have also carried out computations with the three-parameter orbitals of Green *et al.* [42] and the four-parameter wave function of Löwdin [43]. The total cross sections obtained by Green *et al.* [42] and Löwdin [43] wave functions are very close to those obtained by using the Hylleraas and Silverman *et al.* [32] wave functions. Therefore, to avoid clutter, all numerical results are not included here and we have presented only a few numerical values for illustration. The post total cross sections obtained by Green *et al.* [42] and Löwdin [43] wave functions for the p-He collisions at 0.1 MeV are, respectively, 3.69×10^{-17} and 3.68×10^{-17}, whereas at 1 MeV they are 5.65×10^{-21} and 5.61×10^{-21}, and at 10 MeV they are 2.03×10^{-26} and 2.00×10^{-26}. As can be seen by comparing with corresponding results from Table I, the dependence of the total cross sections for the p-He collisions upon these four bound-state wave functions is weak. Similar results are obtained for the prior cross sections.

The relatively small post-prior discrepancy was previously found within four-body continuum distorted wave (CDW-4B) method for double [44] as well as single charge exchange [45] in p-He collisions. As shown by Belkić *et al.* [46], in the case of simultaneous transfer and ionizaton, due to the potential $V_{\rm corr}$ in the corresponding perturbation, the post form is more adequate than its prior counterpart. However, the calculations of Ciappina *et al.* [47,48] within continuum-distorted-wave–eikonal-initial-state (CDW-EIS) model for ion impact ionization of helium have shown that the prior version gives better agreement with experimental data than the post version calculations.

Further, we have evaluated the contribution of the correlation term $V_{\rm corr} = 1/r_{12} - 1/x_1$ which is contained only in the post cross sections. Namely, if we ignore this term in Eq. (7), we obtain the numerical results labeled as Q_1^+ in Table I. The potential $1/r_{12}$ in $V_{\rm corr} = 1/r_{12} - 1/x_1$ represents the direct Coulomb interaction between e_1 and e_2, whereas $1/x_1$ is the asymptotic tail of the $1/r_{12}$, since $r_{12} \to x_1$ at infinitely large x_1 and finite x_2. Hence, the term $V_{\rm corr}$ is precisely the difference between the finite and limiting values of the *same* potential. As such, $V_{\rm corr}$ is a short-range interaction in accordance with the correct boundary conditions [16,17]. Using the relation $r_{12} = |\vec{x}_1 - \vec{x}_2|$, we can develop $1/x_1 = 1/|\vec{r}_{12} - \vec{x}_2|$ in a power series around $\vec{x}_2$ according to $1/x_1 = 1/|\vec{r}_{12} - \vec{x}_2| = 1/r_{12} - \vec{r}_{12} \cdot \vec{x}_2/r_{12}^3 + \cdots$, so that

$$V_{\rm corr} = \frac{1}{r_{12}} - \frac{1}{x_1} = \frac{\vec{r}_{12} \cdot \vec{x}_2}{r_{12}^3} + \cdots .$$

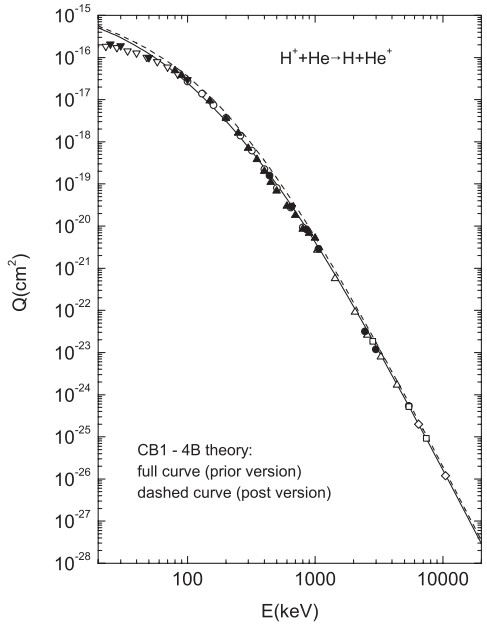

FIG. 1. Total cross sections (in cm^2) as a function of the laboratory incident energy for reaction $p + {}^4\mathrm{He} \longrightarrow \mathrm{H} + {}^4\mathrm{He}^+$. The solid and dashed curves represent the prior and post total cross sections in the CB1-4B method, respectively. Both theoretical curves are obtained with the complete perturbation potentials. The initial ground state of atom He ($1s^2$) is described by means of the two-parameter Silverman *et al.* orbital [32]. Experimental data: ▽ Shah *et al.* [33], △ Schryber [34] ○ Shah and Gilbody [35], □ Horsdal-Pedersen *et al.* [36], ◇ Berkner *et al.* [37], ▲ Williams [38], ▼ Martin *et al.* [39], • Welsh *et al.* [40].

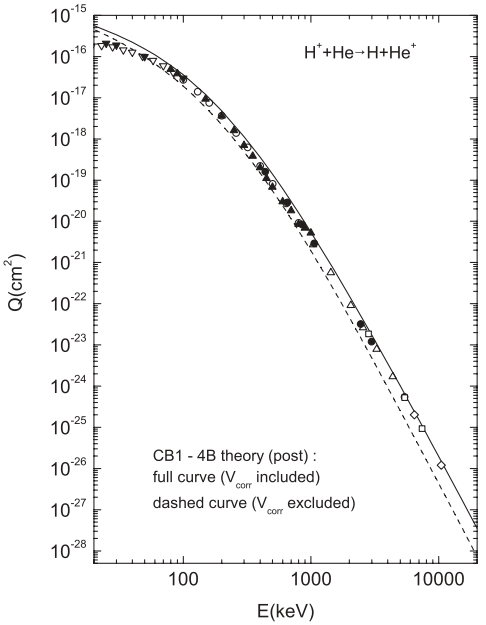

FIG. 2. Total cross sections (in cm^2) as a function of the laboratory incident energy for reaction $p + {}^4\mathrm{He} \longrightarrow \mathrm{H} + {}^4\mathrm{He}^+$. The solid and dashed curves from the CB1-4B method correspond to the cases where the potential $V_{\mathrm{corr}} = 1/r_{12} - 1/x_1$ is included and excluded from the complete perturbation V_f, respectively. The wave function of Silverman *et al.* [32] is used for the initial bound state. Experimental data: the same as in Fig. 1.

This is justified by the small value of the x_2 coordinate (of the order of Bohr radius a_0), since electron e_2 always remains bound in the target. From here we can see that the potential V_{corr} contains information on the dielectronic correlation $e_1 - e_2$. Therefore, V_{corr} can be interpreted as a correlation term. When the potential V_{corr} is placed in the T matrix (9), it plays the role of a perturbation which causes capture of electron e_1.

In order to critically assess the contribution from this term in the framework of the present CB1-4B model, a comparison with measurements is required, and this is carried out on Fig. 2. One can see from Fig. 2 that very good agreement is obtained, provided that the full perturbation V_f is included in the post formulation. When we neglect the relevant term for the dynamic electron correlation $V_{\mathrm{corr}} = 1/r_{12} - 1/x_1$, we obtain the results (the dashed curve in Fig. 2) that underestimate the experimental findings especially at higher impact energies. For example, the relative contribution of this term, expressed via $\gamma = |Q_{if}^+ - Q_1^+|/Q_{if}^+$ for the Silverman *et al.* [32] wave function is 46.9%, 64.7%, and 79.2% at impact energies 100, 1000, and 20 000 keV, respectively. Similar results of γ are obtained when one-parameter orbitals [31] are utilized for the initial state of helium, that is, 45.4%, 68.6%, and 81.0% at the same energies. The presented numerical results about the contribution of the term V_{corr} can be understood as an estimation of the role of the dynamic correlation. However, strictly speaking, by removing V_{corr} from the perturbation V_f, we obtain a transition amplitude in which the proper connection between the remaining part of the perturbation $(V_f - V_{\mathrm{corr}})$ and the corresponding scattering states is not accomplished. However, it should be re-emphasized that V_{corr} is a short-range interaction.

The results of the computations of the CB1-4B total cross sections for reaction (47) at impact energies ranging from 100 to 10 000 keV are presented in Table II (with the same notations as in Table I), as well as in Figs. 3 and 4. As can be seen from Fig. 3, the present CB1-4B approximation is found to be in excellent agreement (above 50 keV/amu) with the available experimental data. The relative difference between the post (solid curve) and prior form (dash-dotted curve) is up to 22%. In the same figure, the present CB1-4B results are compared with the corresponding CDW-4B findings from [53]. As can be expected, at lower energies, the CB1-4B cross sections are much smaller than the corresponding results of the CDW-4B model. A comparison is also made with the continuum-distorted-wave–independent-event model (CDW-IEM) of Dunseath and Crothers [54], derived using the correlated Pluvinage wave function [55] $\varphi_i(\vec{x}_1, \vec{x}_2) = (Z_T^3/\pi)\exp[-Z_T(x_1 + x_2)]\exp(-ikr_{12})_1F_1(1 - i\gamma, 2, 2ikr_{12})$, where $\gamma = -1/(2k)$ and $c(k)$ is the normalization constant, with k being a nonlinear variational parameter. This wave function contains two entirely uncorrelated hydrogenlike wave functions with the unscreened charge Z_T that are multiplied with a corrective r_{12}-dependent term of the form $\exp(-ikr_{12})_1F_1(1 - i\gamma, 2, 2ikr_{12})$. The formulation of Dunseath and Crothers [54] ignores the dynamic correlations altogether, and this may be one of the reasons for its less favorable agreement with the measurements, as is clear from Fig. 3. Moreover, this might also indicate that

TABLE II. Same as in Table I, except for reaction $\alpha + \mathrm{He} \longrightarrow \mathrm{He}^{++}\mathrm{He}^{+}$.

E (keV)	Q_{if}^{-} Hyll.	Q_{if}^{+} Hyll.	Q_{1}^{+} Hyll.	Q_{if}^{-} Silv.	Q_{if}^{+} Silv.	Q_{1}^{+} Silv.
100	5.69[−16]	5.60[−16]	4.20[−16]	5.18[−16]	5.33[−16]	4.04[−16]
150	3.94[−16]	3.95[−16]	2.96[−16]	3.56[−16]	3.75[−16]	2.83[−16]
200	2.84[−16]	2.93[−16]	2.14[−16]	2.54[−16]	2.78[−16]	2.04[−16]
300	1.61[−16]	1.73[−16]	1.21[−16]	1.42[−16]	1.64[−16]	1.14[−16]
400	9.89[−17]	1.09[−16]	7.35[−17]	8.64[−17]	1.03[−16]	6.93[−17]
500	6.42[−17]	7.21[−17]	4.71[−17]	5.56[−17]	6.82[−17]	4.44[−17]
600	4.34[−17]	4.93[−17]	3.14[−17]	3.74[−17]	4.66[−17]	2.96[−17]
700	3.03[−17]	3.47[−17]	2.16[−17]	2.60[−17]	3.28[−17]	2.04[−17]
800	2.17[−17]	2.50[−17]	1.53[−17]	1.86[−17]	2.37[−17]	1.45[−17]
900	1.59[−17]	1.84[−17]	1.11[−17]	1.36[−17]	1.74[−17]	1.05[−17]
1000	1.18[−17]	1.38[−17]	8.16[−18]	1.01[−17]	1.30[−17]	7.77[−18]
1500	3.33[−18]	3.97[−18]	2.21[−18]	2.91[−18]	3.75[−18]	2.14[−18]
2000	1.19[−18]	1.44[−18]	7.68[−19]	1.06[−18]	1.36[−18]	7.57[−19]
3000	2.33[−19]	2.88[−19]	1.45[−19]	2.17[−19]	2.73[−19]	1.47[−19]
4000	6.49[−20]	8.19[−20]	3.96[−20]	6.30[−20]	7.82[−20]	4.11[−20]
5000	2.27[−20]	2.92[−20]	1.36[−20]	2.28[−20]	2.79[−20]	1.44[−20]
6000	9.28[−21]	1.21[−20]	5.48[−21]	9.56[−21]	1.17[−20]	5.89[−21]
7000	4.27[−21]	5.66[−21]	2.49[−21]	4.50[−21]	5.46[−21]	2.70[−21]
8000	2.15[−21]	2.88[−21]	1.23[−21]	2.30[−21]	2.79[−21]	1.35[−21]
9000	1.16[−21]	1.57[−21]	6.59[−22]	1.26[−21]	1.53[−21]	7.27[−22]
10 000	6.64[−22]	9.11[−22]	3.73[−22]	7.34[−22]	8.84[−22]	4.14[−22]

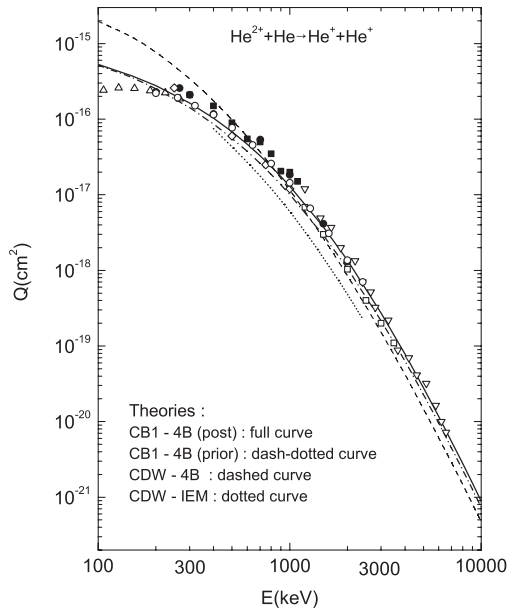

FIG. 3. Total cross sections (in cm^2) as a function of the laboratory incident energy E (keV) for reaction $^4\mathrm{He}^{2+} + {}^4\mathrm{He} \longrightarrow {}^4\mathrm{He}^{+} + {}^4\mathrm{He}^{+}$. The solid and dash-dotted curves represent the post and prior total cross sections of the CB1-4B method with the complete perturbation potential, respectively. The dashed curve refers to the theoretical results of Mančev [53] in the CDW-4B theory. For all the three curves, the initial ground state of He ($1s^2$) is described by means of the Silverman *et al.* [32] orbital. The dotted curve refers to the theoretical results of Dunseath and Crothers [54] in CDW-IEM. Experimental data: ▽ Hvelplund *et al.* [49], □ de Castro Faria *et al.* [50], ○ Shah and Gilbody [35], △ Shah *et al.* [33], ◇ Mergel *et al.* [41], • DuBois [51], ■ Pivovar *et al.* [52].

dynamic electronic correlations in the perturbation potentials that cause the transition are more important than the static ones in the target bound-state wave function. This is also supported by a small discrepancy (not exceeding 6%) between the cross section computed by means of the uncorrelated Hylleras and the radially correlated Silverman *et al.* [32] wave functions, as shown in Table II. Very similar results are obtained by using three-parameter orbitals of Green *et al.* [42] and four-parameter wave function of Löwdin [43].

The role of the V_{corr} term in α-He collisions remains important, as shown in Fig. 4. As can be seen in this figure, the difference between the two curves becomes more significant at higher impact energies. The relative contribution γ of the V_{corr} term is up to 53% when the Silverman *et al.* [32] wave function is utilized, and $\gamma \leqslant 59\%$ is obtained by using the Hylleraas orbital. This might mean that the dynamic electron correlations play a very important role, especially at higher impact energies. A similar conclusion has been previously reached in Refs. [45,53] by using the CDW-4B model for the same collisional systems.

Despite the present numerical computations being restricted to the four wave functions, it should be noted that the presented CB1-4B method can also be extended and adapted for using multiparameter highly correlated wave functions, such those of Byron and Joachain [56], Joachain and Vanderpoorten [57], or Tweed [58], which include a number of CI terms ranging from 12 to 108. These orbitals [56–58] are capable of including most radial and angular correlations, despite the fact that they do not explicitly contain the interelectronic coordinate $\vec{r}_{12}$. Such wave functions [56–58] are convenient for analytical calculations due to their separable form $\varphi_i(\vec{r}_1, \vec{r}_2) = \sum_{k,l} \varphi_k(\vec{r}_1)\varphi_l(\vec{r}_2)$, where $\varphi_{k,l}(\vec{r}_{1,2})$ are unnormalized Slater-type orbitals.

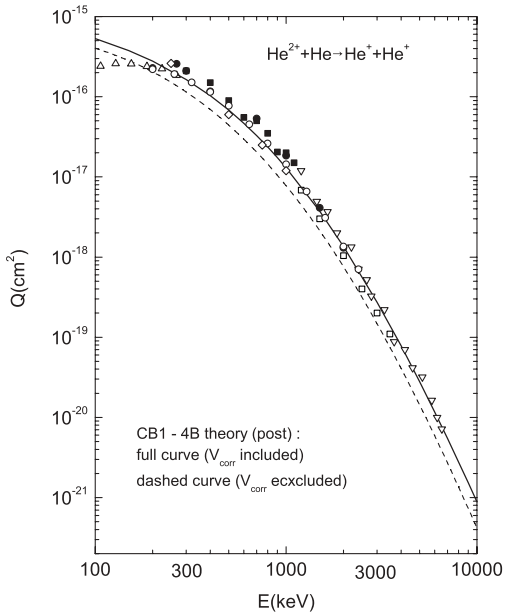

FIG. 4. Total cross sections (in cm^2) as a function of the laboratory incident energy E (keV) for reaction $^4He^{2+} + {}^4He \longrightarrow {}^4He^+ + {}^4He^+$. The solid and dashed curves from the CB1-4B method correspond to the cases where the potential $V_{corr} = 1/r_{12} - 1/x_1$ is included and excluded from the complete perturbation V_f, respectively. The wave function of Silverman *et al.* [32] is used for the initial bound state. Experimental data: the same as in Fig. 3.

Besides very good agreement between theoretical total cross sections obtained by means of the CB1-4B method and a number of experimental data for p-He and α-He collisions, we have also tested our method against very recently published experimental results of Sant'Anna *et al.* [59], as well as Woitke *et al.* [60], for Li^{3+}-He collisions, and good agreement is found. Hence, the presented theoretical results for the total cross sections can be considered as reliable at intermediate and high impact energies. However, in the case of differential cross sections, the CB1-4B model exhibits an unphysical and experimentally unobserved dip due to mutual cancellation among the various terms in the perturbation potentials. A similar problem in the case of differential cross sections appeared when the one-channel distorted wave models were utilized [61].

IV. CONCLUSIONS

We have investigated the problem of single charge exchange in collisions between bare ions and a two-electron atomic system. The analysis is carried out by means of the CB1-4B model. The obtained total cross sections for the investigated p-He and α-He one-electron capture are presently found to be in very good agreement with the available experimental data. This is not surprising, since the four-body version of the CB1-4B model is obtained as a direct extension of its well-established three-body counterpart. In addition to some works [6,8] which argue that in the independent particle approach can explain the processes studied in this work, the present CB1-4B model can be considered as a reliable theory for single capture at intermediate and high impact energies and might bring some information on electronic correlation effects. The obtained results indicate that the term $V_{corr} = 1/r_{12} - 1/x_1$ in the perturbation potential of the post version, which is connected with the dynamic electron correlations, is important.

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APPENDIX

In this appendix we give the final result of the integral $I_{n,\lambda}^{(\vec{p})}$, $(n = 0, 1, 2, 3, 4)$ defined in Eq. (31) of the main text. The standard Nordsieck technique [62], together with the partial differential procedure, yields the following expressions:

$$I_0 = 4\pi\Gamma(1+i\xi)\mathcal{F}_\lambda^{(\vec{p})}, \tag{A1}$$

$$I_1 = 8\pi\Gamma(1+i\xi)D_\lambda^{(\vec{p})}\mathcal{F}_\lambda^{(\vec{p})}\left[1 - i\xi C_\lambda^{(\vec{p})}\right], \tag{A2}$$

$$I_2 = -8\pi\Gamma(1+i\xi)\frac{D_\lambda^{(\vec{p})}\mathcal{F}_\lambda^{(\vec{p})}}{\lambda}\left[A_{\alpha,\lambda}^{(\vec{p})} + i\xi B_{\alpha,\lambda}^{(\vec{p})}\right], \tag{A3}$$

$$I_3 = -16\pi\Gamma(1+i\xi)\frac{\left[D_\lambda^{(\vec{p})}\right]^2\mathcal{F}_\lambda^{(\vec{p})}}{\lambda}\left[A_{\beta,\lambda}^{(\vec{p})} + i\xi B_{\beta,\lambda}^{(\vec{p})}\right], \tag{A4}$$

$$I_4 = 16\pi\Gamma(1+i\xi)\frac{\left[D_\lambda^{(\vec{p})}\right]^2\mathcal{F}_\lambda^{(\vec{p})}}{\lambda^2}\left[A_{\gamma,\lambda}^{(\vec{p})} - i\xi B_{\gamma,\lambda}^{(\vec{p})}\right], \tag{A5}$$

where the symbol Γ stands for the conventional γ function. The other quantities appearing in Eqs. (A1)–(A5) are

$$\mathcal{F}_\lambda^{(\vec{p})} = \frac{\left[B_\lambda^{(\vec{p})}\right]^{i\xi}}{p^2+\lambda^2}, \quad B_\lambda^{(\vec{p})} = \frac{2(v\lambda - i\,\vec{p}\cdot\vec{v})}{p^2+\lambda^2}, \tag{A6}$$

$$C_\lambda^{(\vec{p})} = \frac{v}{\lambda B_\lambda^{(\vec{p})}} - 1, \quad A_\lambda^{(\vec{p})} = \frac{\lambda^2}{p^2+\lambda^2}, \quad D_\lambda^{(\vec{p})} = \frac{A_\lambda^{(\vec{p})}}{\lambda}, \tag{A7}$$

$$A_{\alpha,\lambda}^{(\vec{p})} = 1 - 4A_\lambda^{(\vec{p})}, \quad B_{\alpha,\lambda}^{(\vec{p})} = 1 + 2A_\lambda^{(\vec{p})}C_{\alpha,\lambda}^{(\vec{p})}, \tag{A8}$$

$$C_{\alpha,\lambda}^{(\vec{p})} = C_\lambda^{(\vec{p})}\left[4 + (1-i\xi)C_\lambda^{(\vec{p})}\right], \tag{A9}$$

$$A_{\beta,\lambda}^{(\vec{p})} = 6\left[1 - 2A_\lambda^{(\vec{p})}\right], \quad B_{\beta,\lambda}^{(\vec{p})} = 2A_\lambda^{(\vec{p})}C_{\beta,\lambda}^{(\vec{p})} + 3D_{\beta,\lambda}^{(\vec{p})} \tag{A10}$$

$$C_{\beta,\lambda}^{(\vec{p})} = C_\lambda^{(\vec{p})}\left\{18 + 9(1-i\xi)C_\lambda^{(\vec{p})} + (1-i\xi)(2-i\xi)\left[C_\lambda^{(\vec{p})}\right]^2\right\}, \tag{A11}$$

$$D_{\beta,\lambda}^{(\vec{p})} = 2 - (1+i\xi)C_\lambda^{(\vec{p})},$$

$$A_{\gamma,\lambda}^{(\vec{p})} = 6\left\{16\left[A_\lambda^{(\vec{p})}\right]^2 - 12A_\lambda^{(\vec{p})} + 1\right\}, \tag{A12}$$

$$B_{\gamma,\lambda}^{(\vec{p})} = 4\left[A_\lambda^{(\vec{p})}\right]^2 C_{\gamma,\lambda}^{(\vec{p})} - 12A_\lambda^{(\vec{p})}D_{\gamma,\lambda}^{(\vec{p})} - 3(3+i\xi), \tag{A13}$$

$$C_{\gamma,\lambda}^{(\vec{p})} = C_\lambda^{(\vec{p})}\left\{96 + 72(1-i\xi)C_\lambda^{(\vec{p})} + 16(1-i\xi)(2-i\xi) \times \left[C_\lambda^{(\vec{p})}\right]^2 + (1-i\xi)(2-i\xi)(3-i\xi)\left[C_\lambda^{(\vec{p})}\right]^3\right\}, \tag{A14}$$

$$D_{\gamma,\lambda}^{(\vec{p})} = (1+i\xi)C_\lambda^{(\vec{p})}\left[6 + (1-i\xi)C_\lambda^{(\vec{p})}\right] - 6. \tag{A15}$$

[1] J. McGuire, *Electron Correlation Dynamics in Atomic Collisions* (Cambrige University Press, Cambrige, 1997).

[2] R. Nagano, K. Yabana, T. Tazawa, and Y. Abe, Phys. Rev. A **62**, 062721 (2000).

[3] X. M. Tong, T. Watanabe, D. Kato, and S. Ohtani, Phys. Rev. A **66**, 032709 (2002).

[4] T. Kirchner, H. J. Lüdde, and M. Horbatsch, Phys. Scr. **T110**, 364 (2004).

[5] M. Zapukhlyak, T. Kirchner, H. J. Lüdde, S. Knoop, R. Morgenstern, and R. Hoekstra, J. Phys. B **38**, 2353 (2005).

[6] M. Zapukhlyak, T. Kirchner, A. Hasan, B. Tooke, and M. Schulz, Phys. Rev. A **77**, 012720 (2008).

[7] T. Kirchner, H. J. Lüdde, and M. Horbatsch, Recent Res. Dev. Phys. **5**, 433 (2004).

[8] M. Zapukhlyak and T. Kirchner, Phys. Rev. A **80**, 062705 (2009).

[9] J. F. Reading and A. L. Ford, Phys. Rev. Lett. **58**, 543 (1987).

[10] J. F. Reading and A. L. Ford, J. Phys. B **20**, 3747 (1987).

[11] F. Martin and A. Salin, Phys. Rev. Lett. **76**, 1437 (1996).

[12] F. Martin and A. Salin, Phys. Rev. A **54**, 3990 (1996); **55** 2004 (1997).

[13] C. Diaz, F. Martin, and A. Salin, J. Phys. B **33**, 4373 (2000).

[14] J. F. Reading, T. Bronk, and A. L. Ford, J. Phys. B **29**, 6075 (1996).

[15] Dž. Belkić, R. Gayet, and A. Salin, Phys. Rep. **56**, 279 (1979).

[16] D. Dollard, J. Math. Phys. **5**, 729 (1964).

[17] Dž. Belkić, *Principles of Quantum Scattering Theory* (Institute of Physics, Bristol, 2004).

[18] Dž. Belkić, R. Gayet, J. Hanssen, and A. Salin, J. Phys. B **19**, 2945 (1986).

[19] D. P. Dewangan and J. J. Eichler, J. Phys. B **19**, 2939 (1986).

[20] Dž. Belkić, S. Saini, and H. Taylor, Z. Phys. D **3**, 59 (1986).

[21] Dž. Belkić, S. Saini, and H. S. Taylor, Phys. Rev. A **36**, 1601 (1987).

[22] N. Toshima, T. Ishihara, and J. Eichler, Phys. Rev. A **36**, 2659 (1987).

[23] Dž. Belkić and H. S. Taylor, Phys. Rev. A **35**, 1991 (1987).

[24] Dž. Belkić, Phys. Rev. A **37**, 55 (1988).

[25] Dž. Belkić, Phys. Scr. **40**, 610 (1989); **T28**, 106 (1989).

[26] Dž. Belkić and I. Mančev, Phys. Scr. **42**, 89 (1990).

[27] Dž. Belkić, I. Mančev, and J. Hanssen, Rev. Mod. Phys. **80**, 249 (2008).

[28] Dž. Belkić, *Quantum Theory of High-Energy Ion-Atom Collisions* (Taylor & Francis, London, 2009).

[29] I. Mančev, Phys. Scr. **51**, 762 (1995).

[30] I. Mančev, Phys. Rev. A **54**, 423 (1996).

[31] E. Hylleraas, Z. Phys. **54**, 347 (1929).

[32] J. N. Silverman, O. Platas, and F. A. Matsen, J. Chem. Phys. **32**, 1402 (1960); C. Eckart, Phys. Rev. **36**, 878 (1930).

[33] M. B. Shah, P. McCallion, and H. B. Gilbody, J. Phys. B **22**, 3037 (1989).

[34] U. Schryber, Helv. Phys. Acta **40**, 1023 (1967).

[35] M. B. Shah and H. B. Gilbody, J. Phys. B **18**, 899 (1985).

[36] E. Horsdal-Pedersen, C. L. Cocke, and M. Stockli, Phys. Rev. Lett. **50**, 1910 (1983).

[37] K. H. Berkner, S. N. Kaplan, G. A. Paulikas, and R. V. Pyle, Phys. Rev. **140**, A729 (1965).

[38] J. F. Williams, Phys. Rev. **157**, 97 (1967).

[39] P. J. Martin, K. Arnett, D. M. Blankenship, T. J. Kvale, J. L. Peacher, E. Redd, V. C. Sutcliffe, J. T. Park, C. D. Lin, and J. H. McGuire, Phys. Rev. A **23**, 2858 (1981).

[40] L. M. Welsh, K. H. Berkner, S. N. Kaplan, and R. V. Pyle, Phys. Rev. **158**, 85 (1967).

[41] V. Mergel *et al.* Phys. Rev. Lett. **74**, 2200 (1995).

[42] L. Green, M. Mulder, M. Lewis, and J. W. Woll, Phys. Rev. **93**, 757 (1954).

[43] P. O. Löwdin, Phys. Rev. **90**, 120 (1953).

[44] Dž. Belkić and I. Mančev, Phys. Scr. **47**, 18 (1993).

[45] Dž. Belkić, R. Gayet, J. Hanssen, I. Mančev, and A. Nuñez, Phys. Rev. A **56**, 3675 (1997).

[46] Dž. Belkić, I. Mančev, and V. Mergel, Phys. Rev. A **55**, 378 (1997).

[47] M. F. Ciappina, W. R. Cravero, and C. R. Garibotti, J. Phys. B **36**, 3775 (2003).

[48] M. F. Ciappina and W. R. Cravero, J. Phys. B **39**, 1091 (2006).

[49] P. Hvelplund, J. Heinemei, E. Horsdal-Pedersen, and F. R. Simpson, J. Phys. B **9**, 491 (1976).

[50] N. V. de Castro Faria, F. L. Freire Jr., and A. G. de Pinho, Phys. Rev. A **37**, 280 (1988).

[51] R. D. DuBois, Phys. Rev. A **36**, 2585 (1987).

[52] L. I. Pivovar, V. M. Tabuev, and M. T. Novikov, Zh. Eksp. Teor. Fiz. **41**, 26 (1961) [Sov. Phys. JETP **14**, 20 (1962)].

[53] I. Mančev, Phys. Rev. A **60**, 351 (1999).

[54] K. M. Dunseath and D. S. F. Crothers, J. Phys. B **24**, 5003 (1991).

[55] P. Pluvinage, J. Phys. Radium **12**, 789 (1951).

[56] F. W. Byron and C. J. Joachain, Phys. Rev. Lett. **16**, 1139 (1966).

[57] C. J. Joachain and R. Vanderpoorten, Physica (Amsterdam) **46**, 333 (1970).

[58] R. J. Tweed, J. Phys. B **5**, 810 (1972).

[59] M. M. Sant'Anna, A. C. F. Santos, L. F. S. Coelho, G. Jalbert, N. V. de Castro Faria, F. Zappa, P. Focke, and Dž. Belkić, Phys. Rev. A **80**, 042707 (2009).

[60] O. Woitke, P. A. Závodszky, S. M. Ferguson, J. H. Houck, and J. A. Tanis, Phys. Rev. A **57**, 2692 (1998).

[61] M. S. Schöffler, J. Titze, L. Ph. H. Schmidt, T. Jehnke, N. Neumann, O. Jagutzki, H. Schmidt-Böcking, R. Dörner, and I. Mančev, Phys. Rev. A **79**, 064701 (2009).

[62] A. Nordsieck, Phys. Rev. **93**, 785 (1954).