

Electron correlations in single-electron capture into any state of fast projectiles from heliumlike atomic systems

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State-selective and total single-electron capture cross sections in fast collisions of a bare projectile with a heliumlike target are examined in the four-body formalism. A special emphasis is given to a proper inclusion of dynamic electron-electron correlation effects. For this purpose, the post form of the four-body boundary-corrected first Born approximation (CB1-4B) is utilized. With regard to our related previous study, where the prior version has been considered, in the present work an extensive analytical study of the post-transition amplitude for electron capture into the arbitrary final states $n^f l^f m^f$ of the projectile is carried out. The post-transition amplitude for single charge exchange encompassing symmetric and asymmetric collisions is derived in terms of five-dimensional integrals over real variables. The dielectronic interaction $V_{12} = 1/r_{12} \equiv 1/|\vec{r}_1 - \vec{r}_2|$ explicitly appears in the perturbation potential V_f of the post-transition probability amplitude T_{if}^+ , such that the CB1-4B method can provide information about the relative significance of the dynamic interelectron correlation in the collisions under study. An illustrative computation is performed involving state-selective and total single capture cross sections for the p -He collisions at intermediate and high impact energies. The so-called post-prior discrepancy, which plagues almost all the existing distorted wave approximations, is presently shown to be practically nonexistent in the CB1-4B method. The validity of our findings is critically assessed in comparisons with the available experimental data for both state-selective and total cross sections summed over all the discrete energy levels of the hydrogenlike atom formed with the projectile. Overall, excellent performance of the CB1-4B method is recorded, thus robustly establishing this formalism as the leading first-order description of high-energy single charge exchange, which is a collision of paramount theoretical and practical importance across interdisciplinary fields ranging from astrophysics to medicine.

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I. INTRODUCTION

Electron capture from atomic and molecular targets by the impact of fast ions is a topic of major importance in various basic branches of physics such as astrophysics and plasma physics, as well as in applied areas such as radiotherapy by hadrons and in fusion research. Charge exchange as the source of energy transfer is also a subject in microbiology. The present work is focused on the case of single-electron capture from two-electronic atomic systems interacting with bare ions where four particles in total are involved. We report on our theoretical investigation of single-electron capture process in the typical $Z_P - (Z_T; e_1, e_2)$ collision by using the four-body boundary-corrected first Born (CB1-4B) approximation. The CB1-4B method is a fully quantum mechanical four-body formalism, since it explicitly considers each individual particle and all the interactions among them in the collision under investigation. The CB1-4B theory goes beyond the usual independent-particle frozen-core approximations. Moreover, it strictly preserves the correct boundary conditions in both collisional channels. It is well known that the boundary conditions, or equivalently, the asymptotic convergence problem [1–4] are of essential importance for atomic collisions whenever the aggregates are charged in the asymptotic channels. Such a conclusion has been rigorously reached in formal scattering theory (see, e.g., Ref. [4] and references therein). In general, the correct Coulomb boundary conditions consist of the simultaneous requirement for the correct asymptotic behaviors of all the scattering wave functions and their proper

connection with the corresponding perturbation interactions that must be of short range [1]. The relevance of the Coulomb phase distortions of the asymptotic channel states has been established in comparison with experimental data for many ion-atom collisions.

The first Born approximation with the correct boundary conditions has been introduced within the three-body formalism [3] (hereafter denoted as CB1-3B). Later, the CB1-3B model has successfully been applied to many electron-capture processes [5–19]. These applications of the CB1-3B model have also shown that a first-order theory could be adequate for describing single-electron capture, but only provided that it obeys the proper Coulomb boundary conditions and that it is associated with a nondivergent series development. The initial formulation and implementation of the CB1-4B approximation was carried out for double charge exchange [20,21]. Subsequently, the CB1-4B method was adapted and applied to single-electron capture [22–24]. These computations [20–24] have been performed for the ground-to-ground-state capture. In a recent paper [25], we have carried out an extension of the CB1-4B model in its prior version to encompass electron capture into arbitrary final states of the projectile. A number of quantum-mechanical four-body methods have been proposed to study one- and two-electron transitions for nonrelativistic fast ion-atom collisions with two actively participating electrons, as reviewed in Refs. [26–28].

Beyond the essential importance of the correct boundary conditions, the studies of interelectronic static and dynamic correlations have also played a central role in atomic collision

physics for a long time (see, e.g., Ref. [29]). Static correlations are included in the bound-state wave functions of multielectron targets. Dynamic correlations are due to interelectron Coulomb potentials in the perturbation interactions from the transition amplitudes. In other words, static correlations of electrons are of the spectroscopic type and, as such, are built for isolated atoms with no reference to collisions. By contrast, dynamic correlations are the interelectronic interactions that constitute a part of the overall perturbation potential responsible for transitions between the initial and final states of the colliding atomic systems. Helium atoms and negative hydrogen ions have, to a large extent, been the two most prominent benchmark systems of such studies. For example, using the four-body modified Coulomb-Born (MCB-4B), or equivalently, the four-body continuum distorted wave eikonal initial state (CDW-EIS-4B) approximation, the static correlations have been shown to be of a paramount importance for single-electron detachment in the $p\text{-H}^-$ collisions from the threshold to the high-energy Bethe region and beyond [30,31]. Likewise, the dynamic correlations between electrons have been analyzed by means of the CDW-EIS-4B model and shown to be very significant for single ionization in the $p\text{-He}$ collisions [32]. Further, for transfer ionization in the $\alpha\text{-He}$ collisions, Belkić *et al.* [33,34] used the post version of the four-body continuum distorted wave (CDW-4B) method, in which the dielectronic interaction $V_{12} = 1/r_{12}$ explicitly appears in the perturbation potential V_f . Their results [33,34] prove that there is a substantial improvement of the CDW-4B method over the independent electron models, implying that this success can be attributed solely to the dynamic electron correlation effects. Moreover, the importance of the correlation effects has very recently been examined in the context of time-dependent density functional theory of antiproton-helium collisions [35]. Thus, Ref. [35] has presented the results for single and double ionization in the impact energy range 5–2000 keV. The conclusion that the electron correlation effects play a significant role in antiproton impact ionization of helium has also been reached by Pindzola *et al.* [36] by using the time-dependent close-coupling method. The presence of a negatively charged impact ion in such reactions removes the necessity of considering charge-transfer processes.

Electron correlations in single-electron capture have been analyzed within the CDW-4B theory [37,38] in the $p\text{-He}$, $\alpha\text{-He}$, and $p\text{-Li}^+$ scattering, as well as within the CB1-4B approximation [24] for the $p\text{-He}$ and $\alpha\text{-He}$ collisions. In these studies [24,37,38], the computations have been carried out *only* for the ground-to-ground state capture. Additionally, the obtained results were multiplied by a factor of 1.202 in order to roughly include a contribution from all the excited states. Electron transfer into excited states is expected to play an important role, at least at lower and intermediate impact energies. The contribution from the $e_1\text{-}e_2$ interaction during the collision to single-electron capture into *arbitrary* final states of the projectile has not been previously assessed. Therefore, the main goal of the present work is to examine the relative significance of the role of the dynamic interelectron correlation with the help of the CB1-4B theory. We shall focus on the role of the interelectron ($e_1\text{-}e_2$) potential $V_{12} = 1/r_{12}$ from a dynamic point of view, with the purpose of determining whether electronic correlations remain important for capture into excited states. In order to achieve this goal within the CB1-4B method, one ought to employ the post formalism with the explicit allowance of V_{12} in the complete final perturbation V_f , which appears in the transition amplitude T_{if}^+ .

Atomic units will be used throughout unless otherwise stated.

II. THEORY

The reactions to be studied are of the following type:

$$Z_P + (Z_T; e_1, e_2)_{1s^2} \longrightarrow (Z_P, e_1)_{n^f l^f m^f} + (Z_T, e_2)_{1s}, \quad (1)$$

where Z_K is the charge of the K th nucleus ($K = P, T$) and $n^f l^f m^f$ is the usual set of the three quantum numbers of hydrogenlike atomic systems. The parentheses in Eq. (1) denote the bound states. Let \vec{s}_1 and \vec{s}_2 (\vec{x}_1 and \vec{x}_2) be the position vectors of the first and second electron e_1 and e_2 relative to the nuclear charge of the projectile Z_P (target Z_T), respectively. Further, let \vec{R} be the position vector of Z_T with respect to Z_P .

The post form of the transition amplitude for process (1) in the CB1-4B method is

$$T_{if}^+(\vec{\eta}) = \iiint d\vec{x}_1 d\vec{x}_2 d\vec{R} (\rho v)^{2i Z_P (Z_T - 2)/v} \varphi_{n^f l^f m^f}^*(\vec{s}_1) \varphi_T^*(\vec{x}_2) \left[Z_P \left(\frac{1}{R} - \frac{1}{s_2} \right) + (Z_T - 1) \left(\frac{1}{R} - \frac{1}{x_1} \right) + \left(\frac{1}{r_{12}} - \frac{1}{x_1} \right) \right] \varphi_i(\vec{x}_1, \vec{x}_2) e^{i\vec{k}_i \cdot \vec{r}_i + i\vec{k}_f \cdot \vec{r}_f + i\xi \ln(vR + \vec{v} \cdot \vec{R})}, \quad (2)$$

where $\xi = (Z_P - Z_T + 1)/v$ and $\vec{\rho}$ is the projection of vector \vec{R} onto the XOY plane ($\vec{\rho} = \vec{R} - \vec{Z}$, $\vec{\rho} \cdot \vec{Z} = 0$). Furthermore, \vec{k}_i and \vec{k}_f are the initial and final wave vectors, while $\vec{\eta}$ is the transverse momentum transfer $\vec{\eta} = (\eta \cos \phi_\eta, \eta \sin \phi_\eta, 0)$ with the property $\vec{\eta} \cdot \vec{v} = 0$ and \vec{v} is the incident velocity vector. According to Ref. [3], for the purpose of computing total cross sections, evaluation of the matrix element $T_{if}^+(\vec{\eta})$ can be carried out by omitting the phase factor $(\rho v)^{2i Z_P (Z_T - 2)/v}$ from the outset. Vector \vec{r}_i in Eq. (2) is the relative vector of Z_P

with respect to the center of mass of $(Z_T; e_1, e_2)_{1s^2}$, whereas \vec{r}_f is the position vector of the center of mass of $(Z_P, e_1)_{n^f l^f m^f}$ relative to $(Z_T, e_2)_{1s}$. The vector of the distance between the two electrons e_1 and e_2 is denoted by $\vec{r}_{12} = \vec{x}_1 - \vec{x}_2 = \vec{s}_1 - \vec{s}_2$, so that $r_{12} = |\vec{r}_{12}|$. The wave function of the two-electron ground state of the target $(Z_T; e_1, e_2)_{1s^2}$ is labeled by $\varphi_i(\vec{x}_1, \vec{x}_2)$. Likewise, the bound-state wave functions of the hydrogenlike atomic systems $(Z_P, e_1)_{n^f l^f m^f}$ and $(Z_T, e_2)_{1s}$ are denoted by $\varphi_{n^f l^f m^f}(\vec{s}_1)$ and $\varphi_T(\vec{x}_2)$, respectively.

We shall use the eikonal hypothesis, since the small-angle limit applies to heavy particles:

$$\vec{k}_i \cdot \vec{r}_i + \vec{k}_f \cdot \vec{r}_f = \vec{\alpha} \cdot \vec{s}_1 + \vec{\beta} \cdot \vec{x}_1 = -\vec{v} \cdot \vec{x}_1 - \vec{\alpha} \cdot \vec{R}, \quad (3)$$

where $\vec{\alpha}$ and $\vec{\beta}$ are the linear momentum transfers,

$$\begin{aligned} \vec{\beta} &= -\vec{\eta} - \beta_z \hat{v}, & \vec{\alpha} &= \vec{\eta} - \alpha_z \hat{v}, \\ \vec{\alpha} + \vec{\beta} &= -\vec{v}, & \alpha_z &= v/2 - \Delta E/v, \\ \beta_z &= v/2 + \Delta E/v. \end{aligned} \quad (4)$$

Here, $\hat{v} \equiv \vec{v}/v$ and $\Delta E = E_i - E_f$, where E_i is the binding energy of the two-electron target with $E_f = -Z_P^2/[2(n^f)^2] -$

$Z_T^2/2$. We shall use the general factorized form for φ_i via:

$$\varphi_i(\vec{x}_1, \vec{x}_2) = \sum_{k,l} \varphi_{\alpha k}(\vec{x}_1) \varphi_{\alpha l}(\vec{x}_2), \quad (5)$$

where $\varphi_{\alpha j}(\vec{r}) = N_{\alpha j} \exp(-\alpha_j r)$ with $N_{\alpha j} = a_j \sqrt{N}$ ($j = k, l$) 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 on a concrete choice for the wave function.

The transition amplitude T_{if}^+ from (2) for process (1) can now be written as

$$T_{if}^+ = \sum_{k,l} N_{kl} \{ Z_P [J_R^{(k,l)} - J_{s_2}^{(k,l)}] + (Z_T - 1) [J_R^{(k,l)} - J_{x_1}^{(k,l)}] + [J_{r_{12}}^{(k,l)} - J_{x_1}^{(k,l)}] \}, \quad (6)$$

$$J_{\omega}^{(k,l)} = \int d\vec{R} e^{-i\vec{\alpha} \cdot \vec{R}} (vR + \vec{v} \cdot \vec{R})^{i\xi} W_{\omega}^{(k,l)}(\vec{R}); \quad \omega = R, x_1, s_2, r_{12}, \quad (7)$$

$$W_R^{(k,l)} = \frac{1}{R} \mathcal{B}_k \mathcal{A}_l, \quad W_{s_2}^{(k,l)} = \mathcal{B}_k \mathcal{D}_l, \quad W_{x_1}^{(k,l)} = \mathcal{L}_k \mathcal{A}_l, \quad W_{r_{12}}^{(k,l)} = \frac{1}{2\pi^2} \int \frac{d\vec{\tau}}{\tau^2} \mathcal{B}_{k,\tau} \mathcal{A}_{l,\tau}, \quad (8)$$

$$\mathcal{A}_l = \int d\vec{x}_2 e^{-(Z_T + \alpha_l)x_2} = \frac{8\pi}{(Z_T + \alpha_l)^3}, \quad \mathcal{B}_k = \int d\vec{x}_1 e^{-i\vec{v} \cdot \vec{x}_1 - \alpha_k x_1} \varphi_{n^f l^f m^f}^*(\vec{s}_1), \quad (9)$$

$$\mathcal{A}_{l,\tau} = \int d\vec{x}_2 e^{i\vec{\tau} \cdot \vec{x}_2 - (Z_T + \alpha_l)x_2} = \frac{8\pi(Z_T + \alpha_l)}{[\tau^2 + (Z_T + \alpha_l)^2]^2}, \quad (10)$$

$$\mathcal{D}_l = \int d\vec{x}_2 \frac{e^{-(Z_T + \alpha_l)x_2}}{s_2} = 2\pi(Z_T + \alpha_l) \int_0^1 dt_1 \frac{1-t_1}{\Delta_1^3} (1 + \Delta_1 R) e^{-\Delta_1 R}, \quad (11)$$

$$\mathcal{L}_k = \int d\vec{x}_1 \frac{e^{-i\vec{v} \cdot \vec{x}_1 - \alpha_k x_1}}{x_1} \varphi_{n^f l^f m^f}^*(\vec{s}_1) = \int d\vec{x}_1 \frac{e^{-i\vec{v} \cdot \vec{x}_1 - \alpha_k x_1}}{x_1} \left[\int d\vec{q} e^{-i\vec{q} \cdot \vec{s}_1} \tilde{\varphi}_{n^f l^f m^f}(\vec{q}) \right]^*, \quad (12)$$

$$\mathcal{B}_{k,\tau} = \int d\vec{x}_1 e^{-i(\vec{\tau} + \vec{v}) \cdot \vec{x}_1 - \alpha_k x_1} \varphi_{n^f l^f m^f}^*(\vec{s}_1) = \int d\vec{x}_1 e^{-i(\vec{\tau} + \vec{v}) \cdot \vec{x}_1 - \alpha_k x_1} \left[\int d\vec{q} e^{-i\vec{q} \cdot \vec{s}_1} \tilde{\varphi}_{n^f l^f m^f}(\vec{q}) \right]^*, \quad (13)$$

where $N_{k,l} = (Z_T)^{3/2} N_{\alpha k} N_{\alpha l} / \sqrt{\pi}$ and $\Delta_1 = (Z_T + \alpha_l) \sqrt{1 - t_1}$. In integral $J_{r_{12}}^{(k,l)}$, the well-known Bethe transform can be utilized via $1/r_{12} = (2\pi^2)^{-1} \int d\vec{\tau} \tau^{-2} e^{-i\vec{\tau} \cdot (\vec{x}_1 - \vec{x}_2)}$. Quantity $\tilde{\varphi}_{n^f l^f m^f}(\vec{q})$ in Eqs. (12) and (13) represents the Fourier transform $\tilde{\varphi}_{n^f l^f m^f}(\vec{q}) = (2\pi)^{-3} \int d\vec{s}_1 e^{i\vec{q} \cdot \vec{s}_1} \varphi_{n^f l^f m^f}(\vec{s}_1)$ of the hydrogenlike wave function $\varphi_{n^f l^f m^f}(\vec{s}_1)$. Regarding $\tilde{\varphi}_{n^f l^f m^f}(\vec{q})$, it will prove advantageous to employ this power series representation [39]:

$$\tilde{\varphi}_{n^f l^f m^f}(\vec{q}) = (2\pi)^{-3} N_f^{Z_P} i^{l^f} \sum_{p=0}^{n_r} c_p \frac{\mathcal{Y}_{l^f m^f}(\vec{q})}{(q^2 + a_f^2)^{p+l^f+2}}, \quad (14)$$

$$N_f^{Z_P} = 16\pi Z_P \left[\frac{a_f^3 (n^f + l^f)!}{n^f n_r!} \right]^{1/2} \frac{l^f! (4a_f)^{l^f}}{(2l^f + 1)!}, \quad c_p = \frac{(-n_r)_p (n^f + l^f + 1)_p}{(l^f + 3/2)_p p!} a_f^{2p}, \quad (15)$$

with $n_r = n^f - l^f - 1$ and $a_f = Z_P/n^f$. Here, symbol $\mathcal{Y}_{lm}(\vec{q})$ denotes the regular solid harmonic, i.e., the multipole of the type $\mathcal{Y}_{lm}(\vec{q}) = q^l Y_{lm}(\hat{q})$, where $Y_{lm}(\hat{q})$ is the usual spherical harmonic, whereas $(a)_n$ is the Pochhammer symbol, which is alternatively called the rising factorial $(a)_n = \Gamma(a+n)/\Gamma(a) = a(a+1) \cdots (a+n-1)$ with $(a)_0 = 1$.

In the sequel, we shall generalize the original derivation of Belkić and Taylor [15]. To this end, integrals $\mathcal{B}_{k,\tau}$ and \mathcal{L}_k are written as:

$$\mathcal{B}_{k,\tau} = (2\pi)^{-3} N_f^{Z_P} (-i)^{l^f} 8\pi \alpha_k \sum_{p=0}^{n_r} c_p \mathcal{G}_{k,p}^{(\tau,2)}, \quad \mathcal{L}_k = (2\pi)^{-3} N_f^{Z_P} (-i)^{l^f} 4\pi \sum_{p=0}^{n_r} c_p \mathcal{G}_{k,p}^{(0,1)}, \quad (16)$$

$$\mathcal{G}_{k,p}^{(\tau,2)} = e^{i\vec{\alpha} \cdot \vec{R}} \int d\vec{q} e^{-i\vec{q} \cdot \vec{R}} \frac{\mathcal{Y}_{l^f m^f}^*(\vec{q} - \vec{\alpha})}{(|\vec{q} - \vec{\alpha}|^2 + a_f^2)^{p+l^f+2} [|\vec{q} + (\vec{\beta} - \vec{\tau})|^2 + \alpha_k^2]^2}, \quad (17)$$

$$\mathcal{G}_{k,p}^{(0,1)} = e^{i\vec{\alpha} \cdot \vec{R}} \int d\vec{q} e^{-i\vec{q} \cdot \vec{R}} \frac{\mathcal{Y}_{l^f m^f}^*(\vec{q} - \vec{\alpha})}{(|\vec{q} - \vec{\alpha}|^2 + a_f^2)^{p+l^f+2} (|\vec{q} + \vec{\beta}|^2 + \alpha_k^2)}. \quad (18)$$

First, we shall consider integral $\mathcal{G}_{k,p}^{(\tau,2)}$. Using the Feynman parametrization integral:

$$\frac{1}{A^s B^r} = \frac{(s+r-1)!}{(s-1)!(r-1)!} \int_0^1 dt \frac{t^{s-1}(1-t)^{r-1}}{[At + B(1-t)]^{s+r}} \quad (s, r \geq 1), \quad (19)$$

it follows,

$$\mathcal{G}_{k,p}^{(\tau,2)} = n(n-1) \int_0^1 dt t^{n-2}(1-t) \mathcal{U}_{k,p}^{(\tau)}, \quad \mathcal{U}_{k,p}^{(\tau)} = e^{-i\vec{Q}_{\tau\alpha} \cdot \vec{R}} \int d\vec{q} e^{-i\vec{q} \cdot \vec{R}} \frac{\mathcal{Y}_{l^f m^f}^*(\vec{q} + \vec{Q}_{\tau\alpha})}{(q^2 + \Delta_{\tau}^2)^{n+1}}, \quad (20)$$

$$\vec{Q}_{\tau\alpha} = \vec{Q}_{\tau} - \vec{\alpha} = (1-t)(\vec{\tau} + \vec{v}), \quad \vec{Q}_{\tau} = \vec{Q} + (1-t)\vec{\tau}, \quad \vec{Q} = \vec{\alpha}t - \vec{\beta}(1-t), \quad (21)$$

$$\Delta_{\tau}^2 = |\vec{v} + \vec{\tau}|^2 t(1-t) + a_{\tau}^2 t + \alpha_k^2(1-t), \quad n = p + l^f + 3. \quad (22)$$

In order to perform the angular integration over $\Omega_{\vec{q}} = (\theta_q, \phi_q)$ in Eq. (20), we shall first apply this addition theorem for regular solid harmonics [40,41]:

$$\mathcal{Y}_{l^f m^f}(\vec{q} + \vec{Q}_{\tau\alpha}) = \sum_{l_1^f=0}^{l^f} \sum_{m_1^f=-l_1^f}^{l_1^f} (l_1^f m_1^f | l^f m^f) \mathcal{Y}_{l_1^f m_1^f}(\vec{q}) \mathcal{Y}_{l_2^f m_2^f}(\vec{Q}_{\tau\alpha}), \quad (23)$$

where $l_1^f + l_2^f = l^f$, $m_1^f + m_2^f = m^f$, $-l_j^f \leq m_j^f \leq l_j^f$ ($j = 1, 2$) and,

$$(l_1^f m_1^f | l^f m^f) = \left[4\pi \frac{2l^f + 1}{(2l_1^f + 1)(2l_2^f + 1)} \frac{(l^f + m^f)!}{(l_1^f + m_1^f)!(l_2^f + m_2^f)!} \frac{(l^f - m^f)!}{(l_1^f - m_1^f)!(l_2^f - m_2^f)!} \right]^{1/2}. \quad (24)$$

Applying once again the addition theorem to $\mathcal{Y}_{l_2^f m_2^f}(\vec{Q}_{\tau\alpha})$, we have:

$$\mathcal{Y}_{l_2^f m_2^f}(\vec{Q}_{\tau\alpha}) = \sum_{l_{1s}^f=0}^{l_2^f} \sum_{m_{1s}^f=-l_{1s}^f}^{l_{1s}^f} (l_{1s}^f m_{1s}^f | l_2^f m_2^f) \mathcal{Y}_{l_{1s}^f m_{1s}^f}([1-t]\vec{\tau}) \mathcal{Y}_{l_{2s}^f m_{2s}^f}([1-t]\vec{v}), \quad (25)$$

where $l_{1s}^f + l_{2s}^f = l_2^f$, $m_{1s}^f + m_{2s}^f = m_2^f$, $-l_{js}^f \leq m_{js}^f \leq l_{js}^f$ ($j = 1, 2$) and,

$$(l_{1s}^f m_{1s}^f | l_2^f m_2^f) = \left[4\pi \frac{2l_2^f + 1}{(2l_{1s}^f + 1)(2l_{2s}^f + 1)} \frac{(l_2^f + m_2^f)!}{(l_{1s}^f + m_{1s}^f)!(l_{2s}^f + m_{2s}^f)!} \frac{(l_2^f - m_2^f)!}{(l_{1s}^f - m_{1s}^f)!(l_{2s}^f - m_{2s}^f)!} \right]^{1/2}. \quad (26)$$

Employing the relation $\mathcal{Y}_{l_{2s}^f m_{2s}^f}([1-t]\vec{v}) = (1-t)^{l_{2s}^f} v^{l_{2s}^f} Y_{l_{2s}^f m_{2s}^f}(\hat{v})$ and choosing the velocity vector \vec{v} along the Z axes, the spherical harmonic $Y_{l_{2s}^f m_{2s}^f}(\hat{v})$ in this special case will be nonzero only for $m_{2s}^f = 0$, so that $Y_{l_{2s}^f m_{2s}^f}(\hat{v}) \equiv Y_{l_{2s}^f m_{2s}^f}(0, \phi_v) = \sqrt{(2l_{2s}^f + 1)/(4\pi)} \delta_{0, m_{2s}^f}$, where $\delta_{n, n'}$ is the usual Kronecker δ symbol. In this way, the sum over m_{1s}^f in Eq. (25) disappears altogether and, therefore, the formula for $\mathcal{Y}_{l^f m^f}^*(\vec{q} + \vec{Q}_{\tau\alpha})$ is reduced to:

$$\mathcal{Y}_{l^f m^f}^*(\vec{q} + \vec{Q}_{\tau\alpha}) = \sqrt{4\pi} \sum_{l_1^f=0}^{l^f} \sum_{m_1^f=-l_1^f}^{l_1^f} \sum_{l_{1s}^f=|m_1^f|}^{l_1^f} (l_1^f m_1^f | l^f m^f) (1-t)^{l_{1s}^f} \Omega(l_{1s}^f, \vec{v}) \mathcal{Y}_{l_1^f, -m_1^f}(\vec{q}) \mathcal{Y}_{l_{1s}^f, -m_1^f}([1-t]\vec{\tau}), \quad (27)$$

$$\Omega(l_{1s}^f, \vec{v}) = \frac{(l_{1s}^f | l_2^f m_2^f) v^{l_{1s}^f}}{\sqrt{4\pi} (-1)^{m^f}}, \quad (l_{1s}^f | l_2^f m_2^f) = \left[\frac{2l_2^f + 1}{(2l_{1s}^f + 1)} \frac{(l_2^f + m_2^f)!}{(l_{1s}^f + m_1^f)!} \frac{(l_2^f - m_2^f)!}{(l_{1s}^f - m_1^f)!(l_{2s}^f)^2} \right]^{1/2}. \quad (28)$$

The auxiliary integral $\mathcal{U}_{k,p}^{(\tau)}$ from Eq. (20) can be cast into the form:

$$\mathcal{U}_{k,p}^{(\tau)} = e^{-i\vec{Q}_{\tau\alpha} \cdot \vec{R}} \sum_{l_1^f=0}^{l^f} \sum_{m_1^f=-l_1^f}^{l_1^f} \sum_{l_{1s}^f=|m_1^f|}^{l_1^f} (l_1^f m_1^f | l^f m^f) (1-t)^{l_{1s}^f} \Omega(l_{1s}^f, \vec{v}) \mathcal{Y}_{l_1^f, -m_1^f}([1-t]\vec{\tau}) \mathcal{W}_{k,p}^{(\tau)}, \quad (29)$$

$$\mathcal{W}_{k,p}^{(\tau)} = \sqrt{4\pi} \int d\vec{q} e^{-i\vec{q} \cdot \vec{R}} \frac{\mathcal{Y}_{l_1^f, -m_1^f}(\vec{q})}{(q^2 + \Delta_{\tau}^2)^{n+1}} = 4\pi^{\frac{5}{2}} (-i)^{l^f} \mathcal{F}_{k,p}^{(\tau)} \mathcal{Y}_{l_1^f, -m_1^f}(\vec{R}). \quad (30)$$

In Eq. (30), we used the Rayleigh ansatz $e^{-i\vec{q} \cdot \vec{R}} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^l (-i)^l j_l(qR) Y_{lm}^*(\hat{q}) Y_{lm}(\hat{R})$, where $(2z)^{1/2} j_l(z) = \pi^{1/2} J_{l+1/2}(z)$ and $J_{\nu}(z)$ is the ν th-order Bessel function of the first kind [42]. Above, the following result from Refs. [15,40] is

employed:

$$\mathcal{F}_{k,p}^{(\tau)} = \frac{2}{\pi R^{l_1^f}} \int_0^\infty dq \frac{q^{l_1^f+2} j_{l_1^f}(qR)}{(q^2 + \Delta_\tau^2)^{n+1}} = \frac{\hat{k}_{\nu-1/2}(R\Delta_\tau)}{2^n n! \Delta_\tau^{2n-2l_1^f-1}}, \quad (31)$$

where $\nu = n - l_1^f$. Here, $\hat{k}_\nu(z)$ is the reduced Bessel function $\hat{k}_\nu(z) = \sqrt{2/\pi} z^\nu K_\nu(z)$ and $K_\nu(z)$ is the McDonald function [42]. Therefore, integrals $\mathcal{U}_{k,p}^{(\tau)}$ and $\mathcal{G}_{k,p}^{(\tau,2)}$ can be mapped to:

$$\begin{aligned} \mathcal{U}_{k,p}^{(\tau)} &= \frac{4\pi^{5/2}}{2^n n!} e^{-i\vec{Q}_\tau \cdot \vec{R}} \sum_{l_1^f=0}^{l_1^f} \sum_{m_1^f=-l_1^f}^{l_1^f} \sum_{l_2^f=|m_2^f|}^{l_2^f} (l_1^f m_1^f | l_2^f m_2^f) (1-t)^{l_2^f} \Omega(l_{1s}^f, \vec{v}) (-i)^{l_1^f} \mathcal{Y}_{l_{1s}^f, -m_2^f}([1-t]\vec{\tau}) \frac{B_{l_1^f, -m_1^f}^{(v, \Delta_\tau)}(\vec{R})}{\Delta_\tau^{2n-2l_1^f-1}}, \quad (32) \\ \mathcal{G}_{k,p}^{(\tau,2)} &= \frac{4\pi^{5/2}}{2^n (n-2)!} \sum_{l_1^f=0}^{l_1^f} \sum_{m_1^f=-l_1^f}^{l_1^f} \sum_{l_2^f=|m_2^f|}^{l_2^f} (l_1^f m_1^f | l_2^f m_2^f) \Omega(l_{1s}^f, \vec{v}) (-i)^{l_1^f} \\ &\quad \times \int_0^1 dt t^{n-2} (1-t)^{l_2^f+1} e^{-i\vec{Q}_\tau \cdot \vec{R}} \frac{B_{l_1^f, -m_1^f}^{(v, \Delta_\tau)}(\vec{R})}{\Delta_\tau^{2n-2l_1^f-1}} \mathcal{Y}_{l_{1s}^f, -m_2^f}([1-t]\vec{\tau}), \quad (33) \end{aligned}$$

where $B_{l_1^f, -m_1^f}^{(v, \Delta_\tau)}(\vec{R}) = \hat{k}_{\nu-1/2}(R\Delta_\tau) \mathcal{Y}_{l_{1s}^f, -m_2^f}(\vec{R})$ is the so-called B -function [43]. Substituting Eq. (33) into Eq. (16) and using Eqs. (7), (8) and (10), it follows:

$$\begin{aligned} J_{r_{12}}^{(k,l)} &= \frac{2}{\pi^2} D_{l_1^f}^{(k,l)} \sum_{p=0}^{n_r} \frac{c_p}{2^n (n-2)!} \sum_{l_1^f=0}^{l_1^f} \sum_{m_1^f=-l_1^f}^{l_1^f} \sum_{l_2^f=|m_2^f|}^{l_2^f} (l_1^f m_1^f | l_2^f m_2^f) \Omega(l_{1s}^f, \vec{v}) (-i)^{l_1^f} \\ &\quad \times \int_0^1 dt t^{n-2} (1-t)^{l_2^f+1} \int \frac{d\vec{\tau}}{\Delta_\tau^{2n-2l_1^f-1} \tau^2 [\tau^2 + (Z_T + \alpha_l)^2]^2} \mathcal{Y}_{l_{1s}^f, -m_2^f}([1-t]\vec{\tau}) I_{r_{12}}^{(v, l_1^f)}, \quad (34) \end{aligned}$$

$$D_{l_1^f}^{(k,l)} = 64\pi^{9/2} (-i)^{l_1^f} N_f^{Z_p} (Z_T + \alpha_l) \alpha_k, \quad (35)$$

$$I_{r_{12}}^{(v, l_1^f)} = \frac{1}{(2\pi)^3} \int d\vec{R} e^{-i\vec{Q}_\tau \cdot \vec{R}} (vR + \vec{v} \cdot \vec{R})^{i\xi} B_{l_1^f, -m_1^f}^{(v, \Delta_\tau)}(\vec{R}). \quad (36)$$

Integral $I_{r_{12}}^{(v, l_1^f)}$ has been calculated in Ref. [25] for the prior CB1-4B method with the result:

$$I_{r_{12}}^{(v, l_1^f)} = \frac{(-1)^{l_1^f} (2i)^{l_1^f} (2n_p)!}{2\pi^2} \sum_{p_r=0}^{n_p} \frac{(-n_p)_{p_r}}{n_p!} \frac{2^{p_r-n_p}}{p_r!} \Delta_\tau^{p_r} G_{v, -m_1^f}^{(1, \Delta_\tau)}(\vec{Q}_\tau), \quad (37)$$

$$G_{v, -m_1^f}^{(\lambda, \Delta_\tau)}(\vec{Q}_\tau) = \sum_{k=0}^{p_\lambda} \sum_{l_1=|m_1^f|}^{l_1^f} \Phi_{p_r, v\tau}^{kl_1}(\lambda) \mathcal{Z}_{l_1^f, l_1}(\vec{Q}_\tau \cdot \vec{v}), \quad p_\lambda = p_r + \lambda, \quad (38)$$

where for $\lambda = 1$ and $n_p = n - l_1^f - 1$, we have,

$$\mathcal{Z}_{l_1^f, l_1}(\vec{Q}_\tau \cdot \vec{v}) = (l_1 | l_1^f - m_1^f) (-iv)^{l_2} \mathcal{Y}_{l_1, -m_1^f}(\vec{Q}_\tau), \quad (39)$$

$$(l_1 | l_1^f - m_1^f) = \left[\frac{2l_1^f + 1}{(2l_1 + 1)} \frac{(l_1^f + m_1^f)!}{(l_1 + m_1^f)!} \frac{(l_1^f - m_1^f)!}{(l_1 - m_1^f)! (l_2!)^2} \right]^{1/2}. \quad (40)$$

The remaining quantities appearing in Eq. (38) are defined as:

$$\Phi_{p_r, v\tau}^{kl_1}(\lambda) = (a_\tau^\lambda b_\tau^\lambda) {}_3F_2(-k_\lambda/2, -k_\lambda/2 + 1/2, 1 - i\gamma_1; k + l_1^f + 1, -p_\lambda - l_1^f; 1/A_\tau), \quad (41)$$

$$a_\tau^\lambda = \Gamma(1 + i\xi) (l_1^f + 1)_{p_\lambda} \frac{(2D_\tau)^{p_\lambda} \mathcal{F}_\tau}{(\Delta_\tau^2 + Q_\tau^2)^{l_1^f}}, \quad b_\tau^\lambda = \frac{(1 + i\xi)_{l_1} (-i\xi)_{l_2} (-p_\lambda)_k (i\gamma_2)_k (-1)^k C_\tau^k}{B_\tau^2 (l_1^f + 1)_k k!}, \quad (42)$$

$${}_3F_2(-k_\lambda/2, -k_\lambda/2 + 1/2, 1 - i\gamma_1; k + l_1^f + 1, -p_\lambda - l_1^f; 1/A_\tau) = \sum_{u=0}^{[k_\lambda/2]} \frac{(-k_\lambda/2)_u (-k_\lambda/2 + 1/2)_u (1 - i\gamma_1)_u}{(k + l_1^f + 1)_u (-p_\lambda - l_1^f)_u u!} \left(\frac{1}{A_\tau} \right)^u, \quad (43)$$

$$A_\tau = \frac{\Delta_\tau^2}{\Delta_\tau^2 + Q_\tau^2}, \quad B_\tau = \frac{2(v\Delta_\tau - i\vec{Q}_\tau \cdot \vec{v})}{\Delta_\tau^2 + Q_\tau^2}, \quad C_\tau = \frac{v}{B_\tau \Delta_\tau} - 1, \quad (44)$$

$$D_\tau = \frac{A_\tau}{\Delta_\tau}, \quad \mathcal{F}_\tau = \frac{B_\tau^{\xi}}{\Delta_\tau^2 + Q_\tau^2}, \tag{45}$$

$$k_\lambda = p_\lambda - k, \quad l_1 + l_2 = l_1^f, \quad \gamma_1 = -\xi + il_1, \quad \gamma_2 = -\xi - il_2. \tag{46}$$

In Eq. (43), function ${}_3F_2$ denotes the Clausen generalized hypergeometric polynomial [44] and symbol $[k_\lambda/2]$ is the largest integer contained in fraction $k_\lambda/2$. Hence, the dynamic correlation term is reduced to the following four-dimensional integral:

$$J_{r_{12}}^{(k,l)} = \frac{D_{l_1^f}^{(k,l)}}{\pi^4} \sum_{p=0}^{n_r} \frac{c_p}{2^n(n-2)!} \sum_{l_1^f=0}^{l_1^f} \sum_{m_1^f=-l_1^f}^{l_1^f} \sum_{l_2^f=|m_2^f|}^{l_2^f} (l_1^f m_1^f | l_1^f m_1^f) \Omega(l_{1s}^f, \vec{v}) (-1)^{l_1^f} 2^{l_2^f} \mathcal{M}_{12}^{(v,l_1^f)}, \tag{47}$$

$$\mathcal{M}_{12}^{(v,l_1^f)} = \frac{(2n_p)!}{n_p!} \sum_{p_r=0}^{n_p} \frac{(-n_p)_{p_r}}{(-2n_p)_{p_r}} \frac{2^{p_r-n_p}}{p_r!} \int_0^1 dt t^{n-2} (1-t)^{l_2^f+1} \mathcal{H}_{12}, \tag{48}$$

$$\mathcal{H}_{12} = \int_0^\infty \int_0^\pi \int_0^{2\pi} \frac{\sin \theta_\tau d\tau d\theta_\tau d\phi_\tau}{\Delta_\tau^{2n-2l_1^f-p_r-1} [\tau^2 + (Z_T + \alpha_l)^2]^2} G_{v,-m_1^f}^{(1,\Delta_\tau)}(\vec{Q}_\tau) \mathcal{Y}_{l_{1s}^f, -m_2^f}([1-t]\vec{\tau}). \tag{49}$$

Applying a similar procedure, the auxiliary integral $\mathcal{G}_{k,p}^{(0,1)}$ from Eq. (18) can be reduced to a real one-dimensional integral. As such, quantity $J_{x_1}^{(k,l)}$ from Eq. (7) becomes:

$$J_{x_1}^{(k,l)} = \frac{D_{l_1^f}^{(k,l)}}{\pi^2 \alpha_k (Z_T + \alpha_l)^4} \sum_{p=0}^{n_r} \frac{c_p}{2^{n-1}(n-2)!} \sum_{l_1^f=|m_1^f|}^{l_1^f} (-1)^{l_1^f} 2^{l_1^f} \Omega(l_1^f, \vec{v}) \mathcal{M}_{x_1}^{(v_1,l_1^f)}, \tag{50}$$

$$\mathcal{M}_{x_1}^{(v_1,l_1^f)} = \frac{(2n_p-2)!}{(n_p-1)!} \sum_{p_r=0}^{n_p-1} \frac{(1-n_p)_{p_r}}{(2-2n_p)_{p_r}} \frac{2^{p_r-n_p+1}}{p_r!} \int_0^1 dt \frac{t^{n-2} (1-t)^{l_2^f}}{\Delta^{2(n-1)-2l_1^f-p_r-1}} G_{v_1,-m^f}^{(1,\Delta)}(\vec{Q}), \tag{51}$$

$$\Delta^2 = v^2 t(1-t) + a_f^2 t + \alpha_k^2 (1-t), \quad v_1 = n-1-l_1^f. \tag{52}$$

Quantity $G_{v_1,-m^f}^{(1,\Delta)}(\vec{Q})$ is defined by Eq. (38) except that all the subsequent expressions should use $\{\Delta, \vec{Q}, \vec{\tau} = \vec{0}, v_1, m^f\}$ instead of $\{\Delta_\tau, \vec{Q}_\tau, \vec{\tau}, v, m_1^f\}$.

The remaining integrals $J_R^{(k,l)}$ and $J_{s_2}^{(k,l)}$ from Eq. (7) have previously been calculated in the prior version of the CB1-4B method [25] and the results are:

$$J_R^{(k,l)} = \frac{2D_{l_1^f}^{(k,l)}}{\pi^2 (Z_T + \alpha_l)^4} \sum_{p=0}^{n_r} \frac{c_p}{2^n(n-2)!} \sum_{l_1^f=|m_1^f|}^{l_1^f} (-1)^{l_1^f} 2^{l_1^f} \Omega(l_1^f, \vec{v}) \mathcal{M}_R^{(v,l_1^f)}, \tag{53}$$

$$J_{s_2}^{(k,l)} = \frac{D_{l_1^f}^{(k,l)}}{2\pi^2} \sum_{p=0}^{n_r} \frac{c_p}{2^n(n-2)!} \sum_{l_1^f=|m_1^f|}^{l_1^f} (-1)^{l_1^f} 2^{l_1^f} \Omega(l_1^f, \vec{v}) \mathcal{M}_{s_2}^{(v,l_1^f)}, \tag{54}$$

$$\mathcal{M}_R^{(v,l_1^f)} = \frac{(2n_p)!}{n_p!} \sum_{p_r=0}^{n_p} \frac{(-n_p)_{p_r}}{(-2n_p)_{p_r}} \frac{2^{p_r-n_p}}{p_r!} \int_0^1 dt \frac{t^{n-2} (1-t)^{l_2^f+1}}{\Delta^{2n-2l_1^f-p_r-1}} G_{v,-m^f}^{(0,\Delta)}(\vec{Q}), \tag{55}$$

$$\mathcal{M}_{s_2}^{(v,l_1^f)} = \frac{(2n_p)!}{n_p!} \sum_{p_r=0}^{n_p} \frac{(-n_p)_{p_r}}{(-2n_p)_{p_r}} \frac{2^{p_r-n_p}}{p_r!} \int_0^1 dt_1 \frac{(1-t_1)}{\Delta_1^3} \int_0^1 dt \frac{t^{n-2} (1-t)^{l_2^f+1}}{\Delta^{2n-2l_1^f-p_r-1}} [G_{v,-m^f}^{(1,\Delta_2)}(\vec{Q}) + \Delta_1 G_{v,-m^f}^{(2,\Delta_2)}(\vec{Q})], \tag{56}$$

where $\Delta_2 = \Delta + \Delta_1$. Thus, the final expression for the transition amplitude is given by:

$$\begin{aligned} T_{if}^+(\vec{\eta}) &= \sum_{k,l} \sum_{p=0}^{n_r} \mathcal{N}_{k,l} \frac{c_p}{2^n(n-2)!} \left\{ \sum_{l_1^f=|m_1^f|}^{l_1^f} (-1)^{l_1^f} 2^{l_1^f} \frac{\Omega(l_1^f, \vec{v})}{(Z_T + \alpha_l)^4} \right. \\ &\times \left[Z_p \left(2\mathcal{M}_R^{(v,l_1^f)} - \frac{(Z_T + \alpha_l)^4}{2} \mathcal{M}_{s_2}^{(v,l_1^f)} \right) + 2(Z_T - 1) \left(\mathcal{M}_R^{(v,l_1^f)} - \frac{1}{\alpha_k} \mathcal{M}_{x_1}^{(v_1,l_1^f)} \right) - \frac{2}{\alpha_k} \mathcal{M}_{x_1}^{(v_1,l_1^f)} \right] \\ &\left. + \frac{1}{\pi^2} \sum_{l_1^f=0}^{l_1^f} \sum_{m_1^f=-l_1^f}^{l_1^f} \sum_{l_2^f=|m_2^f|}^{l_2^f} (l_1^f m_1^f | l_1^f m_1^f) (-1)^{l_1^f} 2^{l_1^f} \Omega(l_{1s}^f, \vec{v}) \mathcal{M}_{12}^{(v,l_1^f)} \right\}, \quad \mathcal{N}_{k,l} = \frac{N_{k,l} D_{l_1^f}^{(k,l)}}{\pi^2}. \end{aligned} \tag{57}$$

This completes the calculation of the transition amplitude T_{if}^{\pm} in terms of the five-dimensional integral over real variables $t, t_1, \tau, \theta_{\tau}$, and ϕ_{τ} . The entire dependence of the transition amplitude $T_{if}^{\pm}(\vec{\eta}) \equiv T_{if}^{\pm}(\eta, \phi_{\eta})$ upon the azimuthal angle ϕ_{η} is contained in the single phase factor $\exp(-im^f \phi_{\eta})$. Therefore, in order to obtain the total cross sections, the integration over ϕ_{η} can be carried out analytically, so that:

$$Q_{if}^{\pm}(\pi a_0^2) = \frac{1}{2\pi^2 v^2} \int_0^{\infty} d\eta \eta |T_{if}^{\pm}(\eta, 0)|^2. \quad (58)$$

The remaining integrations over $\eta, t, t_1, \tau, \theta_{\tau}$, and ϕ_{τ} are carried out by numerical quadratures. Except for the integration over $\phi_{\tau} \in [0, 2\pi]$ for which the Gauss-Mehler (GM) quadrature is employed, the Gauss-Legendre (GL) quadrature is applied to the other integrations, after the following change of variables $\tau = (1+x)/(1-x), x \in [-1, +1], \cos \theta_{\tau} = u, u \in [-1, +1], \eta = \sqrt{2(1+y)/(1-y)}$, and $y \in [-1, +1]$. The change of variable in η is the most important, since it concentrates the integration points near the forward cone [16], which gives the dominant contributions due to the eikonal nature of scattering for heavy projectiles. This can be seen by writing $\cos \theta = 1 - (\mu v)^{-2}(1+y)/(1-y)$, where the scattering angle θ is linked to η via $\eta = 2\mu v \sin(\theta/2)$ and μ is the reduced mass of the incident and target nuclei. The singularities at $x = 1$ and $y = 1$ are only superficial, as they disappear altogether after factoring out all the powers of $1-x$ and $1-y$.

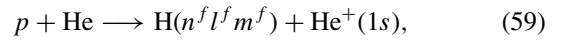
In the present computations, the orders of the GM and GL quadratures, i.e., the numbers N_{GM} and N_{GL} of integration points are varied until convergence to two decimal places has been attained for state-selective and total cross sections. In practice, only $N_{GM} \leq 20$ for the ϕ_{τ} integrals and $N_{GL} \leq 80$ for each of the remaining $t, t_1, \tau, \theta_{\tau}$, and η quadratures proved to be sufficient for the sought accuracy of two decimal places.

From the numerical point of view, it is more convenient to use the prior form of the CB1-4B method for different applications. The prior transition amplitude T_{if}^{-} has recently been derived [25] in terms of a two-dimensional numerical quadrature over real variables, whereas the post transition amplitude T_{if}^{+} , as presently reported, is reduced to integrals over five real variables. Nevertheless, these latter integrals are still advantageous with respect to, e.g., the work of Madison *et al.* [45–49] who computed some extremely time consuming nine-dimensional numerical quadratures for single charge exchange in proton-helium collisions.

III. RESULTS AND DISCUSSIONS

In the present work, we shall use the four-parameter wave function of Löwdin [50] for the ground state of the helium target $\text{He}(1s^2)$. It is given by $\varphi_i(\vec{x}_1, \vec{x}_2) = N(a_1 e^{-b_1 x_1} + a_2 e^{-b_2 x_1})(a_1 e^{-b_1 x_2} + a_2 e^{-b_2 x_2})$, where $a_1 = 2.7626$, $a_2 = 1.9104$, $b_1 = 1.4287$, $b_2 = 2.7022$ with the binding energy $E_i = -2.861525$. The normalization constant N is $\pi N = \{a_1^2/b_1^3 + a_2^2/b_2^3 + 16a_1/(b_1 + b_2)^3\}^{-1}$. The presented algorithm is general, in the sense that it can be applied to both heteronuclear and homonuclear single charge exchanges of type (1). As an illustration, numerical computations are performed for proton-helium charge

exchange:



where symbol Σ denotes the formation of atomic hydrogen $\text{H}(\Sigma)$ in any state. The results of our computations of the state-selective cross sections for atomic hydrogen formation as $\text{H}(2s), \text{H}(2p), \text{H}(3s), \text{H}(3p), \text{H}(3d)$, and $\text{H}(4s)$ are summarized in Tables I–V and Figs. 1–8 at impact energies 20–10 000 keV. In Figs. 1–3, the full curves represent the state-selective cross sections that are obtained with the full perturbation V_f in the T_{if}^{\pm} from (2) as:

$$\begin{aligned} V_f &= \Delta V_{P2} + \Delta V_{T1} + \Delta V_{12}, \quad \Delta V_{12} = V_{12} - V_{12}^{\infty}, \\ V_{12} &= \frac{1}{r_{12}}, \quad V_{12}^{\infty} = \frac{1}{x_1} \\ \Delta V_{P2} &= Z_P \left(\frac{1}{R} - \frac{1}{s_2} \right), \quad \Delta V_{T1} = (Z_T - 1) \left(\frac{1}{R} - \frac{1}{x_1} \right). \end{aligned} \quad (61)$$

The effect of the dynamic electron correlations is explicitly included through $1/r_{12}$ in V_f . For capture into $n^f = 4$, the experimental data [57,59,61] are available only for formation of the $\text{H}(4s)$ state, and a comparison with these measurements is made in Fig. 3. It can be seen from Figs. 1–3 that the obtained theoretical results for formation of $\text{H}(2s), \text{H}(3s)$, and $\text{H}(4s)$ are presently found to be in excellent agreement with the measurements at all impact energies above 60 keV. The cross sections for electron capture into the $2p$ and $3p$ states of atomic hydrogen are compared with the available experimental data in Figs. 1 and 2, respectively. These comparisons show that the theoretical curves slightly overestimate the measurements especially at lower impact energies, whereas at higher energies the CB1-4B method converges towards the experimental data. Such an outcome is anticipated since this is a high-energy method, which is expected to agree better with experiments at larger impact energies. A comparison of the CB1-4B method with the measurements for capture into the $3d$ state of H is made in Fig. 2. Therein, it is found that the theoretical curve overestimates the experimental data at lower impact energies, but at higher energies the CB1-4B method predicts very well the corresponding findings from the measurements.

Total cross sections $Q^{\pm}(\Sigma)$ for electron capture into all the final states of H via formation of $\text{H}(\Sigma)$ are obtained by applying the Oppenheimer $(n^f)^{-3}$ scaling law via:

$$Q^{\pm}(\Sigma) = Q_{1s}^{\pm} + Q_{2s}^{\pm} + Q_{2p}^{\pm} + 2.081(Q_{3s}^{\pm} + Q_{3p}^{\pm} + Q_{3d}^{\pm}). \quad (62)$$

This is justified because the contributions from the higher excited states are found to be negligible. The total cross sections for the p -He collisions in the energy range 20–10000 keV are plotted in Fig. 4. Here, the obtained results of the CB1-4B method are seen to be in excellent agreement with all the available measurements at a very wide interval of impact energies where the cross sections vary within ten orders of magnitude.

Potential ΔV_{12} in the complete perturbation V_f from (61) represents a source of the dynamic electron correlation effect. Specifically, interaction ΔV_{12} is the difference between the finite (V_{12}) and asymptotic (V_{12}^{∞}) values of

TABLE I. Present total cross sections (in units of cm^2) as a function of laboratory impact energy E (keV) for electron capture by protons from $\text{He}(1s^2)$ in process (59). The post form of the CB1-4B method is applied with the complete perturbation potential V_f by using the helium ground-state wave functions of Löwdin [50]. The row labeled “Total” represents the cross sections summed over the bound states of the captured electron $\text{H}(n^f l^f m^f)$ by employing (62). Notation $X[-N]$ implies $X \times 10^{-N}$.

$n^f l^f m^f$	E (keV)						
	20	50	100	150	300	500	
100	4.27[-16]	1.05[-16]	2.21[-17]	6.96[-18]	6.33[-19]	7.88[-20]	
200	2.37[-17]	1.06[-17]	2.80[-18]	9.36[-19]	8.70[-20]	1.07[-20]	
210	3.48[-17]	7.73[-18]	1.35[-18]	3.46[-19]	1.89[-20]	1.48[-21]	
211	1.59[-18]	5.40[-19]	1.29[-19]	3.56[-20]	2.02[-21]	1.60[-22]	
2p	3.80[-17]	8.81[-18]	1.61[-18]	4.17[-19]	2.29[-20]	1.80[-21]	
300	5.89[-18]	2.98[-18]	8.26[-19]	2.80[-19]	2.62[-20]	3.21[-21]	
310	1.02[-17]	2.48[-18]	4.60[-19]	1.20[-19]	6.66[-21]	5.24[-22]	
311	4.54[-19]	1.60[-19]	4.17[-20]	1.19[-20]	6.99[-22]	5.58[-23]	
3p	1.11[-17]	2.79[-18]	5.43[-19]	1.44[-19]	8.05[-21]	6.35[-22]	
320	8.04[-19]	1.71[-19]	2.42[-20]	5.11[-21]	1.78[-22]	9.41[-24]	
321	8.94[-20]	2.10[-20]	4.55[-21]	1.09[-21]	4.12[-23]	2.20[-24]	
322	5.39[-21]	1.91[-21]	4.77[-22]	1.14[-22]	4.17[-24]	2.16[-25]	
3d	9.94[-19]	2.17[-19]	3.43[-20]	7.52[-21]	2.69[-22]	1.42[-23]	
Total	5.26[-16]	1.37[-16]	2.94[-17]	9.21[-18]	8.15[-19]	9.93[-20]	
$n^f l^f m^f$	750	1000	1500	3000	5000	7500	10000
100	1.29[-20]	3.32[-21]	4.50[-22]	1.23[-23]	7.71[-25]	8.06[-26]	1.58[-26]
200	1.72[-21]	4.37[-22]	5.86[-23]	1.58[-24]	9.79[-26]	1.02[-26]	2.01[-27]
210	1.62[-22]	3.09[-23]	2.71[-24]	3.49[-26]	1.25[-27]	8.51[-29]	1.23[-29]
211	1.76[-23]	3.39[-24]	3.03[-25]	3.98[-27]	1.44[-28]	9.78[-30]	1.41[-30]
2p	1.97[-22]	3.77[-23]	3.32[-24]	4.28[-26]	1.54[-27]	1.05[-28]	1.52[-29]
300	5.15[-22]	1.31[-22]	1.75[-23]	4.64[-25]	2.85[-26]	3.02[-27]	6.11[-28]
310	5.72[-23]	1.09[-23]	9.59[-25]	1.23[-26]	4.43[-28]	3.01[-29]	4.36[-30]
311	6.18[-24]	1.19[-24]	1.07[-25]	1.40[-27]	5.11[-29]	3.47[-30]	5.01[-31]
3p	6.96[-23]	1.33[-23]	1.17[-24]	1.51[-26]	5.45[-28]	3.70[-29]	5.36[-30]
320	7.30[-25]	1.08[-25]	6.47[-27]	4.14[-29]	8.75[-31]	3.87[-32]	4.15[-33]
321	1.71[-25]	2.53[-26]	1.53[-27]	9.99[-30]	2.15[-31]	9.59[-33]	1.03[-33]
322	1.64[-26]	2.38[-27]	1.41[-28]	8.88[-31]	1.87[-32]	8.22[-34]	8.76[-35]
3d	1.10[-24]	1.63[-25]	9.81[-27]	6.32[-29]	1.34[-30]	5.95[-32]	6.39[-33]
Total	1.60[-20]	4.09[-21]	5.51[-22]	1.49[-23]	9.31[-25]	9.72[-26]	1.91[-26]

the same e_1 - e_2 potential $1/r_{12}$. The residual potential $1/x_1$ is the limiting value of $1/r_{12}$ at infinitely large x_1 and finite x_2 ($V_{12}^\infty = \{V_{12}\}_{x_1 \gg x_2} \approx 1/x_1$). Such a circumstance implies that potential ΔV_{12} is a *short-range* interaction. This can be made more explicit by using relation $r_{12} = |\vec{x}_1 - \vec{x}_2|$ to develop $1/x_1 = 1/|\vec{r}_{12} - \vec{x}_2|$ in a power series around \vec{x}_2 according to $1/x_1 = 1/|\vec{r}_{12} - \vec{x}_2| = 1/r_{12} - \hat{r}_{12} \cdot \vec{x}_2/r_{12}^2 + \dots$ ($\hat{r}_{12} = \vec{r}_{12}/r_{12}$). Thus, $\Delta V_{12} = 1/r_{12} - 1/x_1 = \gamma/r_{12}^2 + \dots$ ($\gamma = \hat{r}_{12} \cdot \vec{x}_2$), where the asymptotic tail γ/r_{12}^2 of ΔV_{12} is of a short range. This series development is justified by the small value of coordinate x_2 (which is of the order of Bohr radius a_0), since electron e_2 always remains bound in the target in process (1). A modulation of V_{12} by way of V_{12}^∞ within ΔV_{12} is a type of screening of the long-range Coulomb interaction $V_{12} = 1/r_{12}$. Due to such a screening effect, which is responsible for a short range of the combined potential $1/r_{12} - 1/x_1$, the overall relative importance of the role of dynamic correlations via ΔV_{12} can be quantitatively different from the customary expectations when only $1/r_{12}$ is considered. For example, an increase of the impact energy would decrease the collision time and this, in turn, would

weaken all the perturbation interactions, including $1/r_{12}$ in V_f . However, what matters in T_{if}^+ , where transition $i \rightarrow f$ is directly mediated by V_f , is not so much the specific trend and strength of each individual interaction in the final perturbation, be it the interelectronic potential or otherwise. Rather, what counts, in the end, is the overall balance of every participating interaction. This is dictated by the content of the complete perturbation V_f , which includes both attractive and repulsive potentials whose action can lead to constructive as well as destructive interference in T_{if}^+ . The purpose of grouping the individual Coulomb potentials from V_f into three short-range interactions ΔV_{12} , ΔV_{T1} , and ΔV_{P2} according to (61) is to evaluate the relative importance of these potentials, none of which can produce any distortion of the final unperturbed state in the exit channel. This permits switching on and off one or two interactions from the set $\{\Delta V_{12}, \Delta V_{T1}, \Delta V_{P2}\}$ in V_f while still fulfilling the requirement of the so-called asymptotic freedom [1]. According to this crucial principle, an adequate collision theory must deal only with the unperturbed states in the asymptotic regions because they are the only ones that are experimentally accessible in scattering experiments.

TABLE II. Present total cross sections (in units of cm^2) as a function of laboratory impact energy E (keV) for electron capture by protons from $\text{He}(1s^2)$ in process (59). The post form of the CB1-4B method is applied without ΔV_{12} in V_f by using the helium ground-state wave functions of Löwdin [50]. The row labeled “Total” represents the cross sections summed over the bound states of the captured electron $H(n^f l^f m^f)$ by employing (62). Notation $X[-N]$ implies $X \times 10^{-N}$.

$n^f l^f m^f$	E (keV)						
	20	50	100	150	300	500	
100	3.87[-16]	8.34[-17]	1.62[-17]	4.90[-18]	4.07[-19]	4.64[-20]	
200	2.31[-17]	8.30[-18]	2.04[-18]	6.56[-19]	5.62[-20]	6.35[-21]	
210	4.30[-17]	8.46[-18]	1.27[-18]	3.05[-19]	1.53[-20]	1.15[-21]	
211	2.05[-18]	3.90[-19]	7.14[-20]	1.80[-20]	8.70[-22]	5.97[-23]	
2p	4.71[-17]	9.24[-18]	1.42[-18]	3.41[-19]	1.70[-20]	1.27[-21]	
300	5.88[-18]	2.32[-18]	6.01[-19]	1.96[-19]	1.70[-20]	1.91[-21]	
310	1.26[-17]	2.75[-18]	4.38[-19]	1.07[-19]	5.43[-21]	4.09[-22]	
311	5.99[-19]	1.20[-19]	2.33[-20]	6.05[-21]	3.02[-22]	2.09[-23]	
3p	1.38[-17]	2.99[-18]	4.85[-19]	1.19[-19]	6.04[-21]	4.51[-22]	
320	9.93[-19]	1.98[-19]	2.31[-20]	4.43[-21]	1.39[-22]	7.10[-24]	
321	1.23[-19]	1.91[-20]	2.68[-21]	5.66[-22]	1.82[-23]	8.62[-25]	
322	7.80[-21]	1.27[-21]	2.25[-22]	4.95[-23]	1.56[-24]	7.06[-26]	
3d	1.25[-18]	2.39[-19]	2.89[-20]	5.66[-21]	1.79[-22]	8.97[-24]	
Total	5.01[-16]	1.12[-16]	2.20[-17]	6.57[-18]	5.29[-19]	5.90[-20]	
$n^f l^f m^f$	750	1000	1500	3000	5000	7500	10000
100	6.91[-21]	1.65[-21]	1.97[-22]	4.24[-24]	2.25[-25]	2.11[-26]	3.89[-27]
200	9.32[-22]	2.19[-22]	2.58[-23]	5.45[-25]	2.85[-26]	2.63[-27]	4.78[-28]
210	1.22[-22]	2.26[-23]	1.89[-24]	2.14[-26]	6.85[-28]	4.24[-29]	5.80[-30]
211	5.78[-24]	1.01[-24]	7.79[-26]	8.14[-28]	2.59[-29]	1.64[-30]	2.29[-31]
2p	1.33[-22]	2.46[-23]	2.04[-24]	2.30[-26]	7.37[-28]	4.57[-29]	6.26[-30]
300	2.80[-22]	6.58[-23]	7.77[-24]	1.69[-25]	9.03[-27]	7.91[-28]	1.34[-28]
310	4.33[-23]	8.02[-24]	6.69[-25]	7.54[-27]	2.38[-28]	1.44[-29]	1.94[-30]
311	2.03[-24]	3.55[-25]	2.74[-26]	2.86[-28]	9.09[-30]	5.76[-31]	8.07[-32]
3p	4.73[-23]	8.73[-24]	7.24[-25]	8.11[-27]	2.57[-28]	1.56[-29]	2.10[-30]
320	5.46[-25]	8.04[-26]	4.81[-27]	3.01[-29]	6.10[-31]	2.59[-32]	2.72[-33]
321	6.07[-26]	8.36[-27]	4.57[-28]	2.53[-30]	4.87[-32]	2.05[-33]	2.14[-34]
322	4.73[-27]	6.28[-28]	3.25[-29]	1.68[-31]	3.15[-33]	1.31[-34]	1.36[-35]
3d	6.77[-25]	9.84[-26]	5.79[-27]	3.55[-29]	7.13[-31]	3.03[-32]	3.18[-33]
Total	8.66[-21]	2.05[-21]	2.43[-22]	5.18[-24]	2.74[-25]	2.54[-26]	4.66[-27]

In the T matrix element (2), potential ΔV_{12} plays the role of a perturbation, which can cause capture of electron e_1 . In other words, the correlation potential ΔV_{12} can lead to single capture as a separate and competitive mechanism to the remaining interactions ΔV_{T1} and ΔV_{P2} that do not directly invoke the e_1 - e_2 repulsion. In principle, these separate pathways are indistinguishable and should be added coherently, since they can produce the same final state. The importance of the screened dynamic correlations is presently assessed in the transition amplitude T_{if}^+ from (2) by either including or excluding ΔV_{12} in V_f , as shown in Tables I and II, respectively, for the post version of the CB1-4B method. The cross sections without the correlation term ΔV_{12} are also displayed in Figs. 1–3 by the dashed curves for the state-selective cross sections, as well as in Fig. 4 for the total cross sections. The extent to which the screened dynamic electron correlation ΔV_{12} might influence the entire process can at once be seen on Figs. 1–4. Therein, it follows that above 100 keV, where the CB1-4B model is expected to be valid, the discrepancy between the results with the complete perturbation V_f (solid curves) and the corresponding cross sections without ΔV_{12}

(dashed curves) is seen as being large. These discrepancies increase even further with augmentation of the incident energy. Such a pattern indicates that the role of the screened dynamic correlations ΔV_{12} becomes more prominent at higher incident energies.

Table III shows the corresponding cross sections for the prior version of the CB1-4B method with the full perturbation V_i , which does not include directly the electron-electron correlations. Nevertheless, V_i from T_{if}^- is not entirely free from electronic correlations. Quite the contrary, an alternative mechanism of electronic correlations mediated by potential $-Z_P/s_2$ is also present in V_i , which is given by $V_i = Z_P(2/R - 1/s_1 - 1/s_2)$. In analogy with V_f , the complete short-range potential V_i can be expressed as the sum of two short-range interactions via $V_i = \Delta V_{P1} + \Delta V_{P2}$ where $\Delta V_{P1} = Z_P(1/R - 1/s_1)$ and ΔV_{P2} is the same as in V_f , i.e., $\Delta V_{P2} = Z_P(1/R - 1/s_2)$. Regarding the interactions involving one or both electrons, within the description by means of T_{if}^- , electron e_1 can be captured through either Z_P - e_1 or Z_P - e_2 potentials $-Z_P/s_1$ or $-Z_P/s_2$, respectively. Both captures are associated with the kinematical, i.e., the

TABLE III. Present total cross sections (in units of cm^2) as a function of laboratory impact energy E (keV) for electron capture by protons from $\text{He}(1s^2)$ in process (59). The prior form of the CB1-4B method is applied with the complete perturbation potential $V_i = Z_p(2/R - 1/s_1 - 1/s_2)$ where $Z_p = 1$ by using the helium ground-state wave functions of Löwdin [50]. The row labeled “Total” represents the cross sections summed over the bound states of the captured electron $\text{H}(n^f l^f m^f)$ by employing (62). Notation $X[-N]$ implies $X \times 10^{-N}$.

$n^f l^f m^f$	E (keV)					
	20	50	100	150	300	500
100	3.95[-16]	9.77[-17]	2.11[-17]	6.79[-18]	6.42[-19]	8.20[-20]
200	2.24[-17]	9.69[-18]	2.63[-18]	9.02[-19]	8.78[-20]	1.11[-20]
210	3.54[-17]	7.52[-18]	1.30[-18]	3.35[-19]	1.89[-20]	1.51[-21]
211	1.57[-18]	5.08[-19]	1.26[-19]	3.60[-20]	2.14[-21]	1.73[-22]
2p	3.85[-17]	8.53[-18]	1.55[-18]	4.07[-19]	2.31[-20]	1.86[-21]
300	5.60[-18]	2.72[-18]	7.76[-19]	2.70[-19]	2.65[-20]	3.34[-21]
310	1.03[-17]	2.41[-18]	4.41[-19]	1.17[-19]	6.66[-21]	5.36[-22]
311	4.49[-19]	1.51[-19]	4.09[-20]	1.21[-20]	7.42[-22]	6.05[-23]
3p	1.12[-17]	2.72[-18]	5.23[-19]	1.41[-19]	8.15[-21]	6.57[-22]
320	8.28[-19]	1.71[-19]	2.32[-20]	4.92[-21]	1.77[-22]	9.53[-24]
321	9.01[-20]	1.97[-20]	4.36[-21]	1.08[-21]	4.32[-23]	2.37[-24]
322	5.33[-21]	1.75[-21]	4.57[-22]	1.13[-22]	4.32[-24]	2.29[-25]
3d	1.02[-18]	2.14[-19]	3.29[-20]	7.32[-21]	2.72[-22]	1.47[-23]
Total	4.93[-16]	1.28[-16]	2.80[-17]	8.97[-18]	8.26[-19]	1.03[-19]

$n^f l^f m^f$	E (keV)						
	750	1000	1500	3000	5000	7500	10000
100	1.36[-20]	3.50[-21]	4.70[-22]	1.24[-23]	7.48[-25]	7.67[-26]	1.49[-26]
200	1.81[-21]	4.61[-22]	6.12[-23]	1.58[-24]	9.49[-26]	9.69[-27]	1.89[-27]
210	1.68[-22]	3.21[-23]	2.81[-24]	3.51[-26]	1.23[-27]	8.18[-29]	1.18[-29]
211	1.91[-23]	3.66[-24]	3.20[-25]	3.99[-27]	1.40[-28]	9.30[-30]	1.34[-30]
2p	2.06[-22]	3.95[-23]	3.45[-24]	4.31[-26]	1.51[-27]	1.00[-28]	1.44[-29]
300	5.42[-22]	1.38[-22]	1.83[-23]	4.68[-25]	2.78[-26]	2.83[-27]	5.54[-28]
310	5.93[-23]	1.14[-23]	9.94[-25]	1.24[-26]	4.33[-28]	2.89[-29]	4.15[-30]
311	6.71[-24]	1.29[-24]	1.12[-25]	1.40[-27]	4.93[-29]	3.30[-30]	4.74[-31]
3p	7.28[-23]	1.39[-23]	1.22[-24]	1.52[-26]	5.31[-28]	3.55[-29]	5.10[-30]
320	7.48[-25]	1.11[-25]	6.64[-27]	4.16[-29]	8.60[-31]	3.76[-32]	4.00[-33]
321	1.86[-25]	2.73[-26]	1.62[-27]	1.01[-29]	2.09[-31]	9.18[-33]	9.80[-34]
322	1.74[-26]	2.52[-27]	1.46[-28]	8.82[-31]	1.80[-32]	7.84[-34]	8.31[-35]
3d	1.15[-24]	1.71[-25]	1.02[-26]	6.35[-29]	1.31[-30]	5.75[-32]	6.12[-33]
Total	1.69[-20]	4.32[-21]	5.75[-22]	1.50[-23]	9.03[-25]	9.24[-26]	1.80[-26]

velocity matching mechanism. The former proceeds through the direct Z_p-e_1 interaction, which is typical of the well-known

TABLE IV. Present state-selective cross sections (in units of cm^2) for electron capture into the $4s$ state of H by protons from $\text{He}(1s^2)$ in process (59) obtained by using the helium ground-state wave functions of Löwdin [50]. Quantities Q_{4s}^+ and $Q_{4s}^{+(0)}$ refer to the cross sections in the post version of the CB1-4B method with and without ΔV_{12} , respectively. Similarly, Q_{4s}^- denotes the cross section in the prior variant of the CB1-4B method. Notation $X[-N]$ implies $X \times 10^{-N}$.

E (keV)	Q_{4s}^+	$Q_{4s}^{+(0)}$	Q_{4s}^-
20	2.34[-18]	2.36[-18]	2.23[-18]
50	1.23[-18]	9.61[-19]	1.13[-18]
100	3.48[-19]	2.53[-19]	3.27[-19]
150	1.19[-19]	8.31[-20]	1.14[-19]
300	1.11[-20]	7.19[-21]	1.12[-20]
500	1.36[-21]	8.07[-22]	1.42[-21]
750	2.19[-22]	1.16[-22]	2.30[-22]
1000	5.57[-23]	2.67[-23]	5.86[-23]

first-order Oppenheimer-Brinkman-Kramers approximation. By contrast, the latter is initially associated with the collision of Z_p with e_2 , but subsequently e_2 manages, through correlations

TABLE V. Relative contributions from ΔV_{12} for different nl states for process (59). This is quantified via the weighted difference $\chi = |Q_{nl}^+ - Q_{nl}^{+(0)}|/Q_{nl}^+$, where Q_{nl}^+ and $Q_{nl}^{+(0)}$ are the present cross sections for capture into the nl state with and without ΔV_{12} , respectively, obtained by using the helium ground-state wave functions of Löwdin [50].

nl	E (keV)				
	100	500	1000	5000	10000
1s	26.70%	41.12%	50.30%	70.82%	75.38%
2s	27.14%	40.65%	49.89%	70.89%	76.22%
3s	27.24%	40.50%	49.77%	68.32%	78.07%
4s	27.30%	40.66%	52.06%	64.32%	73.55%
2p	11.80%	29.44%	34.75%	52.14%	58.82%
3p	10.68%	28.98%	34.36%	52.84%	60.82%
3d	15.74%	36.83%	39.63%	46.79%	50.23%

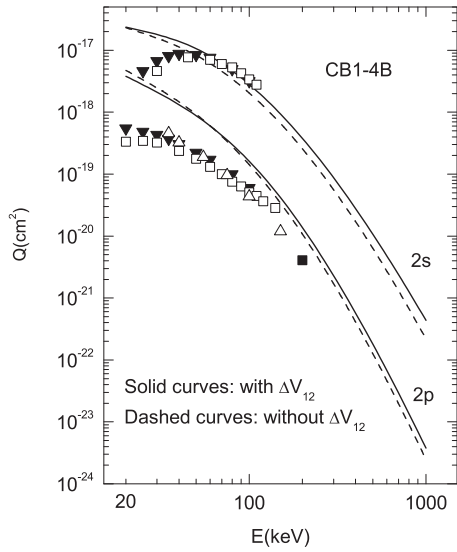


FIG. 1. State-selective cross sections Q_{2s}^+ and Q_{2p}^+ (in units of cm^2) as a function of the laboratory impact energy E (keV) for electron capture by protons from $\text{He}(1s^2)$ in process (59). The solid and dashed curves are the present post cross sections of the CB1-4B method with and without ΔV_{12} in V_f , respectively, obtained by using the helium ground-state wave functions of Löwdin [50]. Experimental data: \blacktriangledown (Q_{2s}, Q_{2p}) Cline *et al.* [51], \square (Q_{2s}, Q_{2p}) Hughes *et al.* [52], \triangle (Q_{2p}) Hippler *et al.* [53], and \blacksquare (Q_{2p}) Hippler *et al.* [54]. Both the theoretical and experimental cross sections for capture into the 2p states of H are divided by 10.

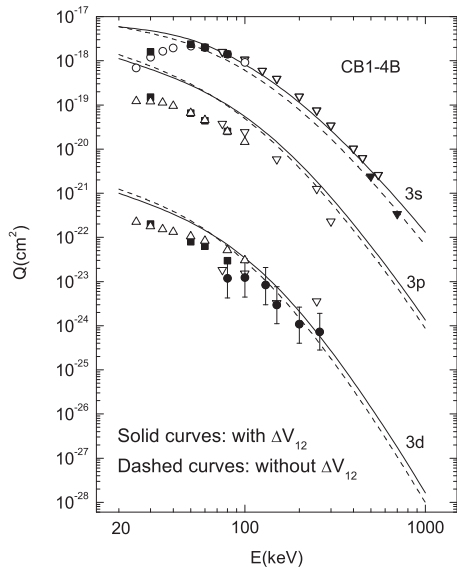


FIG. 2. State-selective cross sections Q_{3s}^+ , Q_{3p}^+ , and Q_{3d}^+ (in units of cm^2) as a function of the laboratory impact energy E (keV) for electron capture by protons from $\text{He}(1s^2)$ in process (59). The solid and dashed curves are the present post cross sections of the CB1-4B method with and without potential ΔV_{12} in V_f , respectively, obtained by using the helium ground-state wave functions of Löwdin [50]. Experimental data: \blacktriangledown (Q_{3s}) Conrads *et al.* [56], \circ (Q_{3s}) Cline *et al.* [51], ∇ (Q_{3s}, Q_{3p}, Q_{3d}) Ford and Thomas [55], \blacksquare (Q_{3s}, Q_{3p}, Q_{3d}) Brower and Pipkin [57], \triangle (Q_{3p}, Q_{3d}) Cline *et al.* [58], and \bullet Edwards and Thomas [60]. Both the theoretical and experimental cross sections for capture into the 3p and 3d states of H are divided by 10 and 1000, respectively.

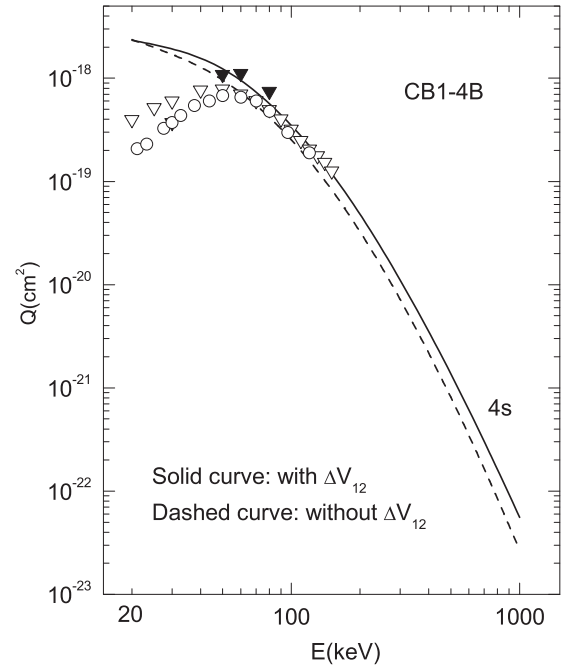


FIG. 3. State-selective cross sections Q_{4s}^+ (in units of cm^2) as a function of the laboratory impact energy E (keV) for electron capture by protons from $\text{He}(1s^2)$ in process (59). The solid and dashed curves are the present post cross sections of the CB1-4B method with and without ΔV_{12} in V_f , respectively, obtained by using the helium ground-state wave functions of Löwdin [50]. Experimental data: ∇ (Q_{4s}) Doughty *et al.* [59], \blacktriangledown (Q_{4s}) Brower and Pipkin [57], and \circ (Q_{4s}) Hughes *et al.* [61].

with e_1 , to transfer the energy received from the projectile to e_1 , which is finally captured by Z_P via the velocity matching mechanism. As stated, potential $-Z_P/s_2$ is also present in V_f from the post form T_{if}^+ of the transition amplitude for process (1). Our computations using T_{if}^- and T_{if}^+ show that the contributions from ΔV_{P2} in these two matrix elements are the same, both in magnitude and the shape of the cross-section curves as a function of impact energy, as it must be. Further, within T_{if}^+ , potentials ΔV_{12} and ΔV_{P2} exhibit a comparable influence onto electron capture at intermediate impact energies 20–200 keV. However, at higher energies above 200 keV, electron capture by way of ΔV_{12} becomes more important than that via ΔV_{P2} . On the other hand, potential ΔV_{12} is dominated by ΔV_{T1} at energies 20–200 keV, but the yield from these two interactions becomes completely comparable above 200 keV and below 1000 keV. Above 1000 keV, the contribution from ΔV_{12} is significantly more important than that from ΔV_{T1} . Overall, relative to both ΔV_{P2} and ΔV_{T1} , potential ΔV_{12} increases its importance with augmentation of the impact energy.

As an illustration, the relative contributions of the correlation term assessed by $\chi = |Q_{nl}^+ - Q_{nl}^{+(0)}|/Q_{nl}^+$ for electron capture into the given nl state at four impact energies are summarized in Table V. Here, Q_{nl}^+ denotes the cross section for capture into the nl state in the case with $\Delta V_{12} \neq 0$, whereas $Q_{nl}^{+(0)}$ refers to the corresponding results with $\Delta V_{12} = 0$ in V_f from the transition amplitude (2). It can be noticed that for the given impact energy and the orbital quantum number

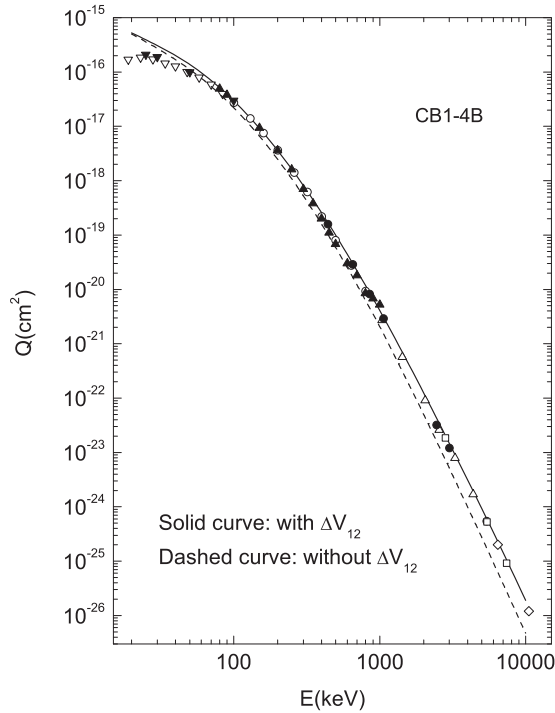


FIG. 4. Total cross sections $Q^+(\Sigma)$ (in units of cm^2) as a function of the laboratory impact energy E (keV) for single capture from the ground state of helium by protons to all states (Σ) of atomic hydrogen $\text{H}(\Sigma)$ in process (60). The solid and the dashed curves are the present cross sections $Q^+(\Sigma)$ from (62) in the post CB1-4B method with and without ΔV_{12} in V_f , respectively, obtained by using the helium ground-state wave functions of Löwdin [50]. Experimental data: ∇ Shah *et al.* [62], \triangle Schryber [63], \circ Shah and Gilbody [64], \square Horsdal-Pedersen *et al.* [65], \diamond Berkner *et al.* [66], \blacktriangle Williams [67], \blacktriangledown Martin *et al.* [68], and \bullet Welsh *et al.* [69].

l , the values for χ are nearly equal for different principal quantum numbers n , especially for lower impact energies. For example, at 100 keV, $\chi \simeq 27\%$ for the $1s, 2s, 3s$, and $4s$ states. As a test of such a trend, we have performed a computation of parameter χ at 100 keV for the $5s$ state, in which case the value $\chi = 26.97\%$ is obtained.

Next, we examine the so-called post-prior discrepancy, which arises from the unequal perturbation potentials ($V_i \neq V_f$) in the transition amplitudes, as well as from the unavailability of the exact bound-state wave function of heliumlike atomic systems. Figure 5 depicts the prior and post total cross sections of the CB1-4B approximation using the same helium wave function of Löwdin [50]. The top pairs of the curves refer to the inclusion of the complete perturbation potentials V_i and V_f . Despite the obvious discrepancy between V_i and V_f , the difference between the results for the post and prior cross sections is very small, as can be seen from Fig. 5. This is an excellent property of the CB1-4B method, since the same physical assumptions are involved in the prior and post forms of this theory. Such a property also holds true for the state-selective cross sections, as can be observed in Figs. 6 and 7, where the post and prior cross sections are plotted for the $2s, 2p$ and $3s, 3p, 3d$ states, respectively. Similar results showing a noticeably weak post-prior discrepancy are also obtained for the $4s$ state, as documented in Table IV. It is

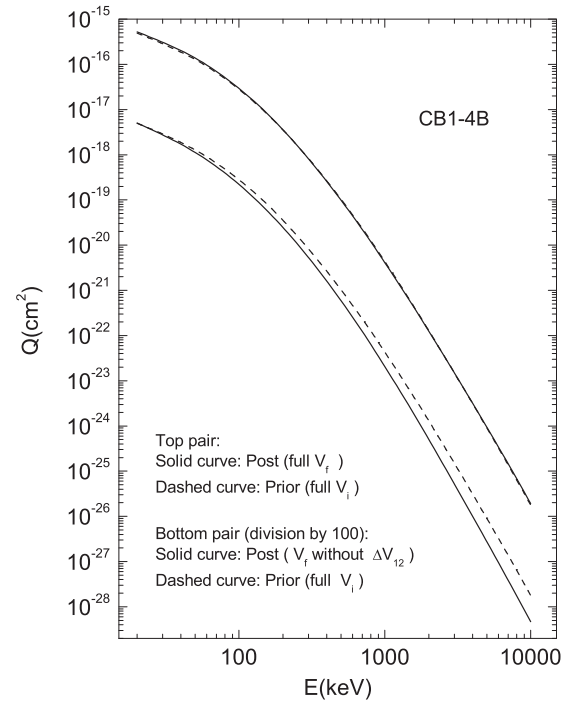


FIG. 5. Total cross sections $Q^\pm(\Sigma)$ (in units of cm^2) as a function of the laboratory impact energy E (keV) for single capture from the ground state of helium by protons in process (60). The pairs of the top and bottom curves are the present post (solid curves) and prior (dashed curves) cross sections $Q^+(\Sigma)$ and $Q^-(\Sigma)$ of the CB1-4B method, obtained by using the helium ground-state wave functions of Löwdin [50]. The prior cross sections in the top and bottom pairs are both with the full perturbation potential V_i . The post cross sections on the top and bottom pairs are with and without ΔV_{12} in V_f , respectively. Both sets of the results for the bottom pair are divided by 100.

important to emphasize that the post-prior discrepancy would persist in the CB1-4B method, if the correlation term $-Z_P/s_2$ is ignored from V_i and V_f and/or if $1/r_{12}$ is neglected in V_f . In other words, all the potentials must be kept throughout, especially including the correlation effects stemming from the direct electron-electron potential ($1/r_{12}$ in T_{if}^+) and indirect electron-electron interaction mediated by way of the projectile ($-Z_P/s_2$ in T_{if}^\pm). Although the difference between the post and prior results with the complete perturbations V_i and V_f is very small, it should be noticed that the two curves are not entirely parallel to each other. This indicates that the post and prior versions of the CB1-4B method exhibit a minor difference in shape for the energy dependence of the cross sections shown in Figs. 6 and 7.

The bottom pairs of the curves in Fig. 5 cast a familiar and quite a different light on the post-prior discrepancy. Here, the prior and post cross sections are divided by 100. The dashed curve is for the full perturbation V_i in the prior version of the results that are, this time, compared with their post counterpart in which, however, the screened dynamic correlation ΔV_{12} is discarded from V_f . A very significant post-prior discrepancy is present with the two bottom curves, in sharp contrast with the corresponding top curves. For charge exchange, precisely this kind of comparison has been the usual practice in the literature for a very long time, when it comes to the alleged detection of

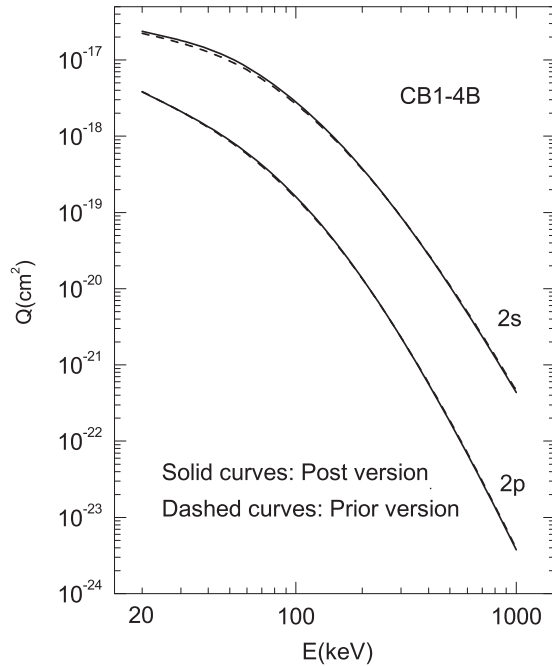


FIG. 6. State-selective cross sections Q_{2s}^{\pm} and Q_{2p}^{\pm} (in units of cm^2) as a function of the laboratory impact energy E (keV) for electron capture by protons from $\text{He}(1s^2)$ in process (59). The solid and dashed curves are the present post $\{Q_{2s}^+, Q_{2p}^+\}$ and prior $\{Q_{2s}^-, Q_{2p}^-\}$ cross sections in the CB1-4B method with the complete perturbation potentials V_f and V_i , respectively, obtained by using the helium ground-state wave functions of Löwdin [50].

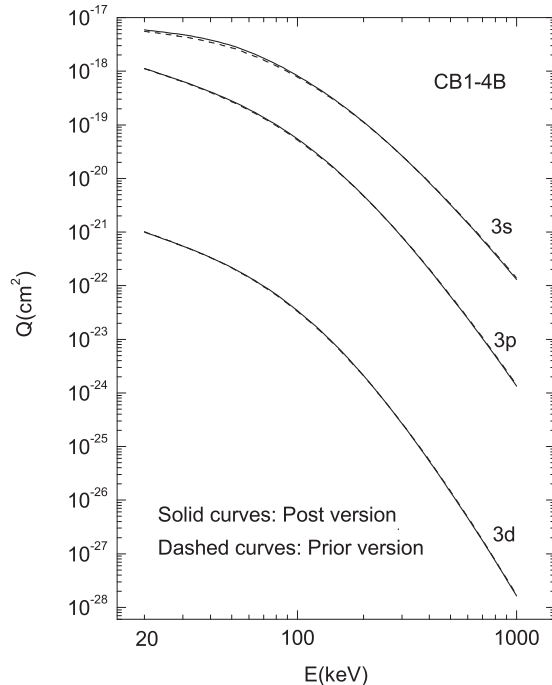


FIG. 7. State-selective cross sections Q_{3s}^{\pm} , Q_{3p}^{\pm} and Q_{3d}^{\pm} (in units of cm^2) as a function of the laboratory impact energy E (keV) for electron capture by protons from $\text{He}(1s^2)$ in process (59). The solid and dashed curves are the present post $\{Q_{3s}^+, Q_{3p}^+, Q_{3d}^+\}$ and prior $\{Q_{3s}^-, Q_{3p}^-, Q_{3d}^-\}$ cross sections of the CB1-4B method with the complete perturbation potentials V_f and V_i , respectively, obtained by using the helium ground-state wave functions of Löwdin [50].

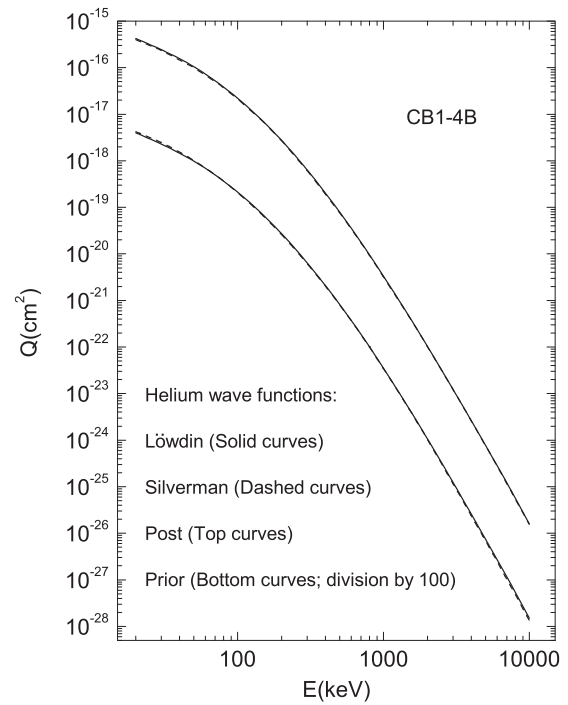


FIG. 8. State-selective cross sections Q_{1s}^{\pm} (in units of cm^2) as a function of the laboratory impact energy E (keV) for electron capture by protons from $\text{He}(1s^2)$ in process (59). The pairs of the top and bottom curves are the present post and prior cross sections of the CB1-4B method with the complete perturbation potential V_f and V_i , respectively. The solid and dashed curves correspond to the helium ground-state wave functions of Löwdin [50] and Silverman *et al.* [70], respectively. Both sets of the results for the bottom pair are divided by 100.

the post-prior discrepancy in a number of approximations (see, e.g., Refs. [71] as well as [72–74]). However, such detections of the post-prior discrepancy could have been an artifact, which the studied method might not possess at all, if the electron-electron repulsion $1/r_{12}$ were a constituent part of the final perturbation V_f in the exit channel of process (1). In the case of the CB1-4B method, this is clearly exemplified by juxtaposing the bottom to the top pairs of the curves in Fig. 5. The post-prior discrepancy, which is considerable without ΔV_{12} in V_f of the post form (the solid curve in the bottom pair), practically disappears altogether when ΔV_{12} is included in V_f (the solid curve in the top pair). Naturally, better physics prefers the full V_f with ΔV_{12} in the post version of the CB1-4B method, as opposed to the choice where ΔV_{12} is ignored, as is usually done for the reason of computational convenience. This preference coheres with experimental data that systematically agree with the post version of the CB1-4B method, where the complete potential V_f contains ΔV_{12} , as seen in Fig. 4. The message conveyed by Fig. 5 is that no valid theory for the Z_p -(Z_T ; e_1, e_2) collisions involving electron capture could be established for the post formalism by leaving out the interelectron interaction from the final perturbation potential V_f in the exit channel.

As mentioned earlier, the other reason for the existence of a post-prior discrepancy in theoretical descriptions of charge exchange is the lack of the exact bound-state heliumlike wave function. In order to test the sensitivity of the CB1-4B method

to the choice of the approximate wave functions for the ground state of the helium target for single-electron capture by protons into the $1s$ state of atomic hydrogen, we refer to Fig. 8. Here, it is seen that the curves obtained by the CB1-4B method using the wave functions of Löwdin [50] and Silverman *et al.* [70] are nearly indistinguishable from each other. Moreover, as is clear from Fig. 8, this conclusion is valid irrespective of whether the post or prior version of the CB1-4B method is employed. The same findings also extend to the excited $H(n^f l^f)$ states formed in the p -He charge-changing collisions, as can be confirmed by comparing the present Table III with Table I from our earlier work [25] using the wave functions of Löwdin [50] and Silverman *et al.* [70], respectively. This is yet another appealing feature of the CB1-4B method, which is only marginally sensitive to the choice of the approximate wave function for the helium target in (59) and (60).

All the present findings about the relative importance of screened dynamic correlations ΔV_{12} for total cross sections integrated over all scattering angles, as computed by means of the CB1-4B method, are fully concordant with the corresponding evaluations using the CDW-4B method [37] for single charge exchange involving heliumlike targets. Such a high degree of coherence between the CB1-4B and CDW-4B methods achieved at intermediate and relatively high impact energy is a very important cross validation of the present results, especially given that we are using a first-order perturbation theory. Therefore, it can be concluded that the CB1-4B method is capable of providing a consistent and systematic quantitative description of single-electron capture in process (1) in good agreement with experimental data at intermediate and high impact energies.

IV. CONCLUSION

We have investigated the problem of single charge exchange in collisions between bare nuclei and heliumlike atomic systems by means of the four-body boundary-corrected first Born (CB1-4B) approximation. An extensive analytical study of the post version of the transition amplitude for electron capture into the arbitrary $n^f l^f m^f$ final states of the projectile is carried out. The post form of the transition amplitude is derived in terms of five-dimensional real integrals for numerical computations. For both the ground- and excited-state capture processes, special attention has been devoted to assessing the role of screened dynamic correlations of the two electrons played by the short-range potential $\Delta V_{12} = V_{12} - V_{12}^\infty$. Interaction V_{12} is the interelectron Coulomb repulsion $1/r_{12}$, which is in the short-range potential ΔV_{12} screened by V_{12}^∞ . Potential V_{12}^∞ is the asymptotic tail of $1/r_{12}$ attained at large distances of the captured electron from the remaining bound electron in the target rest.

An illustrative computation is performed involving the state-selective and total single capture cross sections for the p -He collisions at intermediate and high impact energies.

Thorough comparisons are made between the obtained theoretical results and the related experimental data for electron capture into the excited states of atomic hydrogen, including $H(2s)$, $H(2p)$, $H(3s)$, $H(3p)$, $H(3d)$, and $H(4s)$, as well as for capture into all the final states of atomic hydrogen $H(\Sigma)$. Overall, it is found that the CB1-4B method excellently predicts the corresponding findings from the measurements.

The importance of the screened dynamic correlations has been studied by either including or excluding ΔV_{12} , which appears in the complete perturbation potential V_f of the post variant T_{if}^+ of the transition amplitude. The ensuing results indicate that these electronic correlations are very important for capture to the ground state, as well as to the excited states. Moreover, we proved that the contribution from ΔV_{12} increases with augmenting impact energy relative to the role of the remaining potentials in V_f .

The so-called post-prior discrepancy for charge exchange is a very undesirable feature of many theoretical methods. Its origin is twofold and lies with the unequal perturbation potentials in the entrance and exit channels, as well as with the nonexistence of the exact bound-state wave function of heliumlike atomic systems. The literature on fast-ion atom collisions treated by many methods is abundant on the allegedly detected post-prior discrepancy, which is, however, often an artifact of the adherence to easier computations that neglect the interelectron interaction in the full perturbation potential V_f from the post transition amplitudes. In order to assess the status of the CB1-4B approximation with regard to this important issue, we computed the prior cross sections as well, and compared them with the associated results in the post version of the same method. Despite the existing discrepancy between the initial and final perturbation potentials ($V_i \neq V_f$), our computations show that the results for the prior and post cross sections (both state selective and total) are nearly identical, provided that the electron-electron potential $1/r_{12}$ is taken into account in V_f . Moreover, no appreciable difference is found between the cross sections computed with two different approximate wave functions for the ground state of helium, irrespective of whether the prior or post variant of the CB1-4B method is employed. These findings constitute excellent properties of the CB1-4B approximation, especially given that huge post-prior discrepancies often plague nearly all the available distorted wave approximations.

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