Four-body corrected first Born approximation for single-electron capture into arbitrary states of energetic projectiles

Ivan Mančev,[1] Nenad Milojević,[1] and Dževad Belkić[2]
[1]*Department of Physics, Faculty of Sciences and Mathematics, University of Niš, P. O. Box 224, 18000 Niš, Serbia*
[2]*Karolinska Institute, P. O. Box 260, S-171 76 Stockholm, Sweden*
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Single charge exchange in collisions between fast bare projectiles and heliumlike atomic systems is investigated by means of the four-body boundary-corrected first Born approximation. An extensive analytical study of the general transition amplitude for electron capture into the arbitrary $n^f l^f m^f$ final states of the projectile is carried out. The quantum-mechanical transition amplitude for both symmetric and asymmetric collisions is derived in terms of a two-dimensional numerical quadrature over real variables. An illustrative computation is performed involving state-selective and total single-capture cross sections for p-He and Li^{3+}-He collisions at intermediate and high impact energies. Detailed comparisons with the available measurements are reported with the purpose of further assessing the validity and utility of the four-body corrected first Born method in various applications ranging from fusion research to radiotherapy.

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I. INTRODUCTION

It is well known that ion-atom collisions involve long-range Coulomb potentials that persist even when the scattering particles are at infinite separations from each other. This causes distortion of the unperturbed channel states and modifications of the corresponding perturbation potentials. The long-range nature of the Coulomb interaction yields considerable mathematical difficulties in treating collision processes and requires special attention for unambiguous and proper applications. In a key review paper [1], a long-standing issue was resolved concerning the role of the Coulomb boundary conditions. To this end, the usual scattering theory from nuclear collision physics with short-range interactions had to be substantially reformulated for atomic physics applications involving Coulombic potentials that remain in the asymptotic region of the initial and/or final states. One of the main results of this reformulation [1] was the introduction of a first-order theory, which has subsequently been referred to as the corrected first Born (CB1) approximation. This method satisfies the correct Coulomb boundary conditions in both the entrance and exit channels. The CB1 theory is a first-order term of a divergence-free perturbation expansion of the exact eikonal transition amplitude. The first Born approximation with the correct boundary conditions has been introduced within the three-body formalism [1] (hereafter denoted as the CB1-3B approximation). Over the years, the CB1-3B model has successfully been applied to many electron-capture processes [2–15]. Such computations yielded systematically good agreement with virtually all the existing experimental data on the subject. This represents an essential improvement of the otherwise poor performance of other first-order models for single charge exchange. For example, the Jackson-Schiff (JS1) [16] or the Oppenheimer, Brinkman, and Kramers (OBK1) first-order approximations [17,18] are known to be inadequate for electron capture. Invariably, the inadequacy of the OBK1 and JS1 models was attributed to the fact that they were merely the first-order approximations to the Born perturbation expansion. Moreover, such a claim was used to put into question all the other first-order models for charge exchange. This misconception prompted investigations within several second-order theories, but the real cause of the failure of the OBK1 and JS1 approximations was left unidentified. However, with the emergence of the CB1-3B method [1,2], the allegation of inadequacy of all the first-order theories for charge exchange was invalidated. Thorough applications of the CB1-3B model [2–15] have shown that a first-order theory could indeed be adequate for electron capture, but only provided that it obeys the Coulomb boundary conditions and that it is associated with a nondivergent series development. Neither of these latter two key requirements of atomic collision physics is met in the JS1 or the OBK1 model, and this fact, rather than that they are first-order approximations, was the reason for their failure in comparisons with experiments. Note that in the single case of identical nuclear charges of the projectile and target, $Z_P = Z_T = 1$, dealing with electron capture from atomic hydrogen by protons, the JS1 approximation fortuitously coincides with the CB1 method. For all other values of Z_P and Z_T, the results of the JS1 model deviate from those from the CB1 approximation. This was systematically demonstrated in detailed computations from Ref. [10] for charge exchange $Z_P + H(1s) \rightarrow (Z_P,e)_f + H^+$ with $Z_P = 1$–6. The most striking difference of two orders of magnitude between the total cross sections from the JS1 and CB1 approximations for single-electron capture from the K shell of argon by protons at impact energies 1–12 MeV was reported in Ref. [9], where the latter theory was found to be in excellent agreement with the corresponding experimental data.

In the case of single-electron transfer from a target atom with two or more electrons by a bare projectile, the active electron has often been described using a Roothaan-Hartree-Fock (RHF) orbital in the self-consistent field (SCF) approximation [9–13,15]. Thus, pure four-body problems, such as charge exchange $Z_P - (Z_T; e_1, e_2)_i$, are reduced to effectively three-body problems. In such three-body models, the individual states of the remainder of the target are ignored altogether, in accordance with the single-particle frozen-core approximation. Computation of state-selective cross sections for electron capture from helium by protons has been the subject of investigation in a number of reports. For this

theme of research, different three-body models have been used, such as the CB1-3B [14], the continuum distorted wave (CDW) [19], the continuum intermediate state (CIS) [20], the target continuum distorted wave (TCDW) [21] models, the eikonal (EA) [22], the symmetric eikonal (SE) [23], the impulse eikonal (IA) [24] approximations, the two-center atomic-orbital-expansion approach within the close-coupling (CC) treatment [25], etc. Although interest in four-body models has been considerably revived in recent years [26–30], to our knowledge no computations have thus far been reported on state-selective electron capture from helium by protons using four-body approximations. The present study is meant to bridge this gap.

In general, the correct Coulomb boundary conditions are demanded by the well-known asymptotic convergence problem [1,31,32]. This consists of the simultaneous requirement for the correct asymptotic behaviors of all the scattering wave functions and their proper connection with the corresponding perturbation interactions. Of late, much effort has been focused on four-body theories for nonrelativistic fast-ion–atom collisions with two actively participating electrons. A number of quantum-mechanical four-body methods have been proposed to study one- and two-electron transitions in scattering of completely stripped projectiles on heliumlike atomic systems or in collisions between two hydrogenlike atoms or ions, as recently reviewed in Refs. [26–28].

The formulation and implementation of the four-body boundary-corrected first Born approximation (CB1-4B) approximation was carried out in Refs. [33,34] for double-electron capture. Subsequently, the CB1-4B method was adapted and applied to single-electron capture [35–37]. The CB1-4B theory goes beyond the usual independent-particle frozen-core approximations and consistently obeys the asymptotic convergence criteria of Dollard [31,32] for Coulomb potentials.

Thus far, the CB1-4B method has been applied only to ground-to-ground state capture. This was the case for double-electron capture [33,34] as well as for single-charge exchange [35–37]. The previous results of the CB1-4B method relate to total cross sections for single-electron capture from helium by protons and α particles, involving only the final hydrogenlike states H(1s) and $He^+(1s)$, respectively [37]. This is extended in the present study to encompass electron capture into arbitrary final states of the projectile.

The main goal of the present work is to generalize the CB1-4B theory to single-electron capture by a bare projectile from a heliumlike atomic system into the final arbitrary shells $\{n^f, l^f, m^f\}$ of the transferred electron. Electron transfer into excited states is expected to play an important role, at least at lower and intermediate impact energies. Moreover, our rationale for extending the CB1-4B approximation to include the contributions of various subshells is threefold. *First*, a generalization of the CB1-4B method to any $\{n^f, l^f, m^f\}$ level should test the validity of the main working assumptions of this method which has previously been restricted to ground-to-ground state capture alone [37]. *Second*, in practical applications concerning certain new energy sources, the role played by impurities in neutral-beam heating of tokamak fusion plasmas is currently being examined by using charge-exchange spectroscopy. For this measuring device, information about subshell populations of states formed by charge exchange is necessary. *Third*, while acknowledging the significance of the recent efforts by Madison and coworkers [29,30,38,39] to carry out CPU-time-consuming nine-dimensional numerical quadratures for the related problems using the defining expressions for the transition amplitudes of a selected method, it is likewise important to report the present alternative semianalytical reductions of similar transition amplitudes, yielding computationally efficient two-dimensional quadratures.

Atomic units will be used throughout unless otherwise stated.

II. THEORY

A. The defining prior form of the transition amplitude

We consider single-electron capture in collisions of a completely stripped projectile with a heliumlike target:

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

where Z_K is the charge of the Kth nucleus (K = P,T) and $n^f l^f m^f$ is the usual set of three hydrogenlike quantum numbers. Here, the parentheses symbolize 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 electrons (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 prior form of the transition amplitude for process (1) in the CB1-4B approximation reads as [37]

$$T_{if}(\vec{\eta}) = \iiint d\vec{x}_1 d\vec{x}_2 d\vec{R} \varphi^*_{n^f l^f m^f}(\vec{s}_1)\varphi^*_T(\vec{x}_2) \times \left(\frac{2Z_P}{R} - \frac{Z_P}{s_1} - \frac{Z_P}{s_2}\right) \varphi_i(\vec{x}_1, \vec{x}_2)\, e^{-i\vec{\alpha}\cdot\vec{R} - i\vec{v}\cdot\vec{x}_1} \mathcal{E}(\vec{R}), \qquad (2)$$

where $\mathcal{E}(\vec{R})$ can be either of the following two equivalent expressions:

$$\mathcal{E}(\vec{R}) = \begin{cases} (\rho v)^{2iZ_P(Z_T-2)/v}(vR + \vec{v}\cdot\vec{R})^{i\xi}, \\ (\rho v)^{2i(Z_T-1)(Z_P-1)/v}(vR - \vec{v}\cdot\vec{R})^{-i\xi}. \end{cases} \qquad (3)$$

Here, $\xi = (Z_P - Z_T + 1)/v$ where v is the velocity of the projectile and $\vec{\rho}$ is the projection of vector $\vec{R}$ onto the XOY plane ($\vec{\rho} = \vec{R} - \vec{Z}$, $\vec{\rho}\cdot\vec{Z} = 0$). As has been shown in Ref. [1] for the exact eikonal transition amplitude, the overall multiplying term $(\rho v)^{2iZ_P(Z_T-2)/v}$ or $(\rho v)^{2i(Z_T-1)(Z_P-1)/v}$ does not contribute to the total cross section and can be omitted from further considerations.

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

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

where $\Delta E = E_i - E_f$ with E_i being the binding energy of the two-electron target and $E_f = -Z_P^2/[2(n^f)^2] - Z_T^2/2$. The quantity ΔE, which represents the energy defect for the reaction under study, is often denoted by Q in the related experimental studies and thus, for brevity, referred to as the Q

factor. This notation and nomenclature are avoided in theoretical examinations because of the common practice in which the letter Q usually denotes cross sections. The transverse component of the change in the relative linear momentum of a heavy particle is denoted by $\vec{\eta} = (\eta\cos\phi_\eta, \eta\sin\phi_\eta, 0)$ and has the property $\vec{\eta}\cdot\vec{v} = 0$.

The function $\varphi_i(\vec{x}_1,\vec{x}_2)$ denotes the two-electron ground-state wave function of the atomic system $(Z_T; e_1, e_2)_{1s^2}$. Hereafter, we shall use the general factorized form for the bound state of the heliumlike atomic system:

$$\varphi_i(\vec{x}_1,\vec{x}_2) = \sum_{k,l} \varphi_{\alpha k}(\vec{x}_1)\varphi_{\alpha l}(\vec{x}_2), \tag{4}$$

where $\varphi_{\alpha j}(\vec{r}) = N_{\alpha_j}\exp(-\alpha_j r)$ where $N_{\alpha_j} = a_j\sqrt{N}$ $(j = k, l)$ and N is the normalization constant. The values of the summation indices k and l, as well as of the variationally determined parameters α_j and a_j, depend upon the concrete choice for the wave function. The functions $\varphi_{n^f l^f m^f}(\vec{s}_1)$ and $\varphi_T(\vec{x}_2)$ in Eq. (2) represent the bound-state wave functions of the hydrogenlike atomic systems $(Z_P, e_1)_{n^f l^f m^f}$ and $(Z_T, e_2)_{1s}$, respectively.

In the CB1-4B model, the proper connection between the long-range Coulomb distortion effects and the accompanying perturbation potentials is accomplished according to the well-established principles of scattering theory [32]. As evidenced in abundant applications, imposing the correct Coulomb boundary conditions in the entrance and exit channels is of crucial importance, particularly for ion-atom collisions [28].

B. Analytical method for calculation of the transition amplitude involving arbitrary final excited states of the formed hydrogenlike atomic system

In the derivation presented here, we shall closely follow Ref. [11] with adaptation to process (1). With this goal, the transition amplitude (2) can be reduced to the following form which is amenable to further analytical calculations:

$$T_{if} = Z_P \sum_{k,l} N_{k,l}\left[2J_R^{(k,l)} - J_{s_1}^{(k,l)} - J_{s_2}^{(k,l)}\right], \tag{5}$$

where

$$J_\omega^{(k,l)} = \int d\vec{R}\, e^{-i\vec{\alpha}\cdot\vec{R}}(vR + \vec{v}\cdot\vec{R})^{i\xi}\, W_\omega^{(k,l)}(\vec{R}), \quad (\omega = R, s_1, s_2), \tag{6}$$

$$W_R^{(k,l)} = \frac{1}{R}\mathcal{B}_k\mathcal{A}_l, \quad W_{s_1}^{(k,l)} = \mathcal{C}_k\mathcal{A}_l, \quad W_{s_2}^{(k,l)} = \mathcal{B}_k\mathcal{D}_l, \tag{7}$$

$$\mathcal{A}_l = \int d\vec{x}_2\, e^{-(Z_T+\alpha_l)x_2} = \frac{8\pi}{(Z_T+\alpha_l)^3}, \tag{8}$$

$$\mathcal{D}_l = \int d\vec{x}_2\, e^{-(Z_T+\alpha_l)x_2}\frac{1}{s_2} = 2\pi(Z_T+\alpha_l)\int_0^1 dt_1 \frac{(1-t_1)}{\Delta_1^3} \times (1+\Delta_1 R)e^{-\Delta_1 R}, \tag{9}$$

$$\mathcal{B}_k = \int d\vec{x}_1\, e^{-i\vec{v}\cdot\vec{x}_1-\alpha_k x_1}\varphi^*_{n^f l^f m^f}(\vec{s}_1) = \int d\vec{x}_1\, e^{-i\vec{v}\cdot\vec{x}_1-\alpha_k x_1} \times \left[\int d\vec{q}\, e^{-i\vec{q}\cdot\vec{s}_1}\widetilde{\varphi}_{n^f l^f m^f}(\vec{q})\right]^*, \tag{10}$$

$$\mathcal{C}_k = \int d\vec{x}_1\, e^{-i\vec{v}\cdot\vec{x}_1-\alpha_k x_1}\frac{\varphi^*_{n^f l^f m^f}(\vec{s}_1)}{s_1} = \int d\vec{x}_1\, e^{-i\vec{v}\cdot\vec{x}_1-\alpha_k x_1} \times \left[\int d\vec{q}\, e^{-i\vec{q}\cdot\vec{s}_1}\widetilde{\chi}_{n^f l^f m^f}(\vec{q})\right]^*, \tag{11}$$

with $\chi_{n^f l^f m^f}(\vec{s}_1) = \varphi_{n^f l^f m^f}(\vec{s}_1)/s_1$, $N_{k,l} = (Z_T)^{3/2}N_{\alpha_k}N_{\alpha_l}/\sqrt{\pi}$, and $\Delta_1^2 = (Z_T+\alpha_l)^2(1-t_1)$. Using the Fourier transform $\tilde{f}(\vec{q}) = (2\pi)^{-3}\int d\vec{r}\, e^{i\vec{q}\cdot\vec{r}} f(\vec{r})$ the hydrogenlike wave functions $\varphi_{n^f l^f m^f}(\vec{s}_1)$ and $\chi_{n^f l^f m^f}(\vec{s}_1)$ in the momentum space can be written as [40]

$$\widetilde{\varphi}_{n^f l^f m^f}(\vec{q}) = (2\pi)^{-3}N_f^{Z_P} i^{l^f}\sum_{p=0}^{n_r} c_p \frac{\mathcal{Y}_{l^f m^f}(\vec{q})}{[q^2+(Z_P/n^f)^2]^{p+l^f+2}}, \tag{12}$$

$$\widetilde{\chi}_{n^f l^f m^f}(\vec{q}) = (2\pi)^{-3}\frac{N_f^{Z_P}}{2Z_P} i^{l^f}\sum_{p=0}^{n_r} c_p \frac{\mathcal{Y}_{l^f m^f}(\vec{q})}{[q^2+(Z_P/n^f)^2]^{p+l^f+1}}, \tag{13}$$

where

$$N_f^{Z_P} = 16\pi Z_P\left[\frac{(Z_P/n^f)^3}{n^f}\frac{(n^f+l^f)!}{n_r!}\right]^{1/2}\frac{l^f!(4Z_P/n^f)^{l^f}}{(2l^f+1)!}, \tag{14}$$

$$c_p = \frac{(-n_r)_p(n^f+l^f+1)_p}{(l^f+3/2)_p\, p!}(Z_P/n^f)^{2p}, \quad n_r = n^f - l^f - 1. \tag{15}$$

The quantity $\mathcal{Y}_{lm}(\vec{q})$ denotes the regular solid harmonic $\mathcal{Y}_{lm}(\vec{q}) = q^l Y_{lm}(\hat{\vec{q}})$ where $Y_{lm}(\hat{\vec{q}})$ is the spherical harmonic (see the Appendix for the adopted definitions and phase conventions), whereas $(a)_n$ is the Pochhammer symbol $(a)_n = \Gamma(a+n)/\Gamma(a) = a(a+1)\cdots(a+n-1)$, $(a)_0 = 1$. Using Eqs. (12) and (13), the integrals $\mathcal{B}_k$ and $\mathcal{C}_k$ become

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

with

$$\mathcal{G}^{(\nu)}_{k,p} = e^{i\vec{\alpha}\cdot\vec{R}}\int d\vec{q}\, e^{-i\vec{q}\cdot\vec{R}} \times \frac{\mathcal{Y}^*_{l^f m^f}(\vec{q}-\vec{\alpha})}{\left(|\vec{q}-\vec{\alpha}|^2+a_f^2\right)^{p+l^f+\nu}\left(|\vec{q}+\vec{\beta}|^2+\alpha_k^2\right)^2} \quad (\nu = 1,2), \tag{17}$$

where the translation $\vec{q} \to \vec{q} - \vec{\alpha}$ is made, and $a_f = Z_P/n^f$.

The denominators in the integral (17) can be collected into a single term by means of the Feynman parametrization integral:

$$\frac{1}{A^s B^r} = \frac{(s+r-1)!}{(s-1)!(r-1)!}\int_0^1 dt \times \frac{t^{s-1}(1-t)^{r-1}}{[At+B(1-t)]^{s+r}} \quad (s,r \geqslant 1), \tag{18}$$

$$\mathcal{G}^{(\nu)}_{k,\,p} = (p+l^f+\nu+1)(p+l^f+\nu) \times \int_0^1 dt\, t^{p+l^f+\nu-1}(1-t)\mathcal{U}^{(\nu)}_{k,\,p}, \tag{19}$$

$$\mathcal{U}^{(\nu)}_{k,\,p} = e^{i\vec{\alpha}\cdot\vec{R}}\int d\vec{q}\, e^{-i\vec{q}\cdot\vec{R}}\frac{\mathcal{Y}^*_{l^f m^f}(\vec{q}-\vec{\alpha})}{(|\vec{q}-\vec{Q}|^2+\Delta^2)^{p+l^f+2+\nu}} = e^{-i\vec{Q}_\alpha\cdot\vec{R}}\int d\vec{q}\, e^{-i\vec{q}\cdot\vec{R}}\frac{\mathcal{Y}^*_{l^f m^f}(\vec{q}+\vec{Q}_\alpha)}{(q^2+\Delta^2)^{p+l^f+2+\nu}}, \tag{20}$$

where a variable change $\vec{q} \to \vec{q}+\vec{Q}$ is introduced, and

$$\vec{Q} = \vec{\alpha}t - \vec{\beta}(1-t), \qquad \vec{Q}_\alpha = \vec{Q}-\vec{\alpha} = (1-t)\vec{v}, \tag{21}$$

$$\Delta^2 = v^2 t(1-t) + a_f^2 t + \alpha_k^2(1-t). \tag{22}$$

Furthermore, the addition theorem for regular solid harmonics [41,42] is given by

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

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

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

Employing the relation $\mathcal{Y}_{l_2^f m_2^f}(\vec{Q}_\alpha) = \mathcal{Y}_{l_2^f m_2^f}[(1-t)\vec{v}\,] = (1-t)^{l_2^f} v^{l_2^f} Y_{l_2^f m_2^f}(\hat{\vec{v}})$ and choosing the vector $\vec{v}$ along the Z axes, the spherical harmonic $Y_{l_2^f m_2^f}(\hat{\vec{v}})$ will be nonzero only for $m_2^f = 0$, so that $Y_{l_2^f m_2^f}(\hat{\vec{v}}) = \sqrt{(2l_2^f+1)/(4\pi)}\,\delta_{0,m_2^f}$. In such a case, the sum over m_1^f in Eq. (23) disappears altogether and, therefore, this formula is reduced to

$$\mathcal{Y}^*_{l^f m^f}(\vec{q}+\vec{Q}_\alpha) = \sqrt{4\pi}\sum_{l_1^f=0}^{l^f},\sum_{m_1^f=-l_1^f}^{l_1^f}(1-t)^{l_2^f}\,\Omega\left(l_1^f,\vec{v}\right)\mathcal{Y}_{l_1^f,-m^f}(\vec{q})\delta_{m_1^f,m^f} = \sqrt{4\pi}\sum_{l_1^f=|m^f|}^{l^f}(1-t)^{l_2^f}\,\Omega\left(l_1^f,\vec{v}\right)\mathcal{Y}_{l_1^f,-m^f}(\vec{q}), \tag{25}$$

where

$$\Omega\left(l_1^f,\vec{v}\right) = \left(l_1^f\,|l^f m^f\right)(-1)^{-m^f}v^{l_2^f}/\sqrt{4\pi}, \tag{26}$$

$$\left(l_1^f\,|l^f m^f\right) = \left[\frac{2l^f+1}{(2l_1^f+1)}\frac{(l^f+m^f)!}{(l_1^f+m^f)!}\frac{(l^f-m^f)!}{(l_1^f-m^f)!(l_2^f!)^2}\right]^{1/2}. \tag{27}$$

Under these circumstances, the auxiliary integral $\mathcal{U}^{(\nu)}_{k,\,p}$ from Eq.(20) can be written in the following form:

$$\mathcal{U}^{(\nu)}_{k,\,p} = e^{-i\vec{Q}_\alpha\cdot\vec{R}}\sum_{l_1^f=|m^f|}^{l^f}(1-t)^{l_2^f}\,\Omega\left(l_1^f,\vec{v}\right)\mathcal{W}^{(\nu)}_{k,\,p}, \tag{28}$$

$$\mathcal{W}^{(\nu)}_{k,\,p} = \sqrt{4\pi}\int d\vec{q}\, e^{-i\vec{q}\cdot\vec{R}}\frac{\mathcal{Y}_{l_1^f,-m^f}(\vec{q})}{(q^2+\Delta^2)^{p+l^f+2+\nu}} = (-i)^{l_1^f}\mathcal{L}^{(\nu)}_{k,\,p}\,\mathcal{Y}_{l_1^f,-m^f}(\vec{R}). \tag{29}$$

In Eq. (29), the partial-wave expansion of the plane wave can be used:

$$e^{-i\vec{q}\cdot\vec{R}} = 4\pi\sum_{l=0}^{\infty}\sum_{m=-l}^{l}(-i)^l j_l(qR)Y^*_{lm}(\hat{\vec{q}})Y_{lm}(\hat{\vec{R}}), \tag{30}$$

together with the formula [11,41]

$$\mathcal{L}^{(\nu)}_{k,\,p} = \frac{(4\pi)^{3/2}}{R^{l_1^f}}\int_0^\infty dq\frac{q^{l_1^f+2}j_{l_1^f}(qR)}{(q^2+\Delta^2)^{p+l^f+2+\nu}} = 4\pi^{5/2}\frac{\hat{k}_{\mu_\nu-1/2}(R\Delta)}{2^{n_\nu}n_\nu!\Delta^{2n_\nu-2l_1^f-1}}, \tag{31}$$

with

$$\mu_\nu = p+l^f+1+\nu-l_1^f, \quad n_\nu = n-\sigma_\nu, \tag{32}$$

$$n = p+l^f+3, \quad \sigma_1 = 1, \quad \sigma_2 = 0, \tag{33}$$

where $j_l(x)$ is the spherical Bessel function [43]. Here, $\hat{k}_\delta(z)$ is the reduced Bessel function $\hat{k}_\delta(z) = \sqrt{2/\pi}z^\delta K_\delta(z)$ and $K_\delta(z)$ is the McDonald function [43].

In this way, the integrals $\mathcal{U}^{(\nu)}_{k,\,p}$ and $\mathcal{G}^{(\nu)}_{k,\,p}$ are transformed to

$$\mathcal{U}^{(\nu)}_{k,\,p} = \frac{4\pi^{5/2}}{2^{n_\nu}n_\nu!}e^{-i\vec{Q}_\alpha\cdot\vec{R}}\sum_{l_1^f=|m^f|}^{l^f}(-i)^{l_1^f}(1-t)^{l_2^f} \times \Omega\left(l_1^f,\vec{v}\right)\frac{B^{(\mu_\nu)}_{l_1^f,-m^f}(\vec{R}\Delta)}{\Delta^{2n_\nu-2l_1^f-1}}, \tag{34}$$

$$\mathcal{G}^{(\nu)}_{k,\,p} = \frac{4\pi^{5/2}}{2^{n_\nu}(n_\nu-2)!}\sum_{l_1^f=|m^f|}^{l^f}(-i)^{l_1^f}\,\Omega\big(l_1^f,\vec{v}\big)\int_0^1 dt\,t^{n_\nu-2}$$
$$\times(1-t)^{l_2^f+1}e^{-i\vec{Q}_\alpha\cdot\vec{R}}\,\frac{B^{(\mu_\nu)}_{l_1^f,-m^f}(\vec{R}\Delta)}{\Delta^{2n_\nu-2l_1^f-1}}, \tag{35}$$

where $B^{(\mu_\nu)}_{l_1^f,-m^f}(\vec{R}\Delta)=\hat{k}_{\mu_\nu-1/2}(R\Delta)\mathcal{Y}_{l_1^f,-m^f}(\vec{R})$ is the so-called B function [44]. Inserting Eq. (35) into Eq. (16) and using Eqs. (6) and (7), we have

$$J^{(k,l)}_{\omega} = D^{(k,l)}_{l^f}\sum_{p=0}^{n_r}\frac{c_p}{2^n(n-3)!}\sum_{l_1^f=|m^f|}^{l^f}(-i)^{l_1^f}\,\Omega\big(l_1^f,\vec{v}\big)$$
$$\times\int_0^1 dt\,\frac{t^{n-2}(1-t)^{l_2^f+1}}{\Delta^{2n-2l_1^f-1}}I^{(p,l_1^f)}_{w}, \tag{36}$$

where

$$D^{(k,l)}_{l^f} = 64\pi^{9/2}(-i)^{l^f}N_f^{Z_P}(Z_T+\alpha_l)\alpha_k, \tag{37}$$

$$I^{(p,l_1^f)}_{R} = \frac{4(2\pi)^{-3}}{(Z_T+\alpha_l)^4(n-2)}\int d\vec{R}e^{-i\vec{Q}\cdot\vec{R}}$$
$$\times(vR+\vec{v}\cdot\vec{R})^{i\xi}R^{-1}B^{(\mu_2)}_{l_1^f,-m^f}(\vec{R}\Delta), \tag{38}$$

$$I^{(p,l_1^f)}_{s_1} = \frac{4\Delta^2(2\pi)^{-3}}{Z_P(Z_T+\alpha_l)^4t}\int d\vec{R}\,e^{-i\vec{Q}\cdot\vec{R}}$$
$$\times(vR+\vec{v}\cdot\vec{R})^{i\xi}B^{(\mu_1)}_{l_1^f,-m^f}(\vec{R}\Delta), \tag{39}$$

$$I^{(p,l_1^f)}_{s_2} = \frac{(2\pi)^{-3}}{(n-2)}\int_0^1 dt_1\frac{(1-t_1)}{\Delta_1^3}\int d\vec{R}\,e^{-i\vec{Q}\cdot\vec{R}}(vR+\vec{v}\cdot\vec{R})^{i\xi}$$
$$\times B^{(\mu_2)}_{l_1^f,-m^f}(\vec{R}\Delta)(1+\Delta_1 R)e^{-\Delta_1 R}. \tag{40}$$

In order to obtain the results for the integrals from Eqs. (38)–(40), we shall first express the B function in terms of a linear combination of unnormalized Slater-type orbitals [11,44]:

$$B^{(\mu_\nu)}_{l_1^f,-m^f}(\vec{R}\Delta) = \sum_{p_r=0}^{\mu_\nu-1}b^{\mu_\nu}_{p_r}\Delta^{p_r}\chi^{(p_n)}_{l_1^f,-m^f}(\vec{R}\Delta), \tag{41}$$

where

$$b^{\mu_\nu}_{p_r} = \frac{(2\mu_\nu-p_r-2)!2^{p_r+1-\mu_\nu}}{(\mu_\nu-p_r-1)!p_r!},\quad p_n=p_r+l_1^f+1, \tag{42}$$

$$\chi^{(p_n)}_{l_1^f,-m^f}(\vec{R}\Delta) = R^{p_n-1}e^{-R\Delta}Y_{l_1^f,-m^f}(\hat{\vec{R}}). \tag{43}$$

Next, the Fourier transform of the auxiliary function $\chi^{(p_n,\lambda)}_{l_1^f,-m^f}(\vec{R}\Delta_\tau)$ for $\lambda=0,1,2$, as introduced by

$$\chi^{(p_n,\lambda)}_{l_1^f,-m^f}(\vec{R}\Delta_\tau) = (vR-\vec{v}\cdot\vec{R})^{i\xi}R^{\lambda-1}\chi^{(p_n)}_{l_1^f,-m^f}(\vec{R}\Delta_\tau)$$
$$(\tau=0,2),$$
$$\Delta_0\equiv\Delta,\quad \Delta_2=\Delta+\Delta_1, \tag{44}$$

can be calculated, with the result

$$\widetilde{\chi}^{(p_n,\lambda)}_{l_1^f,-m^f}(\vec{Q}\Delta_\tau)$$
$$= \frac{(-1)^{l_1^f}(2i)^{l_1^f}}{2\pi^2}\sum_{k=0}^{p_\lambda}\sum_{l_1=|m^f|}^{l_1^f}\Phi^{kl_1}_{p_r l_1^f\tau}(\lambda)\mathcal{Z}_{l_1^f l_1}(\vec{Q}\cdot\vec{v}), \tag{45}$$
$$p_\lambda = p_r+\lambda,$$

where

$$\mathcal{Z}_{l_1^f l_1}(\vec{Q}\cdot\vec{v}) = \big(l_1|l_1^f-m^f\big)(-iv)^{l_2}\mathcal{Y}_{l_1,-m^f}(\vec{Q}), \tag{46}$$

$$\big(l_1|l_1^f-m^f\big) = \left[\frac{2l_1^f+1}{(2l_1+1)}\frac{\big(l_1^f+m^f\big)!}{(l_1+m^f)!}\frac{\big(l_1^f-m^f\big)!}{(l_1-m^f)!(l_2!)^2}\right]^{1/2}. \tag{47}$$

The remaining quantities appearing in Eq. (45) are defined as

$$\Phi^{kl_1}_{p_r l_1^f\tau}(\lambda) = \big(a^\lambda_\tau b^\lambda_\tau\big)\,{}_3F_2(-k_\lambda/2,-k_\lambda/2+1/2,1$$
$$-i\gamma_1;k+l_1^f+1,-p_\lambda-l_1^f;1/A_\tau), \tag{48}$$

$$a^\lambda_\tau = \Gamma(1+i\xi)\big(l_1^f+1\big)_{p_\lambda}\frac{(2D_\tau)^{p_\lambda}}{\big(\Delta_\tau^2+Q^2\big)^{l_1^f}}\mathcal{F}_\tau, \tag{49}$$

$$b^\lambda_\tau = \frac{(1+i\xi)_{l_1}(-i\xi)_{l_2}}{B_\tau^{l_2}}\frac{(-p_\lambda)_k(i\gamma_2)_k}{\big(l_1^f+1\big)_k}\frac{(-1)^kC_\tau^k}{k!}, \tag{50}$$

$${}_3F_2(-k_\lambda/2,-k_\lambda/2+1/2,1-i\gamma_1;k+l_1^f+1,-p_\lambda-l_1^f;1/A_\tau)$$
$$= \sum_{u=0}^{[k_\lambda/2]}\frac{(-k_\lambda/2)_u(-k_\lambda/2+1/2)_u(1-i\gamma_1)_u}{\big(k+l_1^f+1\big)_u\big(-p_\lambda-l_1^f\big)_u u!}\left(\frac{1}{A_\tau}\right)^u, \tag{51}$$

where

$$A_\tau = \frac{\Delta_\tau^2}{\Delta_\tau^2+Q^2},\quad B_\tau = \frac{2(v\Delta_\tau-i\vec{Q}\cdot\vec{v})}{\Delta_\tau^2+Q^2},$$
$$C_\tau = \frac{v}{B_\tau\Delta_\tau}-1, \tag{52}$$

$$D_\tau = \frac{A_\tau}{\Delta_\tau},\quad \mathcal{F}_\tau = \frac{B_\tau^{i\xi}}{\Delta_\tau^2+Q^2}, \tag{53}$$

$$k_\lambda = p_\lambda-k,\quad l_1+l_2=l_1^f,$$
$$\gamma_1 = -\xi+il_1,\quad \gamma_2=-\xi-il_2. \tag{54}$$

Here, ${}_3F_2$ is the Clausen generalized hypergeometric polynomial [45] and the symbol $[k_\lambda/2]$ denotes the largest integer contained in the fraction $k_\lambda/2$.

This derivation maps the integrals $J_{\omega}^{(k,l)}$ ($\omega = R, s_1, s_2$) from Eq. (36) into

$$J_R^{(k,l)} = \frac{2D_{l^f}^{(k,l)}}{\pi^2(Z_T+\alpha_l)^4}\sum_{p=0}^{n_r}\frac{c_p}{2^n(n-2)!}\sum_{l_1^f=|m^f|}^{l^f}(-1)^{l_1^f}2^{l_1^f}\Omega\left(l_1^f,\vec{v}\right)\mathcal{M}_R^{(p,l_1^f)}, \tag{55}$$

$$J_{s_1}^{(k,l)} = \frac{D_{l^f}^{(k,l)}}{\pi^2 Z_P(Z_T+\alpha_l)^4}\sum_{p=0}^{n_r}\frac{c_p}{2^{n-1}(n-3)!}\sum_{l_1^f=|m^f|}^{l^f}(-1)^{l_1^f}2^{l_1^f}\Omega\left(l_1^f,\vec{v}\right)\mathcal{M}_{s_1}^{(p,l_1^f)}, \tag{56}$$

$$J_{s_2}^{(k,l)} = \frac{D_{l^f}^{(k,l)}}{2\pi^2}\sum_{p=0}^{n_r}\frac{c_p}{2^n(n-2)!}\sum_{l_1^f=|m^f|}^{l^f}(-1)^{l_1^f}2^{l_1^f}\Omega\left(l_1^f,\vec{v}\right)\mathcal{M}_{s_2}^{(p,l_1^f)}, \tag{57}$$

where

$$\mathcal{M}_R^{(p,l_1^f)} = \frac{(2n_p)!}{n_p!}\sum_{p_r=0}^{n_p}\frac{(-n_p)_{p_r}}{(-2n_p)_{p_r}}\frac{2^{p_r-n_p}}{p_r!}\int_0^1 dt\,\frac{t^{n-2}(1-t)^{l_2^f+1}}{\Delta^{2n-2l_1^f-p_r-1}}G_{l_1^f,-m^f}^{(p_n,0)}(\vec{Q}\Delta), \tag{58}$$

$$\mathcal{M}_{s_1}^{(p,l_1^f)} = \frac{(2n_p-2)!}{(n_p-1)!}\sum_{p_r=0}^{n_p-1}\frac{(1-n_p)_{p_r}}{(2-2n_p)_{p_r}}\frac{2^{p_r-n_p+1}}{p_r!}\int_0^1 dt\,\frac{t^{n-3}(1-t)^{l_2^f+1}}{\Delta^{2(n-1)-2l_1^f-p_r-1}}G_{l_1^f,-m^f}^{(p_n,1)}(\vec{Q}\Delta), \tag{59}$$

$$\mathcal{M}_{s_2}^{(p,l_1^f)} = \frac{(2n_p)!}{n_p!}\sum_{p_r=0}^{n_p}\frac{(-n_p)_{p_r}}{(-2n_p)_{p_r}}\frac{2^{p_r-n_p}}{p_r!}\int_0^1 dt_1\frac{(1-t_1)}{\Delta_1^3}\int_0^1 dt\,\frac{t^{n-2}(1-t)^{l_2^f+1}}{\Delta^{2n-2l_1^f-p_r-1}}\left[G_{l_1^f,-m^f}^{(p_n,1)}(\vec{Q}\Delta_2)+\Delta_1 G_{l_1^f,-m^f}^{(p_n,2)}(\vec{Q}\Delta_2)\right], \tag{60}$$

$$G_{l_1^f,-m^f}^{(p_n,\lambda)}(\vec{Q}\Delta_\tau) = \sum_{k=0}^{p_\lambda}\sum_{l_1=|m^f|}^{l_1^f}\Phi_{p_r l_1^f \tau}^{k l_1}(\lambda)\mathcal{Z}_{l_1^f l_1}(\vec{Q}\cdot\vec{v}), \tag{61}$$

and $n_p = n - l_1^f - 1$. With these results at hand, the final expression for the transition amplitude reads as

$$T_{if} = \sum_{k,l}\sum_{p=0}^{n_r}\sum_{l_1^f=|m^f|}^{l^f}\mathcal{N}_{k,l}\frac{c_p}{2^n(n-3)!}(-1)^{l_1^f}2^{l_1^f}\Omega\left(l_1^f,\vec{v}\right)\left\{\frac{4}{(Z_T+\alpha_l)^4}\left[\frac{2}{n-2}\mathcal{M}_R^{(p,l_1^f)}-\frac{1}{Z_P}\mathcal{M}_{s_1}^{(p,l_1^f)}\right]-\frac{1}{n-2}\mathcal{M}_{s_2}^{(p,l_1^f)}\right\}, \tag{62}$$

where

$$\mathcal{N}_{k,l} = \frac{1}{2\pi^2}Z_P N_{k,l} D_{l^f}^{(k,l)}. \tag{63}$$

This completes the calculation of the transition amplitude T_{if} in terms of the two-dimensional integral over the real variables t and t_1.

C. Cross sections

The total cross section in the CB1-4B method is given by

$$Q_{if}(\pi a_0^2) = \frac{1}{2\pi^2 v^2}\int_0^\infty d\eta\,\eta|T_{if}|^2, \tag{64}$$

where the angular integration of the orientation of the transverse momentum transfer vector $\vec{\eta}$ is performed analytically. The remaining triple integration over η, t, and t_1 must be carried out numerically, and this is achieved at present by means of the Gauss-Legendre quadratures.

III. RESULTS

A. Electron capture from He($1s^2$) by H^+ into any excited hydrogen state of H($n^f l^f m^f$)

The cross sections are computed in the prior version of the CB1-4B method by using the two-parameter wave function of Silverman *et al.* [46] for the ground state of the helium atom: $\varphi_i(\vec{x}_1,\vec{x}_2) = (N/\pi)(e^{-\alpha_1 x_1-\alpha_2 x_2}+e^{-\alpha_2 x_1-\alpha_1 x_2})$, where $N^{-2} = 2[(\alpha_1\alpha_2)^{-3}+(\alpha_1/2+\alpha_2/2)^{-6}]$. Specifically, we will apply the formulas from Sec. II B to the following near-symmetric charge-exchange reactions:

$$p + \mathrm{He} \longrightarrow \mathrm{H}(n^f l^f m^f) + \mathrm{He}^+(1s), \tag{65}$$

$$\mathrm{Li}^{3+} + \mathrm{He} \longrightarrow \mathrm{Li}^{2+}(n^f l^f m^f) + \mathrm{He}^+(1s). \tag{66}$$

The present state-selective cross sections for reaction (65) within the energy range $20 \leqslant E \leqslant 1000$ keV are displayed in Table I as well as Figs. 1–3. The cross sections for electron capture into the $2s$ and $2p$ states are compared with the available experimental data in Fig. 1, whereas those for

TABLE I. Cross sections (in cm^2) as a function of proton incident energy (in keV) for state-selective capture as well as for capture from He($1s^2$) into all the final states of atomic hydrogen according to process (1). The column labeled $n^f l^f m^f$ refers to the state-selective (or partial) cross sections $Q_{n^f l^f m^f}$ and $Q_{n^f l^f}$ for reaction (65). The row denoted "Total" represents the cross sections summed over all the bound states of the H($n^f l^f m^f$) atom by using Eq. (67). The notation $X[-N]$ implies $X \times 10^{-N}$.

	E (keV)					
$n^f l^f m^f$	20	30	50	75	100	150
100	4.21[−16]	2.45[−16]	1.02[−16]	4.24[−17]	2.06[−17]	6.49[−18]
200	2.24[−17]	1.81[−17]	1.05[−17]	5.10[−18]	2.65[−18]	8.71[−19]
210	3.75[−17]	1.98[−17]	7.64[−18]	2.94[−18]	1.29[−18]	3.25[−19]
211	1.52[−18]	9.31[−19]	5.29[−19]	2.54[−19]	1.23[−19]	3.38[−20]
$2p$	4.05[−17]	2.17[−17]	8.70[−18]	3.45[−18]	1.53[−18]	3.93[−19]
300	5.55[−18]	4.73[−18]	2.94[−18]	1.49[−18]	7.87[−19]	2.61[−19]
310	1.09[−17]	6.08[−18]	2.46[−18]	9.84[−19]	4.40[−19]	1.13[−19]
311	4.35[−19]	2.63[−19]	1.57[−19]	8.02[−20]	4.01[−20]	1.14[−20]
$3p$	1.18[−17]	6.61[−18]	2.78[−18]	1.14[−18]	5.20[−19]	1.36[−19]
320	1.03[−18]	5.41[−19]	1.76[−19]	5.81[−20]	2.27[−20]	4.69[−21]
321	9.24[−20]	4.56[−20]	2.07[−20]	9.55[−21]	4.35[−21]	1.02[−21]
322	5.07[−21]	2.76[−21]	1.76[−21]	9.18[−22]	4.34[−22]	1.05[−22]
$3d$	1.23[−18]	6.38[−19]	2.21[−19]	7.90[−20]	3.22[−20]	6.94[−21]
400	2.20[−18]	1.91[−18]	1.22[−18]	6.27[−19]	3.32[−19]	1.11[−19]
410	4.56[−18]	2.58[−18]	1.06[−18]	4.30[−19]	1.94[−19]	5.02[−20]
411	1.81[−19]	1.09[−19]	6.59[−20]	3.43[−20]	1.74[−20]	4.98[−21]
$4p$	4.92[−18]	2.79[−18]	1.19[−18]	4.99[−19]	2.29[−19]	6.02[−20]
420	5.65[−19]	3.05[−19]	1.01[−19]	3.39[−20]	1.34[−20]	2.79[−21]
421	5.06[−20]	2.53[−20]	1.16[−20]	5.44[−21]	2.51[−21]	6.00[−22]
422	2.77[−21]	1.50[−21]	9.59[−22]	5.15[−22]	2.48[−22]	6.08[−23]
$4d$	6.72[−19]	3.59[−19]	1.26[−19]	4.58[−20]	1.89[−20]	4.11[−21]
430	1.32[−20]	7.15[−21]	2.05[−21]	5.91[−22]	2.08[−22]	3.56[−23]
431	2.13[−21]	1.02[−21]	3.63[−22]	1.52[−22]	6.39[−23]	1.26[−23]
432	2.38[−22]	1.14[−22]	5.75[−23]	2.89[−23]	1.29[−23]	2.63[−24]
433	1.30[−23]	6.58[−24]	4.31[−24]	2.32[−24]	1.05[−24]	2.16[−25]
$4f$	1.80[−20]	9.44[−21]	2.90[−21]	9.57[−22]	3.63[−22]	6.66[−23]
Total	5.23[−16]	3.10[−16]	1.34[−16]	5.67[−17]	2.76[−17]	8.60[−18]
	200	300	500	750	1000	
100	2.59[−18]	6.16[−19]	8.05[−20]	1.34[−20]	3.45[−21]	
200	3.51[−19]	8.39[−20]	1.09[−20]	1.79[−21]	4.56[−22]	
210	1.06[−19]	1.82[−20]	1.49[−21]	1.66[−22]	3.18[−23]	
211	1.14[−20]	2.03[−21]	1.68[−22]	1.88[−23]	3.59[−24]	
$2p$	1.29[−19]	2.23[−20]	1.83[−21]	2.04[−22]	3.89[−23]	
300	1.06[−19]	2.53[−20]	3.27[−21]	5.37[−22]	1.36[−22]	
310	3.73[−20]	6.43[−21]	5.28[−22]	5.88[−23]	1.12[−23]	
311	3.91[−21]	7.02[−22]	5.88[−23]	6.60[−24]	1.26[−24]	
$3p$	4.51[−20]	7.84[−21]	6.45[−22]	7.20[−23]	1.38[−23]	
320	1.29[−21]	1.70[−22]	9.42[−24]	7.47[−25]	1.10[−25]	
321	2.97[−22]	4.06[−23]	2.30[−24]	1.82[−25]	2.68[−26]	
322	3.04[−23]	4.09[−24]	2.23 [−25]	1.71[−26]	2.46[−27]	
$3d$	1.95[−21]	2.59[−22]	1.45[−23]	1.15[−24]	1.69[−25]	
400	4.49[−20]	1.07[−20]	1.38[−21]	2.27[−22]	5,79[−23]	
410	1.66[−20]	2.87[−21]	2.35[−22]	2.63[−23]	5.01[−24]	
411	1.72[−21]	3.11[−22]	2.61[−23]	2.93[−24]	5.61[−25]	
$4p$	2.00[−20]	3.49[−21]	2.88[−22]	3.21[−23]	6.13[−24]	
420	7.73[−22]	1.02[−22]	5.66[−24]	4.49[−25]	6.64[−26]	
421	1.76[−22]	2.41[−23]	1.37[−24]	1.09[−25]	1.61[−26]	
422	1.79[−23]	2.42[−24]	1.33[−25]	1.02[−26]	1.47[−27]	
$4d$	1.16[−21]	1.55[−22]	8.68[−24]	6.88[−25]	1.01[−25]	
430	8.36[−24]	8.43[−25]	3.21[−26]	1.83[−27]	2.11[−28]	
431	3.13[−24]	3.27[−25]	1.26[−26]	7.17[−28]	8.18[−29]	
432	6.56[−25]	6.83[−26]	2.56[−27]	1.41[−28]	1.57[−29]	
433	5.37[−26]	5.49 [−27]	1.99[−28]	1.06[−29]	1.16[−30]	
$4f$	1.60[−23]	1.65[−24]	6.30[−26]	3.57[−27]	4.09[−28]	
Total	3.39[−18]	7.92[−19]	1.01[−19]	1.67[−20]	4.26[−21]	

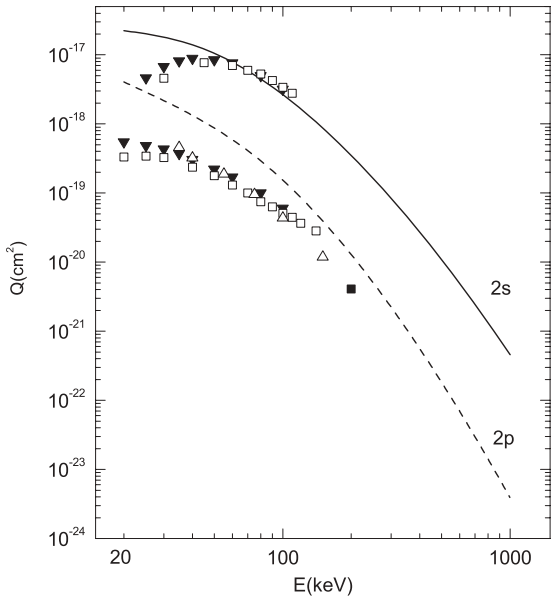

FIG. 1. State-selective cross sections Q_{2s} and Q_{2p} for electron capture by protons from He($1s^2$). The curves represent the theoretical results obtained using the CB1-4B method (present computations). Experimental data: ▼, (Q_{2s}, Q_{2p}) Cline *et al.* [47]; □, (Q_{2s}, Q_{2p}) Hughes *et al.* [48]; △, (Q_{2p}) Hippler *et al.* [49]; and ■, (Q_{2p}) Hippler *et al.* [50]. Both the theoretical and experimental results for Q_{2p} are divided by 10.

capture into $3s$, $3p$, and $3d$ states are depicted in Fig. 2. In Fig. 3, in addition to capture into the H($4s$) state, in which case the experimental data exist, we also show, for completeness,

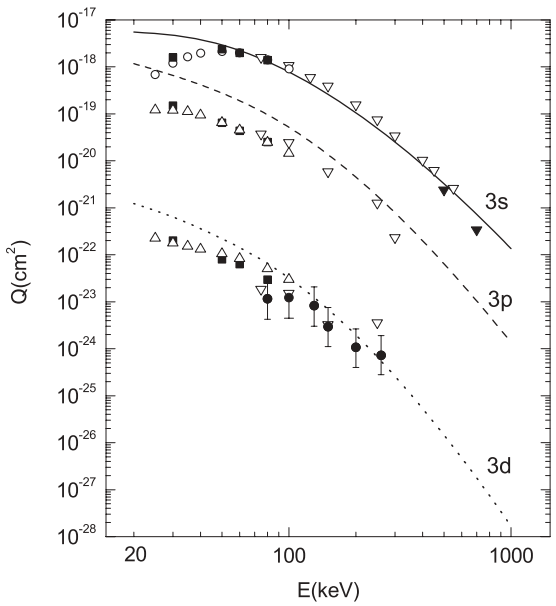

FIG. 2. State-selective cross sections Q_{3s}, Q_{3p}, and Q_{3d} for electron capture by protons from He($1s^2$). The curves represent the theoretical results using the CB1-4B method (present computations). Experimental data: ▼, (Q_{3s}) Conrads *et al.* [51], ○, (Q_{3s}) Cline *et al.* [47]; ▽, (Q_{3s}, Q_{3p}, Q_{3d}) Ford and Thomas [52]; ■, (Q_{3s}, Q_{3p}, Q_{3d}) Brower and Pipkin [53]; △, (Q_{3p}, Q_{3d}) Cline *et al.* [54]; and •, Edwards and Thomas [55]. Both the theoretical and experimental results for Q_{3p} and Q_{3d} are divided by 10 and 1000, respectively.

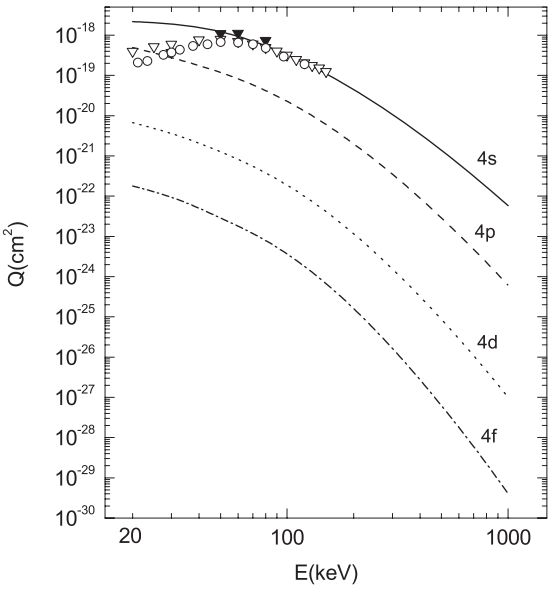

FIG. 3. State-selective cross sections Q_{4s}, Q_{4p}, Q_{4d}, and Q_{4f} for electron capture by protons from He($1s^2$). The curves represent the theoretical results obtained using the CB1-4B method (present computations). Experimental data: ▽, (Q_{4s}) Doughty *et al.* [56]; ▼, (Q_{4s}) Brower *et al.* [53]; and ○, (Q_{4s}) Hughes *et al.* [57]. Theoretical results for Q_{4p} are divided by 10, whereas those for Q_{4d} and Q_{4f} are divided by 100.

the computed cross sections describing the formation of the H($4p$), H($4d$), and H($4f$) states. It can be seen from Figs. 1–3 that the present results for capture into the H($2s$), H($3s$), and H($4s$) states systematically exhibit excellent agreement at all energies above 60 keV. A comparison of results of the CB1-4B method with the measurements for capture into H($2p$) and H($3p$) shows that the theoretical curves slightly overestimate the experimental data. Nevertheless, it is clear that the CB1-4B theory converges towards the experimental data as the impact energy increases, i.e., within the main region of the anticipated validity of this method. The theoretical results for capture into H($3d$) overestimate the experimental data at lower impact energies, but for higher energies the CB1-4B method is in a fairly good agreement with the measurements.

The total cross sections $Q_{\rm tot}$ for capture summed over the final states of atomic hydrogen according to the Oppenheimer $(n^f)^{-3}$ scaling law,

$$Q_{\rm tot} \simeq Q_1 + Q_2 + Q_3 + 2.561\,24 Q_4, \tag{67}$$

where

$$Q_{n^f} = \sum_{l^f=0}^{n^f-1} Q_{n^f l^f}, \quad Q_{n^f l^f} = \sum_{m^f=-l^f}^{+l^f} Q_{n^f l^f m^f}, \tag{68}$$

are shown in Fig. 4 alongside experimental data from a number of measurements. The total cross sections of the CB1-4B approximation are seen to be in very good agreement with all the available measurements in an energy range which remarkably covers nearly three orders of magnitude.

The employed Oppenheimer $(n^f)^{-3}$ scaling law was originally introduced within the OBK1 approximation [18]. However, this practical procedure is not limited to the OBK1

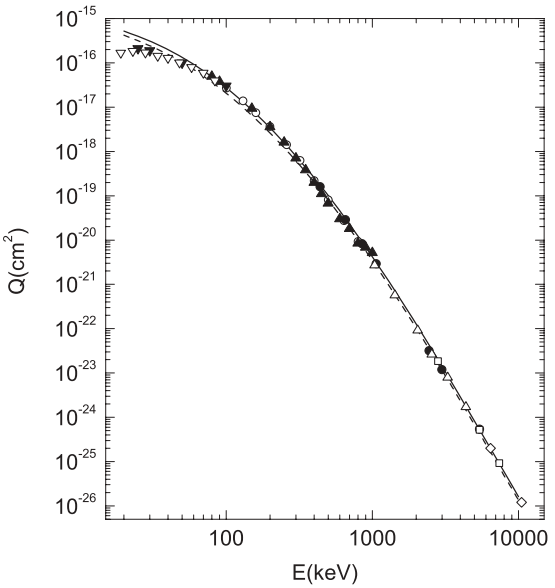

FIG. 4. Total cross sections for electron capture into all the final states H(Σ) from the ground state of helium by protons: $p + \mathrm{He}(^1S) \longrightarrow \mathrm{H}(\Sigma) + \mathrm{He}^+(1s)$. The full curve shows the results for $Q_{\mathrm{tot}} \simeq Q_1 + Q_2 + Q_3 + 2.561\,24 Q_4$ that are from the present computations by means of the CB1-4B approximation. The dashed curve represents $Q_{1s} \equiv Q_1$ from the CB1-4B method. Experimental data: ▽, Shah *et al.* [58]; △, Schryber [59]; ○, Shah and Gilbody [60]; □, Horsdal-Pedersen *et al.* [61]; ◇, Berkner *et al.* [62]; ▲, Williams [63]; ▼, Martin *et al.* [64]; and ●, Welsh *et al.* [65].

model alone. Namely, a number of related studies [10,11,13] have indicated that the Oppenheimer rule is also valid in the CB1-3B approximation. Moreover, this is further confirmed by the present computations using the CB1-4B method. Specifically, our computations were stopped when the total cross sections Q_{tot} became insensitive to the inclusion of more partial cross sections Q_{n^f}. This was the case with $n^f = 4$, as illustrated in Table II for four impact energies: 20, 100, 1000, and 10 000 keV. As can be seen from Table II, inclusion of the higher partial cross sections Q_5 and Q_6 does not influence Q_{tot} which is computed explicitly for $n^f \leqslant 4$ and augmented by the Oppenheimer sum for all the higher excited states. It should be noted that Melezhik *et al.* [66] have also found it useful to employ the Oppenheimer procedure for studying the convergence properties of the quantum time-dependent

TABLE II. Cross sections (in cm^2) for the p-He collisions (1). The $Q_{\mathrm{tot}}(\Sigma_4)$ are calculated by means of Eq. (67), whereas $Q_{\mathrm{tot}}(\Sigma_5) = Q_1 + Q_2 + Q_3 + Q_4 + 3.0493 Q_5$ and $Q_{\mathrm{tot}}(\Sigma_6) = Q_1 + Q_2 + Q_3 + Q_4 + Q_5 + 3.5412 Q_6$. Notation $X[-N]$ implies $X \times 10^{-N}$.

E(keV)	20	100	1000	10000
Q_4	7.80[−18]	5.80[−19]	6.41[−23]	1.99[−28]
$Q_{\mathrm{tot}}(\Sigma_4)$	5.23[−16]	2.76[−17]	4.26[−21]	1.62[−26]
Q_5	3.99[−18]	3.01[−19]	3.27[−23]	9.89[−29]
$Q_{\mathrm{tot}}(\Sigma_5)$	5.23[−16]	2.76[−17]	4.26[−21]	1.62[−26]
Q_6	2.30[−18]	1.75[−19]	1.89[−23]	5.74[−29]
$Q_{\mathrm{tot}}(\Sigma_6)$	5.23[−16]	2.76[−17]	4.26[−21]	1.62[−26]

approach with semiclassical trajectories for stripping processes (including ionization and electron transfer) as well as for excitation in collisions between helium and protons.

The existing experimental data for $Q_{n^f l^f}$ are not directly related to process (65), but instead correspond to $p + \mathrm{He} \longrightarrow \mathrm{H}(n^f l^f) + [\mathrm{He}^+]$, where the square brackets indicate that no information is available on the postcollisional state of the He^+ ion. This means that for a strict comparison with measurements, theories must allow for all possible contributions arising from transitions of the noncaptured electron in the He^+ ion. Earlier computations [67] in the framework of the first Born approximation have shown that the inclusion of the excited states of He^+ does not increase the capture cross sections by more than 5%. The present results support these estimates, indicating that $Q_{2s} > Q_{2p_0}$, $Q_{3s} > Q_{3p_0}$, and $Q_{4s} > Q_{4p_0}$ at energies $E \geqslant 50$ keV, as well as $Q_{2p_0} > Q_{2p_{\pm1}}$, $Q_{3p_0} > Q_{3p_{\pm1}}$, and $Q_{4p_0} > Q_{4p_{\pm1}}$ at all the considered energies. All the shown theoretical cross sections are for total cross sections, but our general program developed for the reported computation can also provide differential cross sections for the cases when $Z_{\mathrm{P}} = 1$ or $Z_{\mathrm{T}} = 2$. It would also be very important to extend the CB1-4B method to encompass the excited states of the residual hydrogenic ion, which is the remainder of the target. This could help clarify the existing huge disagreement between experiment and a four-body distorted-wave theory for simultaneous charge exchange and target excitation in proton-helium collisions at intermediate impact energies [39]. Recently, differential cross sections were reported for electron transfer in proton-helium collisions at 630, 1000, and 1200 keV with a sufficient resolution to distinguish certain final electronic states [68]. These results were obtained by means of the cold-target recoil-ion momentum spectroscopy technique (COLTRIMS) and a spectrometer optimized for high momentum resolution. Specifically, the COLTRIMS technique can measure the recoil-ion momentum in coincidence with the charge state of the projectile ion in the exit collisional channel. These coincidences were utilized to separate various capture channels, while the recoil-ion momentum was used to obtain the energy defect or the earlier mentioned Q value and the angular distributions. Such Q values were subsequently employed to identify the populated states of these channels and the angular distributions that helped identify the capture mechanisms. At the projectile energies 630, 1000, and 1200 keV, this experiment [68] revealed that for the electronic states of the single-capture process $p + \mathrm{He} \rightarrow H(n) + \mathrm{He}^+(n')$, with simultaneous target excitation ($n = 1, n' \geqslant 2$), the branching ratio was 3.9%, 4.7%, and 5.2%, respectively. Conclusions of this type have also been reached by Alessi *et al.* [69–71] in their similar recent measurements using the same COLTRIMS technique.

B. Electron capture from $\mathrm{He}(1s^2)$ by Li^{3+} into any excited hydrogenlike state of $\mathrm{Li}^{2+}(n^f l^f m^f)$

Along the lines of Sec. III A and using the same formulas from Sec. II B, we shall also examine electron capture from $\mathrm{He}(1s^2)$ by Li^{3+} in the energy range from 50 to 5000 keV/amu. The obtained results are shown in Fig. 5. The present cross sections from the CB1-4B method are in excellent agreement with the measurements [60,72–74]. In the same figure, the

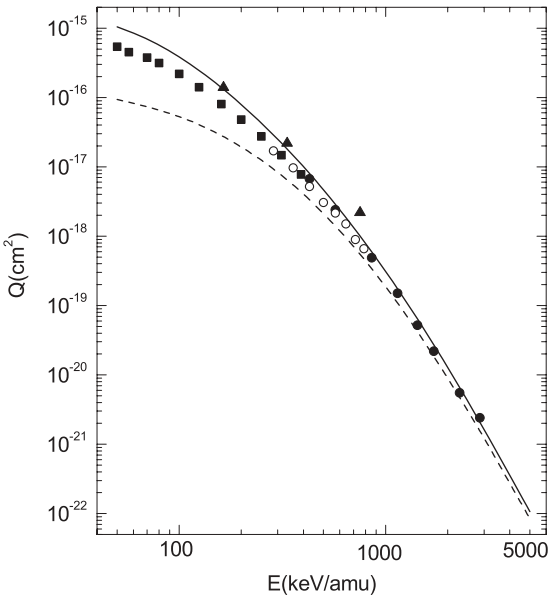

FIG. 5. Total cross sections for electron capture into all the final states $Li^{2+}(\Sigma)$ from the ground state of helium by Li^{3+} ions: $Li^{3+} + He(^1S) \longrightarrow Li^{2+}(\Sigma) + He^+(1s)$. The full curve shows the results for $Q_{tot} \simeq Q_1 + Q_2 + Q_3 + 2.561\,24 Q_4$ that are presently computed by means of the CB1-4B approximation. The dashed curve represents $Q_{1s} \equiv Q_1$ from the CB1-4B method. Experimental data: ■, Shah and Gilbody [60]; ●, Woitke *et al.* [72]; ○, Sant'Anna *et al.* [73]; and ▲, Dmitriev *et al.* [74].

cross sections for capture into the $1s$ state are depicted. As expected, the contribution from the excited states is more significant at lower than at higher impact energies.

C. Relevance of the present methodology to interdisciplinary applications

The formalism of the present work can find useful applications in particle transport physics for computations of energy losses of heavy ions during their passage through matter, as needed in, e.g., fusion research and radiotherapy for cancer treatment [27]. For example, in therapy by energetic light ions, the present general results with the Slater-type orbitals can be extended to encompass electron capture from molecular targets to further the recent generalization of the CB1 method to tissuelike targets, such as water [75–78]. Detailed stochastic simulations of energy losses of ions during their passage through matter, including tissue and tissuelike media, is customarily carried out by various Monte Carlo (MC) codes, as discussed in, e.g., Refs. [27,79,80]. Every MC code requires the input cross sections for binary atomic and nuclear collisions. Moreover, the overall trust in and adequacy of the MC simulations depend critically on the accuracy and reliability of these input cross sections. Once equipped with the input cross sections, the existing MC codes can begin to produce the sought event histograms through statistical assessments of energy losses of the given incident, primary particles as well as their secondaries and tertiaries and particles of high-order generation. The MC simulations effectively approximate true transport of ions through matter. Here, the prescribed event threshold for discriminating among various channels is used to predict whether the interaction at a considered point in space for the available energy would lead to nuclear transmutations or other types of nuclear reaction or to atomic transitions (excitation, electron capture, ionization, or other atomic processes) through which energy loss of all the involved particles could occur. In MC algorithms, specific particle interactions could be examined through, e.g., the ratios of various input cross sections. Evidently, there cannot be any substantial progress in studying ion transport phenomena by MC modeling without heavy reliance upon the most accurate databases for cross sections. These should preferentially come from first-principle theories for atomic and nuclear collisions that determine the stopping powers for ions in their penetration through matter. Hence, an important improvement in theoretical descriptions of the traversal of fast heavy ions through matter would be to incorporate the cross sections and stopping powers from the pertinent atomic collisions into all the existing MC codes. The most relevant part in these energy loss simulations, where the methodology from the present study would be of direct use, is the contribution to the databases for electron capture into excited states by multiply charged ions. Capture cross sections attain their maxima near the Massey resonance condition $Z_P \approx n^f$, such that for higher nuclear charges Z_P of the projectile, the major contribution stems from excited states with larger values of the principal quantum number n^f. Such collisional events with excited-state capture become very important when the fast, multiply charged ions from the entrance to the medium slow down considerably near the Bragg peak, at which location the major energy is deposited, yielding the main biological effect on the irradiated tissue. Hence, in addition to ionization and excitation, near the end of the ions' paths (the so-called range), electron capture and electron loss become competitive channels for energy deposition in the traversed matter. Prior to reaching their range in the immediate vicinity of the Bragg peak, ions readily capture electrons, only to promptly lose them via electron loss processes. Before being eventually brought to rest, such conversions from partially or fully dressed ions to partially or completely stripped projectiles occur literally thousands of times close to the Bragg peak. Such pre-equilibrium phenomena are capable of significantly altering the overall energy balance and energy losses of radiotherapeutic ions in tissue. For this special application, it is important to have reliable databases for excited-state electron capture involving light-ion projectiles ($Z_P \leqslant 8$) that are currently used in hospital-based accelerator facilities in several countries worldwide [27]. The corrected first Born approximation from the present work would adequately deal with this particular need. The same theoretical databases are also necessary for evaluation of the overall energy balance in processes involving charge exchange studied within plasma physics, astrophysics, and fusion research. For instance, one of the major obstacles to ion plasma stability is ion neutralization through electron capture. To remove such causes of instability, one needs to eliminate substances from the ion plasma environment that have the largest cross section for charge exchange, which predominantly occurs into excited states for multiply charged ions. Here too the present general program for the CB1-4B method can come to the rescue. It is important that the remarkable computational efficiency of

our program with triple quadratures for total cross sections is of great relevance for the said MC simulations that need fast sampling from the supplied cross-section expressions. This is in sharp contrast to the corresponding ten-dimensional numerical integrations from the four-body distorted-wave method from Refs. [29,38,39].

IV. CONCLUSIONS

The high-energy four-body first Born approximation with the correct boundary conditions (CB1-4B) is a consistently designed first-order perturbation theory for charge exchange, starting from the basic principles of atomic scattering [31,32]. Here, the word "consistent" implies that the unperturbed channel states and the perturbing potentials are determined in accordance with the Coulomb boundary conditions for two charged aggregates, which are widely separated [31,32]. Previous examinations in this method were limited exclusively to the ground state of the captured electron $\{n^f,l^f,m^f\} = \{1,0,0\}$. Considering single-electron capture from heliumlike targets by bare projectiles, the present study goes beyond such restrictions and extends the computational feasibility of the CB1-4B method to any possible triple of the final-state hydrogenlike quantum numbers $\{n^f,l^f,m^f\}$. With this goal, we have carried out an analytical reduction of the original nine-dimensional integral for the transition amplitude to a straightforward and efficient two-dimensional numerical quadrature over real variables that are left after the Feynman parametrization of the usual two denominators encountered in the momentum-space analysis. No further integration is needed for differential cross sections. Total cross sections necessitate an additional numerical quadrature over the transverse component of the momentum transfer.

A general computer program was written based on the obtained semianalytical expressions for arbitrary nuclear charges of the completely stripped projectile and two-electron atomic or ionic targets. This program is presently used to compute total cross sections for electron capture into the atomic hydrogen states $H(n^f l^f)$ by fast protons from helium. The theoretical results obtained are compared with the related experimental data that are available for several state-selective transitions, as well as for electron capture into all the final states $H(\Sigma)$. It is observed that the CB1-4B method systematically predicts very well the corresponding findings from measurements. The same method is also applied to single-charge exchange in fast collisions of Li^{3+} ions with helium, and the ensuing total cross sections are reported to agree very well with experimental data in a wide range of impact energies. This is encouraging and it motivates a further extension of the CB1-4B method to two-electron transitions with simultaneous electron capture and excitation of the remaining hydrogenlike target in proton-helium collisions. Such a generalization is particularly needed in light of the current discrepancy between experiments and a four-body distorted-wave method.

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APPENDIX

For completeness and definiteness regarding different existing phase conventions, the complex-valued spherical harmonics used in the derivation in the main text are of the same form as in Ref. [11]: $Y_{l,m}(\theta,\phi) = \mathcal{P}_{l,m}(\cos\theta)\Phi_m(\phi)$, where $\Phi_m(\phi) = e^{im\phi}/\sqrt{2\pi}$. Here, $\mathcal{P}_{lm}$ is the associated normalized Legendre function of the first kind:

$$\mathcal{P}_{l,m}(z) = (-1)^m \sqrt{\frac{2l+1}{2}\frac{(l-m)!}{(l+m)!}}(1-z^2)^{m/2} \times \left(\frac{d}{dz}\right)^{l+m}\frac{(z^2-1)^l}{2^l l!}, \tag{A1}$$

with the magnetic quantum number symmetry $\mathcal{P}_{l,-m}(z) = (-1)^m\mathcal{P}_{l,m}(z)$ and $Y_{l,-m}(z) = (-1)^m Y^*_{l,m}(z)$. The right-hand side of Eq. (A1) is well defined for $l+m \geqslant 0$, i.e., $m \geqslant -l$. Therefore, Eq. (A1) holds true for both positive and negative values of m where $-l \leqslant m \leqslant l$.

The associated normalized Legendre function of the first kind can be expressed via the associated Legendre function $P_{l,m}(z) = (1-z^2)^{m/2}(d/dz)^{l+m}[(z^2-1)^l/2^l l!]$:

$$\mathcal{P}_{l,m}(z) = (-1)^m\sqrt{\frac{2l+1}{2}\frac{(l-m)!}{(l+m)!}}P_{l,m}(z). \tag{A2}$$

These definitions of polynomials $P_{l,m}$ and $\mathcal{P}_{l,m}$ are valid for zero, positive, and negative integer values of m, where $|m| \leqslant l$. Moreover, the polynomials $P_{l,-m}$ and $P_{l,m}$, which satisfy the same differential equation, differ only by a constant multiplier through the relationship [43]

$$P_{l,-m}(z) = (-1)^m\frac{(l-m)!}{(l+m)!}P_{l,m}(z). \tag{A3}$$

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