Intermediate ionization continua for double charge exchange at high impact energies

Dževad Belkić
Manne Siegbahn Institute of Physics, S-104 05 Stockholm, Sweden
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We investigate the problem of two-electron capture from heliumlike atomic systems by bare nuclei $Z_P+(Z_T;e_1,e_2)_i \rightarrow (Z_P;e_1,e_2)_f+Z_T$ at high incident energies, using the four-body formalism of the first- and second-order theories. Our goal is to establish the relative importance of the *intermediate* ionization continua of the two electrons in comparison with the usual *direct* path of the double electron transfer. For this purpose we presently introduce the boundary-corrected continuum-intermediate-state (BCIS) approximation, which preserves all the features of two-electron capture as a genuine four-body problem. The proposed second-order theory provides a fully adequate description of the fact that, in an intermediate stage of collision, both electrons move in the field of the two Coulomb centers. The previously devised boundary-corrected first Born (CB1) approximation can be obtained as a further simplification of the BCIS model if the invoked two-electron Coulomb waves are replaced by their long-range logarithmic phase factors defined in terms of the corresponding interaggregate separation R. The BCIS method is implemented on the symmetric resonant double charge exchange in collisions between α particles and He($1s^2$) at impact energies $E \geq 900$ keV. The obtained results for the differential and total cross sections are compared with the available experimental data and satisfactory agreement is recorded. As the incident energy increases, a dramatic improvement is obtained in going from the CB1 to the BCIS approximation, since the latter closely follows the measurement, whereas the former overestimates the observed total cross sections by two orders of magnitude.

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I. INTRODUCTION

Double charge exchange in collisions between bare nuclei and heliumlike atomic systems has been the subject of numerous theoretical investigations at intermediate and high impact energies. Most of the previous studies proceed through the use of McGuire and Weaver's [1] independent-particle model (IPM) [2–16], in which the interelectron Coulomb interaction is replaced by an appropriate average field, such as the well-known Roothaan-Hartree-Fock atomic model potential [17,18]. The essence of the IPM is in treating double charge exchange as two independent single-electron transfers. This implies that the overall transition probability for the total event is reduced to the product of the two partial probabilities for each of the invoked electrons. Such a model ignores some of the finest physical effects, namely, electronic correlations which make the double charge transfer fundamentally different from the single-electron capture process [19]. Electron correlation effects can be roughly incorporated within Crothers and McCarroll's [20–23] independent *event* model which, however, still determines the total probability as the product of the two individual probabilities.

A substantially different approach to the problem of high-energy two-electron transfer has recently been undertaken by Belkić and Mančev [24,25], who introduced the four-body extension of Cheshire's [26] second-order continuum-distorted-wave (CDW) method. This CDW theory is a strict generalization of the single charge exchange formalism to double-electron transfer with no further approximations and without recourse to the IPM nor to the probability product theorem. The CDW approximation of Refs. [24,25] naturally incorporates the usual *static* as well as *dynamic* correlation effects and preserves the correct boundary conditions. Such a four-body CDW model is found to yield excellent agreement with the experimental data on total cross sections for H^- formation in H^+-He double-electron transfer [24,25]. Another second-order distorted-wave model of the impulse approximation type has been proposed by Gravielle and Miraglia [27]. Their approximation also takes full account of the electronic correlation effects and the product of single-electron probabilities is not imposed as the starting point of the development. It should be remarked, however, that despite the fact that the methods of Refs. [24,25,27] go beyond the IPM by resorting to the four-body distorted-wave formalism, only the CDW theory possesses the total scattering wave functions with adequate asymptotic behaviors at large interaggregate separations. We recall that the impulse approximation always violates the correct boundary conditions and this is particularly true for the channel in which it explicitly allows for the continuum intermediate states [28] for both single [29] and double charge exchange [27].

Much more than single-electron capture, two-electron transfer requires inclusion of the second- and higher-order effects via double or multiple scattering phenomena at high energies. This is because (i) the high-energy cross sections for double charge exchange are considerably smaller than the corresponding data for single-electron capture, so that any (even small) deficiency of theories is expected to induce significant errors in the final results. In addition, (ii) unlike the single-electron capture from

heliumlike atoms or ions by completely stripped projectiles, double charge exchange in the same collisional systems always promotes *two* active electrons, for which more variants of the double Thomas scattering could actually take place [30] as the incident velocity is augmented. This couple of arguments leads us to the conclusion that the first-order theories for two-electron transfer should have a sizably smaller upper energy limit of their applicability than in the case of single charge exchange. According to the well-documented evidence concerning the one-electron capture processes, the total cross sections obtained by means of the boundary-corrected first Born (CB1) approximation [31–49] have been observed to be systematically in excellent agreement with the measurements at intermediate (≥ 100 keV/amu) and high energies but, of course, below the region where the Thomas double scattering becomes important. Due to reason (i) above we expect that for double charge exchange, the breakdown of the first-order perturbation theories should occur even at those higher impact energies for which the Thomas double scattering is negligible. Indeed, the four-body CB1 approximation introduced by Belkić [50,51] revealed that this first-order theory is fully satisfactory only in a limited intermediate-energy range, hence the need for the introduction of second-order theories for double charge exchange. The CDW approximation does not transparently separate the contributions coming from the first- and second-order effects. The four-body generalization of the boundary-corrected second Born (CB2) approximation from single [52–56] to double charge exchange would be a highly recommended method which could tell us, in a perfectly clear manner, about the relative importance of the neatly separated first- and second-order terms. However, such a CB2 model is very difficult to implement without obligatorily resorting to statistical methods of the Monte Carlo type [57,58], which would require a tremendously large amount of (industrial) CPU computer time. Therefore, it is important to devise a theory which would overcome the above limitations of the CDW and CB2 model by (1) transparently incorporating first- as well as second-order effects and (2) providing a relatively easy framework for numerical computations. This is achieved in the present work, where the boundary-corrected continuum-intermediate-state (BCIS) approximation is developed. From the computational point of view, the BCIS method is as easy as the CDW approach, since in both cases the transition amplitudes are reduced to the readily obtainable triple numerical quadratures in impulse space. On the other hand, an inspection of the transition probabilities in the BCIS and CB1 methods reveals that they both have *the same* perturbation potentials. Furthermore, the total scattering wave functions of the BCIS and CB1 models are the same in *one* of the asymptotic channels (entrance or exit, depending upon whether we are considering the *prior* or *post* form of the transition amplitudes). The only difference is, however, in the other channel since the BCIS method employs the electronic continuum intermediate (Coulomb) wave functions centered on the projectile or target nucleus. A product of two such full Coulomb waves each containing explicit *electronic* coordinates always appears in the BCIS model. As a further simplification of the BCIS theory, we can formally obtain the CB1 method in which the product of the Coulomb waves is replaced by its appropriate logarithmic phase factors, but in the vector variable $\mathbf{R}$ of the interaggregate separation. Hence, any difference found between the results of the CB1 and BCIS theories ought to be directly attributed to the importance of the *full* Coulomb electronic continuum intermediate states. Whether such a difference could also be numerically relevant is another question, which will be answered in the present study by providing comparisons between the theory and experiment.

Atomic units will be used throughout unless stated otherwise.

II. THEORY

We examine a collision in which the nucleus P of charge Z_P is impinging upon a heliumlike atomic system consisting of two electrons e_1 and e_2 bound to the nucleus T of charge Z_T, i.e.,

$$Z_P+(Z_T;e_1,e_2)_i \rightarrow (Z_P;e_1,e_2)_f+Z_T \ . \tag{2.1}$$

The parentheses in the double-charge-exchange process (2.1) symbolize the bound state, whose quantum numbers are given by the collective label i or f. Let us denote by $\mathbf{R}$ the position vector of P relative to T. Further, the position vectors of $e_{1,2}$ relative to P, T and the middle point of the internuclear axis R will respectively be represented by $\mathbf{s}_{1,2}$, $\mathbf{x}_{1,2}$, and $\mathbf{r}_{1,2}$, so that the interelectron distance r_{12} can be introduced by $r_{12}=|\mathbf{r}_1-\mathbf{r}_2|$, where $\mathbf{r}_{12}=\mathbf{x}_1-\mathbf{x}_2=\mathbf{s}_1-\mathbf{s}_2$. We adopt the well-known impact parameter formalism of the scattering theory, in which the relative internuclear motion is described by a classical rectilinear trajectory $\mathbf{R}=\boldsymbol{\rho}+\mathbf{v}t$, where t denotes time. The target nucleus T is assumed to be at rest, so that the constant relative velocity vector $\mathbf{v}$ will, in fact, be the incident speed. The so-called impact parameter ρ has its customary meaning, with the important constraint $\boldsymbol{\rho}\cdot\mathbf{v}=0$.

The full scattering states $\Psi_{if}^{\pm}(\mathbf{r}_1,\mathbf{r}_2;t)$ of the entire four-body system with outgoing or incoming boundary conditions are described by the time-dependent Schrödinger equation:

$$\left[H-i\frac{\partial}{\partial t}\right]\Psi_{i,f}^{\pm}(\mathbf{r}_1,\mathbf{r}_2;t)=0 \ , \tag{2.2a}$$

where $H=H_0+V$ is the total Hamiltonian given as the sum of the kinetic-energy operator H_0 and the complete interaction potential V:

$$\begin{aligned} H_0&=-\tfrac{1}{2}\nabla_{r_1}^2-\tfrac{1}{2}\nabla_{r_2}^2 \ , \\ V&=\frac{Z_PZ_T}{R}-\frac{Z_P}{s_1}-\frac{Z_P}{s_2}-\frac{Z_T}{x_1}-\frac{Z_T}{x_2}+\frac{1}{r_{12}} \ . \end{aligned} \tag{2.2b}$$

For rearrangement collisions such as the two-electron transfer process (2.1), it is useful to split the operator H into two equivalent forms: $H=H_i+V_i=H_f+V_f$, where

$H_{i,f}$ are the entrance and exit channel Hamiltonians, whereas $V_{i,f}$ represent the corresponding perturbation interactions:

$$H_i = H_0 + V_T \equiv H_0 - \frac{Z_T}{x_1} - \frac{Z_T}{x_2} + \frac{1}{r_{12}},$$
$$V_i = \frac{Z_P Z_T}{R} - \frac{Z_P}{s_1} - \frac{Z_P}{s_2}, \tag{2.3a}$$
$$H_f = H_0 + V_P \equiv H_0 - \frac{Z_P}{s_1} - \frac{Z_P}{s_2} + \frac{1}{r_{12}},$$
$$V_f = \frac{Z_P Z_T}{R} - \frac{Z_T}{x_1} - \frac{Z_T}{x_2}. \tag{2.3b}$$

The impact parameter dependent transition probability $\mathcal{P}_{if}^{\pm}(\boldsymbol{\rho})$ for the double-electron capture reaction (2.1) is defined as the square of the absolute value of the transition amplitudes $\mathcal{A}_{if}^{\pm}(\boldsymbol{\rho})$, i.e., $\mathcal{P}_{if}^{\pm}(\boldsymbol{\rho}) = |\mathcal{A}_{if}^{\pm}(\boldsymbol{\rho})|^2$. The quantities $\mathcal{A}_{if}^{\pm}(\boldsymbol{\rho})$ are given as the projection of the total wave functions $\Psi_{i,f}^{\pm}$ onto the final Φ_f^- or initial Φ_i^+ asymptotic states in the pertinent limit $t \to +\infty$ or $t \to -\infty$:

$$\mathcal{A}_{if}^{+}(\boldsymbol{\rho}) = \lim_{t \to +\infty} \langle \Phi_f^- | \Psi_i^+ \rangle = \lim_{t \to +\infty} \int\int d\mathbf{r}_1 d\mathbf{r}_2 \Phi_f^{-*}(\mathbf{r}_1, \mathbf{r}_2; t) \Psi_i^+(\mathbf{r}_1, \mathbf{r}_2; t), \tag{2.4a}$$

$$\mathcal{A}_{if}^{-}(\boldsymbol{\rho}) = \lim_{t \to -\infty} \langle \Psi_f^- | \Phi_i^+ \rangle = \lim_{t \to -\infty} \int\int d\mathbf{r}_1 d\mathbf{r}_2 \Psi_f^{-*}(\mathbf{r}_1, \mathbf{r}_2; t) \Phi_i^+(\mathbf{r}_1, \mathbf{r}_2; t). \tag{2.4b}$$

The initial and final asymptotic states $\Phi_{i,f}^{\pm}$ are introduced by [59]

$$\Phi_{i,f}^{\pm}(\mathbf{r}_1, \mathbf{r}_1; t) = \Phi_{i,f}(\mathbf{r}_1, \mathbf{r}_1; t) \mathcal{H}^{\pm}(\mathbf{R}), \tag{2.5a}$$

where $\mathcal{H}^{\pm}(\mathbf{R}) = \exp[\pm i \nu_i \ln(vR \mp v^2 t)]$ and

$$\Phi_{i,f}(\mathbf{r}_1, \mathbf{r}_1; t) = \varphi_{i,f}(\mathbf{x}_1, \mathbf{x}_2) e^{-i(E_{i,f} t + v^2 t/4 \pm \mathbf{v} \cdot \mathbf{r}_1/2 \pm \mathbf{v} \cdot \mathbf{r}_2/2)}, \tag{2.5b}$$

with $\nu_i = Z_P(Z_T - 2)/v$, $\nu_f = Z_T(Z_P - 2)/v$, and $v = |\mathbf{v}|$. In general, the *prior* $\mathcal{P}_{if}^{-}(\boldsymbol{\rho})$ and *post* $\mathcal{P}_{if}^{+}(\boldsymbol{\rho})$ forms of the transition probability are different from each other due to the unavailability of the exact bound state wave functions $\varphi_{i,f}$ for the two-electron systems. In a case study [50], appropriate corrections were introduced with the purpose of consistently defining the initial and final unperturbed channel states $\Phi_{i,f}$, irrespective of whether or not the bound state wave functions $\varphi_{i,f}$ satisfy the *exact* eigenvalue problems: $(H_i - E_i)\varphi_i(\mathbf{x}_1, \mathbf{x}_2) = 0$ and $(H_f - E_f)\varphi_f(\mathbf{s}_1, \mathbf{s}_2) = 0$, where E_i and E_f are the corresponding *exact* binding energies. These corrections appear in the transition amplitudes as certain perturbation potential operators, which are demonstrated [50] to provide corrections of the order of $\sim(10-15)\%$ and as such will be ignored in the present work. The asymptotic channel states $\Phi_{i,f}^{\pm}$ from (2.5a) are the solutions of the following equations:

$$\left[H_{i,f}^a - i \frac{\partial}{\partial t} \right] \Phi_{i,f}^{+}(\mathbf{r}_1, \mathbf{r}_2; t) = 0, \tag{2.6}$$

where $H_{i,f}^a = H_{i,f} + V_{i,f}^a$ with $V_{i,f}^a$ being the asymptotic $(R \to \infty)$ values of the perturbations $V_{i,f}$, i.e., $V_i^a = Z_P(Z_T - 2)/R$ and $V_f^a = Z_T(Z_P - 2)/R$.

We shall next introduce the distorted waves $\chi_{i,f}^{\pm}$ as a solution of the following differential equations:

$$\left[H_{i,f} - U_{i,f} - i \frac{\partial}{\partial t} \right] \chi_{i,f}^{\pm}(\mathbf{r}_1, \mathbf{r}_2; t) = 0, \tag{2.7a}$$

where $U_{i,f}$ are certain distorting potential operators, which must be chosen in accordance with the imposition of the correct boundary conditions,

$$\lim_{t \to \mp \infty} \chi_{i,f}^{\pm}(\mathbf{r}_1, \mathbf{r}_2; t) = \lim_{t \to \mp \infty} \Phi_{i,f}^{\pm}(\mathbf{r}_1, \mathbf{r}_2; t). \tag{2.7b}$$

It is then easily shown that the *post* transition amplitude $\mathcal{A}_{if}^{+}(\boldsymbol{\rho})$ can be written as

$$\mathcal{A}_{if}^{+}(\boldsymbol{\rho}) = -i \int_{-\infty}^{+\infty} dt \int\int d\mathbf{r}_1 d\mathbf{r}_2 [(V_f + U_f) \chi_f^{-}(\mathbf{r}_1; \mathbf{r}_2; t)]^* \times \Psi_i^+(\mathbf{r}_1, \mathbf{r}_2; t), \tag{2.8a}$$

provided that $\lim_{t \to -\infty} \int\int d\mathbf{r}_1 d\mathbf{r}_2 \chi_f^{-*} \Psi_i^+ = 0$. Similarly, the *prior* form $\mathcal{A}_{if}^{-}(\boldsymbol{\rho})$ of the transition amplitude becomes

$$\mathcal{A}_{if}^{-}(\boldsymbol{\rho}) = -i \int_{-\infty}^{+\infty} dt \int\int d\mathbf{r}_1 d\mathbf{r}_2 \Psi_f^{-*}(\mathbf{r}_1; \mathbf{r}_2; t) \times [(V_i + U_i) \chi_i^{+}(\mathbf{r}_1; \mathbf{r}_2; t)], \tag{2.8b}$$

if the following condition is fulfilled: $\lim_{t \to +\infty} \int\int d\mathbf{r}_1 d\mathbf{r}_2 \Psi_f^{-*} \chi_i^+ = 0$. The corresponding *post* and *prior* total cross sections are defined as follows:

$$Q_{if}^{\pm}(a_0^2) = \int d\boldsymbol{\rho} |\mathcal{A}_{if}^{\pm}(\boldsymbol{\rho})|^2. \tag{2.9}$$

In obtaining the transition amplitude $\mathcal{A}_{if}^{+}(\boldsymbol{\rho})$, we shall presently make the following approximation for the complete scattering wave function Ψ_i^+ and distorted wave χ_f^-:

$$\Psi_i^+(\mathbf{r}_1, \mathbf{r}_2; t) \approx \chi_i^+(\mathbf{r}_1, \mathbf{r}_2; t), \qquad \chi_f^-(\mathbf{r}_1, \mathbf{r}_2; t) \approx \Phi_f^-(\mathbf{r}_1, \mathbf{r}_2; t). \tag{2.10a}$$

The distorting potential U_f consistent with the choice (2.10a) is given by

$$U_f = -V_f^a. \tag{2.10b}$$

Next we look for the distorted waves $\chi_i^+(\mathbf{r}_1, \mathbf{r}_2; t)$ in the following simple factorized form:

$$\chi_i^+(\mathbf{r}_1, \mathbf{r}_2; t) = \Phi_i(\mathbf{r}_1, \mathbf{r}_2; t) \mathcal{L}_i^+. \tag{2.11a}$$

Upon inserting (2.11a) into Eq. (2.7a), it is at once seen that the function $\mathcal{L}_i^+$ satisfies the equation [59]

$$\left[\frac{1}{2}\nabla_1^2+\frac{1}{2}\nabla_2^2+\frac{Z_P}{s_1}+\frac{Z_P}{s_2}-\frac{Z_PZ_T}{R}+i\frac{\partial}{\partial t}-\frac{i}{2}\mathbf{v}\cdot\nabla_1-\frac{i}{2}\mathbf{v}\cdot\nabla_2+U_i\right]\mathcal{L}_i^+=0\ . \tag{2.11b}$$

The distorted wave χ_i^+ from (2.11a) will possess the correct asymptotic behavior (2.7b) if Eq. (2.11b) is solved subject to the boundary condition

$$\lim_{t\to-\infty}\mathcal{L}_i^+=\lim_{t\to-\infty}e^{-i[E_it+(1/4)v^2t+(1/2)\mathbf{v}\cdot\mathbf{r}_1+(1/2)\mathbf{v}\cdot\mathbf{r}_2-\nu_i\ln(vR-v^2t)]}\ . \tag{2.11c}$$

The present choice of the distorting potential U_i is identical to that of the four-body CDW approximation [24,25]:

$$U_i=-V_i+\sum_{j=1}^{2}\nabla_j\varphi_i(\mathbf{x}_1,\mathbf{x}_2)\cdot\nabla_j\circ\frac{1}{\varphi_i(\mathbf{x}_1,\mathbf{x}_2)}\ , \tag{2.11d}$$

where the symbol $\circ$ indicates that any function from the domain of the definition of operator U_i must be given in a form which factorizes out the initial orbital φ_i. This requirement guarantees that the operator U_i will not have any singularity at the eventual nodes of the function φ_i. The merit of choice (2.11d) is that it makes Eq. (2.11b) solvable *exactly* in the form

$$\mathcal{L}_i=[N^+(\nu_P)]^2\mathcal{G}^+{}_1F_1(i\nu_P,1,ivs_1+i\mathbf{v}\cdot\mathbf{s}_1)\times{}_1F_1(i\nu_P,1,ivs_2+i\mathbf{v}\cdot\mathbf{s}_2)\ , \tag{2.12a}$$

where $\mathcal{G}^\pm=\exp[\pm i\nu_{PT}\ln(vR\mp v^2t)]$ with ${}_1F_1$ standing for the usual symbol for the Kummer confluent hypergeometric function [60], $\nu_{PT}=Z_PZ_T/v$ and

$$N^\pm(\nu_K)=\Gamma(1\mp i\nu_K)e^{\pi\nu_K/2},\quad \nu_K=Z_K/v\ (K=P,T)\ . \tag{2.12b}$$

Since the following relation holds true,

$$\lim_{t\to-\infty}(vR-v^2t)=\lim_{t\to-\infty}(vs_j+\mathbf{v}\cdot\mathbf{s}_j)\ (j=1,2)\ , \tag{2.12c}$$

it is immediately obvious that the boundary condition (2.11c) of function $\mathcal{L}_i$ is fulfilled. In this manner, the simultaneous choices (2.10a), (2.10b), and (2.11d) determine the boundary-corrected continuum-intermediate-state approximation. Hence, the *post* form of the transition amplitude in the BCIS method is given by

$$\mathcal{A}_{if}^+(\boldsymbol{\rho})=-i[N^+(\nu_P)]^2\int_{-\infty}^{+\infty}dt\int\int d\mathbf{r}_1d\mathbf{r}_2\Phi_f^{-*}V_f^d\Phi_i\mathcal{G}^+{}_1F_1(i\nu_P,1,ivs_1+i\mathbf{v}\cdot\mathbf{s}_1){}_1F_1(i\nu_P,1,ivs_2+i\mathbf{v}\cdot\mathbf{s}_2)\ , \tag{2.13a}$$

where

$$V_f^d\equiv V_f+U_f=Z_T\left[\frac{2}{R}-\frac{1}{x_1}-\frac{1}{x_2}\right]\ . \tag{2.13b}$$

Similarly, we shall briefly proceed to determine the *prior* form of the transition amplitude within the BCIS approximation. This time, the choices of the distorting potentials U_i and U_f are given by

$$U_i=-V_i^a,\quad U_f=-V_f+\sum_{j=1}^{2}\nabla_j\varphi_f(\mathbf{s}_1,\mathbf{s}_2)\cdot\nabla_j\circ\frac{1}{\varphi_f(\mathbf{s}_1,\mathbf{s}_2)}\ , \tag{2.14a}$$

so that

$$\mathcal{A}_{if}^-(\boldsymbol{\rho})=-i[N^{-*}(\nu_T)]^2\int_{-\infty}^{+\infty}dt\int\int d\mathbf{r}_1d\mathbf{r}_2\Phi_f^*\mathcal{G}^{-*}V_i^d\Phi_i^+{}_1F_1(i\nu_T,1,ivx_1+i\mathbf{v}\cdot\mathbf{x}_1){}_1F_1(i\nu_T,1,ivx_2+i\mathbf{v}\cdot\mathbf{x}_2)\ , \tag{2.14b}$$

where

$$V_i^d\equiv V_i+U_i=Z_P\left[\frac{2}{R}-\frac{1}{s_1}-\frac{1}{s_2}\right]\ . \tag{2.14c}$$

Concerning the symbol $\circ$ in Eq. (2.14a), a remark similar to the one made after Eq. (2.11d) applies to the functions from the domain of definition of operator U_f. Also, both the initial and final scattering state wave functions occurring in the *prior* form of the BCIS approximation satisfy the proper boundary conditions, as readily verified by means of the relation (2.12c) and

$$\lim_{t\to+\infty}(vR+v^2t)=\lim_{t\to+\infty}(vx_j+\mathbf{v}\cdot\mathbf{x}_j)\ (j=1,2)\ . \tag{2.15}$$

Given the final results (2.13a) and (2.14b), the corresponding full quantum-mechanical transition amplitudes $T_{if}^\pm(\boldsymbol{\eta})$ are obtained from the Fourier transforms:

$$R_{if}^\pm(\boldsymbol{\eta})=\frac{1}{2\pi}\int d\boldsymbol{\rho}\,e^{i\boldsymbol{\eta}\cdot\boldsymbol{\rho}}\mathcal{A}_{if}^\pm(\boldsymbol{\rho})\ , \tag{2.16}$$

where $R_{if}^\pm(\boldsymbol{\eta})=T_{if}^\pm(\boldsymbol{\eta})/2\pi v$ and $\boldsymbol{\eta}=(\eta\cos\phi_\eta,\eta\sin\phi_\eta,0)$ is the transverse momentum transfer. Written in a compact and physically transparent way, the expressions from (2.16) become

$$\begin{aligned}T_{if}^+(\boldsymbol{\eta})&=\langle f^-,\mathbf{q}_T|V_f^d|i^+\rangle\ ,\\ T_{if}^-(\boldsymbol{\eta})&=\langle f^-|V_i^d|i^+,\mathbf{q}_P\rangle\ ,\end{aligned} \tag{2.17}$$

where

$$\langle \mathbf{R};\mathbf{s}_1,\mathbf{s}_2|f^-,\mathbf{q}_T\rangle = e^{-2i\mathbf{q}_T\cdot\mathbf{R}}\mathcal{H}^-(\mathbf{R})\varphi_f(\mathbf{s}_1,\mathbf{s}_2)$$
$$= e^{-2i\mathbf{q}_T\cdot\mathbf{R}-(i/v)Z_T(Z_P-2)\ln(vR+\mathbf{v}\cdot\mathbf{R})}\varphi_f(\mathbf{s}_1,\mathbf{s}_2)\ , \tag{2.18a}$$

$$\langle \mathbf{R};\mathbf{x}_1,\mathbf{x}_2|i^-\rangle = \mathcal{G}^+(\mathbf{R})\varphi_f(\mathbf{x}_1,\mathbf{x}_2)\varphi^+_{-\mathbf{v}}(\mathbf{s}_1)\varphi^+_{-\mathbf{v}}(\mathbf{s}_2)$$
$$= e^{(i/v)Z_PZ_T\ln(vR-\mathbf{v}\cdot\mathbf{R})}\varphi_i(\mathbf{x}_1,\mathbf{x}_2)\varphi^+_{-\mathbf{v}}(\mathbf{s}_1)\varphi^+_{-\mathbf{v}}(\mathbf{s}_2)\ , \tag{2.18b}$$

$$\langle \mathbf{R};\mathbf{s}_1,\mathbf{s}_2|f^-\rangle = \mathcal{G}^-(\mathbf{R})\varphi_f(\mathbf{s}_1,\mathbf{s}_2)\varphi^-_{\mathbf{v}}(\mathbf{x}_1)\varphi^-_{\mathbf{v}}(\mathbf{x}_2)$$
$$= e^{-(i/v)Z_PZ_T\ln(vR+\mathbf{v}\cdot\mathbf{R})}\varphi_f(\mathbf{s}_1,\mathbf{s}_2)\varphi^-_{\mathbf{v}}(\mathbf{x}_1)\varphi^-_{\mathbf{v}}(\mathbf{x}_2)\ , \tag{2.18c}$$

$$\langle \mathbf{R};\mathbf{x}_1,\mathbf{x}_2|i^+,\mathbf{q}_P\rangle = e^{-2i\mathbf{q}_P\cdot\mathbf{R}}\mathcal{H}^+(\mathbf{R})\varphi_i(\mathbf{x}_1,\mathbf{x}_2)$$
$$= e^{-2i\mathbf{q}_P\cdot\mathbf{R}+(i/v)Z_P(Z_T-2)\ln(vR-\mathbf{v}\cdot\mathbf{R})}\varphi_i(\mathbf{x}_1,\mathbf{x}_2)\ , \tag{2.18d}$$

and

$$2\mathbf{q}_T\cdot\mathbf{R}-\mathbf{v}\cdot(\mathbf{s}_1+\mathbf{s}_2) = -2\mathbf{q}_P\cdot\mathbf{R}-\mathbf{v}\cdot(\mathbf{x}_1+\mathbf{x}_2)\ , \tag{2.19a}$$

$$2\mathbf{q}_{P,T} = \pm\boldsymbol{\eta}-q^{\pm}\hat{\mathbf{v}},\quad q^{\pm}=v\pm\frac{E_f-E_i}{v}\ . \tag{2.19b}$$

Quantities $\varphi^+_{-\mathbf{v}}(\mathbf{s}_j)$ and $\varphi^-_{\mathbf{v}}(\mathbf{x}_j)$ appearing in Eqs. (2.18b) and (2.18c) are the well-known electronic continuum Coulomb functions in the attractive fields $-Z_P/s_j$ and $-Z_T/x_j$ with outgoing and incoming boundary conditions, respectively,

$$\varphi^{\pm}_{\mathbf{p}}(\mathbf{r}) = [e^{\pi Z/2p}\Gamma(1\mp iZ/p)]e^{i\mathbf{p}\cdot\mathbf{r}}$$
$$\times {}_1F_1(\pm iZ/p,1,\pm ipr-i\mathbf{p}\cdot\mathbf{r})\ . \tag{2.20}$$

Matrix element $T^-_{if}(\boldsymbol{\eta})$ from (2.17) which represents the *prior* form of the transition amplitude can be interpreted in the following plausible way. The incident particle scatters on each of the three constituents of the target $(Z_T;e_1,e_2)_i$. In the entrance channel, collision between the projectile P and target $(T,2e)$ results in the *accumulation* of the Coulombic phase factor $\mathcal{H}^+=\exp[(i/v)Z_P(Z_T-2)\ln(vR-\mathbf{v}\cdot\mathbf{R})]$. On the other hand, in the exit channel, the scattered projectile P interacts with the target nucleus accumulating the phase factor $\mathcal{G}^-=\exp[-(i/v)Z_PZ_T\ln(vR+\mathbf{v}\cdot\mathbf{R})]$. At the same time, the interaction of P with the two electrons e_1 and e_2 leads to double ionization of the target $(T,2e)$. The ionized electrons propagate in the Coulomb field of Z_P in a particular direction with the momentums $\boldsymbol{\kappa}_1=\boldsymbol{\kappa}_2=\mathbf{v}$. Finally, the capture of the two electrons occurs from these intermediate ionizing states (capture *from* the continuum) because the electrons are traveling together with the projectile in the same direction and the attractive force between Z_P and $e_{1,2}$ is sufficient to bind them together into the heliumlike atomic system $(Z_p;e_1,e_2)_f$. This is a quantum version of the well-known Thomas classical double scattering. An analogous and symmetric situation can also be pictured in the case of the *post* form from $T^+_{if}(\boldsymbol{\eta})$ of the transition amplitude given in (2.17).

For the purpose of making the analytical part of the calculation easier, we shall reduce the product of the two Coulomb logarithmic terms $\mathcal{H}^{-*}\mathcal{G}^+$ and $\mathcal{G}^{-*}\mathcal{H}^+$ in Eq. (2.17) to only a single phase factor relevant for the computation of the *total* cross sections:

$$\mathcal{H}^{-*}\mathcal{G}^+ = e^{(i/v)Z_T(Z_P-2)\ln(vR+\mathbf{v}\cdot\mathbf{R})}e^{(i/v)Z_PZ_T\ln(vR-\mathbf{v}\cdot\mathbf{R})}$$
$$= (\rho v)^{2iZ_PZ_T/v}e^{-i\xi_T\ln(vR+\mathbf{v}\cdot\mathbf{R})}\ , \tag{2.21a}$$

$$\mathcal{G}^{-*}\mathcal{H}^+ = e^{(i/v)Z_PZ_T\ln(vR+\mathbf{v}\cdot\mathbf{R})}e^{(i/v)Z_P(Z_T-2)\ln(vR-\mathbf{v}\cdot\mathbf{R})}$$
$$= (\rho v)^{2iZ_PZ_T/v}e^{-i\xi_P\ln(vR-\mathbf{v}\cdot\mathbf{R})}\ , \tag{2.21b}$$

where $\xi_K=2\nu_K=2Z_K/v$ $(K=P,T)$. The corresponding *post* and *prior* forms of the total cross sections are subsequently found to read as

$$Q^{\pm}_{if}(a_0^2) = \int d\boldsymbol{\eta}\left|\frac{\bar{T}^{\pm}_{if}(\boldsymbol{\eta})}{2\pi v}\right|^2\ , \tag{2.22}$$

respectively, where

$$\bar{T}^+_{if}(\boldsymbol{\eta}) = \bar{N}^+\int\int\int d\mathbf{R}\,d\mathbf{x}_1d\mathbf{x}_2e^{2i\mathbf{q}_T\cdot\mathbf{R}-i\mathbf{v}\cdot(\mathbf{s}_1+\mathbf{s}_2)}(vR+\mathbf{v}\cdot\mathbf{R})^{-i\xi_T}\varphi^*_f(\mathbf{s}_1,\mathbf{s}_2)\varphi_i(\mathbf{x}_1,\mathbf{x}_2)$$
$$\times\left[\frac{2}{R}-\frac{1}{x_1}-\frac{1}{x_2}\right]{}_1F_1(i\nu_P,1,ivs_1+i\mathbf{v}\cdot\mathbf{s}_1){}_1F_1(i\nu_P,1,ivs_2+i\mathbf{v}\cdot\mathbf{s}_2)\ , \tag{2.23a}$$

$$\bar{T}^-_{if}(\boldsymbol{\eta}) = \bar{N}^-\int\int\int d\mathbf{R}\,d\mathbf{s}_1d\mathbf{s}_2e^{-2i\mathbf{q}_P\cdot\mathbf{R}-i\mathbf{v}\cdot(\mathbf{x}_1+\mathbf{x}_2)}(vR-\mathbf{v}\cdot\mathbf{R})^{-i\xi_P}\varphi^*_f(\mathbf{s}_1,\mathbf{s}_2)\varphi_i(\mathbf{x}_1,\mathbf{x}_2)$$
$$\times\left[\frac{2}{R}-\frac{1}{s_1}-\frac{1}{s_2}\right]{}_1F_1(i\nu_T,1,ivx_1+i\mathbf{v}\cdot\mathbf{x}_1){}_1F_1(i\nu_T,1,ivx_2+i\mathbf{v}\cdot\mathbf{x}_2)\ , \tag{2.23b}$$

with $\bar{N}^{\pm}=Z_{T,P}[N^{\pm}(\nu_{P,T})]^2$. We see that the integrands in Eq. (2.22) are independent of the internuclear Coulomb potential $V_{PT}=Z_P Z_T/R$. The only function in the transition amplitudes of the BCIS method which incorporates the term V_{PT} is the phase factor $(\rho v)^{2iZ_P Z_T/v}$ which, however, gives no contribution to the total cross sections [28]. Notice that the four-body CB1 approximation can formally be obtained from (2.23a) and (2.23b) replacing the confluent hypergeometric functions ${}_1F_1(i\nu_P,1,ivs_j+i\mathbf{v}\cdot\mathbf{s}_j)$, ${}_1F_1(i\nu_T,1,ivx_j+i\mathbf{v}\cdot\mathbf{x}_j)$ by their asymptotic forms $\exp[-i\nu_P\ln(vs_j+\mathbf{v}\cdot\mathbf{s}_j)]$, $\exp[-i\nu_T\ln(vx_j+\mathbf{v}\cdot\mathbf{x}_j)]$, with subsequent use of the limits $t\to\mp\infty$ by means of (2.12c) and (2.15), and finally retaining the Coulombic phases $\exp[-i\nu_P\ln(vR-\mathbf{v}\cdot\mathbf{R})]$, $\exp[-i\nu_T\ln(vR+\mathbf{v}\cdot\mathbf{R})]$, respectively. Despite the appearance of the functions depending upon the vector of the internuclear distance ($\mathbf{R}$), these latter two Coulomb logarithmic terms are also asymptotic *electronic* phases, since $\mathbf{s}_j$, $\mathbf{x}_j$ $(j=1,2)$ are indistinguishable from $\mp\mathbf{R}$ as $t\to\mp\infty$.

In addition to the total cross sections $Q_{if}^{\pm}$, we are presently interested in the computation of the angular distributions of the projectiles scattered into the solid angle $\Omega=\{\theta,\phi\}$ around the direction of incidence, which is situated along the initial wave vector $\mathbf{k}_i$. As usual, the eikonal differential cross sections $dQ_{if}^{\pm}/d\Omega$ are defined in the center-of-mass system by the relation

$$\frac{dQ_{if}^{\pm}}{d\Omega}=\frac{\mu_i\mu_f}{4\pi^2}\frac{k_f}{k_i}|T_{if}^{\pm}(\eta)|^2(a_0^2/sr)\ , \tag{2.24}$$

where μ_i and μ_f are the reduced masses of the aggregates $[P;(T,2e)]$ and $[T;(P,2e)]$, respectively. The ratio k_f/k_i of the magnitudes of the final and initial wave vectors in Eq. (2.24) is close to unity, since the heavy projectiles scatter mainly in the forward direction at high impact energies. The scattering angle θ is identified from the relation: $\eta=2\mu v\sin(\theta/2)$, where μ is the reduced mass of the projectile and target nucleus. Calculation of the angular distributions $dQ_{if}^{\pm}/d\Omega$ becomes particularly convenient in the BCIS approximation when either of the two-electron atoms is neutral, i.e., for $Z_P=2$ or $Z_T=2$. In such a case, the products of the logarithmic Coulomb phase factors from (2.21a) and (2.21b) will again reduce to the single term $\mathcal{H}^{-*}\mathcal{G}^{+}=\exp[2(i/v)Z_T\ln(vR-\mathbf{v}\cdot\mathbf{R})]$ or $\mathcal{G}^{-*}\mathcal{H}^{+}=\exp[2(i/v)Z_P\ln(vR+\mathbf{v}\cdot\mathbf{R})]$. Hence, a trivial modification of the parameters $\xi_{P,T}$ and the signs $\mp$ of the term $\mathbf{v}\cdot\mathbf{R}$ in the function $\ln(vR\mp\mathbf{v}\cdot\mathbf{R})$ from Eqs. (2.21a) and (2.21b) enables us to obtain both differential and total cross sections from the same algorithm associated with the BCIS method. An analogous but simpler reasoning also applies to the CB1 approximation.

III. CALCULATION OF MATRIX ELEMENTS $\bar{T}_{if}^{\pm}(\eta)$: METHOD 1

Let us first outline the present method 1 for the calculation of the scattering integrals contained in the matrix elements $\bar{T}_{if}^{\pm}(\eta)$ from (2.23a) and (2.23b). For this purpose, it will prove convenient to employ the following integral representation for the logarithmic Coulomb phase factors $(vR\pm\mathbf{v}\cdot\mathbf{R})^{-i\xi_K}$ with $K=P,T$:

$$(vR\pm\mathbf{v}\cdot\mathbf{R})^{-i\xi_K}=-\frac{\mathcal{N}(\xi_K)}{2\pi i}\oint_C^{(0^+,\infty^+)}d\tau(-\tau)^{i\xi_K-1}e^{-i(vR\pm\mathbf{v}\cdot\mathbf{R})\tau}\ , \tag{3.1}$$

where $\mathcal{N}(\xi_K)=\Gamma(1-i\xi_K)e^{-\pi\xi_K/2}$ $(K=P,T)$. Here C represents an *open* contour encircling counterclockwise (positive direction) the branch point singularity at the point $\tau=0$. There is a branch cut along the positive real axis in the complex τ plane connected with Eq. (3.1). For the two confluent hypergeometric functions in Eqs. (2.23a) and (2.23b), we shall used the mixed quadrature techniques by expressing ${}_1F_1(i\nu_K,1,i\xi_{K1})$ and ${}_1F_1(i\nu_K,1,i\xi_{K2})$ through the contour integral representation and the real quadrature, respectively, as follows:

$${}_1F_1(i\nu_K,1,i\xi_1^K)=\frac{1}{2\pi i}\oint_{C_1}^{(0^+,1^+)}d\tau_1\tau_1^{i\nu_K-1}(\tau_1-1)^{-i\nu_K}e^{i\tau_1\xi_1^K}\ , \tag{3.2a}$$

$${}_1F_1(i\nu_K,1,i\xi_2^K)=\frac{1}{B(i\nu_K,1-i\nu_K)}\int_0^1 d\tau_2\tau_2^{i\nu_K-1}(1-\tau_2)^{-i\nu_K}e^{i\tau_2\xi_2^K}\ , \tag{3.2b}$$

where $\xi_j^P=vs_j+\mathbf{v}\cdot\mathbf{s}_j$, $\xi_j^T=vx_j+\mathbf{v}\cdot\mathbf{x}_j$ $(j=1,2)$, and $B(x,y)$ is the beta function defined in terms of the gamma functions $\Gamma(x)$ and $\Gamma(y)$ by [60]

$$B(x,y)=\frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}=\int_0^1 dz\, z^{x-1}(1-z)^{y-1}\ . \tag{3.2c}$$

The contour C_1 in Eq. (3.2a) is *closed* and encircles in the positive direction the two branch point singularities at $\tau_1=0$ and $\tau_1=1$. In connection with Eq. (3.2a), the complex τ_1 plane possesses a branch cut along the segment from 0 to 1 on the positive part of the real axis. Furthermore, at the point where the contour crosses the real axis to the right-hand side of $\tau_1=1$, we have that $\arg\tau_1=0=\arg(1-\tau_1)$. Inserting (3.1), (3.2a), and (3.2b) into (2.23a) and (2.23b) we obtain the expressions for $\bar{T}_{if}^{\pm}(\eta)$. These read as follows:

$$\bar{T}_{if}^{\pm}(\eta)=N^{+}(\nu_{P,T})\mathcal{M}_{P,T}^{\pm}\int_0^1\frac{d\tau_2}{\tau_2}h^{\pm}(\tau_2)G_{if}^{\pm}(\eta;\tau_2)\ , \tag{3.3a}$$

where we utilized the property $N^{-*}(\nu_K)=N^{+}(\nu_K)$,

$$G_{if}^{\pm}(\eta;\tau_2)=N(\nu_{P,T};\xi_{T,P})\oint_C^{(0^+,\infty^+)}d\tau\oint_{C_1}^{(0^+,1^+)}d\tau_1 f(\nu_{P,T};\xi_{T,P};\tau,\tau_1)g_{if}^{\pm}(\eta;\tau,\tau_1,\tau_2)\ , \tag{3.3b}$$

$$N(\nu;\xi)=\frac{N^+(\nu)\mathcal{N}(\xi)}{4\pi^2},\quad \mathcal{M}_K^{\pm}=\frac{1}{B(i\nu_K,1-i\nu_K)}\ , \tag{3.3c}$$

$$f(\nu;\xi;\tau,\tau_1)=(-\tau)^{i\xi-1}\tau_1^{i\nu-1}(\tau_1-1)^{-i\nu},\quad h^{\pm}(\tau_2)=\left[\frac{\tau_2}{1-\tau_2}\right]^{i\nu_{P,T}}\ , \tag{3.3d}$$

with $N^+(y)$ given in (2.12b) and

$$g_{if}^{\pm}(\eta;\tau,\tau_1,\tau_2)=Z_{T,P}\int\int\int d\mathbf{R}\,d\boldsymbol{\omega}_1 d\boldsymbol{\omega}_2\varphi_f^*(\mathbf{s}_1,\mathbf{s}_2)e^{-i(vR\pm\mathbf{v}\cdot\mathbf{R})\tau}$$
$$\times\exp[\mp 2i\mathbf{q}_{P,T}\cdot\mathbf{R}-i\mathbf{v}\cdot(\boldsymbol{\omega}_1+\boldsymbol{\omega}_2)+i\tau_1\zeta_1^{P,T}+i\tau_2\zeta_2^{P,T}]\left[\frac{2}{R}-\frac{1}{\omega_1}-\frac{1}{\omega_2}\right]\varphi_i(\mathbf{x}_1,\mathbf{x}_2)\ . \tag{3.4}$$

Here the vector $\boldsymbol{\omega}_j$ becomes $\mathbf{x}_j$ and $\mathbf{s}_j$ for the assignments $+$ and $-$ of the superscript, respectively ($j=1,2$). Method 1 consists of subdividing the nine-dimensional integrals given by Eqs. (3.4) in such a way that we first carry out the quadratures over the electronic matrix elements and then perform the remaining outermost integration over $\mathbf{R}$. Thus, we shall have

$$g_{if}^{\pm}(\eta;\tau,\tau_1,\tau_2)=\int d\mathbf{R}\,e^{\mp 2i\mathbf{q}_{P,T}\cdot\mathbf{R}-i(vR\pm\mathbf{v}\cdot\mathbf{R})\tau}\mathcal{F}_{if}^{\pm}(\mathbf{R})\ , \tag{3.5a}$$

where

$$\mathcal{F}_{if}^{\pm}(\mathbf{R})=Z_{T,P}\int\int d\boldsymbol{\omega}_1 d\boldsymbol{\omega}_2\varphi_f^*(\mathbf{s}_1,\mathbf{s}_2)\left[\frac{2}{R}-\frac{1}{\omega_1}-\frac{1}{\omega_2}\right]$$
$$\times\exp[-i\mathbf{v}\cdot(\boldsymbol{\omega}_1+\boldsymbol{\omega}_2)+i\tau_1\zeta_1^{P,T}$$
$$+i\tau_2\zeta_2^{P,T}]\varphi_i(\mathbf{x}_1,\mathbf{x}_2)\ . \tag{3.5b}$$

The illustrative explicit calculation of the integrals $G_{if}^{\pm}(\eta;\tau_2)$ from Eqs. (3.3b) will be carried out by using the well-known uncorrelated one-parameter wave functions for the heliumlike atomic systems given by

$$\varphi_i(\mathbf{x}_1,\mathbf{x}_2)=\phi_\alpha(\mathbf{x}_1)\phi_\alpha(\mathbf{x}_2)\ ,$$
$$\varphi_f(\mathbf{s}_1,\mathbf{s}_2)=\phi_\beta(\mathbf{s}_1)\phi_\beta(\mathbf{s}_2)\ , \tag{3.6a}$$

with the corresponding *approximate* binding energies $-\alpha^2,-\beta^2$ used instead of the exact $E_{i,f}$ (variational or experimental) values and

$$\phi_\alpha(\mathbf{x}_j)=\left[\frac{\alpha^3}{\pi}\right]^{1/2}e^{-\alpha x_j},$$
$$\phi_\beta(\mathbf{s}_j)=\left[\frac{\beta^3}{\pi}\right]^{1/2}e^{-\beta s_j}\quad (j=1,2)\ , \tag{3.6b}$$

$$\alpha=Z_T-a_S,\quad \beta=Z_P-b_S,\quad a_S=b_S=5/16=0.3125\ . \tag{3.6c}$$

Parameters α and β are the effective charges of the target and projectile nucleus defined by (3.6c) in terms of $Z_{T,P}$ and the inner Slater screening $a_S=b_S=0.3125$. Hence Eq. (3.5b) can be put into the following forms:

$$\mathcal{F}_{if}^{\pm}(\mathbf{R})=-2Z_{T,P}[\mathcal{A}^{\pm}(\mathbf{R})-\mathcal{B}^{\pm}(\mathbf{R})]\ , \tag{3.7a}$$

with

$$\mathcal{A}^{\pm}(\mathbf{R})=\mathcal{A}_{1,1}^{\pm}(\mathbf{R})\mathcal{A}_{2,0}^{\pm}(\mathbf{R}),$$
$$\mathcal{B}^{\pm}(\mathbf{R})=\frac{1}{R}\mathcal{A}_{1,0}^{\pm}(\mathbf{R})\mathcal{A}_{2,0}^{\pm}(\mathbf{R})\ , \tag{3.7b}$$

$$\mathcal{A}_{j,k}^{\pm}(\mathbf{R})=\int d\boldsymbol{\omega}_j\frac{1}{\omega_j^k}\chi_{\alpha\beta}^{\pm}(\boldsymbol{\omega}_j,\mathbf{R})\quad (k=0,1)\ , \tag{3.7c}$$

where the superscript $\pm$ are respectively associated with the vectors $\boldsymbol{\omega}_j=\mathbf{x}_j,\mathbf{s}_j$ ($j=1,2$),

$$\chi_{\alpha\beta}^{+}(\mathbf{x}_j,\mathbf{R})=e^{-i\mathbf{v}\cdot\mathbf{x}_j+i[v|\mathbf{x}_j-\mathbf{R}|+\mathbf{v}\cdot(\mathbf{x}_j-\mathbf{R})]\tau_j}\varphi_\alpha(\mathbf{x}_j)\varphi_\beta^*(\mathbf{x}_j-\mathbf{R})\ , \tag{3.8a}$$

$$\chi_{\alpha\beta}^{-}(\mathbf{s}_j,\mathbf{R})=e^{-i\mathbf{v}\cdot\mathbf{s}_j+i[v|\mathbf{s}_j+\mathbf{R}|+\mathbf{v}\cdot(\mathbf{s}_j+\mathbf{R})]\tau_j}\varphi_\alpha(\mathbf{s}_j+\mathbf{R})\varphi_\beta^*(\mathbf{s}_j)\ . \tag{3.8b}$$

The two-center scattering integrals in Eq. (3.7c) are carried out by using the standard Fourier transform: $\tilde{f}(\mathbf{p})=(2\pi)^{-3}\int d\mathbf{r}\,e^{i\mathbf{p}\cdot\mathbf{r}}f(\mathbf{r})$ and its corresponding inverse expression $f(\mathbf{r})=\int d\mathbf{p}\,e^{-i\mathbf{p}\cdot\mathbf{r}}\tilde{f}(\mathbf{p})$. This yields

$$\mathcal{A}_{j,k}^{+}(\mathbf{R})=4\frac{(2\alpha)^{1-k}\beta_j}{\pi}N_{\alpha\beta}e^{i\mathbf{q}_P\cdot\mathbf{R}}\int d\mathbf{q}_j\frac{e^{-i\mathbf{q}_j\cdot\mathbf{R}}}{(|\mathbf{q}_j-\mathbf{q}_{Pj}|^2+\beta_j^2)^2(|\mathbf{q}_j+\mathbf{q}_T|^2+\alpha^2)^{2-k}}\ , \tag{3.9a}$$

$$\mathcal{A}_{j,k}^{-}(\mathbf{R})=4\frac{(2\beta)^{1-k}\alpha_j}{\pi}N_{\alpha\beta}e^{-i\mathbf{q}_T\cdot\mathbf{R}}\int d\mathbf{q}_j\frac{e^{-i\mathbf{q}_j\cdot\mathbf{R}}}{(|\mathbf{q}_j-\mathbf{q}_P|^2+\beta^2)^{2-k}(|\mathbf{q}_j+\mathbf{q}_{Tj}|^2+\alpha_j^2)^2}\ , \tag{3.9b}$$

where $N_{\alpha\beta}=N_\alpha N_\beta^*$, $\mathbf{q}_{Kj}=\mathbf{q}_K+\tau_j\mathbf{v}$ $(j=1,2,\ k=1,2)$, and

$$\mathbf{q}_{Pj}+\mathbf{q}_T=-(1-\tau_j)\mathbf{v}\equiv-\mathbf{v}_j=\mathbf{q}_{Tj}+\mathbf{q}_P,\quad \alpha_j=\alpha-i\tau_j v,\quad \beta_j=\beta-i\tau_j v\ . \tag{3.10}$$

Inserting the results (3.7a)–(3.7c), and (3.9b) into Eq. (3.5a), we carry out the integration over variable $\mathbf{R}$, so that the expressions for $G_{if}^{\pm}(\boldsymbol{\eta};\tau_2)$ from (3.3b) become

$$G_{if}^{+}(\boldsymbol{\eta};\tau_2)=-2Z_T[\,A_{2,1}^{(2,2)}(2)-A_{2,2}^{(2,2)}(1)]\ , \tag{3.11a}$$

$$G_{if}^{-}(\boldsymbol{\eta};\tau_2)=-2Z_P[B_{1,2}^{(2,2)}(2)-B_{2,2}^{(2,2)}(1)]\ , \tag{3.11b}$$

where

$$A_{n_1,n_2}^{(m_1,m_2)}(n)=\frac{256}{\pi}\alpha^{3-n}N_{\alpha\beta}^2N(\nu_P;\xi_T)\oint_C^{(0^+,\infty^+)}d\tau\oint_{C_1}^{(0^+,1^+)}d\tau_1\beta_1\beta_2(iv\tau)^{n-1}$$
$$\times f(\nu_P;\xi_T;\tau,\tau_1)\int\int\frac{d\mathbf{q}_1d\mathbf{q}_2}{(|\mathbf{q}_1-\mathbf{q}_{P1}|^2+\beta_1^2)^{n_1}(|\mathbf{q}_1+\mathbf{q}_T|^2+\alpha^2)^{m_1}}$$
$$\times\frac{1}{(|\mathbf{q}_2-\mathbf{q}_{P2}|^2+\beta_2^2)^{n_2}(|\mathbf{q}_2+\mathbf{q}_T|^2+\alpha^2)^{m_2}(|\mathbf{q}_1+\mathbf{q}_2+\tau\mathbf{v}|^2-\tau^2v^2)^n} \tag{3.12a}$$

and

$$B_{n_1,n_2}^{(m_1,m_2)}(n)=\frac{256}{\pi}\beta^{3-n}N_{\alpha\beta}^2N(\nu_T;\xi_P)\oint_C^{(0^+,\infty^+)}d\tau\oint_{C_1}^{(0^+,1^+)}d\tau_1\alpha_1\alpha_2(iv\tau)^{n-1}$$
$$\times f(\nu_T;\xi_P;\tau,\tau_1)\int\int\frac{d\mathbf{q}_1d\mathbf{q}_2}{(|\mathbf{q}_1-\mathbf{q}_P|^2+\beta^2)^{n_1}(|\mathbf{q}_1+\mathbf{q}_{T1}|^2+\alpha_1^2)^{m_1}}$$
$$\times\frac{1}{(|\mathbf{q}_2-\mathbf{q}_P|^2+\beta^2)^{n_2}(|\mathbf{q}_2+\mathbf{q}_{T2}|^2+\alpha_2^2)^{m_2}(|\mathbf{q}_1+\mathbf{q}_2+\tau\mathbf{v}|^2-\tau^2v^2)^n}\ . \tag{3.12b}$$

In particular, we have that

$$A_{2,1}^{(2,2)}(2)=\mathcal{N}_{\alpha\beta}[\mathcal{O}Z_{\gamma_\lambda;\beta_{b1},\beta_{b2}}^{(a_1,a_2)}(\nu_P,\xi_T;-\tau\mathbf{v};\mathbf{q}_{P1},-\mathbf{q}_T,\mathbf{q}_{P2},-\mathbf{q}_T)]'\ , \tag{3.13a}$$

$$A_{2,2}^{(2,2)}(1)=\mathcal{N}_{\alpha\beta}[\mathcal{O}'Z_{\gamma_\lambda;\beta_{b1},\beta_{b2}}^{(a_1,a_2)}(\nu_P,\xi_T;-\tau\mathbf{v};\mathbf{q}_{P1},-\mathbf{q}_T,\mathbf{q}_{P2},-\mathbf{q}_T)]'\ , \tag{3.13b}$$

$$B_{1,2}^{(2,2)}(2)=\mathcal{N}_{\alpha\beta}[\mathcal{O}''Z_{\gamma_\lambda;b1,b2}^{(\alpha_{a1},\alpha_{a2})}(\nu_T,\xi_P;-\tau\mathbf{v};\mathbf{q}_P,-\mathbf{q}_{T1},\mathbf{q}_P,-\mathbf{q}_{T2})]'\ , \tag{3.13c}$$

$$B_{2,2}^{(2,2)}(1)=\mathcal{N}_{\alpha\beta}[\mathcal{O}'Z_{\gamma_\lambda;b1,b2}^{(\alpha_{a1},\alpha_{a2})}(\nu_T,\xi_P;-\tau\mathbf{v};\mathbf{q}_P,-\mathbf{q}_{T1},\mathbf{q}_P,-\mathbf{q}_{T1})]'\ , \tag{3.13d}$$

with $\mathcal{N}_{\alpha\beta}=(16/\pi)N_{\alpha\beta}^2$ and

$$\gamma_\lambda=\lambda+iv\tau,\quad \alpha_{aj}=a_j-iv\tau_j,\quad \beta_{bj}=b_j-iv\tau_j\quad (j=1,2)\ , \tag{3.14a}$$

$$\mathcal{O}=\frac{\partial^4}{\partial b_1\partial b_2\partial a_2\partial\lambda},\quad \mathcal{O}'=\frac{\partial^4}{\partial b_1\partial b_2\partial a_1\partial a_2},\quad \mathcal{O}''=\frac{\partial^4}{\partial a_1\partial a_2\partial b_2\partial\lambda}\ , \tag{3.14b}$$

where the symbol [ ]′ signifies that once all the partial differentiations are completed, the content of the square brackets must be taken at the following sets of the values of the invoked parameters: $\{\lambda=0;a_{1,2}=\alpha,b_{1,2}=\beta\}$,

$$Z_{\gamma;\gamma_1,\gamma_2}^{(\delta_1,\delta_2)}(\nu,\xi,\mathbf{q};\mathbf{p}_1,\boldsymbol{\kappa}_1;\mathbf{p}_2,\boldsymbol{\kappa}_2)=N(\nu;\xi)\oint_C^{(0^+,\infty^+)}d\tau\oint_{C_1}^{(0^+,1^+)}d\tau_1f(\nu;\xi;\tau,\tau_1)$$
$$\times\int\int\frac{d\mathbf{q}_1d\mathbf{q}_2}{(|\mathbf{q}_1-\mathbf{p}_1|^2+\gamma_1^2)(|\mathbf{q}_1-\boldsymbol{\kappa}_1|^2+\delta_1^2)}$$
$$\times\frac{1}{(|\mathbf{q}_2-\mathbf{p}_2|^2+\gamma_2^2)(|\mathbf{q}_2-\boldsymbol{\kappa}_2|^2+\delta_2^2)(|\mathbf{q}_1+\mathbf{q}_2-\mathbf{q}|^2+\gamma^2)}\ . \tag{3.15}$$

We show in Appendix A that this eightfold integral can analytically be reduced to a two-dimensional quadrature. Thus, for example, in the case of Eqs. (3.13a) and (3.13b) we obtain

$$Z^{(a_1,a_2)}_{\gamma_\lambda;\beta_{b1},\beta_{b2}}(\nu_P,\xi_T;-\tau\mathbf{v};\mathbf{q}_{P1},-\mathbf{q}_T,\mathbf{q}_{P2},-\mathbf{q}_T) = \frac{\pi^3}{2}\int_0^1 \frac{dt_2}{\Delta_2}\int_0^1 dt\,\mathcal{N}(t,t_2)\,, \tag{3.16a}$$

where

$$\mathcal{N}(t,t_2)=\frac{2\pi}{\alpha'}N^+(\nu_P)N^{-*}(\xi_T) \times\left[\frac{\alpha'}{\beta'}\right]^{i\xi_T}\left[\frac{\alpha'}{\gamma'}\right]^{i\nu_P}{}_2F_1(i\xi_T,i\nu_P;1;x)\,, \tag{3.16b}$$

with $N^-(\xi_T)=\Gamma(1+i\xi_T)e^{\pi\xi_T/2}$ and where ${}_2F_1$ is the standard Gauss hypergeometric function [60] of one variable $x=1-\alpha'\delta'/\beta'\gamma'$. All the other quantities entering into Eqs. (3.16a) and (3.16b) are listed in Appendix A. An analogous result is obtained for the integrals (3.13c) and (3.13d) by repeating the same procedure. Hence by performing the straightforward partial differentiations indicated in Eqs. (3.13a)–(3.13d), we can conclude that method 1 finally provides the basic matrix elements $\bar{T}^{\pm}_{if}(\boldsymbol{\eta})$ from (3.3a) in the form of the *three-dimensional* integrals over real variables τ_2, t_2, and t, which all range from 0 to 1, as can be seen from Eqs. (3.3a), (3.11a), (3.11b), (3.16a), and (3.27a).

IV. CALCULATION OF MATRIX ELEMENTS $\bar{T}^{\pm}_{if}(\boldsymbol{\eta})$: METHOD 2

In this section we shall develop an alternative method for calculation of the basic matrix elements $\bar{T}^{\pm}_{if}(\boldsymbol{\eta})$ from Eqs. (2.23a) and (2.23b). This procedure, hereafter called method 2, will depart from the two real integral representations of the type (3.2b) for both confluent hypergeometric functions ${}_1F_1(i\nu_K,1,i\zeta^K_j)$ with $j=1,2$. Then we shall have

$$\bar{T}^{\pm}_{if}(\boldsymbol{\eta})=[N^+(\nu_{P,T})]^2(\mathcal{M}^{\pm}_{P,T})^2\int_0^1\int_0^1 d\tau_1 d\tau_2 f^{\pm}(\tau_1,\tau_2) \times\bar{T}^{\pm}_{if}(\boldsymbol{\eta};\tau_1,\tau_2)\,, \tag{4.1}$$

where

$$f^{\pm}(\tau_1,\tau_2)=f^{\pm}(\tau_1)f^{\pm}(\tau_2)\,, \tag{4.2}$$

$$f^{\pm}(\tau_j)=\frac{1}{\tau_j}h^{\pm}(\tau_j),\quad h^{\pm}(\tau_j)=\left[\frac{\tau_j}{1-\tau_j}\right]^{i\nu_{P,T}}, \tag{4.3}$$

and

$$\bar{T}^{\pm}_{if}(\boldsymbol{\eta};\tau_1,\tau_2)=Z_T\int\int\int d\mathbf{R}\,d\boldsymbol{\omega}_1 d\boldsymbol{\omega}_2\varphi^*_f(\mathbf{s}_1,\mathbf{s}_2)(vR\pm\mathbf{v}\cdot\mathbf{R})^{-i\xi_{T,P}} \times\exp[\mp 2i\mathbf{q}_{P,T}\cdot\mathbf{R}-i\mathbf{v}\cdot(\boldsymbol{\omega}_1+\boldsymbol{\omega}_2)+i\zeta^{P,T}_1\tau_1+i\zeta^{P,T}_2\tau_2]\left[\frac{2}{R}-\frac{1}{\omega_1}-\frac{1}{\omega_2}\right]\varphi_i(\mathbf{x}_1,\mathbf{x}_2)\,, \tag{4.4}$$

with $N^+(\nu_{P,T})$ and $\mathcal{M}^{\pm}_K$ given respectively in Eqs. (2.12b) and (3.3c). Here the vectors $\boldsymbol{\omega}_1$ and $\boldsymbol{\omega}_2$ have the same meaning as in Eq. (3.4). In method 2, we again first carry out the integrations over the electronic coordinates, thus leaving the remaining outermost integral over $\mathbf{R}$ for the end of the calculation. Hence,

$$\bar{T}^{\pm}_{if}(\boldsymbol{\eta};\tau_1,\tau_2)=\int d\mathbf{R}\,e^{\mp 2i\mathbf{q}_{P,T}\cdot\mathbf{R}}(vR\pm\mathbf{v}\cdot\mathbf{R})^{-i\xi_{T,P}}\mathcal{F}^{\pm}_{if}(\mathbf{R})\,, \tag{4.5}$$

where quantities $\mathcal{F}^{\pm}_{if}(\mathbf{R})$ are defined in Eq. (3.5b). Of course, in deriving the results for $\mathcal{F}^{\pm}_{if}(\mathbf{R})$ with the one-parameter orbitals (3.6a), we will again encounter integrals (3.9a) and (3.9b). This time, however, we shall perform the integrations over $\mathbf{q}_{1,2}$ *before* carrying out the $\mathbf{R}$ integral, in the same manner as in our previous work concerned with the CB1 approximation [51]. To this end, we need the Feynman parametrization integral:

$$\frac{1}{A^nB^m}=\frac{(n+m-1)!}{(n-1)!(m-1)!}\int_0^1 dt\,t^{n-1}(1-t)^{m-1}[At+B(1-t)]^{-n-m}\,, \tag{4.6}$$

where n,m are certain integer numbers. Then we can carry out the integration over $\mathbf{q}_{1,2}$ with the help of the expressions [36]

$$\int d\mathbf{q}\frac{e^{i\mathbf{q}\cdot\mathbf{R}}}{(|\mathbf{q}-\mathbf{p}|^2+\lambda^2)^3}=\frac{\pi^2}{4\lambda^3}(1+\lambda R)e^{i\mathbf{p}\cdot\mathbf{R}-\lambda R}\,, \tag{4.7a}$$

$$\int d\mathbf{q}\frac{e^{i\mathbf{q}\cdot\mathbf{R}}}{(|\mathbf{q}-\mathbf{p}|^2+\lambda^2)^4}=\frac{\pi^2}{24\lambda^5}(3+3\lambda R+\lambda^2R^2)e^{i\mathbf{p}\cdot\mathbf{R}-\lambda R}\,, \tag{4.7b}$$

with $\mathbf{q}$ being a real vector and $\mathrm{Re}\lambda>0$. In this manner we arrive at the following results for integrals (3.9a) and (3.9b):

$$\mathcal{A}^{+}_{j,k}(\mathbf{R})=2\pi\beta_j\alpha^{1-k}N_{\alpha\beta}e^{i\mathbf{q}_P\cdot\mathbf{R}}C^{+}_{2-k}(\mathbf{R})\,, \tag{4.8a}$$

$$\mathcal{A}^{-}_{j,k}(\mathbf{R})=2\pi\alpha_j\beta^{1-k}N_{\alpha\beta}e^{-i\mathbf{q}_T\cdot\mathbf{R}}C^{-}_{2-k}(\mathbf{R})\,, \tag{4.8b}$$

with $N_{\alpha\beta}=N_\alpha N_\beta^*$,

$$C_1^\pm(\mathbf{R})=\int_0^1 dt_1 \frac{t_1^\pm}{(\Delta_1^\pm)^3}(1+\Delta_1^\pm R)\exp(-i\mathbf{Q}_1^\pm\cdot\mathbf{R}-\Delta_1^\pm R)\ , \tag{4.9a}$$

$$C_2^\pm(\mathbf{R})=\int_0^1 dt_2 \frac{t_2(1-t_2)}{(\Delta_2^\pm)^5}[3+3\Delta_2^\pm R+(\Delta_2^\pm)^2R^2]\exp(-i\mathbf{Q}_2^\pm\cdot\mathbf{R}-\Delta_2^\pm R)\ , \tag{4.9b}$$

and $t_1^+=t_1$, $t^-=1-t_1$,

$$\mathbf{Q}_j^+=\mathbf{q}_{Pj}t_j-\mathbf{q}_T(1-t_j),\quad \mathbf{Q}_j^-=\mathbf{q}_P t_j-\mathbf{q}_{Tj}(1-t_j),\quad \mathbf{q}_{Kj}=\mathbf{q}_K+\tau_j\mathbf{v}\ , \tag{4.10a}$$

$$(\Delta_j^\pm)^2=v_j^2t_j(1-t_j)+\{\beta_j^2,\beta^2\}t_j+\{\alpha^2,\alpha_j^2\}(1-t_j),\quad \Delta_j^\pm=+\sqrt{(\Delta_j^\pm)^2}\ , \tag{4.10b}$$

where $\mathrm{Re}[(\Delta_j^\pm)^2]>0$ and quantities α_j, β_j are given in Eq. (3.10). With the help of these results, the matrix elements $\mathcal{A}^\pm$ and $\mathcal{B}^\pm$ from Eq. (3.7b) become

$$\mathcal{A}^\pm(\mathbf{R})=4\pi^2 x^\pm N_{\alpha\beta}^2 e^{\pm 2i\mathbf{q}_{P,T}\cdot\mathbf{R}}A^\pm(\mathbf{R})\ , \tag{4.11a}$$

$$\mathcal{B}^\pm(\mathbf{R})=\frac{4\pi^2}{R}y^\pm N_{\alpha\beta}^2 e^{\pm 2i\mathbf{q}_{P,T}\cdot\mathbf{R}}B^\pm(\mathbf{R})\ , \tag{4.11b}$$

where

$$A^\pm(\mathbf{R})=\int_0^1\int_0^1 dt_1dt_2\frac{t_1^\pm t_2(1-t_2)}{(\Delta_1^\pm)^3(\Delta_2^\pm)^5}e^{-i\mathbf{Q}^\pm\cdot\mathbf{R}-\Delta^\pm R}(1+\Delta_1^\pm R)[3+3\Delta_2^\pm R+(\Delta_2^\pm)^2R^2]\ , \tag{4.12a}$$

$$B^\pm(\mathbf{R})=\int_0^1\int_0^1 dt_1dt_2\frac{t_1t_2(1-t_1)(1-t_2)}{(\Delta_1^\pm)^5(\Delta_2^\pm)^5}e^{-i\mathbf{Q}^\pm\cdot\mathbf{R}-\Delta^\pm R}[3+3\Delta_1^\pm R+(\Delta_1^\pm)^2R^2][3+3\Delta_2^\pm R+(\Delta_2^\pm)^2R^2]\ , \tag{4.12b}$$

$$x^\pm=z^\pm v^\pm,\quad y^\pm=x^\pm z^\pm,\quad z^+=\alpha,\quad z^-=\beta,\quad v^+=\beta_1\beta_2,\quad v^-=\alpha_1\alpha_2\ , \tag{4.12c}$$

$$\mathbf{Q}^\pm=\mathbf{Q}_1^\pm+\mathbf{Q}_2^\pm,\quad \Delta^\pm=\Delta_1^\pm+\Delta_2^\pm\ . \tag{4.12d}$$

This analysis fully determines the objects $\mathcal{F}_{if}^\pm(\mathbf{R})$ from Eq. (3.7a). However, for the specification of the matrix elements $\overline{T}_{if}^\pm(\boldsymbol{\eta};\tau_1,\tau_2)$ from Eqs. (4.1) and (4.4), the results of the following auxiliary integrals are required:

$$\begin{aligned}I^\pm&\equiv\int d\mathbf{R}\,e^{-i\mathbf{Q}^\pm\cdot\mathbf{R}-\Delta^\pm R}(1+\Delta_1^\pm R)[3+3\Delta_2^\pm R+(\Delta_2^\pm)^2R^2](vR\pm\mathbf{v}\cdot\mathbf{R})^{-i\xi_{T,P}}\\&=3I_1^\pm+3\Delta^\pm I_2^\pm+\Delta_2^\pm(3\Delta_1^\pm+\Delta_2^\pm)I_3^\pm+\Delta_1^\pm(\Delta_2^\pm)^2I_4^\pm\ ,\end{aligned} \tag{4.13a}$$

$$\begin{aligned}J^\pm&\equiv\int\frac{d\mathbf{R}}{R}e^{-i\mathbf{Q}^\pm\cdot\mathbf{R}-\Delta^\pm R}[3+3\Delta_1^\pm R+(\Delta_1^\pm)^2R^2][3+3\Delta_2^\pm R+(\Delta_2^\pm)^2R^2](vR\pm\mathbf{v}\cdot\mathbf{R})^{-i\xi_{T,P}}\\&=9I_0^\pm+9\Delta^\pm I_1^\pm+3[(\Delta_1^\pm)^2+3\Delta_1^\pm\Delta_2^\pm+(\Delta_2^\pm)^2]I_2^\pm+3\Delta_1^\pm\Delta_2^\pm\Delta^\pm I_3^\pm+(\Delta_1^\pm)^2(\Delta_2^\pm)^2I_4^\pm\ ,\end{aligned} \tag{4.13b}$$

where

$$I_n^\pm=\int d\mathbf{R}\,e^{-i\mathbf{Q}^\pm\cdot\mathbf{R}-\Delta^\pm R}R^{n-1}(vR\pm\mathbf{v}\cdot\mathbf{R})^{-i\xi_{T,P}}\ . \tag{4.13c}$$

Once a detailed algebra is accomplished by means of the partial differentiation technique, we obtain the following results of a simpler version of the Nordsieck [36,61] integrals $I_n^\pm$ for $n\le 4$:

$$I_0^\pm=4\pi\Gamma(1-i\xi_{T,P})\mathcal{F}^\pm\ , \tag{4.14a}$$

$$I_1^\pm=8\pi\Gamma(1-i\xi_{T,P})D\mathcal{F}^\pm(1+i\xi_{T,P}C^\pm)\ , \tag{4.14b}$$

$$I_2^\pm=-8\pi\Gamma(1-i\xi_{T,P})\frac{D^\pm\mathcal{F}^\pm}{\Delta^\pm}(A_\alpha^\pm-i\xi_{T,P}B_\alpha^\pm)\ , \tag{4.14c}$$

$$I_3^\pm=-16\pi\Gamma(1-i\xi_{T,P})\frac{(D^\pm)^2\mathcal{F}^\pm}{\Delta^\pm}(A_\beta^\pm-i\xi_{T,P}B_\beta^\pm)\ , \tag{4.14d}$$

$$I_4^\pm=16\pi\Gamma(1-i\xi_{T,P})\frac{(D^\pm)^2\mathcal{F}^\pm}{(\Delta^\pm)^2}(A_\gamma^\pm+i\xi_{T,P}B_\gamma^\pm)\ , \tag{4.14e}$$

and

$$\mathcal{F}^{\pm}=\lambda^{\pm}(B^{\pm})^{-i\xi_{T,P}},\quad \lambda^{\pm}=\frac{1}{(Q^{\pm})^2+(\Delta^{\pm})^2},\quad B^{\pm}=2\lambda^{\pm}(v\Delta^{\pm}\mp i\mathbf{Q}^{\pm}\cdot\mathbf{v}) , \tag{4.15a}$$

$$C^{\pm}=\frac{v}{B^{\pm}\Delta^{\pm}}-1,\quad D^{\pm}=\frac{A^{\pm}}{\Delta^{\pm}}=\lambda^{\pm}\Delta^{\pm},\quad A^{\pm}=\lambda^{\pm}(\Delta^{\pm})^2 , \tag{4.15b}$$

$$A_{\alpha}^{\pm}=1-4A^{\pm},\quad B_{\alpha}^{\pm}=1+2A^{\pm}C_{\alpha}^{\pm},\quad C_{\alpha}^{\pm}=C^{\pm}[4+(1+i\xi_{T,P})C^{\pm}] , \tag{4.15c}$$

$$A_{\beta}^{\pm}=6(1-2A^{\pm}),\quad B_{\beta}^{\pm}=2A^{\pm}C_{\beta}^{\pm}+3D_{\beta}^{\pm},\quad D_{\beta}^{\pm}=2-(1-i\xi_{T,P})C^{\pm} , \tag{4.15d}$$

$$C_{\beta}^{\pm}=C^{\pm}[18+9(1+i\xi_{T,P})C^{\pm}+(1+i\xi_{T,P})(2+i\xi_{T,P})(C^{\pm})^2] , \tag{4.16a}$$

$$A_{\gamma}^{\pm}=6[16(A^{\pm})^2-12A^{\pm}+1] , \tag{4.16b}$$

$$B_{\gamma}^{\pm}=4(A^{\pm})^2C_{\gamma}^{\pm}-12A^{\pm}D_{\gamma}^{\pm}+3(3-i\xi_{T,P}) , \tag{4.16c}$$

$$C_{\gamma}^{\pm}=C^{\pm}[96+72(1+i\xi_{T,P})C^{\pm}+16(1+i\xi_{T,P})(2+i\xi_{T,P})(C^{\pm})^2+(1+i\xi_{T,P})(2+i\xi_{T,P})(3+i\xi_{T,P})(C^{\pm})^3] , \tag{4.16d}$$

$$D_{\gamma}^{\pm}=(1-i\xi_{T,P})C^{\pm}[6+(1+i\xi_{T,P})C^{\pm}]-6 . \tag{4.16e}$$

Thus, the auxiliary integrals $I^{\pm}$ and $J^{\pm}$ from Eqs. (4.13a) and (4.13b) take the form

$$I^{\pm}=8\pi\Gamma(1-i\xi_{T,P})D^{\pm}\mathcal{F}^{\pm}(\gamma_0^{\pm}+i\xi_{T,P}\delta_0^{\pm}) , \tag{4.17a}$$

$$J^{\pm}=12\pi\Gamma(1-i\xi_{T,P})\mathcal{F}^{\pm}(\nu^{\pm}+i\xi_{T,P}\mu^{\pm}) , \tag{4.17b}$$

where

$$\gamma_0^{\pm}=3(1-A_{\alpha}^{\pm})-2\Delta_2^{\pm}(3\Delta_1^{\pm}+\Delta_2^{\pm})A_{\beta}^{\pm}\frac{D^{\pm}}{\Delta^{\pm}}+2\Delta_1^{\pm}(\Delta_2^{\pm})^2A_{\gamma}^{\pm}\frac{D^{\pm}}{(\Delta^{\pm})^2} , \tag{4.17c}$$

$$\delta_0^{\pm}=3(C^{\pm}+B_{\alpha}^{\pm})+2\Delta_2^{\pm}(3\Delta_1^{\pm}+\Delta_2^{\pm})B_{\beta}^{\pm}\frac{D^{\pm}}{\Delta^{\pm}}+2\Delta_1^{\pm}(\Delta_2^{\pm})^2B_{\gamma}^{\pm}\frac{D^{\pm}}{(\Delta^{\pm})^2} , \tag{4.17d}$$

$$\begin{aligned}\nu^{\pm}&=3+6\lambda^{\pm}(\Delta^{\pm})^2-2[(\Delta_1^{\pm})^2+3\Delta_1^{\pm}\Delta_2^{\pm}+(\Delta_2^{\pm})^2]\lambda^{\pm}A_{\alpha}^{\pm}-4\Delta_1^{\pm}\Delta_2^{\pm}(\lambda^{\pm})^2(\Delta^{\pm})^2A_{\beta}^{\pm}+\tfrac{4}{3}(\Delta_1^{\pm})^2(\Delta_2^{\pm})^2(\lambda^{\pm})^2A_{\gamma}^{\pm}\\&=3+2[2(\Delta_1^{\pm})^2+3\Delta_1^{\pm}\Delta_2^{\pm}+2(\Delta_2^{\pm})^2]\lambda^{\pm}+8[(\Delta_1^{\pm})^4+2(\Delta_1^{\pm})^3\Delta_2^{\pm}+3(\Delta_1^{\pm})^2(\Delta_2^{\pm})^2+2\Delta_1^{\pm}(\Delta_2^{\pm})^3+(\Delta_2^{\pm})^4](\lambda^{\pm})^2\\&\quad+48\Delta_1^{\pm}\Delta_2^{\pm}[(\Delta_1^{\pm})^2+(\Delta_2^{\pm})^2](\Delta^{\pm})^2(\lambda^{\pm})^3+128(\Delta_1^{\pm})^2(\Delta_2^{\pm})^2(\Delta^{\pm})^4(\lambda^{\pm})^4 ,\end{aligned} \tag{4.18a}$$

$$\mu^{\pm}=2\lambda^{\pm}\{3C^{\pm}(\Delta^{\pm})^2+[(\Delta_1^{\pm})^2+3\Delta_1^{\pm}\Delta_2^{\pm}+(\Delta_2^{\pm})^2]B_{\alpha}^{\pm}+2\Delta_1^{\pm}\Delta_2^{\pm}\lambda^{\pm}(\Delta^{\pm})^2B_{\beta}^{\pm}+\tfrac{2}{3}(\Delta_1^{\pm})^2(\Delta_2^{\pm})^2\lambda^{\pm}B_{\gamma}^{\pm}\} . \tag{4.18b}$$

These expressions enable us to write the quantities $\overline{T}_{if}^{\pm}(\boldsymbol{\eta};\tau_1,\tau_2)$ from Eq. (4.4) as follows:

$$\frac{\overline{T}_{if}^{\pm}(\boldsymbol{\eta};\tau_1,\tau_2)}{2\pi v}=-\mathcal{N}^{\pm}\int_0^1\int_0^1 dt_1dt_2\frac{t_1^{\pm}t_2(1-t_2)}{(\Delta_1^{\pm})^3(\Delta_2^{\pm})^5}\mathcal{F}^{\pm}(\mathcal{H}^{\pm}+i\xi_{T,P}\mathcal{G}^{\pm}) , \tag{4.19}$$

where

$$\mathcal{H}^{\pm}=8(\lambda^{\pm})^2\gamma^{\pm}-\epsilon^{\pm}\nu^{\pm},\quad \mathcal{G}^{\pm}=8(\lambda^{\pm})^2\delta^{\pm}-\epsilon^{\pm}\mu^{\pm} , \tag{4.20a}$$

$$\gamma^{\pm}=(\Delta_1^{\pm})^3+2\Delta_2^{\pm}(\Delta^{\pm})^2[3(\Delta_1^{\pm})^2-2\Delta_1^{\pm}\Delta_2^{\pm}+(\Delta_2^{\pm})^2]\lambda^{\pm}+16\Delta_1^{\pm}(\Delta_2^{\pm})^2(\Delta^{\pm})^4(\lambda^{\pm})^2 , \tag{4.20b}$$

$$\delta^{\pm}=\frac{1}{4\lambda^{\pm}}\Delta^{\pm}(C^{\pm}+B_{\alpha}^{\pm})+\frac{1}{6}\Delta^{\pm}\Delta_2^{\pm}(3\Delta_1^{\pm}+\Delta_2^{\pm})B_{\beta}^{\pm}+\frac{1}{6}\Delta_1^{\pm}(\Delta_2^{\pm})^2B_{\gamma}^{\pm} , \tag{4.20c}$$

$$\mathcal{N}^{\pm}=\frac{48Z_{T,P}}{v}(\alpha\beta)^3z^{\pm}(z^{\mp}-i\tau_1v)(z^{\mp}-i\tau_2v),\quad \epsilon^{\pm}=\frac{z^{\pm}t_1^{\mp}}{(\Delta_1^{\pm})^2} . \tag{4.20d}$$

This step of the analysis completes the calculation of the matrix elements $\overline{T}_{if}^{\pm}(\boldsymbol{\eta};\tau_1,\tau_2)$ in terms of the two-dimensional integrals over the real variables t_1 and t_2 both belonging to the interval [0,1]. Thus the final results of method 2 for the basic quantities $\overline{T}_{if}^{\pm}(\boldsymbol{\eta})$ from Eq. (4.1) are given by *four-dimensional* numerical quadratures over the real variables $\tau_{1,2}\in[0,1]$ and $t_{1,2}\in[0,1]$. Hence, this procedure of the calculation is less efficient than method 1 from the preceding section. Nevertheless, method 2 has its own merits because it can be extended to the excited states and highly correlated configuration interaction (CI) orbitals [62,63] in a much easier manner

than in the case of method 1. In the present work, method 2 will serve as an independent check of the numerical results obtained by means of method 1.

V. THE RESULTS OF THE NUMERICAL COMPUTATIONS

We emphasize that from the results presented in Sec. IV for the BCIS method, one could also readily deduce the corresponding formulas relating to the CB1 approximation. This is accomplished by setting the Sommerfeld parameter ν_K equal to zero in the Coulomb continuum intermediate states and redefining appropriately [50,51] the constant ξ_K. In this way the present algorithm developed for the BCIS theory is easily adjusted to yield the results in the CB1 model also. We observe from Eqs. (4.1), (4.4), and (4.19), that the quantities $\overline{T}_{if}^{\pm}(\eta)$ do not depend upon the azimuthal angle ϕ_η, i.e., $\overline{T}_{if}^{\pm}(\boldsymbol{\eta})=\overline{T}_{if}^{\pm}(\eta)$ and, therefore,

$$Q_{if}^{\pm}(\pi a_0^2)=\frac{1}{2\pi^2 v^2}\int_0^{\infty} d\eta\,\eta|\overline{T}_{if}^{\pm}(\eta)|^2 . \tag{5.1}$$

Here, rather than performing the remaining quadrature over η by the usual *scaled* Gauss-Laguerre method, we shall resort to an appropriate change of variable with the purpose of concentrating the integration points near the forward cone [34], where the total cross section peaks: $\eta=\sqrt{2(1+u)/(1-u)}$, with $u\in[-1,+1]$. This yields

$$Q_{if}^{\pm}(\pi a_0^2)=N_{\xi_{T,P}}^{\pm}N_{P,T}\int_{-1}^{+1}du\,|\mathcal{T}_{if}^{\pm}(u)|^2 , \tag{5.2}$$

where the quantities $N_{P,T}$ and $\mathcal{T}_{if}^{\pm}(u)$ are defined in Appendix B. In particular, method 2 provides the matrix element $\mathcal{T}_{if}^{\pm}(u)$ as a *four-dimensional* real quadrature from 0 to 1. The present algorithm developed to compute the total cross section (5.3) through the *five-dimensional* quadrature is thoroughly described in Appendix C.

As an illustration of the presently proposed BCIS approximation, the differential and total cross sections are computed for the following symmetric double charge exchange:

$$^4\mathrm{He}^{2+}+{}^4\mathrm{He}(1s^2)\rightarrow{}^4\mathrm{He}(1s^2)+{}^4\mathrm{He}^{2+} , \tag{5.3}$$

for which there is no *post-prior* discrepancy. The results obtained are shown in Tables I and II and Figs. 1 and 2. We shall first inspect the differential cross sections in Fig. 1 at 1.5 MeV by comparing the experimental data of Schuch *et al.* [16] with the present results obtained in the BCIS and CB1 approximations. The CB1 method exhibits an unphysical and experimentally unobserved dip at $\theta_{\mathrm{lab}}\approx 0.112$ mrad. At this particular scattering angle, perturbation potentials V_f^d and V_i^d from Eqs. (2.13b) and (2.14c) vanish identically due to the cancellation of the contributions of the opposite signs coming from the terms $+2/R$ and $-1/\omega_1-1/\omega_2$, where $\omega_j=x_j$ or $\omega_j=s_j$. As seen from Fig. 1, in a narrow cone near the forward direction, which otherwise contributes dominantly to the observables $Q_{if}^{\pm}$, the differential cross sections of the CB1 approximation grossly overestimate the experimental findings. On the other hand, the BCIS theory is observed in Fig. 1 to provide a substantial improvement over the CB1 model. First of all, the dip in the angular distribution obtained in the BCIS method disappears, despite the fact that perturbation potentials $V_{f,i}^d$ are also present in the transition amplitudes $T_{if}^{\pm(\mathrm{BCIS})}$. The reason for this is in the interference of the dip due to the vanishing of the potential V_i^d or V_f^d and a minimum produced by the presence of the two continuum intermediate states $\varphi_{\mathbf{v}}^{-}(\mathbf{x}_{1,2})$ or $\varphi_{-\mathbf{v}}^{+}(\mathbf{s}_{1,2})$. In addition to the eikonal strong forward peaking, there are two additional structures in the curve predicted by the BCIS model, namely, a minimum and maximum at $\theta_{\mathrm{lab}}\approx 0.14$ mrad and $\theta_{\mathrm{lab}}\approx 0.21$ mrad, respectively. Thomas double

TABLE I. Theoretical differential cross sections $dQ_{if}^{\pm}/d\Omega\equiv(dQ_{if}^{\pm}/d\Omega)_{\mathrm{lab}}$ (cm^2/sr) as a function of the laboratory scattering angle $\theta\equiv\theta_{\mathrm{lab}}$ (mrad) at incident energy 1.5 MeV for the double-charge-exchange reaction $^4\mathrm{He}^{2+}+{}^4\mathrm{He}(1s^2)\rightarrow{}^4\mathrm{He}^{2+}(1s^2)+{}^4\mathrm{He}^{2+}$. The displayed results are obtained by means of the present boundary-corrected continuum-intermediate-state (BCIS) method using the uncorrelated one-parameter orbitals of the type $(Z^3/\pi)e^{-Z(r_1+r_2)}$ for the initial and final helium bound states with the effective nuclear charge $Z=1.6875$. The *prior* and *post* differential cross sections $dQ_{if}^{-}/d\Omega$ and $dQ_{if}^{+}/d\Omega$ are identical to each other for the reaction under study and they are denoted by the common label $dQ/d\Omega\equiv dQ_{if}^{\pm}/d\Omega$. The numbers in brackets denote multiplicative powers of ten.

θ	$\frac{dQ}{d\Omega}$	θ	$\frac{dQ}{d\Omega}$
0.0000	5.31[−13]	0.2300	1.16[−14]
0.0125	4.97[−13]	0.2400	1.13[−14]
0.0250	4.09[−13]	0.2500	1.08[−14]
0.0375	2.98[−13]	0.2750	9.43[−15]
0.0500	1.95[−13]	0.3000	8.00[−15]
0.0625	1.16[−13]	0.3250	6.69[−15]
0.0750	6.54[−14]	0.3500	5.57[−15]
0.0875	3.60[−14]	0.3750	4.62[−15]
0.1000	2.06[−14]	0.4000	3.84[−15]
0.1050	1.70[−14]	0.4250	3.19[−15]
0.1100	1.43[−14]	0.4500	2.66[−15]
0.1150	1.24[−14]	0.4750	2.23[−15]
0.1200	1.10[−14]	0.5000	1.87[−15]
0.1250	1.01[−14]	0.5250	1.58[−15]
0.1300	9.57[−15]	0.5500	1.34[−15]
0.1350	9.24[−15]	0.5750	1.14[−15]
0.1400	9.11[−15]	0.6000	9.74[−16]
0.1450	9.12[−15]	0.6250	8.37[−16]
0.1500	9.23[−15]	0.6500	7.23[−16]
0.1550	9.43[−15]	0.6750	6.27[−16]
0.1600	9.68[−15]	0.7000	5.46[−16]
0.1750	1.06[−14]	0.7250	4.78[−16]
0.1800	1.09[−14]	0.7500	4.19[−16]
0.1850	1.11[−14]	0.7750	3.70[−16]
0.1900	1.14[−14]	0.8000	3.27[−16]
0.1950	1.15[−14]	0.8250	2.90[−16]
0.2000	1.17[−14]	0.8500	2.58[−16]
0.2100	1.18[−14]	0.8750	2.31[−16]
0.2200	1.18[−14]	0.9000	2.07[−16]
0.2250	1.17[−14]		

TABLE II. Theoretical total cross sections $Q_{if}^{\pm}$ (cm^2), as a function of the laboratory incident energy E (keV) for double-charge-exchange reaction $^4He^{2+}+{}^4He(1s^2)\rightarrow{}^4He^{2+}(1s^2)+{}^4He^{2+}$. The displayed results are obtained by means of the present boundary-corrected continuum-intermediate-state (BCIS) method and the boundary-corrected first Born (CB1) approximation of Ref. [50] using the uncorrelated one-parameter orbitals of the type $(Z^3/\pi)e^{-Z(r_1+r_2)}$ for the initial and final helium bound states with the effective nuclear charge $Z=1.6875$. The *prior* and *post* total cross sections Q_{if}^{-} and Q_{if}^{+} are identical to each other for the reaction under study and they are denoted by the common label $Q\equiv Q_{if}^{\pm}$.

	Q (cm^2)	
E (keV)	BCIS	CB1
900	1.89[−19]	8.11[−19]
1000	1.10[−19]	5.16[−19]
1250	3.19[−20]	1.87[−19]
1500	1.05[−20]	7.75[−20]
1750	3.89[−21]	3.54[−20]
2000	1.57[−21]	1.75[−20]
2500	3.17[−22]	5.10[−21]
3000	7.96[−23]	1.78[−21]
3500	2.37[−23]	7.07[−22]
4000	8.11[−24]	3.12[−22]
5000	1.31[−24]	7.65[−23]
6000	2.95[−25]	2.35[−23]
7000	8.69[−26]	8.55[−24]

scattering for reaction (5.3) takes place at $\theta_{lab}\approx 0.24$ mrad, but the energy of 1.5 MeV is too small to exhibit this effect clearly in the measurement. Otherwise, as can be seen from Fig. 1, overall agreement between the BCIS method and the experimental data can be considered as fairly good. We should point out that the measured findings on $dQ/d\Omega$ relate to double capture into all (ground and excited) states of He, whereas the theory accounts only for the transition $1s^2\rightarrow 1s^2$. The minimum in the full curve in Fig. 1 would be partially filled in by inclusion of the excited states of He. A similar effect has previously been noticed in Ref. [33] in the case of single-electron capture treated within the CB1 model. The main purpose of Fig. 1 is to clearly demonstrate the influence of the electronic intermediate ionization continua onto the differential cross-section data by direct comparison between the results of the *four-body* versions of the BCIS and CB1 methods. Nevertheless, it would be instructive to plot on the same figure the corresponding findings of the independent-particle model, which has successfully been used in the previous computations. Hence, we show in Fig. 1 the angular distribution obtained using a version of the CDW approximation, devised by Deco and Grün [13,16] within the IPM and configuration-interaction (CI) wave functions. There are some undulations in the differential cross sections $dQ^{CDW}/d\Omega$ similar to those reported previously in Ref. [28] in the case of one-electron capture by protons from helium. Around the critical angle $\theta_{lab}\approx 0.24$ mrad, only a shoulder is seen in the dotted curve of the CDW model, since the impact energy is too small to exhibit a net effect of the Thomas double scattering. None of the theoretical curves displayed in Fig. 1 are folded with the experimental angular resolution function. Once this folding is accomplished, as exemplified in Ref. [16], the convoluted data of Deco and Grün's IPM model of the CDW theory are significantly reduced only at the scattering angles from $\theta_{lab}=0.01$ mrad to $\theta_{lab}\approx 0.1$ mrad. This reduction is smooth, ranging from a factor of ~ 3.1 at $\theta_{lab}=0.01$ mrad to ~ 1.2 at $\theta_{lab}=0.1$ mrad. A similar behavior is expected to be found also in the present BCIS approximation.

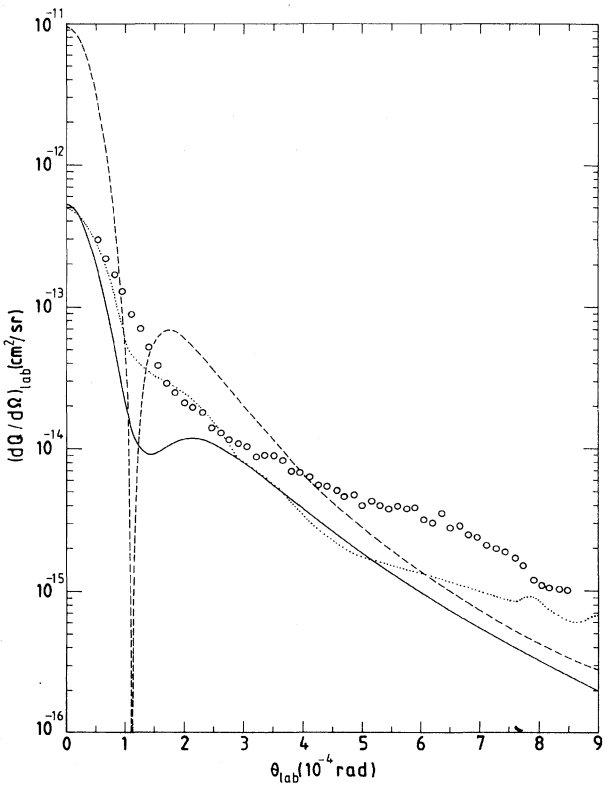

FIG. 1. Differential cross sections $dQ_{if}^{\pm}/d\Omega\equiv(dQ_{if}^{\pm}/d\Omega)_{lab}$ (cm^2/sr), as a function of scattering angle $\theta\equiv\theta_{lab}$ (mrad) in the laboratory frame of reference at incident energy $E=1.5$ MeV for the double-charge-exchange reaction: $^4He^{2+}+{}^4He\rightarrow{}^4He+{}^4He^{2+}$. The displayed theoretical curves relate only to the transition $1s^2\rightarrow 1s^2$. The full line represents the results of the present boundary-corrected continuum-intermediate-state method. The dashed line is due to the boundary-corrected first Born approximation introduced in Refs. [50,51] for two-electron transfer. Both computations employ the uncorrelated one-parameter orbitals of the type $(Z^3/\pi)e^{-Z(r_1+r_2)}$ with the effective nuclear charge $Z=1.6875$ for the initial and final bound states of helium. The *prior* and *post* differential cross sections $dQ_{if}^{-}/d\Omega$ and $dQ_{if}^{+}/d\Omega$ are identical to each other for the reaction under study and they are denoted by the common label $dQ/d\Omega\equiv dQ_{if}^{\pm}/d\Omega$. The dotted line represents the results of Deco and Grün's independent-particle model of the CDW approximation with the CI wave functions (Refs. [13,16]). None of the quoted theoretical data are folded with the experimental resolution function. Experimental data (including double capture into all bound states of He): ∘ , Schuch *et al.* (Ref. [16]).

The total cross sections for process (5.4) are shown in Fig. 2 at impact energies ranging from 900 keV to 6 MeV. We have also extended the computation of Ref. [50] and obtained the results of the total cross sections by using the boundary-corrected first Born (CB1) approximation in the energy range $E \in [0.9,6]$ MeV. We emphasize again that the perturbation potentials $V_{i,f}^{d}$ are the same in the CB1 and BCIS theories. Both methods satisfy the correct boundary conditions in the entrance and exit channels of the general reaction (2.1). However, unlike the CB1 approach, the second-order BCIS method takes *full* account of the Coulomb continuum intermediate states of both electrons in either the entrance or exit channels. Hence, by comparing these two theories, we would learn about the relative importance of these intermediate ionization electronic continua. The outcome of such a comparison is evident and self-explanatory from Fig. 2. The BCIS method provides the cross sections which are much smaller than the corresponding results of the CB1 approximation throughout the energy range under consideration. The difference between the findings of the BCIS and CB1 methods increases as the impact energy is augmented reaching even *two orders* of magnitudes at 6 MeV. Such a pattern is explained by the following argument. The two electrons are *intermediately* found in the on-shell continuum states of the projectile nucleus before the actual double capture takes place. Since the electrons are *not* staying in these continuum states in the *final* stage of the collision, the probability for double-electron transfer to a discrete state in the projectile Coulomb field is *reduced*. The obtained reduction seen in Fig. 2 is so significant that the mechanism of having the two electrons in the continuum intermediate states, as in the BCIS method, becomes dominant over the simple picture of the CB1 model, according to which the electrons are *free* in the intermediate stage of collision involving double charge exchange. A comparison between the present results and the available experimental data on total cross sections is also displayed in Fig. 2. The BCIS method is found to be in satisfactory agreement with the measurement. Also shown in Fig. 1 are the total cross sections of the Deco-Grün [13,16] IPM model of the CDW approximation with the CI wave functions, which compares favorably with the experiment. It is seen in Fig. 1 that the most dramatic improvement of the BCIS over CB1 approximation is observed at impact energies belonging to the interval [0.9, 3] MeV. At the two largest energies (5 and 6 MeV) considered in the experiment of Ref. [16], the results of the BCIS model are seen from Fig. 2 to significantly overestimate the measured data. This is partially due to the fact that the BCIS method allows for the full electronic continuum intermediate states only in *one* channel (entrance or exit). If we account for these intermediate ionization continua symmetrically in both asymptotic channels, as properly done within the four-body CDW approximation [24,25], then the total cross sections should be further reduced in relation to the BCIS method. This follows from an argument analogous to the one put forward in the above discussion concerning the relation between the CB1 and BCIS models. The other reason for a possible explanation of the discrepancy between the BCIS theory and the measurement at 5 and 6 MeV is an experimental underestimation of the true total cross sections, namely, the results reported in Ref. [16] at these two energies relate to the "partial" cross sections Q_p defined by $Q_p \equiv 2\pi \int_0^{\theta_m} d\theta (dQ/d\theta)$, where θ_m is a certain maximal value of the acceptance angle. Schuch *et al.* [16] have determined θ_m with confidence at 1.5 MeV, since they measured the differential cross sections at this energy. That same value of θ_m was also used at 4 and 6 MeV at which, however, no data on $dQ/d\theta$ were recorded in Ref. [16]. A correction due to the proper

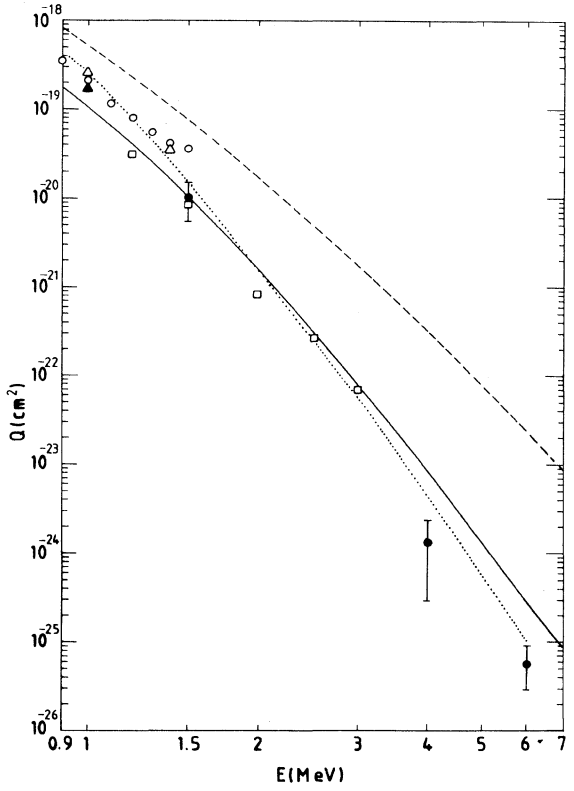

FIG. 2. Total cross sections, as a function of laboratory incident energy E (keV) for the double-charge-exchange reaction: $^4He^{2+} + {}^4He \rightarrow {}^4He + {}^4He^{2+}$. The depicted theoretical curves relate only to the translation $1s^2 \rightarrow 1s^2$. The full line represents the results of the present boundary-corrected continuum-intermediate-state method. The dashed line is due to the boundary-corrected first born approximation introduced in Refs. [50,51] for two-electron transfer. Both computations employ the uncorrelated one-parameter orbitals of the type $(Z^3/\pi)e^{-Z(r_1+r_2)}$ with the effective nuclear charge $Z=1.6875$ for the initial and final bound states of helium. The *prior* and *post* total cross sections Q_{if}^{-} and Q_{if}^{+} are identical to each other for the reaction under study and they are denoted by the common label $Q \equiv Q_{if}^{\pm}$. The dotted line represents the results of Deco and Grün's independent-particle model of the CDW approximation with the CI wave functions (Refs. [13,16]). Experimental data (including double capture into all bound states of He): ○, Pivovar, Novikov, and Tubaev (Ref. [77]); Δ, McDaniel *et al.* (Ref. [78]); ∇, DuBois (Ref. [79]); □, Castro de Faria, Freire, and de Pinho (Ref. [80]); and ●, Schuch *et al.* (Ref. [16]).

determination of θ_m at 5 and 6 MeV could enlarge the error bar seen in Fig. 2 by another estimated [16,64] amount of roughly 30%.

VI. CONCLUSION

We have studied the role of the intermediate ionization continua in the problem of the two-electron capture from heliumlike atomic systems by bare nuclei at high impact energies. The analysis is accomplished within the distorted-wave four-body formalism by devising a second-order model termed as the boundary-corrected continuum-intermediate-state approximation. The total scattering wave functions of the four-body BCIS theory satisfy the proper boundary conditions in *both* initial and final asymptotic channels. In addition to the long-range Coulomb distortions of the plane waves for the relative motion of the two charged aggregates, we account for the intermediate ionization continua of the two electrons in either the entrance or exit channel depending upon whether we are dealing with the post or prior form of the transition amplitude. The effect of these continuum intermediate states is observed to be striking in the case of the symmetric resonant double charge transfer in α-He($1s^2$) collision at high energies. Reduction of the total cross sections for about *two orders* of magnitude at high energies is recorded in the BCIS method in comparison with the corresponding results of the boundary-corrected first Born model, which incorporates only the direct collisional path without any double-electron scattering effects. As to testing the theory against the measurement, the BCIS approximation is found to yield results which are in good agreement with the available experimental data on differential and total cross sections for two-electron capture from helium by α particles at high incident energies. More work is required to firmly establish the validity of the present second-order method in comparison with the experimental data on asymmetric collision systems exhibiting double charge exchange, as well as with other second-order theories, notably the rigorous four-body extension of the continuum-distorted-wave theory recently devised by Belkić and Mančev [24,25].

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APPENDIX A

Here we calculate the integral (3.15) from the main text. We first utilize the Feynman parametrization technique, such as

$$\frac{1}{(|\mathbf{q}_2-\mathbf{p}_2|^2+\gamma_2^2)(|\mathbf{q}_2-\boldsymbol{\kappa}_2|^2+\delta_2^2)} = \int_0^1 dt_2 \frac{1}{(|\mathbf{q}_2-\mathbf{Q}_2|^2+\Delta_2^2)^2} , \tag{A1a}$$

where

$$\begin{aligned} \mathbf{Q}_2 &= \mathbf{p}_2 t_2 + \boldsymbol{\kappa}_2(1-t_2), \\ \Delta_2^2 &= |\mathbf{p}_2-\boldsymbol{\kappa}_2|^2 t_2(1-t_2)+\gamma_2^2 t_2+\delta_2^2(1-t_2) . \end{aligned} \tag{A1b}$$

Inserting (A1) into Eq. (3.15) we arrive at the following expression:

$$Z^{(\delta_1,\delta_2)}_{\gamma;\gamma_1,\gamma_2}(\nu,\xi,\mathbf{q};\mathbf{p}_1,\boldsymbol{\kappa}_1;\mathbf{p}_2,\boldsymbol{\kappa}_2) = N(\nu;\xi) \oint_C^{(0^+,\infty^+)} d\tau \oint_{C_1}^{(0^+,1^+)} d\tau_1 f(\nu;\xi;\tau,\tau_1) \int_0^1 dt_2 K(t_2) , \tag{A2a}$$

where

$$K(t_2) = \int d\mathbf{q}_1 \frac{L(t_2,\mathbf{q}_1)}{(|\mathbf{q}_1-\mathbf{p}_1|^2+\gamma_1^2)(|\mathbf{q}_1-\boldsymbol{\kappa}_1|^2+\delta_1^2)} , \tag{A2b}$$

and

$$L(t_2,\mathbf{q}_1) = \int d\mathbf{q}_2 \frac{1}{(|\mathbf{q}_2-\mathbf{Q}_2|^2+\Delta_2^2)^2(|\mathbf{q}_1+\mathbf{q}_2-\mathbf{q}|^2+\gamma^2)} . \tag{A2c}$$

Using the simple analytical result of the two-denominator integral in the form [65–67]

$$\int d\mathbf{p} \frac{1}{(p^2+\lambda^2)(|\mathbf{p}-\boldsymbol{\omega}|^2+\mu^2)^2} = \frac{\pi^2}{\mu} \frac{1}{\omega^2+(\lambda+\mu)^2} , \tag{A3a}$$

we deduce

$$L(t_2,\mathbf{q}_1) = \frac{\pi^2}{\Delta_2} \frac{1}{|\mathbf{q}_1-\mathbf{Q}|^2+\Delta^2} , \tag{A3b}$$

where $\mathbf{Q}=\mathbf{q}-\mathbf{Q}_2$ and $\Delta=\gamma+\Delta_2$. Therefore, Eq. (A2b) becomes

$$K(t_2) = \frac{\pi^2}{\Delta_2} \int d\mathbf{q}_1 \frac{1}{(|\mathbf{q}_1-\mathbf{p}_1|^2+\gamma_1^2)(|\mathbf{q}_1-\boldsymbol{\kappa}_1|^2+\delta_1^2)(|\mathbf{q}_1-\mathbf{Q}|^2+\Delta^2)} . \tag{A4a}$$

This is the well-known Dalitz [65] three-denominator integral whose general result was obtained by Lewis [66] (for the most general Dalitz-Lewis integrals involving the momentum space hydrogenic orbitals with spherical harmonics encountered in applications within the CB2 approximation, see Belkić [67]):

$$\int d\mathbf{p}\frac{1}{(p^2+\lambda^2)(|\mathbf{p}-\mathbf{p}_1|^2+\mu_1^2)(|\mathbf{p}-\mathbf{p}_2|^2+\mu_2^2)}=2\pi^2\int_0^\infty dt\frac{1}{\alpha_0 t^2+2\beta_0 t+\gamma_0}$$
$$=\frac{\pi^2}{\sqrt{\beta_0^2-\alpha_0\gamma_0}}\ln\left[\frac{\beta_0+\sqrt{\beta_0^2-\alpha_0\gamma_0}}{\beta_0-\sqrt{\beta_0^2-\alpha_0\gamma_0}}\right], \tag{A4b}$$

where

$$\alpha_0=\mu_1(z_1^{1/2}+z_2^{1/2})[p_2^2+(\lambda+\mu_2)^2], \tag{A5a}$$
$$\beta_0=\lambda\mu_1\mu_2(2+z_1+z_2)+\mu_2(\lambda^2+p_1^2+\mu_1^2)+\mu_1(\lambda^2+p_2^2+\mu_2^2), \tag{A5b}$$
$$\gamma_0=\mu_2(z_1^{1/2}+z_2^{1/2})[p_1^2+(\lambda+\mu_1)^2], \tag{A5c}$$

and

$$z_{1,2}=\frac{1}{2\mu_1\mu_2}\{|\mathbf{p}_1-\mathbf{p}_2|^2+\mu_1^2+\mu_2^2\mp\sqrt{[|\mathbf{p}_1-\mathbf{p}_2|^2+\mu_1^2+\mu_2^2]^2-4\mu_1^2\mu_2^2}\}. \tag{A5d}$$

If we employ the final analytical result of the Dalitz-Lewis integral (A4b) in terms of the elementary logarithmic function, we would afterwards be forced to carry out the integrals over τ and τ_1 in Eq. (A2a) by means of the numerical methods. However, as it will be shown shortly, these two integrations (τ,τ_1) can be carried out analytically, provided that we utilize the intermediate expression in (A4b) given as a real quadrature over t from 0 to ∞. By so doing, we shall first introduce the change of variable $t'=\mu_1(z_1^{1/2}+z_2^{1/2})t$ in the integral over t in Eq. (A4b) and obtain the result

$$\int d\mathbf{p}\frac{1}{(p^2+\lambda^2)(|\mathbf{p}-\mathbf{p}_1|^2+\mu_1^2)(|\mathbf{p}-\mathbf{p}_2|^2+\mu_2^2)}=2\pi^2\int_0^\infty dt\frac{1}{At^2+2Bt+C}, \tag{A6a}$$

with

$$A=|\mathbf{p}_1-\mathbf{p}_2|^2+(\mu_1+\mu_2)^2, \tag{A6b}$$
$$B=\lambda A+\mu_2(\lambda^2+p_1^2+\mu_1^2)+\mu_1(\lambda^2+p_2^2+\mu_2^2), \tag{A6c}$$
$$C=[p_1^2+(\lambda+\mu_1)^2][p_2^2+(\lambda+\mu_2)^2]. \tag{A6d}$$

In this manner, integral $K(t_2)$ from Eq. (A4a) reads as follows:

$$K(t_2)=\frac{\pi^2}{\Delta^2}\int d\mathbf{q}_1\frac{1}{(q_1^2+\delta_1^2)(|\mathbf{q}_1-\mathbf{u}_1|^2+\gamma_1^2)(|\mathbf{q}_1-\mathbf{w}_1|^2+\Delta^2)}$$
$$=\frac{2\pi^4}{\Delta_2}\int_0^\infty dt\frac{1}{at^2+2bt+c}, \tag{A7a}$$

where

$$a=|\mathbf{u}_1-\mathbf{w}_1|^2+(\gamma_1+\Delta)^2=|\mathbf{p}_1-\mathbf{Q}|^2+(\gamma_1+\Delta)^2, \tag{A7b}$$
$$b=a\delta_1+(\delta_1^2+u_1^2+\gamma_1^2)\Delta+(\delta_1^2+w_1^2+\Delta^2)\gamma_1, \tag{A7c}$$
$$c=[u_1^2+(\delta_1+\gamma_1)^2][w_1^2+(\delta_1+\Delta)^2], \tag{A7d}$$
$$\mathbf{u}_1=\mathbf{p}_1-\boldsymbol{\kappa}_1,\quad \mathbf{w}_1=\mathbf{Q}-\boldsymbol{\kappa}_1,\quad u_1=|\mathbf{u}_1|,\quad w_1=|\mathbf{w}_1|. \tag{A7e}$$

Inserting the result (A7a) into Eq. (A2a), we arrive at the expression

$$Z^{(\delta_1,\delta_2)}_{\gamma;\gamma_1,\gamma_2}(\nu,\xi,\mathbf{q};\mathbf{p}_1,\boldsymbol{\kappa}_1;\mathbf{p}_2,\boldsymbol{\kappa}_2)=2\pi^4N(\nu;\xi)\oint_C^{(0^+,\infty^+)}d\tau\oint_{C_1}^{(0^+,1^+)}d\tau_1 f(\nu;\xi;\tau,\tau_1)\int_0^1\frac{dt_2}{\Delta_2}\int_0^\infty dt\frac{1}{at^2+2bt+c}. \tag{A8}$$

In the particular case of Eqs. (3.13a) and (3.13b) of the main text, we shall have

$$Z^{(a_1,a_2)}_{\gamma_\lambda;\beta_{b1},\beta_{b2}}(\nu_P,\xi_T;-\tau\mathbf{v};\mathbf{q}_{P1},-\mathbf{q}_T,\mathbf{q}_{P2},-\mathbf{q}_T)$$
$$=2\pi^4N(\nu_P;\xi_T)\oint_C^{(0^+,\infty^+)}d\tau\oint_{C_1}^{(0^+,1^+)}d\tau_1 f(\nu_P;\xi_T;\tau,\tau_1)\int_0^1\frac{dt_2}{\Delta_2}\int_0^\infty dt\frac{1}{a't^2+2b't+c'}, \tag{A9a}$$

where

$$a'=a_\alpha-2a_\beta\tau+2a_\gamma\tau_1-2a_\delta\tau\tau_1 , \tag{A9b}$$

$$b'=b_\alpha-2b_\beta\tau+2b_\gamma\tau_1-2b_\delta\tau\tau_1 , \tag{A9c}$$

$$c'=c_\alpha-2c_\beta\tau+2c_\gamma\tau_1-2c_\delta\tau\tau_1 , \tag{A9d}$$

and

$$a_\alpha=w_T^2+\xi_b^2,\quad \xi_b=\xi+b_1,\quad \xi=\lambda+\Delta_2 , \tag{A10a}$$

$$a_\beta=\mathbf{w}_T\cdot\mathbf{v}-iv\xi_a,\quad a_\gamma=-\mathbf{w}_T\cdot\mathbf{v}-iv\xi_a,\quad a_\delta=-2v^2 , \tag{A10b}$$

$$\mathbf{w}_T=\mathbf{u}_T+\mathbf{v},\quad \mathbf{u}_T=2\mathbf{q}_T+t_2'\mathbf{v},\quad t_2'=(1-\tau_2)t_2 , \tag{A10c}$$

$$b_\alpha=b_1\omega_\alpha+a_1a_\alpha+\zeta\gamma_\alpha,\quad \omega_\alpha=a_1^2+\xi^2+u_T^2,\quad \gamma_\alpha=v^2+b_1^2+a_1^2 , \tag{A11a}$$

$$b_\beta=a_1a_\beta+b_1\omega_\beta-\tfrac{1}{2}iv\gamma_\alpha,\quad \omega_\beta=\mathbf{u}_T\cdot\mathbf{v}-iv\zeta , \tag{A11b}$$

$$b_\gamma=a_1a_\gamma+\zeta\gamma_\beta-\tfrac{1}{2}iv\omega_\alpha,\quad \gamma_\beta=-v^2-ivb_1 , \tag{A11c}$$

$$b_\delta=a_1a_\delta-iv(\gamma_\beta+\omega_\beta) , \tag{A11d}$$

$$c_\alpha=\sigma_\alpha\rho_\alpha,\quad \sigma_\alpha=v^2+c_1^2,\quad \rho_\alpha=\xi_a^2+u_T^2,\quad \zeta_a=\zeta+a_1 , \tag{A12a}$$

$$c_\beta=\sigma_\alpha\rho_\beta,\quad \rho_\beta=\mathbf{u}_T\cdot\mathbf{v}-iv\zeta_a , \tag{A12b}$$

$$c_\gamma=i\sigma_\beta\rho_\alpha,\quad \sigma_\beta=iv^2-c_1v , \tag{A12c}$$

$$c_\delta=2i\sigma_\beta\rho_\beta,\quad c_1=a_1+b_1 . \tag{A12d}$$

For the purpose of having an integral over the *finite* lower and upper limits, which are more convenient for subsequent numerical computations than the original interval $[0,\infty]$, we shall change the integration variable in Eq. (A9a) according to $t'=t/(1+t)$ so that

$$Z^{(a_1,a_2)}_{\gamma_\lambda;\beta_{b1},\beta_{b2}}(\nu_P,\xi_T;-\tau\mathbf{v};\mathbf{q}_{P1},-\mathbf{q}_T,\mathbf{q}_{P2},-\mathbf{q}_T) = \frac{\pi^3}{2}\int_0^1\frac{dt_2}{\Delta_2}\int_0^1 dt\,\mathcal{N}(t,t_2) , \tag{A13a}$$

where

$$\mathcal{N}(t,t_2)=-\frac{N}{2\pi}\oint_C^{(0^+,\infty^+)}d\tau\oint_{C_1}^{(0^+,1^+)}d\tau_1\frac{(-\tau)^{i\xi_T-1}\tau_1^{i\nu_P-1}(\tau_1-1)^{-i\nu_P}}{(\delta'-\beta')\tau\tau_1+\beta'\tau+(\alpha'-\gamma')\tau_1-\alpha'} , \tag{A13b}$$

with $N=N^+(\nu_P)\mathcal{N}(\xi_T)$,

$$\alpha'=\tfrac{1}{2}[(a_\alpha-2b_\alpha+c_\alpha)t^2+2(b_\alpha-c_\alpha)t+c_\alpha] , \tag{A14a}$$

$$\beta'=(a_\beta-2b_\beta+c_\beta)t^2+2(b_\beta-c_\beta)t+c_\beta , \tag{A14b}$$

$$\gamma'=(a_\gamma-2b_\gamma+c_\gamma)t^2+2(b_\gamma-c_\gamma)t+c_\gamma+\alpha' , \tag{A14c}$$

$$\delta'=(a_\delta-2b_\delta+c_\delta)t^2+2(b_\delta-c_\delta)t+c_\delta+\beta' . \tag{A14d}$$

The quantity $\mathcal{N}(t,t_2)$ belongs to the class of the well-known Nordsieck [61] integrals, whose final result is presently obtained as the following concise expression:

$$\mathcal{N}(t,t_2)=\frac{2\pi}{\alpha'}N^+(\nu_P)N^{-*}(\xi_T)\left[\frac{\alpha'}{\beta'}\right]^{i\xi_T}\times\left[\frac{\alpha'}{\gamma'}\right]^{i\nu_P}{}_2F_1(i\xi_T,i\nu_P;1;x) , \tag{A15}$$

with $N^-(\xi_T)=\Gamma(1+i\xi_T)e^{\pi\xi_T/2}$ and where ${}_2F_1$ is the standard Gauss hypergeometric function [60] of one variable,

$$x=1-\frac{\alpha'\delta'}{\beta'\gamma'} . \tag{A16}$$

Note that Nordsieck [61] unnecessarily limited himself to small values of the so-called damping parameter λ appearing as the exponential term $e^{-\lambda r}$ in his space integral of the bremsstrahlung matrix element. This subsequently led some authors [68] to conjecture that Nordsieck's [61] powerful complex contour method is valid only for infinitesimally small positive values λ. Such a limitation is, however, only a matter of convenience and can be avoided by the argument of analytical continuation. Borowitz and Klein [69] realized that the Nordsieck [61] technique also remains valid for noninfinitesimal values of parameter λ and this fact was utilized intensively in the case of the excitation problem in atomic scattering [69–71], as well as in single-charge-exchange reactions [72,73].

APPENDIX B

In this appendix we provide a list of the quantities encountered in Eq. (5.3) of the main text. Thus, we have

$$N_K=|N(\nu_K)|^4=\left[e^{\pi\nu_K}\frac{\pi\nu_K}{\sinh(\pi\nu_K)}\right]^2 , \tag{B1a}$$

$$N^\pm_{\xi_K}=4N_\pm^2 n_{\xi_K},\quad n_{\xi_K}=\frac{\pi\xi_K}{\sinh(\pi\xi_K)},\quad N_\pm=\frac{48Z_{T,P}}{v}(\alpha\beta)^3z^\pm , \tag{B1b}$$

where $|N^+(\nu_K)|=|N^-(\nu_K)|\equiv|N(\nu_K)|$ and

$$\mathcal{T}_{if}^\pm(u)=(\mathcal{M}_{P,T}^\pm)^2\int_0^1\int_0^1 d\tau_1 d\tau_2 f^\pm(\tau_1,\tau_2)F^\pm(\tau_1,\tau_2) . \tag{B1c}$$

Further,

$$F_{if}^\pm(\tau_1,\tau_2)=v^\pm\int_0^1\int_0^1 dt_1dt_2t_1^\pm t_2(1-t_2)\mathcal{U}^\pm(u) , \tag{B2}$$

$$\mathcal{U}^\pm(u)=(B^\pm)^{-i\xi_{T,P}}\frac{\lambda^\pm}{(\Delta_1^\pm)^3(\Delta_2^\pm)^5}(\mathcal{H}^\pm+i\xi_{T,P}\mathcal{G}^\pm) , \tag{B3a}$$

$$\mathcal{H}^{\pm}=8u_1^2(\lambda^{\pm})^2\gamma^{\pm}-\epsilon^{\pm}\nu^{\pm},\quad \mathcal{G}^{\pm}=8(\lambda^{\pm})^2\delta^{\pm}-\epsilon^{\pm}\mu^{\pm}\ , \tag{B3b}$$

$$\gamma^{\pm}=(\Delta_1^{\pm})^3+2\Delta_2^{\pm}(\Delta^{\pm})^2[3(\Delta_1^{\pm})^2-2\Delta_1^{\pm}\Delta_2^{\pm}+(\Delta_2^{\pm})^2]u_1\lambda^{\pm}$$
$$+16\Delta_1^{\pm}(\Delta_2^{\pm})^2(\Delta^{\pm})^4(u_1\lambda_1^{\pm})^2\ , \tag{B3c}$$

$$\delta^{\pm}=\frac{1}{4\lambda^{\pm}}\Delta^{\pm}(C^{\pm}+B_{\alpha}^{\pm})$$
$$+\frac{1}{6}\Delta^{\pm}\Delta_2^{\pm}(3\Delta_1^{\pm}+\Delta_2^{\pm})B_{\beta}^{\pm}+\frac{1}{6}\Delta_1^{\pm}(\Delta_2^{\pm})^2B_{\gamma}^{\pm}\ , \tag{B3d}$$

$$\nu^{\pm}=3+2[2(\Delta_1^{\pm})^2+3\Delta_1^{\pm}\Delta_2^{\pm}+2(\Delta_2^{\pm})^2]u_1\lambda^{\pm}$$
$$+8[(\Delta_1^{\pm})^4+2(\Delta_1^{\pm})^3\Delta_2^{\pm}+3(\Delta_1^{\pm})^2(\Delta_2^{\pm})^2$$
$$+2\Delta_1^{\pm}(\Delta_2^{\pm})^3+(\Delta_2^{\pm})^4](u_1\lambda^{\pm})^2$$
$$+48\Delta_1^{\pm}\Delta_2^{\pm}[(\Delta_1^{\pm})^2+(\Delta_2^{\pm})^2](\Delta^{\pm})^2(u_1\lambda^{\pm})^3$$
$$+128(\Delta_1^{\pm})^2(\Delta_2^{\pm})^2(\Delta^{\pm})^4(u_1\lambda^{\pm})^4\ , \tag{B4a}$$

$$\mu^{\pm}=2\lambda^{\pm}\{3C^{\pm}(\Delta^{\pm})^2+[(\Delta_1^{\pm})^2+3\Delta_1^{\pm}\Delta_2^{\pm}+(\Delta_2^{\pm})^2]B_{\alpha}^{\pm}$$
$$+2\Delta_1^{\pm}\Delta_2^{\pm}\lambda^{\pm}(\Delta^{\pm})^2B_{\beta}^{\pm}+\tfrac{2}{3}(\Delta_1^{\pm})^2(\Delta_2^{\pm})^2\lambda^{\pm}B_{\gamma}^{\pm}\}\ , \tag{B4b}$$

$$\lambda^{\pm}=\frac{1}{a^{\pm}+2u_1b^{\pm}}\ , \tag{B4c}$$

$$a^{\pm}=q_{\alpha}t_0+q_{\beta}t+2q_P^2t_1t_2-2t_0'\mathbf{q}_P\cdot\mathbf{q}_T$$
$$+2q_T^2(1-t_1)(1-t_2)+2u_1\Delta_1^{\pm}\Delta_2^{\pm}\ , \tag{B4d}$$

$$b^{+}=t_1t_2(v^2\tau_1\tau_2+\tau_0\mathbf{q}_P\cdot\mathbf{v})+(\mathbf{q}_P\cdot\mathbf{v}-i\beta v)\tau^{+}$$
$$-\mathbf{q}_T\cdot\mathbf{v}(\tau^{+}-\tau_0t_1t_2)\ , \tag{B5a}$$

$$b^{-}=(1-t_1)(1-t_2)(v^2\tau_1\tau_2+\tau_0\mathbf{q}_T\cdot\mathbf{v})+(\mathbf{q}_T\cdot\mathbf{v}-i\alpha v)\tau^{-}$$
$$-\mathbf{q}_P\cdot\mathbf{v}(\tau_0'-\tau_0t_1t_2)\ , \tag{B5b}$$

$$2\mathbf{q}_P\cdot\mathbf{v}=-vq^{+},\quad 2\mathbf{q}_T\cdot\mathbf{v}=-vq^{-},\quad \epsilon^{\pm}=\frac{z^{\pm}t_1^{\mp}}{(\Delta_1^{\pm})^2}\ , \tag{B5c}$$

$$4q_{T,P}^2=2(1+u)+(q^{\mp})^2u_1,$$
$$4\mathbf{q}_T\cdot\mathbf{q}_P=-2(1+u)+q^{+}q^{-}u_1\ , \tag{B5d}$$

$$q_{\alpha}=q_T^2+u_1\alpha^2,\quad q_{\beta}=q_P^2+u_1\beta^2,\quad u_1=1-u,\quad t=t_1+t_2\ , \tag{B6a}$$

$$t_0=2-t,\quad \tau^{+}=\tau_1t_1+\tau_2t_2,\quad \tau_0=\tau_1+\tau_2,$$
$$q^{\pm}=v\pm\frac{\alpha^2-\beta^2}{v}\ , \tag{B6b}$$

$$\tau_0'=\tau_1t_2+\tau_2t_1,\quad \tau^{-}=\tau_1(1-t_1)+\tau_2(1-t_2)=\tau_0-\tau^{+},$$
$$t_0'=t-2t_1t_2\ , \tag{B6c}$$

$$(\Delta_j^{\pm})^2=v_j^2t_j(1-t_j)+\{\beta_j^2,\beta^2\}t_j+\{\alpha^2,\alpha_j^2\}(1-t_j),$$
$$\Delta_j^{\pm}=+\sqrt{(\Delta_j^{\pm})^2}\ , \tag{B7a}$$

$$\Delta^{\pm}=\Delta_1^{\pm}+\Delta_2^{\pm},\quad \xi_K=2\nu_K\quad (K=P,T)\ , \tag{B7b}$$

$$C^{\pm}=\frac{v}{B^{\pm}\Delta^{\pm}}-u_1,\quad B^{\pm}=2\lambda^{\pm}(v\Delta^{\pm}\mp i\mathbf{Q}^{\pm}\cdot\mathbf{v})\ , \tag{B7c}$$

$$\mathbf{Q}^{+}\cdot\mathbf{v}=-2\mathbf{q}_T\cdot\mathbf{v}-v^2t^{+},\quad t^{+}=t-\tau^{+}\ , \tag{B8a}$$

$$\mathbf{Q}^{-}\cdot\mathbf{v}=-2\mathbf{q}_T\cdot\mathbf{v}-v^2t^{-},\quad t^{-}=t+\tau^{-}\ , \tag{B8b}$$

$$B_{\alpha}^{\pm}=u_1+2A^{\pm}C_{\alpha},\quad A^{\pm}=\lambda^{\pm}(\Delta^{\pm})^2,$$
$$C_{\alpha}^{\pm}=C^{\pm}[4u_1+(1+i\xi_{T,P})C^{\pm}]\ , \tag{B8c}$$

$$B_{\beta}^{\pm}=2A^{\pm}C_{\beta}^{\pm}+3u_1D_{\beta}^{\pm},$$
$$D_{\beta}^{\pm}=2u_1-(1-i\xi_{T,P})C^{\pm}\ , \tag{B8d}$$

$$C_{\beta}^{\pm}=C^{\pm}[18u_1^2+9(1+i\xi_{T,P})u_1C^{\pm}$$
$$+(1+i\xi_{T,P})(2+i\xi_{T,P})(C^{\pm})^2]\ , \tag{B9a}$$

$$B_{\gamma}^{\pm}=4(A^{\pm})^2C_{\gamma}^{\pm}-12u_1A^{\pm}D_{\gamma}^{\pm}+3(3-i\xi_{T,P})u_1^2\ , \tag{B9b}$$

$$C_{\gamma}^{\pm}=C^{\pm}[96u_1^3+72(1+i\xi_{T,P})u_1^2C^{\pm}$$
$$+16(1+i\xi_{T,P})(2+i\xi_{T,P})u_1(C^{\pm})^2$$
$$+(1+i\xi_{T,P})(2+i\xi_{T,P})(3+i\xi_{T,P})(C^{\pm})^3]\ , \tag{B9c}$$

$$D_{\gamma}^{\pm}=(1-i\xi_{T,P})C^{\pm}[6u_1+(1+i\xi_{T,P})C^{\pm}]-6u_1^2\ . \tag{B9d}$$

APPENDIX C

Here we shall outline the details of the present algorithm pertinent only to method 2, since it is more complicated than method 1. The numerical work invoked in method 1 can be directly set up by analogy to the device which we are going to expose. The functions $f^{\pm}(\tau_1,\tau_2)$ defined in Eqs. (4.2) and (4.3) possess the *integrable* branch-point singularities at $\tau_{1,2}=0$ and $\tau_{1,2}=1$. The standard Cauchy regularization of the whole integrand in Eq. (B1c) can be readily accomplished by first rewriting the expressions for $\mathcal{T}_{if}^{\pm}(u)$ in the following way:

$$\mathcal{T}_{if}^{\pm}(u)=\mathcal{M}_{P,T}^{\pm}\int_0^1\frac{d\tau_2}{\tau_2}h^{\pm}(\tau_2)X^{\pm}(\tau_2)\ , \tag{C1a}$$

where

$$X^{\pm}(\tau_2)=\mathcal{M}_{P,T}^{\pm}\int_0^1\frac{d\tau_1}{\tau_1}h^{\pm}(\tau_1)F^{\pm}(\tau_1,\tau_2)\ , \tag{C1b}$$

where quantities $F^{\pm}$ are defined in Eq. (B2). Then the Cauchy subtraction procedure for simultaneous regularization of the branch-point singularities at $\tau_{1,2}=0$ *and* $\tau_{1,2}=1$ implies

$$X^{\pm}(\tau_2)=\mathcal{M}_{P,T}^{\pm}\left\{\int_0^1d\tau_1h^{\pm}(\tau_1)\frac{F^{\pm}(\tau_1,\tau_2)-\tau_1[F^{\pm}(1,\tau_2)-F^{\pm}(0,\tau_2)]-F^{\pm}(0,\tau_2)}{\tau_1}\right.$$
$$\left.+[F^{\pm}(1,\tau_2)-F^{\pm}(0,\tau_2)]\int_0^1d\tau_1h^{\pm}(\tau_1)+F^{\pm}(0,\tau_2)\int_0^1\frac{d\tau_1}{\tau_1}h^{\pm}(\tau_1)\right\}\ . \tag{C2a}$$

The two last integrals in Eq. (C2a) can be calculated analytically by means of the β function (3.2c) with the results

$$\mathcal{M}_{P,T}^{\pm}\int_0^1 d\tau_1 h^{\pm}(\tau_1)=i\nu_{P,T},$$
$$\mathcal{M}_{P,T}^{\pm}\int_0^1 \frac{d\tau_1}{\tau_1} h^{\pm}(\tau_1)=1\ , \tag{C2b}$$

so that

$$X^{\pm}(\tau_2)=X_{\alpha}^{\pm}(\tau_2)+\frac{i}{\pi}\sinh(\pi\nu_{P,T})\int_0^1 d\tau_1 X_{\beta}^{\pm}(\tau_1,\tau_2)\ , \tag{C3a}$$

where

$$X_{\alpha}^{\pm}(\tau_2)=F^{\pm}(0,\tau_2)+i\nu_{P,T}X_{\gamma}^{\pm}(\tau_2)\ , \tag{C3b}$$

$$X_{\beta}^{\pm}(\tau_1,\tau_2)=h^{\pm}(\tau_1)\frac{F^{\pm}(\tau_1,\tau_2)-\tau_1 X_{\gamma}^{\pm}(\tau_2)-F^{\pm}(0,\tau_2)}{\tau_1}\ , \tag{C3c}$$

$$X_{\gamma}^{\pm}(\tau_2)=F^{\pm}(1,\tau_2)-F^{\pm}(0,\tau_2)\ . \tag{C3d}$$

An entirely analogous technique applied to the integral over the variable τ_2 yields the final results:

$$\mathcal{T}_{if}^{\pm}(u)=V_{\alpha}^{\pm}+\frac{i}{\pi}\sinh(\pi\nu_{P,T})\int_0^1 d\tau_2 V_{\beta}^{\pm}(\tau_2)\ , \tag{C4a}$$

with

$$V_{\alpha}^{\pm}=X^{\pm}(0)+i\nu_{P,T}V_{\gamma}^{\pm}\ , \tag{C4b}$$

$$V_{\beta}^{\pm}(\tau_2)=h^{\pm}(\tau_2)\frac{X^{\pm}(\tau_2)-\tau_2 V_{\gamma}^{\pm}-X^{\pm}(0)}{\tau_2}\ , \tag{C4c}$$

$$V_{\gamma}^{\pm}=X^{\pm}(1)-X^{\pm}(0)\ . \tag{C4d}$$

These Cauchy regularized integrations over τ_1 and τ_2 are now well adopted for the present application of the universal Gauss-Legendre variable-order numerical quadratures. We also employ the same quadrature rule to the other three integrations over the variables $t_{1,2}\in[0,1]$ and $u\in[-1,+1]$ in Eq. (5.2) of the main text.

Another convenient method [74] to handle the singularities at $\tau_{1,2}=0$ and $\tau_{1,2}=1$ is further implemented in our computations, namely, we first split the interval $\tau_j\in[0,1]$ into two subintervals $[0,1/2]$ and $[1/2,1]$ for $j=1,2$. Then we change the integration variables in the first and the second subintervals according to $\tau_j=\frac{1}{2}e^{-u_j}$ and $\tau_j=1-\frac{1}{2}e^{-u_j}$, respectively. This yields

$$\mathcal{T}_{if}^{\pm}(u)=\bar{X}^{\pm}(0)+\frac{i}{2\pi}\sinh(\pi\nu_{P,T})\int_0^{\infty} du_2 e^{-u_2}[\bar{V}_{\beta}^{\pm}(e^{-u_2}/2)+\bar{V}_{\beta}^{\pm}(1-e^{-u_2}/2)]\ , \tag{C5a}$$

where

$$\bar{X}^{\pm}(\tau_2)=F^{\pm}(0,\tau_2)+\frac{i}{2\pi}\sinh(\pi\nu_{T,P})\int_0^{\infty} du_1 e^{-u_1}[\bar{X}_{\beta}^{\pm}(e^{-u_1}/2,\tau_2)+\bar{X}_{\beta}^{\pm}(1-e^{-u_1}/2,\tau_2)]\ , \tag{C5b}$$

$$\bar{V}_{\beta}^{\pm}(\tau_2)=h^{\pm}(\tau_2)\frac{\bar{X}^{\pm}(\tau_2)-\bar{X}^{\pm}(0)}{\tau_2}\ , \tag{C5c}$$

$$\bar{X}^{\pm}(\tau_1,\tau_2)=h^{\pm}(\tau_1)\frac{F^{\pm}(\tau_1,\tau_2)-F^{\pm}(0,\tau_2)}{\tau_1}\ . \tag{C5d}$$

The integrals over the variables u_j $(j=1,2)$ have the branch-point singularity at $\tau_j=\infty$. This singularity, however, is never reached in practical computations due to the presence of the overall multiplying cutoff function e^{-u_j} in the integrands in Eqs. (C5a) and (C5b). This time we apply the scaled Gauss-Laguerre quadrature methods to compute the integrals over u_1 and u_2. Here, a scaling of the type

$$\int_0^{\infty} du_j e^{-u_j} f(u_j)=\frac{1}{\lambda_j}\int_0^{\infty} du_j e^{-u_j/\lambda_j} f(u_j/\lambda_j) \tag{C6}$$

is required to obtain the accurate result with the low-order Gauss-Laguerre quadrature. Some numerical experiment is necessary to select the optimal values of the scaling parameters $\lambda_j\geq 0$. Only certain values $\lambda_j^{(\mathrm{opt})}$ of λ_j are retained, which make the final result insensitive to variation of λ_j around $\lambda_j^{(\mathrm{opt})}$ $(j=1,2)$. Note that in most applications in atomic physics, the Gauss-Laguerre quadrature rule necessitates a scaling of the type (C6) in order to stabilize the convergence while increasing the number of the integration points. When the order of this quadrature method is augmented, the upper integration limit, which in practice always remains finite, is also increased. For this reason, the larger number of the quadrature pivots does not necessarily yield a better result. This is particularly true if the function under the integral sign possesses one or more maxima and otherwise is negligible elsewhere, as recorded in most applications of atomic scattering theory. In such a case, by taking a larger set of integration points one would also spend a considerable amount of the CPU time computing the values of the integrand which essentially do not contribute to the final result of the integral with a prescribed accuracy. The change of integration variable $u_j\rightarrow u_j/\lambda_j$ in (C6) scales the Gauss-Laguerre quadrature points to the region where the integrand $f(u_j)$ peaks, provided that the optimal values $\lambda_j^{(\mathrm{opt})}$ of the parameter λ_j are chosen.

We have also implemented yet another method of computation of integrals of the type

$$I_j = \int_0^1 d\tau_j \tau_j^{i\nu_K - 1}(1-\tau_j)^{-i\nu_K} f(\tau_j) , \quad \text{(C7)}$$

where $f(\tau_j)$ is a regular function in the interval $\tau_j \in [0,1]$. This alternative procedure consists of isolating the singularities at $\tau_j = 0$ and $\tau_j = 1$ by splitting the interval [0,1] into three subintervals according to $[0,1] = [0,\epsilon_j] + [\epsilon_j, 1-\epsilon_j] + [1-\epsilon_j, 1]$, where ϵ_j is a positive infinitesimally small number:

$$I_j = \left[\int_0^{\epsilon_j} + \int_{\epsilon_j}^{1-\epsilon_j} + \int_{1-\epsilon_j}^{1} \right] d\tau_j \tau_j^{i\nu_K - 1}(1-\tau_j)^{-i\nu_K} f(\tau_j) . \quad \text{(C8)}$$

Now the whole integrand $\tau_j^{i\nu_K - 1}(1-\tau_j)^{-i\nu_K} f(\tau_j) \equiv g_K(\tau_j) f(\tau_j)$ in the second integral over the middle interval $[\epsilon_j, 1-\epsilon_j]$ becomes regular and smooth, so that the standard Gauss-Legendre quadrature can be directly used in this case. On the other hand, the first and the third integral on the right-hand side of Eq. (C8) are calculated analytically. This is accomplished by expressing the integrand $g_K(\tau_j) f(\tau_j)$ as a series expansion in powers of τ_j and $1-\tau_j$ for $\tau_j \in [0,\epsilon_j]$ and $\tau_j \in [1-\epsilon_j, 1]$, respectively. The coefficients of these power-series expansions are determined numerically from an efficient Aitken algorithm originally devised in Ref. [75]. In this way, the first and third integrals in (C8) become a trivial task with simple analytical results.

It should be remarked, however, that due to the frequent occurrence of integrals of the type (C7) in the application of the distorted-wave scattering theory to realistic problems, there is a need for a general purpose algorithm. Although the three methods for the computation of integral (C7) discussed above are presently thoroughly tested and proven convenient, since they all yield the same results, we are convinced that the most efficient quadrature method would be the one which will generate the integration points by directly incorporating the troublesome terms $g_K(\tau_j)$ into the appropriate weight functions. Such an accomplishment should be feasible with the help of the Jacobi polynomials, despite the singularities of the function $g_K(\tau_j)$ at $\tau_j = 0$ and $\tau_j = 1$. Recall that, similarly, while computing the integral of the type $\int_{-1}^{+1} dx\, u(x) f(x)$, where $f(x)$ is a regular function and $u(x) = 1/\sqrt{1-x^2}$, the term $u(x)$ can readily be included in the weight function of the Chebyshev [76] quadrature methods even though $u(x)$ becomes singular at $x = \pm 1$.

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