Exact second-order Born approximation with correct boundary conditions for symmetric charge exchange

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Symmetric (homonuclear) charge transfer between completely stripped projectiles and hydrogenlike atoms is studied by means of the second-order Born approximation (CB2) with the correct boundary conditions. Along the integration path, the transition amplitude $T_{if}^{\rm CB2}$ exhibits so-called *movable singularities,* such as branch points and poles. A powerful method is presented which demonstrates that these singularities are integrable, not only for the resulting cross sections, but also for every individual matrix element. The resulting algorithm is very efficient, since the exact differential cross sections of the CB2 method are readily obtained through only two-dimensional numerical quadratures. The present theory is applied to symmetric resonant charge exchange in $H^+ + H(1s) \rightarrow H(1s) + H^+$ collisions at several impact energies, and the results are found to be in satisfactory agreement with the experimental data of Martin *et al.* [Phys. Rev. A **23**, 3357 (1981)] and Vogt *et al.* [Phys. Rev. Lett. **57**, 2256 (1986)].

I. INTRODUCTION

After a long-standing controversy, it has recently been shown[1–11] that the first-order perturbation theories of charge exchange are adequate for the total cross sections at intermediate and moderately high impact energies. This important conclusion holds true only if the correct boundary conditions[12,13] of the three-body problem are preserved, and provided that the incident energy is not favorable for the Thomas double scattering. Except at very high energies, where the double scattering of the electron with each of the two Coulomb centers becomes increasingly significant, the total cross sections are predominantly determined by an extremely narrow cone in the forward direction. A single-collision mechanism, which represents the sole basis of the first-order theories, proves sufficient for an adequate description of the angular distributions near the forward direction. Away from a narrow forward cone, however, the first order (CB1) of the perturbation Born series with the correct boundary conditions ceases to yield accurate differential cross sections.[3] This is due to strong cancellation of the contributions which come from the two parts of the perturbation potential with the opposite signs. As a result of this cancellation, an unphysical and experimentally unobserved dip appears at intermediate scattering angles for any impact energy.

Due to the above deficiency of the CB1 approach, it is necessary to compute the differential cross sections through at least the second order (CB2) of the perturbation Born series with the correct boundary conditions.[14–17] Indeed, as recently shown by Belkić,[14,15] in the case of the reaction $H^+ + H(1s) \rightarrow H(1s) + H^+$, the dip is removed from the angular distributions of projectiles at $E \geq 60$ keV, by performing the *exact* numerical computations within the CB2 approximation. These findings have subsequently been confirmed by Decker and Eicher,[18] who also extended the CB2 theory to the asymmetric case. Naturally, the second-order theories become indispensible for both the differential and total cross sections at sufficiently high energies for which the Thomas double scattering dominates the single-collision mechanism. For these reasons, it is of considerable importance to devise a powerful and expedient method for exhaustive *exact* numerical computations by means of the CB2 approximation. This is particularly demanding, in view of the troublesome *movable* singularities in repeated integrals. Specifically, the branch-point singularities of the free-particle Green's function represent the major difficulty for *direct* multiple numerical quadratures.[19–21] Therefore, an alternative algorithm is sought, which would successfully eliminate these singularities *before* the transition amplitude of the CB2 approximation is subjected to the numerical quadratures. Such a procedure is devised and implemented in the present paper. Atomic units will be used throughout unless otherwise stated.

II. THEORY

Charge exchange between completely stripped projectiles and hydrogenlike atoms is customarily symbolized as follows:

$$Z_P + (Z_T, e)_i \rightarrow (Z_P, e)_f + Z_T \ , \qquad (2.1)$$

where Z_K $(K = P, T)$ is the charge of the Kth nucleus and k $(k = i, f)$ is the usual triple of the quantum numbers, i.e., $k = n_k l_k m_k$. In the present paper, we shall restrict analysis to the symmetric (homonuclear) collisions of reaction (2.1), in which case $Z_P = Z_T$. Let us first introduce the Fourier transform $\tilde{f}(\mathbf{q})$ by

$$\tilde{f}(\mathbf{q}) = (2\pi)^{-3} \int d\mathbf{r}\, f(\mathbf{r}) \exp(i\mathbf{q}\cdot\mathbf{r}) \ , \qquad (2.2)$$

and define, for our later purpose, several important quantities, such as the binding energy defect ΔE, as well as the reduced momentum transfers $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$, i.e.,

$$\Delta E = E_i^T - E_f^P,\quad E_k^K = -\frac{1}{2}\left[\frac{Z_K}{n_k}\right]^2 \quad (k=i,f,\quad K=T,P) \tag{2.3a}$$

$$\boldsymbol{\alpha} = \boldsymbol{\eta} + \alpha_z \hat{\mathbf{v}},\quad \boldsymbol{\beta} = -\boldsymbol{\eta} + \beta_z \hat{\mathbf{v}};\quad \boldsymbol{\eta}\cdot\mathbf{v} = 0 \tag{2.3b}$$

$$\alpha_z = -\frac{v}{2} + \frac{\Delta E}{v},\quad \beta_z = -\frac{v}{2} - \frac{\Delta E}{v}\ . \tag{2.3c}$$

Here $\mathbf{v}$ is the incident velocity and $\boldsymbol{\eta}$ is the transverse momentum transfer,

$$\boldsymbol{\eta} = \eta(\cos\varphi_\eta, \sin\varphi_\eta, 0)\ . \tag{2.3d}$$

In the CB2 approximation,[14–18] the transition amplitude for the symmetric case of reaction (2.1) is given by the following *eikonal* expression:

$$T_{if}^{\mathrm{CB2}} = T_{if}^{\mathrm{CB1}} + S_{if} \tag{2.4a}$$

$$\equiv \langle \Phi_f | V_i' | \Phi_i \rangle + S_{if} \tag{2.4b}$$

$$\equiv \langle \Phi_f | V_i' | \Phi_i \rangle + \langle \Phi_f | V_f' G_{0e}^{+} V_i' | \Phi_i \rangle\ , \tag{2.4c}$$

where G_{0e}^{+} is the eikonal Green's function for the three noninteracting (free) particles,

$$G_{0e}^{+} = \frac{1}{E_i^T + \frac{1}{2}\nabla_{r_T}^2 + (\mathbf{k}_i + i\nabla_{r_i})\cdot\mathbf{v} + i\epsilon},\quad \epsilon \to 0+\ . \tag{2.5a}$$

Quantities Φ_i and Φ_f represent the usual unperturbed initial and final channel states, which are given by the products of the plane waves for the relative motion of the heavy particles and the discrete hydrogenlike wave functions:

$$\Phi_i = \varphi_i(\mathbf{r}_T)\exp(i\mathbf{k}_i\cdot\mathbf{r}_i)\ ,\qquad \Phi_f = \varphi_f(\mathbf{r}_P)\exp(-i\mathbf{k}_f\cdot\mathbf{r}_f)\ , \tag{2.5b}$$

where $\mathbf{r}_K$ is the relative vector of the electron with respect to the Kth nucleus, $\mathbf{k}_i$ and $\mathbf{k}_f$ are the initial and final wave vectors. The relative vector of nucleus Z_P with respect to the center of mass of the system $(Z_T,e)_i$ is denoted by $\mathbf{r}_i$. An analogous vector $\mathbf{r}_f$ is introduced in the exit channel of reaction (2.1) for relating the nucleus Z_T to the center of mass of the newly formed hydrogenlike atom $(Z_P,e)_f$. Perturbations V_i' and V_f' in the entrance and exit channel are defined by

$$V_i' = V_P(r_P) - V_P(R),\quad V_f' = V_T(r_T) - V_T(R)\ , \tag{2.5c}$$

where $V_K(r) = -Z_K/r$, with R being the internuclear distance.

We presently adopt the "prior" version of the transition amplitudes in Eqs. (2.4a)–(2.4c). The same results, however, would be obtained by using the "post" formulation, since the CB2 approximation does not exhibit the so-called "post-prior" discrepancy. The term T_{if}^{CB1} in Eqs. (2.4a)–(2.4c) represents the contribution from the first Born (CB1) method with the correct boundary conditions[1–12]

$$T_{if}^{\mathrm{CB1}} = (2\pi)^6 \left\{ -\frac{1}{2}\left[\beta^2 + \left[\frac{Z_T}{n_i}\right]^2\right] \tilde{\varphi}_f^{*}(-\boldsymbol{\alpha})\tilde{\varphi}_i(\boldsymbol{\beta}) + \int d\mathbf{p}\, \tilde{\varphi}_f^{*}(\mathbf{p}-\boldsymbol{\alpha})\widetilde{W}_P(-\mathbf{p})\tilde{\varphi}_i(\mathbf{p}+\boldsymbol{\beta}) \right\}\ , \tag{2.6}$$

where $\tilde{\varphi}_i(\mathbf{q})$ and $\tilde{\varphi}_f(\mathbf{q})$ are, respectively, the initial- and final-state hydrogenlike wave functions in momentum space and $\widetilde{W}_K(\mathbf{q})$ is the Fourier transform of the potential:

$$W_K(R) = -V_K(R) = \frac{Z_K}{R}\ . \tag{2.7}$$

The remaining part S_{if} of the transition amplitude T_{if}^{CB2} is seen from Eqs. (2.4b) and (2.4c) to contain four matrix elements, i.e.,

$$S_{if} = I_{if}(V_T,V_P) + [I_{if}(V_T,W_P) + I_{if}(W_T,V_P) + I_{if}(W_T,W_P)]\ , \tag{2.8}$$

with $V_K \equiv V_K(r_K)$, $W_K \equiv W_K(R)$,

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$$I_{if}(V_T,V_P) = (2\pi)^6 \int\int d\mathbf{p}\, d\mathbf{q}\, \tilde{\varphi}_f^{*}(\mathbf{p}-\boldsymbol{\alpha}) E_{\mathbf{p},\mathbf{q}}^{-1} \tilde{V}_T(-\mathbf{q}) \tilde{V}_P(\mathbf{p}) \tilde{\varphi}_i(\mathbf{q}+\boldsymbol{\beta})\ , \tag{2.9a}$$

$$I_{if}(V_T,W_P) = (2\pi)^6 \int\int d\mathbf{p}\, d\mathbf{q}\, \tilde{\varphi}_f^{*}(\mathbf{p}-\boldsymbol{\alpha}) E_{\mathbf{p},\mathbf{q}}^{-1} \tilde{V}_T(-\mathbf{q}) \widetilde{W}_P(-\mathbf{p}) \tilde{\varphi}_i(\mathbf{q}+\boldsymbol{\beta}+\mathbf{p})\ , \tag{2.9b}$$

$$I_{if}(W_T,V_P) = (2\pi)^6 \int\int d\mathbf{p}\, d\mathbf{q}\, \tilde{\varphi}_f^{*}(\mathbf{p}-\boldsymbol{\alpha}+\mathbf{q}) E_{\mathbf{p},\mathbf{q}}^{-1} \widetilde{W}_T(-\mathbf{q}) \tilde{V}_P(\mathbf{p}) \tilde{\varphi}_i(\mathbf{q}+\boldsymbol{\beta})\ , \tag{2.9c}$$

$$I_{if}(W_T,W_P) = (2\pi)^6 \int\int d\mathbf{p}\, d\mathbf{q}\, \tilde{\varphi}_f^{*}(\mathbf{p}-\boldsymbol{\alpha}+\mathbf{q}) E_{\mathbf{p},\mathbf{q}}^{-1} \widetilde{W}_T(-\mathbf{q}) \widetilde{W}_P(-\mathbf{p}) \tilde{\varphi}_i(\mathbf{q}+\boldsymbol{\beta}+\mathbf{p})\ , \tag{2.9d}$$

where

$$E_{\mathbf{p},\mathbf{q}} = \begin{cases} -2(|\mathbf{p}-\boldsymbol{\alpha}+\mathbf{q}|^2 + \epsilon_{\mathbf{q}}^2), & \epsilon_{\mathbf{q}}^2 = Z_P^2 - 2\mathbf{q}\cdot\mathbf{v} - i\epsilon \quad (2.10\mathrm{a}) \\ -2(|\mathbf{q}+\boldsymbol{\beta}+\mathbf{p}|^2 + \epsilon_{\mathbf{p}}^2)\ , & \epsilon_{\mathbf{p}}^2 = Z_T^2 + 2\mathbf{p}\cdot\mathbf{v} - i\epsilon \quad (2.10\mathrm{b}) \end{cases}$$

and $\alpha^2 + (Z_P/n_f)^2 = \beta^2 + (Z_T/n_i)^2$.

In the following, for the purpose of illustration, we shall outline the method of calculation of the resonant transition, involving only the initial and final ground states, i.e., $i=f=1s$. In such a case, integrals (2.6) and (2.9a) and (2.9b) simplify as follows:

$$T_{if}^{\rm CB1}=64\pi(Z_PZ_T)^{5/2}\left[-\tfrac{1}{2}(\alpha^2+Z_P^2)^{-2}(\beta^2+Z_T^2)^{-1}-\frac{Z_P'}{2\pi^2}\int d\mathbf{p}\,p^{-2}(|\mathbf{p}-\boldsymbol{\alpha}|^2+Z_P^2)^{-2}(|\mathbf{p}+\boldsymbol{\beta}|^2+Z_T^2)^{-2}\right], \quad (2.11)$$

$$I_{if}(V_T,V_P)=-32(Z_PZ_T)^{5/2}(Z_TZ_P)I(V_T,V_P)\,, \quad (2.12a)$$

$$I_{if}(V_T,W_P)=+32(Z_PZ_T)^{5/2}(Z_TZ_P')I(V_T,W_P)\,, \quad (2.12b)$$

$$I_{if}(W_T,V_P)=+32(Z_PZ_T)^{5/2}(Z_T'Z_P)I(W_T,V_P)\,, \quad (2.12c)$$

$$I_{if}(W_T,W_P)=-32(Z_PZ_T)^{5/2}(Z_T'Z_P')I(W_T,W_P)\,, \quad (2.12d)$$

with $Z_K'=Z_K$ and

$$I_{if}(V_T,V_P)=\int\int\frac{d\mathbf{p}\,d\mathbf{q}}{p^2q^2}[(|\mathbf{p}-\boldsymbol{\alpha}|^2+Z_P^2)(|\mathbf{q}+\boldsymbol{\beta}|^2+Z_T^2)]^{-2}A_{\mathbf{p},\mathbf{q}}^{-1}\,, \quad (2.13a)$$

$$I_{if}(V_T,W_P)=\int\int\frac{d\mathbf{p}\,d\mathbf{q}}{p^2q^2}[(|\mathbf{p}-\boldsymbol{\alpha}|^2+Z_P^2)(|\mathbf{q}+\boldsymbol{\beta}+\mathbf{p}|^2+Z_T^2)]^{-2}A_{\mathbf{p},\mathbf{q}}^{-1}\,, \quad (2.13b)$$

$$I_{if}(W_T,V_P)=\int\int\frac{d\mathbf{p}\,d\mathbf{q}}{p^2q^2}[(|\mathbf{p}-\boldsymbol{\alpha}+\mathbf{q}|^2+Z_P^2)(|\mathbf{q}+\boldsymbol{\beta}|^2+Z_T^2)]^{-2}A_{\mathbf{p},\mathbf{q}}^{-1}\,, \quad (2.13c)$$

$$I_{if}(W_T,W_P)=\int\int\frac{d\mathbf{p}\,d\mathbf{q}}{p^2q^2}[(|\mathbf{p}-\boldsymbol{\alpha}+\mathbf{q}|^2+Z_P^2)(|\mathbf{q}+\boldsymbol{\beta}+\mathbf{p}|^2+Z_T^2)]^{-2}A_{\mathbf{p},\mathbf{q}}^{-1}\,, \quad (2.13d)$$

where $A_{\mathbf{p},\mathbf{q}}=\pi^3E_{\mathbf{p},\mathbf{q}}$.

The equality $Z_P=Z_T$ is understood throughout, since we are considering the symmetric version of reaction (2.1). In other words Eqs. (2.11), (2.12a)–(2.12d), and (2.13a)–(2.13d) do not apply to heteronuclear collisions ($Z_P\neq Z_T$) *within the CB2 approximation.* The only reason for treating the labels Z_P and Z_T as if they were different from each other is that the above formulas also supply the transition amplitudes $T_{if}^{\rm JS1}$ and $T_{if}^{\rm JS2}$ of the first[22,23]- and second[21]-order Jackson-Schiff approximation. This is done by merely setting $Z_P'=Z_T'=Z_PZ_T$, for *both* the symmetric and asymmetric case of process (2.1). Unlike the present theory, however, the Jackson-Schiff approximation in *any* order of the perturbation expansion exhibits the *incorrect* boundary conditions for $Z_P=Z_T$ or $Z_P\neq Z_T$, with the only exception concerning the H^+-H charge exchange. It is only in this latter case ($Z_P=Z_T=1$) that the CBn and JSn ($n=1,2,3,\dots$) methods are coincidently identical to each other. It is now well estalished[1–11] that the JS1 approximation is inadequate, because of the incorrect boundary conditions for every case but $Z_P=Z_T=1$. Hence, pursuit using the Jackson-Schiff-Born series is not justified. In particular, we do not expect that the JS2 theory would yield quantitatively acceptable results for any collision but H^+-H charge transfer. Nevertheless, it would be interesting to see whether the difference between the JS2 and CB2 approximations is smaller than in the comparison of the JS1 with the CB1 model. The *symmetric* case ($Z_P=Z_T\neq 1$) of reaction (2.1) is particularly convenient for comparison between the JS2 and CB2 methods, since the same program can be used by appropriately specifying the parameter Z_K' as being equal to Z_PZ_T or to $Z_K(K=P,T)$.

III. CALCULATION OF THE INTEGRAL $I(V_T,V_P)$

We shall first change variables in the integral $I(V_T,V_P)$ according to $\mathbf{p}'=\mathbf{p}+\mathbf{q}-\boldsymbol{\alpha}$ and $\mathbf{q}'=-\mathbf{q}-\boldsymbol{\beta}$, and subsequently rewrite Eq. (2.13a) as follows:

$$I(V_T,V_P)=\frac{1}{\pi^3}\int\int d\mathbf{p}\,d\mathbf{q}[|\mathbf{q}+\boldsymbol{\beta}|^2(q^2+b^2)^2\times(p^2+\gamma^2)D_{\mathbf{p},\mathbf{q}}]^{-1}\,, \quad (3.1)$$

where $a=Z_P$, $b=Z_T(a=b)$, and

$$D_{\mathbf{p},\mathbf{q}}=(|\mathbf{p}+\boldsymbol{\beta}+\mathbf{q}|^2+a^2)^2|\mathbf{p}+\mathbf{q}-\mathbf{v}|^2\,, \quad (3.2a)$$

$$\gamma^2=a^2+2(\mathbf{q}+\boldsymbol{\beta})\cdot\mathbf{v}-i\epsilon \quad ({\rm Re}\gamma>0,\ \epsilon\to 0+)\,. \quad (3.2b)$$

For a convenient representation of the quantity $1/D_{\mathbf{p},\mathbf{q}}$, we shall employ the following identity:

$$A^{-n-1}B^{-m-1}=\frac{(n+m+1)!}{n!m!}\int_0^\infty dt\,t^m(A+Bt)^{-n-m-2}\,, \quad (3.3)$$

which can readily be obtained from the integral form of the Gauss hypergeometric function ${}_2F_1$ (see ref. 24):

$${}_2F_1(a,b,c;1-x)=\frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)}\times\int_0^\infty dt\,t^{a-1}(1+t)^{b-c}(1+xt)^{-b}\,. \quad (3.4)$$

Hence,

$$D_{\mathbf{p},\mathbf{q}}^{-1}=2\int_0^\infty dt\,t_0^3(|\mathbf{p}+\mathbf{Q}|^2+\Delta^2)^{-3}\,, \quad (3.5)$$

where $t_0=1/(1+t)$ and

$$\mathbf{Q}=\mathbf{q}+(\boldsymbol{\beta}-\mathbf{v}t)t_0,\quad \Delta^2=t_0^2[\alpha^2t+a^2(1+t)]\,. \quad (3.6)$$

Inserting (3.5) into Eq. (3.1) and carrying out the integration over $\mathbf{p}$, we obtain

$$I(V_T,V_P)=\int_0^\infty dt\,t_0^3\mathcal{F}(t)\,, \quad (3.7)$$

with

$$\mathcal{F}(t)=\frac{1}{\pi}\int d\mathbf{q}|\mathbf{q}+\boldsymbol{\beta}|^{-2}f(\mathbf{q})\equiv\frac{1}{\pi}\int d\mathbf{q}\,g(\mathbf{q}) , \quad (3.8)$$

$$f(\mathbf{q})=(q^2+b^2)^{-2}[\tfrac{1}{2}\Delta^{-3}\Omega^{-1}+(\gamma+\Delta)\Delta^{-2}\Omega^{-2}] , \quad (3.9a)$$

where

$$\Omega=Q^2+(\gamma+\Delta)^2 . \quad (3.9b)$$

Here we made use of the following result for the two-denominator Dalitz-Lewis integral:[24–26]

$$\frac{1}{\pi^2}\int d\mathbf{p}(p^2+x^2)^{-1}(|\mathbf{p}+\mathbf{Q}|^2+y^2)^{-3} =(4y^3\mathcal{R})^{-1}+(x+y)(2y^2\mathcal{R}^2)^{-1} , \quad (3.10)$$

where $\mathcal{R}=Q^2(x+y)^2$.

Before we proceed to further integrations in (3.8), it is very important to study the analytic properties of the function $g(\mathbf{q})$ in the $\mathbf{q}$ space. In particular, $g(\mathbf{q})$ exhibits branch-point singularities at those values of the variable $\mathbf{q}$ for which the following equality is satisfied:

$$\gamma^2=0 . \quad (3.11)$$

Choosing $\mathbf{v}=(0,0,v)$ and taking the limit $\epsilon\to0+$, it follows from Eq. (3.11) that the branch-point singularity occurs at

$$q_z=-\frac{a^2+2\beta_z v}{2v}\equiv Q_\beta . \quad (3.12)$$

It can be easily shown that

$$Q_\beta=\frac{v^2-b^2}{2v} . \quad (3.13)$$

This singularity can be removed from $g(\mathbf{q})$ by introducing a change of variable proposed by Wadehra, Shakeshaft, and Macek[27] within the BK2 (BK denotes Brinkman-Kramers) model:

$$q_z=\frac{\tau|\tau|}{2v}+Q_\beta , \quad (3.14)$$

which implies

$$\gamma^2=\tau|\tau|-i\epsilon, \quad \epsilon\to0+ . \quad (3.15)$$

Care should be exercised with respect to change of the integration variable given by Eq. (3.14). Namely, considering an arbitrary definite integral $J=\int_a^b dx\, u(x)$, it is convenient to perform the transformation $y=\varphi(x)$. Then, writing $dy=\varphi'(x)dx$, we shall have $\int_a^b dx\, u(x) =\int_A^B dy\, u(\phi(y))/\varphi'(\phi(y))$, *provided that* $\varphi'(x)$ *is continuous for each* $x\in[a,b]$. Here the primes denote the first derivatives, the function ϕ is the inverse of φ, i.e., $x=\phi(y)$, and $A=\varphi(a)$, $B=\varphi(b)$. In the present case $q_z=\tau|\tau|/(2v)+Q_\beta\equiv\varphi(\tau)$, so that $\varphi'(\tau)=\tau/v$ for $\tau\geq0$ and $\varphi'(\tau)=-\tau/v$ for $\tau\leq0$. Hence, $\varphi'(\tau)$ is continuous everywhere on the τ axis, *including* $\tau=0$ and, therefore, equating the integrals over the variables q_z and τ is justified. However, before writing the integral over q_z in Eq. (3.8) in terms of the new variable τ, it is necessary to appropriately split the interval $q_z\in[-\infty,+\infty]$, so that the two resulting integrals over τ cover the regions $\tau\leq0$ and $\tau\geq0$. Restating Eq. (3.14) as $\tau|\tau|=2v(q_z-Q_\beta)$, we shall provisionally assume that $Q_\beta\geq0$, which corresponds to $v\geq Z_T$. Thus, we shall have $\tau\leq0$ for $q_z\leq Q_\beta$ and $\tau\geq0$ for $q_z\geq Q_\beta$. Therefore, the interval $q_z\in[-\infty,+\infty]$ should be split according to $q_z\in[-\infty,Q_\beta]+q_z\in[Q_\beta,+\infty]$. In the former range $q_z\in[-\infty,Q_\beta]$, we have $\tau\leq0$, i.e., $\tau=-\sqrt{2v(Q_\beta-q_z)}$, so that $q_z\in[-\infty,Q_\beta]\to\tau\in[-\infty,0]$. Similarly, the second region $q_z\in[Q_\beta,+\infty]$ corresponds to $\tau\geq0$, i.e., $\tau=+\sqrt{2v(q_z-Q_\beta)}$ and, therefore, $q_z\in[Q_\beta,+\infty]\to\tau\in[0,+\infty]$. Finally, it remains to be demonstrated that this analysis eliminates the branch-point singularity (3.11) from $g(\mathbf{q})$. This is accomplished provided that

$$\Omega\neq0, \quad \forall\tau\in[-\infty,+\infty], \quad \forall t\in[0,+\infty] . \quad (3.16)$$

In order to prove (3.16), we shall separately consider two cases, where $\tau\leq0$ and $\tau\geq0$. The correct branch of the square root of the complex number γ is uniquely determined from the condition $\mathrm{Re}\gamma>0$, in the limit $\epsilon\to0+$. Writing $\gamma=\pm\sqrt{\tau|\tau|-i\epsilon}$ and subsequently developing the square root in the power-series expansion in the limit $\epsilon\to0+$, we shall have

$$\gamma=\tau\sqrt{\mathrm{sgn}(\tau)}, \quad \mathrm{sgn}(\tau)=\frac{|\tau|}{\tau} . \quad (3.17)$$

For convenience, the triple integral in Eq. (3.8) will be carried out in the cylindrical coordinates, i.e., $\mathbf{q}=(\mathbf{q}_\rho,q_z)$, where $\mathbf{q}_\rho=(q_\rho,\phi)$. Hence, we obtain

$$\Omega=\begin{cases} X+iY, & \tau\leq0 \quad (3.18a)\\ T^2+\left[\dfrac{\tau^2}{2v}-t_\beta\right]^2+(\tau+\Delta)^2, & \tau\geq0 \quad (3.18b)\end{cases}$$

where

$$X=\frac{\tau^4}{4v^2}+(t_\beta-v)\frac{\tau^2}{v}+T^2+\Delta^2+t_\beta^2, \quad Y=2\tau\Delta , \quad (3.19a)$$

$$\mathbf{T}=\mathbf{q}_\rho-\boldsymbol{\eta}t_0, \quad t_\beta=t_0\frac{a^2+(b^2+v^2)t}{2v} . \quad (3.19b)$$

It is easily verified that $T^2+[\tau^2/(2v)-t_\beta]^2+(\tau+\Delta)^2>0$ $(\tau\geq0)$, even when τ and Δ are simultaneously equal to zero. Further, one can readily show that the quantities X and Y from Eq. (3.19a) are never simultaneously equal to zero. Therefore, it follows from Eqs. (3.18a) and (3.18b) that $\Omega\neq0$ $\forall\tau\in[-\infty,+\infty]$, $\forall t\in[0,+\infty]$. Hence, we proved condition (3.16). Here we recall that the term $1/\Omega$ stems from the action of the free-particle propagator G_{0e}^+ onto the set of plane waves for the relative motion of heavy particles in an intermediate stage of collision. The branch-point singularities of the quantity $1/\Omega$ are typical for the continuum-intermediate states, which become progressively important as the incident energy increases, due to the dominant role of the ionization channel. Thus, especially at high energies, these singularities become very unwieldy for computation. The transformation (3.14) is successful in removing the branch-point singularities from the integral $I(V_T,V_P)$. After this regularization, the function $\mathcal{F}(t)$ from Eq. (3.8) takes the following form:

$$\mathcal{F}(t)=\frac{\mathcal{F}^{(1)}(t)}{2\Delta^3}+\frac{\mathcal{F}^{(2)}(t)}{\Delta^2}\ , \qquad (3.20)$$

where

$$\mathcal{F}^{(l)}(t)=\frac{1}{v}[\mathcal{F}_1^{(l)}(t)+\mathcal{F}_2^{(l)}(t)] \qquad (3.21)$$

and

$$\mathcal{F}_1^{(l)}(t)=-\int_{-\infty}^{0}d\tau\,\tau\mathcal{H}_1^{(l)}(t,\tau)[\delta_{l,1}+(\Delta+i\tau)\delta_{l,2}]\ , \qquad (3.22a)$$

$$\mathcal{F}_2^{(l)}(t)=+\int_{0}^{+\infty}d\tau\,\tau\mathcal{H}_2^{(l)}(t,\tau)[\delta_{l,1}+(\Delta+\tau)\delta_{l,2}]\ , \qquad (3.22b)$$

with $\delta_{l,l'}$ being the Kronecker δ symbol, i.e., $\delta_{l,l'}=1$ if $l=l'$ and $\delta_{l,l'}=0$ for $l\neq l'$. Further, we have

$$\mathcal{H}_j^{(l)}(t,\tau)=\int_0^\infty dq_\rho q_\rho(q_\rho^2+b_j^2)^{-2}\frac{1}{\pi}\int_0^{2\pi}d\phi(q_\rho^2-2\eta q_\rho\cos\phi'+C_{1\beta j})^{-1}(q_\rho^2-2t_0\eta q_\rho\cos\phi'+C_{2\beta j})^{-l}\ , \qquad (3.23)$$

with $\phi'=\phi-\phi_\eta$ and

$$C_{1\beta j}=\eta^2+\tau_{\beta j}^2,\quad \tau_{\beta j}=-\frac{a^2+\delta_j\tau^2}{2v}\ , \qquad (3.24a)$$

$$C_{2\beta j}=t_0^2\eta^2+\left[t_\beta+\delta_j\frac{\tau^2}{2v}\right]^2+(\Delta+\tau\delta_j^c)^2\ ,$$

$$\delta_j^c=i\delta_{j,1}+\delta_{j,2}\ , \qquad (3.24b)$$

$$b_j^2=\tau_j^2+b^2,\quad \tau_j=Q_\beta-\delta_j\frac{\tau^2}{2v},\quad \delta_j=\delta_{j,1}-\delta_{j,2}\ , \qquad (3.24c)$$

where $j=1$ for $\tau\le 0$ and $j=2$ for $\tau\ge 0$ in the case of the integrals (3.22a) and (3.22b), respectively. After employing the usual fractal decomposition of the two denominators in Eq. (3.23), i.e.,

$$\frac{\beta_1\alpha_2-\beta_2\alpha_1}{(\alpha_1+\beta_1\cos\phi')(\alpha_2+\beta_2\cos\phi')}=\frac{\beta_1}{\alpha_1+\beta_1\cos\phi'}-\frac{\beta_2}{\alpha_2+\beta_2\cos\phi'}\ , \qquad (3.24d)$$

we shall encounter a linear combination of the following integrals (see Sec. V):

$$\frac{1}{2\pi}\int_0^{2\pi}d\phi\frac{1}{A-B\eta\cos(\phi-\phi_\eta)}=\frac{1}{\sqrt{A^2-B^2\eta^2}}\ ,\quad A^2>B^2\eta^2\ . \qquad (3.24e)$$

Hence, we can write

$$\mathcal{H}_j^{(1)}(t,\tau)=2\int_0^\infty dq_\rho q_\rho\frac{\mathcal{S}_{1\beta j}^{1/2}(q_\rho)-t_0\mathcal{S}_{2\beta j}^{1/2}(q_\rho)}{(q_\rho^2+b_j^2)^2(\delta q_\rho^2+t_j)}\ , \qquad (3.25a)$$

$$\mathcal{H}_j^{(2)}(t,\tau)=2\int_0^\infty dq_\rho q_\rho\left[\frac{\mathcal{S}_{1\beta j}^{1/2}(q_\rho)-t_0\mathcal{S}_{2\beta j}^{1/2}(q_\rho)}{(q_\rho^2+b_j^2)^2(\delta q_\rho^2+t_j)^2}-t_0\frac{(q_\rho^2+C_{2\beta j})\mathcal{S}_{2\beta j}^{3/2}(q_\rho)}{(q_\rho^2+b_j^2)^2(\delta q_\rho^2+t_j)}\right]\ , \qquad (3.25b)$$

where $\delta=tt_0$, and

$$t_j=C_{2\beta j}-t_0C_{1\beta j} \qquad (3.26a)$$

$$=t_0\left[t_0\mathcal{T}(t)+t\left[\frac{\tau^2}{2v}\right]^2+\tau\left[2D\delta_j^c-\tau\delta_j\frac{2v^2+(v^2-b^2)t}{2v^2}\right]\right]\equiv t_0t_j'\ , \qquad (3.26b)$$

$$\mathcal{T}(t)=\left[\frac{b^2+v^2}{2v}\right]^2t^2+\left[a^2+\left[\frac{b^2+v^2}{2v}\right]^2\right]t+a^2>0\ , \qquad (3.26c)$$

$$\mathrm{Re}t_j'>0,\quad \forall\tau\in[-\infty,+\infty],\quad \forall t\in[0,\infty]\ , \qquad (3.26d)$$

$$D=\sqrt{a^2+T_\alpha t}\ , \qquad (3.26e)$$

$$T_\alpha=\alpha^2+a^2,\quad T_\beta=\beta^2+b^2\quad (T_\alpha=T_\beta)\ , \qquad (3.26f)$$

$$\mathcal{S}_{1\beta j}^{-1}(q_\rho)=(q_\rho^2+C_{1\beta j})^2-4\eta^2q_\rho^2\ , \qquad (3.26g)$$

$$\mathcal{S}_{2\beta j}^{-1}(q_\rho)=(q_\rho^2+C_{2\beta j})^2-4t_0^2\eta^2q_\rho^2\ . \qquad (3.26h)$$

The remaining one-dimensional integrals over q_ρ in Eqs. (3.25a) and (3.25b) can also be analytically calculated by using appropriate changes of variables. We shall first make a fractal decomposition of the type

$$\frac{1}{(q_\rho^2+b_j^2)(\delta q_\rho^2+t_j)}=\frac{1}{D_{\beta j}}\left[\frac{1}{q_\rho^2+b_j^2}-\frac{\delta}{\delta q_\rho^2+t_j}\right]\ , \qquad (3.27a)$$

where

$$D_{\beta j}=t_j-\delta b_j^2 \qquad (3.27b)$$

$$=t_0D'_{\beta j} \qquad (3.27c)$$

$$\equiv t_0(-\tau^2\delta_j+2\tau\delta_j^cD+a^2)\ , \qquad (3.27d)$$

$$\mathrm{Re}D'_{\beta j}>0,\quad \forall\tau\in[-\infty,+\infty],\quad \forall t\in[0,\infty]\ . \qquad (3.27e)$$

Higher-order terms $(q_\rho^2+b_j^2)^{-2}(\delta q_\rho^2+t_j)^{-1}$ and

$(q_\rho^2+b_j^2)^{-2}(\delta q_\rho^2+t_j)^{-2}$ are generated by repeating transformation (3.27). In this way, several integrals are obtained whose inegrands differ from the corresponding functions in (3.25a) and (3.25b) only in that the *product* $(q_\rho^2+b_j^2)^{-l}(\delta q_\rho^2+t_j)^{-l'}$ is replaced by an appropriate *linear combination* of terms $(q_\rho^2+b_j^2)^{-l''}$ and $(\delta q_\rho^2+b_j^2)^{-l'''}$, where l, l', l'', and l''' are integers. It is in these integrals with the single binomial term $(q_\rho^2+b_j^2)$ or $(\delta q_\rho^2+b_j^2)$ in the denominator that we set $q_\rho^2=u$ or $\delta q_\rho^2=u$, respectively. Hence, we can write

$$\mathcal{H}_j^{(1)}(t,\tau)=\frac{1}{D_{\beta j}}\mathcal{L}_{1\beta j,1}^{(0,2)}(b_j^2)-\frac{\delta}{D_{\beta j}^2}\mathcal{L}_{1\beta j,1}^{(0,1)}(b_j^2)-\frac{t_0}{D_{\beta j}}\mathcal{L}_{1\beta j,1}^{(0,1)}(b_j^2)-\frac{t_0}{D_{\beta j}}\mathcal{L}_{2\beta j,1}^{(0,2)}(b_j^2)+\frac{t_0\delta}{D_{\beta j}^2}\mathcal{L}_{2\beta j,1}^{(0,1)}(b_j^2)$$
$$+\frac{\delta^2}{D_{\beta j}^2}\mathcal{L}_{1\beta j,\delta}^{(0,1)}(t_j)-\frac{t_0\delta^2}{D_{\beta j}^2}\mathcal{L}_{2\beta j,\delta}^{(0,1)}(t_j)\ , \tag{3.28a}$$

and

$$\mathcal{H}_j^{(2)}(t,\tau)=\frac{1}{D_{\beta j}^2}\mathcal{L}_{1\beta j,1}^{(0,2)}(b_j^2)-\frac{2\delta}{D_{\beta j}^3}\mathcal{L}_{1\beta j,1}^{(0,1)}(b_j^2)-\frac{t_0}{D_{\beta j}^2}\mathcal{L}_{2\beta j,1}^{(0,2)}(b_j^2)+\frac{2t_0\delta}{D_{\beta j}^3}\mathcal{L}_{2\beta j,1}^{(0,1)}(b_j^2)+\frac{2\delta^2}{D_{\beta j}^3}\mathcal{L}_{1\beta j,\delta}^{(0,1)}(t_j)+\frac{\delta^2}{D_{\beta j}^2}\mathcal{L}_{1\beta j,\delta}^{(0,2)}(t_j)$$
$$-\frac{2t_0\delta^2}{D_{\beta j}^3}\mathcal{L}_{2\beta j,\delta}^{(0,1)}(t_j)-\frac{t_0\delta^2}{D_{\beta j}^2}\mathcal{L}_{2\beta j,\delta}^{(0,2)}(t_j)-\frac{t_0}{D_{\beta j}}\mathcal{L}_{2\beta j,1}^{(1,1)}(b_j^2)-\frac{t_0C'_{2\beta j}}{D_{\beta j}}\mathcal{L}_{2\beta j,1}^{(1,2)}(b_j^2)+\frac{t_0\delta}{D_{\beta j}^2}\mathcal{K}_{2\beta j,1}^{(1)}+\frac{t_0\delta C'_{2\beta j}}{D_{\beta j}^2}\mathcal{L}_{2\beta j,1}^{(1,1)}(b_j^2)$$
$$-\frac{t_0\delta^3}{D_{\beta j}^2}\mathcal{K}_{2\beta j,\delta}^{(1)}-\frac{t_0\delta^3C'_{2\beta j}}{D_{\beta j}^2}\mathcal{L}_{2\beta j,\delta}^{(1,1)}(t_j)\ , \tag{3.28b}$$

where $C'_{k\beta j}=C_{k\beta j}-b_j^2$ and

$$\mathcal{K}_{k\beta j,x}^{(n)}=\int_0^\infty du\ R_{k\beta j,x}^{-n-1/2}(u),\quad n\ge 1\quad (=1,2,3,\dots)\ , \tag{3.29a}$$

$$\mathcal{L}_{k\beta j,x}^{(n,m)}(y)=\int_0^\infty du(u+y)^{-m}R_{k\beta j,x}^{-n-1/2}(u),\qquad n\ge 0,\quad m\ge 1\ , \tag{3.29b}$$

$$R_{k\beta j,x}(u)=G_{k\beta j,x}+F_{k\beta j,x}u+u^2\ , \tag{3.30a}$$

$$G_{k\beta j,x}=(xC_{k\beta j})^2\ ,$$
$$F_{k\beta j,x}=x[-4\eta^2(\delta_{k,1}+t_0^2\delta_{k,2})+2C_{k\beta j}]\ . \tag{3.30b}$$

The basic integral $\mathcal{L}_{k\beta j,x}^{(0,1)}(y)$ is calculated in the Appendix, with the result

$$\mathcal{L}_{k\beta j,x}^{(0,1)}(y)=R_{k\beta j,x}^{-1/2}(-y)\times\ln\left[\frac{G_{k\beta j,x}^{1/2}+y+R_{k\beta j,x}^{1/2}(-y)}{G_{k\beta j,x}^{1/2}+y-R_{k\beta j,x}^{1/2}(-y)}\right]. \tag{3.31a}$$

Higher-order terms from Eq. (3.29b) with $n>0$ and $m\ge 2$ can be obtained recursively, so that (see Prudnikov, Bričkov, and Maričev,[28] Nos. 1.2.53/1 and 1.2.53.10)

$$\mathcal{L}_{k\beta j,x}^{(0,2)}(y)=R_{k\beta j,x}^{-1}(-y)\left[\frac{1}{y}G_{k\beta j,x}^{1/2}-1-F'_{k\beta j,x}\mathcal{L}_{k\beta j,x}^{(0,1)}(y)\right], \tag{3.31b}$$

$$\mathcal{L}_{k\beta j,x}^{(0,3)}(y)=\tfrac{1}{2}R_{k\beta j,x}^{-1}(-y)\left[\frac{1}{y^2}G_{k\beta j,x}^{1/2}-3F'_{k\beta j,x}\mathcal{L}_{k\beta j,x}^{(0,2)}(y)-\mathcal{L}_{k\beta j,x}^{(0,1)}(y)\right], \tag{3.31c}$$

$$\mathcal{L}_{k\beta j,x}^{(1,1)}(y)=-R_{k\beta j,x}^{-1}(-y)[G_{k\beta j,x}^{-1/2}-\mathcal{L}_{k\beta j,x}^{(0,1)}(y)+F'_{k\beta j,x}\mathcal{K}_{k\beta j,x}^{(1)}]\ , \tag{3.31d}$$

$$\mathcal{L}_{k\beta j,x}^{(1,2)}(y)=R_{k\beta j,x}^{-1}(-y)\left[\frac{1}{y}G_{k\beta j,x}^{-1/2}-3F'_{k\beta j,x}\mathcal{L}_{k\beta j,x}^{(1,1)}(y)-2\mathcal{K}_{k\beta j,x}^{(1)}\right], \tag{3.31e}$$

where $F'_{k\beta j,x}=(F_{k\beta j,x}-2y)/2$ and (see Prudnikov, Bričkov, and Maričev,[28] No. 1.2.52/15)

$$\mathcal{K}_{k\beta j,x}^{(1)}=\frac{2}{\sqrt{G_{k\beta j,x}}(2\sqrt{G_{k\beta j,x}}+F_{k\beta j,x})}\ . \tag{3.32}$$

The integral (3.31c) will be required in Secs. 4–6. This completes the reduction of the integral $I(V_T,V_P)$ to the two-dimensional numerical quadratures, i.e.,

$$I(V_T,V_P)=I^{(-)}(V_T,V_P)+I^{(+)}(V_T,V_P)\ , \tag{3.33a}$$

$$I^{(-)}(V_T,V_P)=-\frac{1}{v}\int_{-\infty}^0 d\tau\,\tau\mathcal{H}_1(\tau)\ , \tag{3.33b}$$

$$I^{(+)}(V_T,V_P)=+\frac{1}{v}\int_0^{+\infty} d\tau\,\tau\mathcal{H}_2(\tau)\ , \tag{3.33c}$$

$$\mathcal{H}_j(\tau)=\int_0^\infty dt\frac{t_0^3}{\Delta^2}\left[\frac{1}{2\Delta}\mathcal{H}_j^{(1)}(t,\tau)+(\Delta+\tau\delta_j^c)\mathcal{H}_j^{(2)}(t,\tau)\right], \tag{3.33d}$$

where $\mathcal{H}_j^{(1)}(t,\tau)$ and $\mathcal{H}_j^{(2)}(t,\tau)$ are, respectively given by Eqs. (3.28a) and (3.28b).

There is yet another singularity in the function $g(\mathbf{q})$, namely, a pole at

$$\mathbf{q}=-\boldsymbol{\beta}\ , \tag{3.34}$$

for which the Fourier transform $\tilde{V}_T(-\mathbf{q}-\boldsymbol{\beta})=-Z_T|\mathbf{q}+\boldsymbol{\beta}|^{-2}/(2\pi^2)$ is divergent. More precisely, this singularity occurs *only* in the integral $I^{(+)}(V_T,V_P)$, if the equations $\mathbf{q}_\rho=\boldsymbol{\eta}$ and $\tau=a$ are simultaneously satisfied:

$$|\mathbf{q}+\boldsymbol{\beta}|^2=\begin{cases}|\mathbf{q}_\rho-\boldsymbol{\eta}|^2+\tau_{\beta j}^2 & (3.35\text{a})\\ |\mathbf{q}_\rho-\boldsymbol{\eta}|^2+\left[\dfrac{-a^2-\tau^2}{2v}\right]^2>0 \quad (j=1,\ \tau\le 0) & (3.35\text{b})\\ |\mathbf{q}_\rho-\boldsymbol{\eta}|^2+\left[\dfrac{-a^2+\tau^2}{2v}\right]^2\ge 0 \quad (j=2,\ \tau\ge 0)\ . & (3.35\text{c})\end{cases}$$

It is obvious from Eq. (3.35a) that, for any finite velocity, the integral $I^{(-)}(V_T,V_P)$ is regular at $\mathbf{q}=-\boldsymbol{\beta}$, and the computation can safely be carried out directly from Eq. (3.33b). As to the integral $I^{(+)}(V_T,V_P)$, however, regularization will be accomplished by means of the Cauchy "subtraction technique" (see, e.g., Sloan[29]):

$$\int d\mathbf{q}\frac{f(\mathbf{q})}{|\mathbf{q}+\boldsymbol{\beta}|^2}=\int d\mathbf{q}\frac{f(\mathbf{q})-f(-\boldsymbol{\beta})}{|\mathbf{q}+\boldsymbol{\beta}|^2}+f(-\boldsymbol{\beta})\int d\mathbf{q}\frac{1}{|\mathbf{q}+\boldsymbol{\beta}|^2}\ , \tag{3.36}$$

where the new integrand $[f(\mathbf{q})-f(-\boldsymbol{\beta})]|\mathbf{q}+\boldsymbol{\beta}|^{-2}$ is a well-behaved function as $\mathbf{q}\to-\boldsymbol{\beta}$. Inspection of the integral $I^{(+)}(V_T,V_P)$ will reveal that the function $\mathcal{H}_2(\tau)$ given by Eq. (3.43d) originates from the following expression:

$$\mathcal{H}_2(\tau)=\frac{1}{\pi}\int_0^\infty dq_\rho q_\rho\int_0^{2\pi}d\phi\, f\left[q_\rho,\phi,Q_\beta+\frac{\tau^2}{2v}\right]|\mathbf{q}+\boldsymbol{\beta}|^{-2}\ , \tag{3.37}$$

where $f(\mathbf{q})$ is written as $f(q_\rho,\phi,q_z)$ with $q_z=Q_\beta+\tau^2/(2v)$. We shall hereafter use the notation $\mathbf{q}^{\beta,\tau}$ to abbreviate the vector $\mathbf{q}$ having the quantity $Q_\beta+\tau^2/(2v)$ as the q_z component:

$$\mathbf{q}^{\beta,\tau}=\left[q_\rho,\phi,Q_\beta+\frac{\tau^2}{2v}\right]\ . \tag{3.38}$$

Thus,

$$\mathcal{H}_2(\tau)=\frac{1}{\pi}\int_0^\infty dq_\rho q_\rho\int_0^{2\pi}d\phi\frac{f(\mathbf{q}^{\beta,\tau})-f(-\boldsymbol{\beta})}{|\mathbf{q}^{\beta,\tau}+\boldsymbol{\beta}|^2}+f(-\boldsymbol{\beta})X_T(\boldsymbol{\beta},\tau)\ , \tag{3.39}$$

where

$$X_T(\boldsymbol{\beta},\tau)=\frac{1}{\pi}\int_0^\infty dq_\rho q_\rho\int_0^{2\pi}d\phi\frac{1}{|\mathbf{q}^{\beta,\tau}+\boldsymbol{\beta}|^2}\ . \tag{3.40}$$

Using the result (3.24e) as well as formula 2.261 of Ref. 30 to perform the integrations in Eq. (3.40), we obtain

$$I^{(+)}(V_T,V_P)=\frac{1}{v}\int_0^\infty d\tau\,\tau\left[\mathcal{H}_2(\tau)+2f(-\boldsymbol{\beta})\ln\left|\frac{\tau^2-a^2}{v}\right|\right]-\frac{2}{v}f(-\boldsymbol{\beta})\int_0^\infty d\tau\,\tau\ln\left|\frac{\tau^2-a^2}{v}\right|\ , \tag{3.41}$$

where $\mathcal{H}_2(\tau)$ is given by Eq. (3.33d) and

$$f(-\boldsymbol{\beta})=\frac{T_\beta+2a^2}{4a^3T_\beta^4}\ . \tag{3.42}$$

The integrand $\mathcal{H}_2(\tau)-f(-\boldsymbol{\beta})\ln[(\tau^2-a^2)/v]^{-2}$ in (3.41) is regular for each $\tau\in[0,+\infty]$. However, a serious loss of accuracy at $\tau\approx a$ in the numerical computation of the first integral over τ in Eq. (3.41) will occur if one proceeds by keeping the original asymmetric interval $\tau\in[0,+\infty]$. This difficulty can easily be circumvented by splitting the interval $\tau\in[0,+\infty]$ into two parts according to $\tau\in[0,+\infty]=\tau\in[0,2a]+\tau\in[2a,+\infty]$. Then, employing formula 2.723/1 of Ref. 30, we finally can write

$$I^{(+)}(V_T,V_P)=\frac{1}{v}\int_0^{2a}d\tau\,\tau\left[\mathcal{H}_2(\tau)+2f(-\boldsymbol{\beta})\ln\left|\frac{\tau^2-a^2}{v}\right|\right]+\left[X_T(\boldsymbol{\beta})+\frac{1}{v}\int_{2a}^{+\infty}d\tau\,\tau\mathcal{H}_2(\tau)\right]\ , \tag{3.43}$$

with

$$X_T(\boldsymbol{\beta})=-\left[\frac{2}{v}\right]f(-\boldsymbol{\beta})\int_0^{2a}d\tau\,\tau\ln\left|\frac{\tau^2-a^2}{v}\right| \tag{3.44a}$$

$$=-\left[\frac{4a^2}{v}\right]f(-\boldsymbol{\beta})\ln\frac{3^{3/4}a^2}{ev}\ , \tag{3.44b}$$

where e is the base of the natural logarithm ($e=2.718\,281\,8\ldots$). Both integrals over τ in Eq. (3.43) can now readily be carried out by using the standard numerical quadratures. In particular, the first integration over τ in Eq. (3.43) covering the *symmetric* interval $\tau\in[0,2a]$ around point $\tau=a$, and possessing the function $\mathcal{H}_2(\tau)-f(-\boldsymbol{\beta})\ln[(\tau^2-a^2)/v]^{-2}$ as the integrand must be performed by an even-order symmetric quadrature rule (e.g., Gauss-Legendre, see Ref. 29).

Thus, we have shown that the integral $I(V_T,V_P)$ can be computed through two-dimensional numerical quadratures. The result is given in Eq. (3.33a) as the sum of two parts $I^{(-)}(V_T,V_P)$ and $I^{(+)}(V_T,V_P)$. The *two* singularities (3.11) and (3.34) are successfully removed from both contributions provided that $I^{(-)}(V_T,V_P)$ and $I^{(+)}(V_T,V_P)$ are, respectively, computed from Eqs. (3.33b) and (3.43).

IV. CALCULATIONS OF THE INTEGRAL $I(V_T,W_P)$

Considering the integral (2.9b), let us make the following change of variables: $\mathbf{p}'=\boldsymbol{\alpha}-\mathbf{p}\to-\mathbf{q}$, $\mathbf{q}'=-\mathbf{q}\to+\mathbf{p}$. Thus, we can write

$$I(V_T,W_P)=\frac{1}{\pi^3}\int\int d\mathbf{p}\,d\mathbf{q}[|\mathbf{q}+\boldsymbol{\alpha}|^2(q^2+a^2)^2p^2D_{\mathbf{p},\mathbf{q}}]^{-1}\ , \tag{4.1}$$

where

$$D_{\mathbf{p},\mathbf{q}}=(|\mathbf{p}+\mathbf{q}-\mathbf{v}|^2+b^2)^2(|\mathbf{p}+\mathbf{q}-\mathbf{v}|^2+\gamma^2)\ , \tag{4.2a}$$

$$\gamma^2=b^2+2(\mathbf{q}+\boldsymbol{\alpha})\cdot\mathbf{v}-i\epsilon\quad(\mathrm{Re}\gamma>0,\ \epsilon\to0+)\ . \tag{4.2b}$$

Using integral representation (3.3) for the term $1/D_{\mathbf{p},\mathbf{q}}$, which is a part of the integrand in Eq. (4.1), we obtain

$$I(V_T,W_P)=\int_0^\infty dt\ tt_0^3\mathcal{F}(t)\ , \tag{4.3}$$

where $t_0=1/(1+t)$ and

$$\mathcal{F}(t)=\frac{1}{\pi}\int d\mathbf{q}|\mathbf{q}+\boldsymbol{\alpha}|^{-2}f(\mathbf{q})\equiv\frac{1}{\pi}\int d\mathbf{q}\,g(\mathbf{q})\ , \tag{4.4}$$

$$f(\mathbf{q})=\frac{2}{\pi^2}(q^2+a^2)^{-2}\int d\mathbf{p}[p^2(|\mathbf{p}+\mathbf{Q}|^2+\Delta^2)^3]^{-1} \tag{4.5a}$$

$$=(q^2+a^2)^{-2}(\tfrac{1}{2}\Delta^{-3}\Omega^{-1}+\Delta^{-1}\Omega^{-2})\ , \tag{4.5b}$$

$$\Omega=Q^2+\Delta^2,\quad \mathbf{Q}=\mathbf{q}-\mathbf{v},\quad \Delta^2=(\gamma^2+b^2t)t_0\ . \tag{4.6}$$

The result (4.5b) for the function $f(\mathbf{q})$ is obtained by means of Eq. (3.10). The function $g(\mathbf{q})$ defined in Eq. (4.4) possesses a branch-point singularity at

$$\gamma^2=0\ , \tag{4.7}$$

as well as a pole for

$$\mathbf{q}=-\boldsymbol{\alpha}\ . \tag{4.8}$$

The singularity (4.7) is removed by the following change of variable:

$$q_z=\frac{\tau|\tau|}{2v}+Q_\alpha\ , \tag{4.9}$$

where

$$Q_\alpha=-\frac{b^2+2\alpha_zv}{2v}=\frac{v^2-a^2}{2v}\ . \tag{4.10}$$

This yields

$$\gamma^2=\tau|\tau|-i\epsilon,\quad \epsilon\to0+\ , \tag{4.11}$$

so that

$$\Omega=\begin{cases} q_\rho^2+\left[Q_\alpha-\dfrac{\tau^2}{2v}\right]^2+a^2+(b^2+\tau^2)\delta-i\epsilon, & \tau\le0 \quad (4.12\text{a})\\ q_\rho^2+\left[Q_\alpha+\dfrac{\tau^2}{2v}-v\right]^2+(b^2t+\tau^2)t_0-i\epsilon, & \tau\ge0\ , \quad (4.12\text{b})\end{cases}$$

where $\delta=tt_0$. Analogous to the preceding section, we shall be considering the cylindrical coordinates of the vector $\mathbf{q}$. Further, the incident velocity vector $\mathbf{v}$ will remain in the Z direction throughout the calculation of *each matrix element* in both the CB1 and CB2 approximation. In the case of Eq. (4.12a), where $\tau\le0$, we see that $\Omega>0$ in the limit $\epsilon\to0+$, since $a=Z_P>0$. Similarly, it is immediately evident from Eq. (4.12b) that $\Omega>0$, for $\tau\ge0$ *and* $t>0$, as $\epsilon\to0+$. In the particular case with $\tau=0=t$, we employ the following relation: $Q_\alpha-v=-(a^2+v^2)/(2v)$, which reduces Eq. (4.12b) to $\Omega=q_\rho^2+(a^2+v^2)/(2v)>0$. Hence, we can conclude that, in the limit $\epsilon\to0+$

$$\Omega>0,\quad \forall\tau\in[-\infty,+\infty],\quad \forall t\in[0,+\infty]\ . \tag{4.13}$$

The rest of the calculation proceeds along the lines described in Sec. III, with the final result

$$I(V_T,W_P)=I^{(-)}(V_T,W_P)+I^{(+)}(V_T,W_P)\ , \tag{4.14a}$$

$$I^{(-)}(V_T,W_P)=-\frac{1}{v}\int_{-\infty}^0 d\tau\,\tau\mathcal{H}_1(\tau)\ , \tag{4.14b}$$

$$I^{(+)}(V_T,W_P)=+\frac{1}{v}\int_0^{+\infty} d\tau\,\tau\mathcal{H}_2(\tau)\ , \tag{4.14c}$$

$$\mathcal{H}_j(\tau)=\frac{1}{2}\mathcal{H}_j^{(1,3)}(\tau)+\mathcal{H}_j^{(2,1)}(\tau)\ , \tag{4.14d}$$

$$\mathcal{H}_j^{(k,m)}(\tau)=\int_0^\infty dt\ t\frac{t_0^3}{\Delta_j^m}\mathcal{H}_j^{(k)}(t,\tau) \tag{4.14e}$$

$$=\int_0^\infty dt\ tt_0^{3-m/2}(b^2t-\delta_j\tau^2-i\epsilon)^{-m/2}\times\mathcal{H}_j^{(k)}(t,\tau)\ , \tag{4.14f}$$

$$\mathcal{H}_j^{(1)}(t,\tau)=-\frac{1}{D_j}\mathcal{L}_{\alpha j}^{(0,2)}(a_j^2)-\frac{1}{D_j^2}\mathcal{L}_{\alpha j}^{(0,1)}(a_j^2)+\frac{1}{D_j^2}\mathcal{L}_{\alpha j}^{(0,1)}(C_j^2)\ , \tag{4.14g}$$

$$\mathcal{H}_j^{(2)}(t,\tau)=\frac{1}{D_j^2}\mathcal{L}_{\alpha j}^{(0,2)}(a_j^2)+\frac{2}{D_j^3}\mathcal{L}_{\alpha j}^{(0,1)}(a_j^2)-\frac{2}{D_j^3}\mathcal{L}_{\alpha j}^{(0,1)}(C_j^2)+\frac{1}{D_j^2}\mathcal{L}_{\alpha j}^{(0,2)}(C_j^2)\ , \tag{4.14h}$$

where $b=Z_T(Z_T=Z_P)$ and

$$\mathcal{L}_{\alpha j}^{(n,m)}(y)=\int_0^\infty du\,(u+y)^{-m}\times R_{\alpha j}^{-n-1/2}(u),\quad n\geq 0,\quad m\geq 1 \tag{4.15a}$$

$$R_{\alpha j}(u)=G_{\alpha j}+F_{\alpha j}u+u^2\ , \tag{4.15b}$$

$$G_{\alpha j}=C_{\alpha j}^2,\quad F_{\alpha j}=-4\eta^2+2C_{\alpha j}\ , \tag{4.15c}$$

$$C_{\alpha j}=\eta^2+\tau_{\alpha j}^2,\quad \tau_{\alpha j}=-\frac{b^2+\delta_j\tau^2}{2v}\ , \tag{4.15d}$$

$$C_1^2=\tau_1^2+a^2+(b^2+\tau^2)\delta\ , \tag{4.15e}$$

$$C_2^2=(\tau_2-v)^2+(b^2t+\tau^2)t_0\ , \tag{4.15f}$$

$$a_j^2=\tau_j^2+a^2,\quad \tau_j=Q_\alpha-\delta_j\frac{\tau^2}{2v},\quad \delta_j=\delta_{j,1}-\delta_{j,2}\ , \tag{4.15g}$$

$$D_j=a_j^2-C_j^2,\quad \Delta_j^2=(b^2t-\delta_j\tau^2)t_0-i\epsilon\ . \tag{4.15h}$$

The integral (4.15a) is of the form (3.29b), i.e., $\mathcal{L}_{\alpha j}^{(n,m)}(y)\equiv\mathcal{L}_{1\alpha j,1}^{(n,m)}(y)$, so that we can also use the result (3.31a)–(3.31e) for this section with the appropriate specification of the parameters.

The auxiliary integral $\mathcal{H}_j(\tau)$ given by Eq. (4.14d) is more complicated than its counterpart (3.33d). This is because of the acquired branch-point singularities of (4.14d) coming from term Δ_j in the denominator of the integrand in Eq. (4.14e) or (4.14f). However, these singularities are also integrable. To this end we first rewrite the integral (4.14d) as follows:

$$\mathcal{H}_j(\tau)=\tfrac{1}{2}\mathcal{H}_{j,3}^{(1,3)}(\tau)+\mathcal{H}_{j,1}^{(2,1)}(\tau)\quad (j=1,2)\ , \tag{4.16}$$

with

$$\mathcal{H}_{j,j'}^{(k,m)}(\tau)=\frac{1}{b^m}\int_0^\infty dt\, t t_0^{3-j'/2}(t-\delta_j t_0'-i\epsilon)^{-m/2}\times\mathcal{H}_j^{(k)}(t,\tau)\ , \tag{4.17}$$

where $t_0'=\tau^2/b^2$. Further, we calculate only the integral $\mathcal{H}_{j,j'}^{(k,1)}(\tau)$, since

$$\mathcal{H}_{j,j'}^{(k,3)}(\tau)=\delta_j\left[\frac{2}{b^2}\right]\frac{\partial}{\partial t_0'}\mathcal{H}_{j,j'}^{(k,1)}(\tau)\ . \tag{4.18}$$

Requiring that $\mathrm{Re}(t-\delta_j t_0'-i\epsilon)^{1/2}>0$, we shall have, as $\epsilon\to 0+$,

$$\lim_{\epsilon\to 0+}(t-t_0'-i\epsilon)^{1/2}=\begin{cases}-i(t_0'-t)^{1/2}, & t\leq t_0' \quad (4.19\text{a})\\ +(t-t_0')^{1/2}, & t\geq t_0'\ . \quad (4.19\text{b})\end{cases}$$

This implies

$$b\mathcal{H}_{1,j'}^{(k,1)}(\tau)=i\int_0^{t_0'}dt\, t t_0^{3-j'/2}(t_0'-t)^{-1/2}\mathcal{H}_1^{(k)}(t,\tau)+\int_{t_0'}^\infty dt\, t t_0^{3-j'/2}(t-t_0')^{-1/2}\mathcal{H}_1^{(k)}(t,\tau)\ . \tag{4.20}$$

The first and the second terms in Eq. (4.20) belong to a class of so-called improper integrals. They can easily be regularized by making a change of variable $t'^2=t_0'-t$ in the first and $t'^2=t-t_0'$ in the second integral of Eq. (4.20). Hence, the regularized form of $\mathcal{H}_{1,j'}^{(k,1)}$ reads as follows:

$$b\mathcal{H}_{1,j'}^{(k,1)}(\tau)=2i\int_0^{\sqrt{t_0'}}dt(t_0'-t^2)(1+t_0'-t^2)^{-3+j'/2}\mathcal{H}_1^{(k)}(t_0'-t^2,\tau)+2\int_0^\infty dt(t_0'+t^2)(1+t_0'+t^2)^{-3+j'/2}\mathcal{H}_1^{(k)}(t_0'+t^2,\tau)\ . \tag{4.21}$$

Using Eqs. (4.18) and (4.21), together with the following relation (Ref. 28, No. 2.1.2/11),

$$\frac{\partial}{\partial x}\int_s^S dy\, f(x,y)=f(x,S)\frac{\partial S}{\partial x}-f(x,s)\frac{\partial s}{\partial x}+\int_s^S dy\frac{\partial}{\partial x}f(x,y)\ , \tag{4.22}$$

we can readily calculate the quantity $\mathcal{H}_{1,j'}^{(k,3)}(\tau)$. The final result is

$$b^2\mathcal{H}_{1,3}^{(k,3)}(\tau)=i\int_0^{\sqrt{t_0'}}dt[2(2-t_0'+t^2)(1+t_0'-t^2)^{-5/2}\mathcal{H}_1^{(k)}(t_0'-t^2,\tau)+4(t_0'-t^2)(1+t_0'-t^2)^{-3/2}\mathcal{H}_1^{(k)\prime}(t_0'-t^2,\tau)]+\int_0^\infty dt[2(2-t_0'-t^2)(1+t_0'+t^2)^{-5/2}\mathcal{H}_1^{(k)}(t_0'+t^2,\tau)+4(t_0'+t^2)(1+t_0'+t^2)^{-3/2}\mathcal{H}_1^{(k)\prime}(t_0'+t^2,\tau)]\ , \tag{4.23}$$

where

$$\mathcal{H}_j^{(1)\prime}(t,\tau)=(T_j/D_j)\left[-\frac{1}{D_j}\mathcal{L}_{\alpha j}^{(0,2)}(a_j^2)-\frac{2}{D_j^2}\mathcal{L}_{\alpha j}^{(0,1)}(a_j^2)+\frac{2}{D_j^2}\mathcal{L}_{\alpha j}^{(0,1)}(C_j^2)-\frac{1}{D_j}\mathcal{L}_{\alpha j}^{(0,2)}(C_j^2)\right]\ , \tag{4.24a}$$

$$\mathcal{H}_j^{(2)'}(t,\tau)=(T_j/D_j)\left[\frac{2}{D_j^2}\mathcal{L}_{\alpha j}^{(0,2)}(a_j^2)+\frac{6}{D_j^3}\mathcal{L}_{\alpha j}^{(0,1)}(a_j^2)-\frac{6}{D_j^3}\mathcal{L}_{\alpha j}^{(0,1)}(C_j^2)+\frac{4}{D_j^2}\mathcal{L}_{\alpha j}^{(0,2)}(C_j^2)-\frac{2}{D_j}\mathcal{L}_{\alpha j}^{(0,3)}(C_j^2)\right], \tag{4.24b}$$

with

$$T_j=(b^2+\delta_j\tau^2)t_0^2 . \tag{4.25}$$

Thus, inserting the results (4.20) and (4.23) into Eq. (4.16), we obtain the following expression for $\mathcal{H}_1(\tau)$, which is free from branch-point singularities:

$$b\mathcal{H}_1(\tau)=2i\int_0^{\sqrt{t_0'}}dt\,\mathcal{H}_1^-(t,\tau)+2\int_0^{\infty}dt\,\mathcal{H}_1^+(t,\tau) , \tag{4.26}$$

where

$$\mathcal{H}_j^{\pm}(t,\tau)=\frac{t_j^{\pm}}{(1+t_j^{\pm})^{5/2}}\mathcal{H}_j^{(2)}(t_j^{\pm},\tau)+\frac{2-t_j^{\pm}}{2b^2(1+t_j^{\pm})^{5/2}}\mathcal{H}_j^{(1)}(t_j^{\pm},\tau)+\frac{t_j^{\pm}}{b^2(1+t_j^{\pm})^{3/2}}\mathcal{H}_j^{(1)'}(t_j^{\pm},\tau)\quad (j=1,2) , \tag{4.27}$$

and

$$t_j^{\pm}=\delta_j(t_0'\pm t^2) . \tag{4.28}$$

The case with $j=2$ ($\tau\geq 0$) is investigated in an analogous manner, but without splitting the original integration limit $t\in[0,\infty]$ in Eq. (4.17). Hence, changing the integration variable in Eq. (4.17) according to $t'^2=t+t_0'$ and using Eqs. (4.18), (4.22), and (4.27), we obtain the quantity $\mathcal{H}_2(\tau)$ in the following form of the regular integral, i.e., without the branch-point singularities, as $\epsilon\to 0+$:

$$b\mathcal{H}_2(\tau)=2\int_{\sqrt{t_0'}}^{\infty}dt\,\mathcal{H}_2^-(t,\tau) . \tag{4.29}$$

Substituting the regularized integrals (4.26) and (4.29) into Eqs. (4.14b) and (4.14c), respectively, we are in a position to consider the only remaining singularity (4.8), which is due to divergence of Fourier transform $\tilde{W}_P(-\mathbf{q}-\boldsymbol{\alpha})$. Since we have

$$|\mathbf{q}+\boldsymbol{\alpha}|^2=|\mathbf{q}_\rho+\boldsymbol{\eta}|^2+\tau_{\alpha j}^2 \tag{4.30}$$

$$=\begin{cases}|\mathbf{q}_\rho+\boldsymbol{\eta}|^2+\left[\dfrac{-b^2-\tau^2}{2v}\right]^2>0\quad (j=1,\ \tau\leq 0) & (4.31a)\\[2ex] |\mathbf{q}_\rho+\boldsymbol{\eta}|^2+\left[\dfrac{-b^2+\tau^2}{2v}\right]^2\geq 0\quad (j=2,\ \tau\geq 0) , & (4.31b)\end{cases}$$

it follows that only the integral $I^{(+)}(V_T,W_P)$ is singular at $\mathbf{q}=-\boldsymbol{\alpha}$. Hence, repeating the same "subtraction" procedure as in Sec. III, we arrive at

$$I^{(+)}(V_T,W_P)=\frac{1}{v}\int_0^{2b}d\tau\,\tau\left[\mathcal{H}_2(\tau)+2f(-\boldsymbol{\alpha})\ln\left|\frac{\tau^2-b^2}{v}\right|\right]+\left[X_P(\boldsymbol{\alpha})+\frac{1}{v}\int_{2b}^{+\infty}d\tau\,\tau\mathcal{H}_2(\tau)\right] , \tag{4.32}$$

where $\mathcal{H}_2(\tau)$ is given by Eq. (4.29) and

$$X_P(\boldsymbol{\alpha})=-\left[\frac{4b^2}{v}\right]f(-\boldsymbol{\alpha})\ln\frac{3^{3/4}b^2}{ev} , \tag{4.33}$$

$$f(-\boldsymbol{\alpha})=\frac{T_\beta+2b^2}{4b^3T_\beta^4} . \tag{4.34}$$

Subsequent numerical quadratures in Eq. (4.32) should be carried out in the same manner as in Eq. (3.43). The integral $I^{(-)}(V_T,W_P)$, however, is obtained directly from Eqs. (4.14b) and (4.26).

V. CALCULATION OF THE INTEGRAL $I(W_T,V_P)$

Setting $\mathbf{p}\to-\mathbf{q}$ and $\mathbf{q}\to-\mathbf{p}$ in Eq. (2.13c), we shall have

$$I(W_T,V_P)=\int\int\frac{d\mathbf{p}\,d\mathbf{q}}{p^2q^2}\left[\left[\left|\mathbf{p}-\boldsymbol{\beta}\right|^2+b^2\right]\times(|\mathbf{p}+\boldsymbol{\alpha}+\mathbf{q}|^2+a^2)\right]^{-2}B_{\mathbf{p},\mathbf{q}}^{-1} , \tag{5.1}$$

where

$$\frac{1}{\pi^3}B_{\mathbf{p},\mathbf{q}}=|\mathbf{p}+\boldsymbol{\alpha}+\mathbf{q}|^2+(a^2+2\mathbf{p}\cdot\mathbf{v}-i\epsilon)$$

$$\equiv|\mathbf{p}+\boldsymbol{\alpha}+\mathbf{q}|^2+E_{\mathbf{p}}^2 \; . \tag{5.2}$$

In the case under study, which encompasses the symmetric collision ($Z_P=Z_T$) and the resonance transition ($i=f=1s$), we have $a=b$, so that

$$E_{\mathbf{p}}^2\equiv\epsilon_{\mathbf{p}}^2=b^2+2\mathbf{p}\cdot\mathbf{v}-i\epsilon \tag{5.3a}$$

and

$$\boldsymbol{\alpha}=\boldsymbol{\eta}-\tfrac{1}{2}\mathbf{v}, \quad \boldsymbol{\beta}=-\boldsymbol{\eta}-\tfrac{1}{2}\mathbf{v} \; . \tag{5.3b}$$

This implies, for $a=b$,

$$I(W_T,V_P)=I^{\beta,\alpha}(V_T,W_P) \; , \tag{5.4}$$

where $I^{\alpha,\beta}(V_T,W_P)$ is given by Eq. (2.13b), i.e.,

$$I^{\alpha,\beta}(V_T,W_P)=I(V_T,W_P) \; . \tag{5.5}$$

Since $\boldsymbol{\eta}\cdot\mathbf{v}=0$ the integral $I(V_T,W_P)$ is invariant to the transformation $\boldsymbol{\alpha}\leftrightarrow\boldsymbol{\beta}$, if substituting $+\boldsymbol{\eta}$ by $-\boldsymbol{\eta}$ leaves $I(V_T,W_P)$ unaltered. The only place where the signs $\pm$ in front of $\boldsymbol{\eta}$ intervene in the calculation of $I(V_T,W_P)$ is in the integration over ϕ in the cylindrical coordinates $\mathbf{q}=(\mathbf{q}_\rho,\phi)$. The integral in question appearing in $I(V_T,W_P)$ is of the following type:

$$J(\boldsymbol{\eta})=\frac{1}{2\pi}\int_0^{2\pi}d\phi\frac{1}{A-2\mathbf{q}\cdot\boldsymbol{\eta}}$$

$$=\frac{1}{2\pi}\int_0^{2\pi}d\phi\frac{1}{A-B\eta\cos(\phi-\phi_\eta)} \; . \tag{5.6}$$

where $B=2q_\rho$. Changing the integration variable ϕ according to $\exp(i\phi)=z$ and passing to the complex z-plane, we can write:

$$J(\boldsymbol{\eta})=\frac{e^{i\phi_\eta}}{B\eta\pi i}\oint_C\frac{1}{(z-z_1)(z-z_2)} \; , \tag{5.7}$$

where

$$z_{1/2}=\left[\frac{-A\pm\sqrt{A^2-B^2\eta^2}}{B\eta}\right]e^{i\phi_\eta} \; . \tag{5.8}$$

If $A^2>B^2\eta^2$, it follows that $|z_1|<1$ and $|z_2|>1$, in which case contour C is a closed counterclockwise semicircle of unit radius around the origin in the upper half of the complex z plane. Applying the Cauchy theorem of residuum, we shall have

$$J(\boldsymbol{\eta})=\frac{1}{\sqrt{A^2-B^2\eta^2}} \; . \tag{5.9}$$

Carrying out the same procedure to the integral

$$J(-\boldsymbol{\eta})=\frac{1}{2\pi}\int_0^{2\pi}d\phi\frac{1}{A+2\mathbf{q}\cdot\boldsymbol{\eta}}$$

$$=\frac{1}{2\pi}\int_0^{2\pi}d\phi\frac{1}{A+B\eta\cos(\phi-\phi_\eta)} \; , \tag{5.10}$$

we obtain the rhs of Eq. (5.9) for $J(-\boldsymbol{\eta})$, provided that $A^2>B^2\eta^2$, so that

$$J(-\boldsymbol{\eta})=J(\boldsymbol{\eta}) \; . \tag{5.11}$$

This result implies

$$I^{\beta,\alpha}(V_T,W_P)=I^{\alpha,\beta}(V_T,W_P) \; . \tag{5.12}$$

Hence, comparing Eqs. (5.4) and (5.12) with each other, we conclude that, for $i=f=1s$,

$$I(W_T,V_P)=I(V_T,W_P) \; . \tag{5.13}$$

This is expected because of the complete symmetry of the problem under study.

VI. CALCULATION OF THE INTEGRAL $I(W_T,W_P)$

Changing the integration variable (2.9d) according to $\mathbf{p}'=\boldsymbol{\alpha}-\mathbf{p}\to-\mathbf{q}$, $\mathbf{q}'=-\mathbf{q}\to+\mathbf{p}$, we can write

$$I(W_T,W_P)=\frac{1}{\pi^3}\int\int d\mathbf{p}\,d\mathbf{q}[|\mathbf{q}+\boldsymbol{\alpha}|^2(|\mathbf{p}+\mathbf{q}|^2+a^2)^2p^2D_{\mathbf{p},\mathbf{q}}]^{-1} \; , \tag{6.1}$$

where

$$D_{\mathbf{p},\mathbf{q}}=(|\mathbf{p}+\mathbf{q}-\mathbf{v}|^2+b^2)^2(|\mathbf{p}+\mathbf{q}-\mathbf{v}|^2+\gamma^2) \; , \tag{6.2a}$$

$$\gamma^2=b^2+2(\mathbf{q}+\boldsymbol{\alpha})\cdot\mathbf{v}-i\epsilon \quad (\mathrm{Re}\gamma>0, \; \epsilon\to 0+) \; . \tag{6.2b}$$

Using the fractional decomposition of the two constituents in $1/D_{\mathbf{p},\mathbf{q}}$, together with the integral representation (3.3), we obtain

$$I(W_T,W_P)=\int_0^\infty dt\, t_0^3\mathcal{F}(t) \; , \tag{6.3}$$

where $t_0=1/(1+t)$,

$$\mathcal{F}(t)=6\delta\mathcal{F}^{(1)}(t)-\mathcal{G}^{(1)}(t)+\mathcal{G}^{(2)}(t) \; , \tag{6.4a}$$

$$\mathcal{F}^{(1)}(t)=\frac{1}{\pi}\int\frac{d\mathbf{q}}{\gamma_q}|\mathbf{q}+\boldsymbol{\alpha}|^{-2}(\tfrac{1}{8}\Delta_1^{-5}\Omega_1^{-1}+\tfrac{1}{6}\Delta_1^{-3}\Omega_1^{-2}+\tfrac{1}{3}\Delta_1^{-1}\Omega_1^{-3}) \; , \tag{6.4b}$$

$$\mathcal{G}^{(j')}(t)=\frac{1}{\pi}\int\frac{d\mathbf{q}}{\gamma_q^2}|\mathbf{q}+\boldsymbol{\alpha}|^{-2}(\tfrac{1}{2}\Delta_{j'}^{-3}\Omega_{j'}^{-1}+\Delta_{j'}^{-1}\Omega_{j'}^{-2}) \; , \tag{6.4c}$$

with $\delta=tt_0$ and

$$\Omega_{j'}=Q^2+\Delta_{j'}^2 \; , \tag{6.4d}$$

$$\mathbf{Q}=\mathbf{q}-\mathbf{v}\delta, \quad \gamma_q=b^2-\gamma^2 \; , \tag{6.4e}$$

$$\Delta_{j'}^2=\{v^2t+[a^2+(b^2\delta_{j',1}+\gamma^2\delta_{j',2})t](1+t)\}t_0^2 \ . \quad (6.4f)$$

Here the integrals over $\mathbf{p}$ are carried out by means of Eq. (3.10), as well as with the help of the following result:

$$\frac{1}{\pi^2}\int d\mathbf{p}(p^2+x^2)^{-1}(|\mathbf{p}+\mathbf{Q}|^2+y^2)^{-4} =(8y^5\mathcal{R})^{-1}+(3x+2y)(12y^4\mathcal{R}^2)^{-1} +(x+y)^2(3y^3\mathcal{R}^3)^{-1} \ , \quad (6.5)$$

where $\mathcal{R}=Q^2+(x+y)^2$. The function $\mathcal{F}(t)$ given by Eq. (6.4a) possesses branch-point singularities at

$$\gamma^2=0 \ , \quad (6.6)$$

which is removed by the substitution

$$q_z=\frac{\tau|\tau|}{2v}+Q_\alpha \ , \quad (6.7a)$$

where

$$Q_\alpha=-\frac{b^2+2\alpha_z v}{2v}=\frac{v^2-a^2}{2v} \ . \quad (6.7b)$$

In this way, quantity γ^2 acquires the form

$$\gamma^2=\tau|\tau|-i\epsilon, \quad \epsilon\to 0+ \ . \quad (6.8)$$

Letting $\epsilon\to 0+$, we arrive at

$$\Omega_{j'}=\begin{cases}\left[q_p^2+\left[Q_\alpha-\frac{\tau^2}{2v}-v\delta\delta_{j',1}\right]^2\right]+D_{j'}^2, & \tau<0 \quad (6.9a)\\ \left[q_p^2+\left[Q_\alpha+\frac{\tau^2}{2v}-v\delta\delta_{j',1}\right]^2\right]+D_{j'}^2, & \tau\ge 0 \quad (6.9b)\end{cases}$$

where $j'=1,2$ and

$$D_1^2=\Delta_1^2=v^2tt_0^2+(a^2+b^2t)t_0>0 \ , \quad (6.10a)$$

$$D_2^2=a^2>0 \ . \quad (6.10b)$$

Hence, the substitution (6.7a) removes branch-point singularity (6.6), since

$$\Omega_{j'}>0, \quad j'=1,2, \quad \forall\tau\in[-\infty,+\infty], \quad \forall t\in[0,+\infty] \ . \quad (6.11)$$

Thus,

$$I(W_T,W_P)=I^{(-)}(W_T,W_P)+I^{(+)}(W_T,W_P) \ , \quad (6.12a)$$

$$I^{(-)}(W_T,W_P)=-\frac{1}{v}\int_{-\infty}^{0}d\tau\,\tau\mathcal{H}_1(\tau) \ , \quad (6.12b)$$

$$I^{(+)}(W_T,W_P)=+\frac{1}{v}\int_{0}^{+\infty}d\tau\,\tau\mathcal{H}_2(\tau) \ , \quad (6.12c)$$

$$\mathcal{H}_j(\tau)=\int_0^\infty dt\, t_0^3\mathcal{H}_j(t,\tau)+\mathcal{G}_j(\tau)\mathcal{J}_j^{(3)}(\tau)+\mathcal{G}_j'(\tau)\mathcal{J}_j^{(1)}(\tau) \ , \quad (6.12d)$$

$$\mathcal{H}_j(t,\tau)=\delta\left[\frac{3}{4\Gamma_j\Delta_1^5}\mathcal{L}_{\alpha j}^{(0,1)}(C_{j1}^2)+\frac{1}{\Gamma_j\Delta_1^3}\mathcal{L}_{\alpha j}^{(0,2)}(C_{j1}^2)+\frac{2}{\Gamma_j\Delta_1}\mathcal{L}_{\alpha j}^{(0,3)}(C_{j1}^2)\right] -\frac{1}{2\Gamma_j^2\Delta_1^3}\mathcal{L}_{\alpha j}^{(0,1)}(C_{j1}^2)-\frac{1}{\Gamma_j^2\Delta_1}\mathcal{L}_{\alpha j}^{(0,2)}(C_{j1}^2) \ , \quad (6.12e)$$

$$\mathcal{G}_j(\tau)=\frac{1}{2\Gamma_j^2}\mathcal{L}_{\alpha j}^{(0,1)}(C_{j2}^2) \ , \quad (6.12f)$$

$$\mathcal{G}_j'(\tau)=\frac{1}{\Gamma_j^2}\mathcal{L}_{\alpha j}^{(0,2)}(C_{j2}^2) \ , \quad (6.12g)$$

$$\mathcal{J}_j^{(m)}(\tau)=\int_0^\infty dt\frac{t_0^{3-m}}{C_j^m} \ , \quad (6.12h)$$

$$C_{jj'}^2=(\tau_j-v\delta\delta_{j',1})^2+\Delta_1^2\delta_{j',1}+a^2\delta_{j',2}>0 \ , \quad (6.12i)$$

$$\Gamma_j=b^2+\delta_j\tau^2-i\epsilon, \quad \tau_j=Q_\alpha-\delta_j\frac{\tau^2}{2v} \ , \quad (612j)$$

$$C_j^2=v^2t+(a^2-\delta_j\tau^2t)(1+t)-i\epsilon, \quad \delta_j=\delta_{j,1}-\delta_{j,2} \ . \quad (6.12k)$$

The function $\mathcal{L}_{\alpha j}^{(n,m)}(y)$ is given by Eq. (4.15a), together with the accompanying quantities defined in Eqs. (4.15b), (4.15c), and (4.15d). Since the equality $C_j=0$ [see Eq. (6.12b)] can be satisfied within the integration limits $t,|\tau|\in[0,+\infty]$, we encounter the so-called improper integrals in Eq. (6.12h). Considering first the case $j=1$ (i.e., $\tau\le 0$), we write

$$C_1^2=-\tau^2(t-t_1)(t-t_2)-i\epsilon \ , \quad (6.13a)$$

where t_1 and t_2 are the roots of the equation $C_1^2=0$, i.e.,

$$t_{1/2}=\frac{1}{2\tau^2}\{(v^2+a^2-\tau^2)\pm[(v^2+a^2-\tau^2)^2+4a^2\tau^2]^{1/2}\} \ . \quad (6.13b)$$

Here $t_1<0$ and $t_2>0$ for any $\tau\in[-\infty,0]$. Therefore,

$$\mathcal{J}_1^{(3)}(\tau)=-\frac{2}{\tau^3}\frac{\partial}{\partial t_2}J^{(0)}(\tau) \ , \quad (6.14a)$$

$$J^{(0)}(\tau)=\int_0^\infty dt\frac{1}{(t-t_1)^{3/2}(t_2-t-i\epsilon)^{1/2}} \ . \quad (6.14b)$$

Splitting the interval from 0 to ∞ into two subintervals $[0,t_2]$ and $[t_2,+\infty]$, we shall have, in the limit $\epsilon\to 0+$,

$$J^{(0)}(\tau)=\int_0^{t_2}dt(t-t_1)^{-3/2}(t_2-t)^{-1/2} +i\int_{t_2}^\infty dt(t-t_1)^{-3/2}(t-t_2)^{-1/2} \ . \quad (6.15)$$

Introducing a change of variable $t_2-t=t'^2$ in the first and $t-t_2=t'^2$ in the second integral of Eq. (6.15), we obtain

$$J^{(0)}(\tau)=2\left[\left[-\frac{t_2}{t_1}\right]^{1/2}+i\right]\frac{\tau^2}{\sqrt{\bar{\omega}_1}}, \tag{6.16}$$

where

$$\bar{\omega}_1=\omega_1^2+4a^2\tau^2, \quad \omega_1=v^2+a^2-\tau^2 . \tag{6.17a}$$

Hence,

$$\mathcal{J}_1^{(3)}(\tau)=2\left[2i\tau+\frac{\omega_1}{a}\right]\Big/\bar{\omega}_1 . \tag{6.17b}$$

The improper integral $\mathcal{J}_1^{(1)}(\tau)$ can also be calculated in a closed form by first setting $t'=1/(1+t)$, in which case

$$\mathcal{J}_1^{(1)}(\tau)=\int_0^1 dt'\frac{t'}{C_1'}, \tag{6.18a}$$

where

$$C'^2=\begin{cases}v^2t'(1-t')+a^2t'-\tau^2(1-t')-i\epsilon , & (6.18b)\\ v^2(t_1'-t')(t'-t_2'-i\epsilon) , & (6.18c)\end{cases}$$

$$t'_{1/2}=\frac{1}{2v^2}[(v^2+a^2+\tau^2)\pm\sqrt{\bar{\omega}_1'}] , \tag{6.19}$$

$$\bar{\omega}_1'=(v^2+a^2+\tau^2)^2-4v^2\tau^2$$
$$=[(v-\tau)^2+a^2][(v+\tau)^2+a^2]>0 \tag{6.19a}$$

$$t_1'>1, \quad t_2'\in[0,1) . \tag{6.19b}$$

Using Eq. (6.18c) and taking the limit $\epsilon\to 0+$, we can write

$$\mathcal{J}_1^{(1)}(\tau)=\frac{1}{v}\left[i\int_0^{t_2'}dt't'(t_1'-t')^{-1/2}(t_2'-t')^{-1/2} + \int_{t_2'}^1 dt't'(t_1'-t')^{-1/2}(t'-t_2')^{-1/2}\right] . \tag{6.20}$$

Making a change of variable such as $t''^2=t_2'-t'$ in the first and $t''^2=t'-t_2'$ in the second integral of Eq. (6.19), together with the help of formulas 2.271/3 and 2.271/4 of Ref. 30, we obtain

$$\mathcal{J}_1^{(1)}(\tau)=\frac{1}{v}\left[\frac{1}{v^2}\omega_1'(i\ln\bar{D}+\arcsin\bar{D}') -\frac{i\tau}{v}-\sqrt{(t_1'-1)(1-t_2')}\right] , \tag{6.21}$$

where

$$\omega_1'=v^2+a^2+\tau^2, \quad \bar{D}=v\frac{\sqrt{t_1'}+\sqrt{t_2'}}{(\bar{\omega}_1')^{1/4}}, \quad \bar{D}'=v\frac{\sqrt{1-t_2'}}{(\bar{\omega}_1')^{1/4}} . \tag{6.22}$$

Both quantities $\mathcal{J}_1^{(3)}(\tau)$ and $\mathcal{J}_1^{(1)}(\tau)$, given by Eqs. (6.17b) and (6.21), respectively, are well-behaved functions for any $\tau\in[-\infty,0]$. Finally, we shall perform a similar analysis for $j=2$ $(\tau\geq 0)$ and analytically calculate the integral $\mathcal{J}_2^{(m)}(\tau)$ for $m=1$ and 3. Letting $\epsilon\to 0+$, it follows that

$$\mathcal{J}_2^{(3)}(\tau)=\frac{1}{\tau^3}\int_0^\infty dt(t-\hat{t}_1)^{-3/2}(t-\hat{t}_2)^{-3/2} , \tag{6.23}$$

where

$$\hat{t}_{1/2}=\frac{1}{2\tau^2}[-(v^2+a^2+\tau^2)\pm\sqrt{\bar{\omega}_2}]; \quad \hat{t}_1<0, \quad \hat{t}_2<0 , \tag{6.24}$$

$$\bar{\omega}_2=(v^2+a^2+\tau^2)^2-4a^2\tau^2$$
$$=[v^2+(a-\tau)^2][v^2+(a+\tau)^2]>0 . \tag{6.25}$$

Setting $z^2=t-\hat{t}_2$ into the integral (6.23) and using formula 2.275/9 of Ref. 28, we shall have

$$\mathcal{J}_2^{(3)}(\tau)=2\frac{v^2+(a-\tau)^2}{a\bar{\omega}_2}=\frac{2}{a}[v^2+(a+\tau)^2]^{-1} . \tag{6.26}$$

In the case of the integral $\mathcal{J}_2^{(1)}(\tau)$, we first introduce a change of variable such as $\hat{t}'=1/(1+t)$, so that

$$\mathcal{J}_2^{(1)}(\tau)=\int_0^1 d\hat{t}'\frac{\hat{t}'}{\hat{C}_2'} , \tag{6.27a}$$

where

$$\hat{C}_2'^2=v^2\hat{t}'(1-\hat{t}')+a^2\hat{t}'+\tau^2(1-\hat{t}') , \tag{6.27b}$$

$$=v^2(\hat{t}'-\hat{t}_1')(\hat{t}_2'-\hat{t}') , \tag{6.27c}$$

$$\hat{t}'_{1/2}=\frac{1}{2v^2}[(a^2+v^2-\tau^2)\mp\sqrt{\bar{\omega}_2'}], \quad \hat{t}_1'\leq 0, \quad \hat{t}_2'>1 , \tag{6.27d}$$

$$\bar{\omega}_2'=(a^2+v^2-\tau^2)^2+4v^2\tau^2>0 . \tag{6.27e}$$

Lastly, we set $z^2=\hat{t}_1$ into Eq. (6.27a) and subsequently employ formulas 2.271/4 and 1.625/5 of Ref. 30 to obtain

$$\mathcal{J}_2^{(1)}(\tau)=\frac{2}{v}\arccos\bar{D}_2' , \tag{6.28a}$$

where

$$\bar{D}_2'=\frac{v^2}{\sqrt{\bar{\omega}_2'}}\{[\hat{t}_2'(\hat{t}_2'-1)]^{1/2}+[-\hat{t}_1'(1-\hat{t}_1')]^{1/2}\} . \tag{6.28b}$$

It is immediately clear from Eqs. (6.26) and (6.28a) that the quantities $\mathcal{J}_2^{(3)}(\tau)$ and $\mathcal{J}_2^{(1)}(\tau)$ are regular, i.e., well-behaved functions for any $\tau\in[0,+\infty]$. This calculation completes the elimination of all the branch-point singularities from the function $\mathcal{H}_j(\tau)$ for any $\tau\in[-\infty,+\infty]$, where the constituents $\mathcal{J}_j^{(3)}(\tau)$ and $\mathcal{J}_j^{(1)}(\tau)$ are given by Eqs. (6.17b), (6.21), (6.26), and (6.28a).

Finally, the only remaining singularity of the integral $I(W_T,W_P)$ is a pole at

$$\mathbf{q}=-\boldsymbol{\alpha}\ , \tag{6.29}$$

which originates from divergence of $\tilde{W}_P(-\mathbf{q}-\boldsymbol{\alpha})$. Between the two constituent parts $I^{(-)}(W_T,W_P)$ and $I^{(+)}(W_T,W_P)$ of $I(W_T,W_P)$, only $I^{(+)}(W_T,W_P)$ possesses a pole at $\mathbf{q}=-\boldsymbol{\alpha}$ [see Eqs. (4.31a) and (4.31b)]. This singularity is removed in the same manner as in the preceeding sections, with the final result

$$I^{(+)}(W_T,W_P)=\frac{1}{v}\int_0^{2b}d\tau\,\tau\left[\mathcal{H}_2(\tau)+2f(-\boldsymbol{\alpha})\ln\left|\frac{\tau^2-b^2}{v}\right|\right]+\left[X_P(\boldsymbol{\alpha})+\frac{1}{v}\int_{2b}^{+\infty}d\tau\,\tau\mathcal{H}_2(\tau)\right]\ , \tag{6.30}$$

where $\mathcal{H}_2(\tau)$ is given by Eq. (6.12d),

$$X_P(\boldsymbol{\alpha})=-\left[\frac{4b^2}{v}\right]f(-\boldsymbol{\alpha})\ln\frac{3^{3/4}b^2}{ev}\ , \tag{6.31}$$

and

$$f(-\boldsymbol{\alpha})=\frac{1}{\pi^2}\int d\mathbf{p}[p^2(|\mathbf{p}-\boldsymbol{\alpha}|^2+a^2)^2(|\mathbf{p}+\boldsymbol{\beta}|^2+b^2)^3]^{-1}\ , \tag{6.32a}$$

$$f(-\boldsymbol{\alpha})=\frac{3}{T_\beta^4}\left[\frac{b}{4v^2}-\frac{4b^2-v^2}{8v^3}\arctan\frac{v}{2b}\right]+\frac{3}{2T_\beta^3}\left[\frac{1}{v^3}\arctan\frac{v}{2b}-\frac{2b}{v^2(v^2+4b^2)}\right]+\frac{3}{2bT_\beta^2(v^2+4b^2)}+\frac{20b^2+v^2}{4b^3T_\beta(v^2+4b^2)^3}\ , \tag{6.32b}$$

where T_β is given in (3.26f). Here we emphasize that the numerical quadratures in Eq. (6.30) should be performed in the same manner as in Eq. (3.53).

Before ending this section and for reasons of completeness, we shall give the matrix element required in the calculation of the CB1 transition amplitude (2.11). For this purpose, the necessary three-denominator Dalitz-Lewis integral[24–26] is of the type (6.32b), and reads as follows:

$$\mathcal{D}=\frac{1}{\pi^2}\int d\mathbf{p}[p^2(|\mathbf{p}-\boldsymbol{\alpha}|^2+a^2)^2(|\mathbf{p}+\boldsymbol{\beta}|^2+b^2)^2]^{-1}=\frac{1}{T_\beta^3}\left[\frac{b}{v^2}-\frac{4b^2-v^2}{2v^3}\arctan\frac{v}{2b}\right]+\frac{2}{T_\beta^2}\left[\frac{1}{v^3}\arctan\frac{v}{2b}-\frac{2b}{v^2(v^2+4b^2)}\right]+\frac{2}{bT_\beta(v^2+4b^2)^2}\ , \tag{6.33}$$

where Eq. (3.26f) is used.

VII. NUMERICAL RESULTS

In the numerical computations of integrals whose range is $x\in[\hat{C},\hat{P}\infty]$, where $\hat{C}$ is a finite constant and $\hat{P}=+$ or $-$, we find it highly convenient to introduce the following change of variable:

$$t=\tan\left[\frac{\vartheta}{2}\right]\ . \tag{7.1}$$

Such a "tangential grid" transforms the former semi-infinite integrals into the quadratures over the finite range, because

$$\vartheta\in[2\arctan(\hat{C}),\hat{P}\pi]\ . \tag{7.2}$$

Since the constant $\hat{C}$ is allowed to take the value zero, we see that all the semi-infinite integrals from the previous sections can be subjected to change of variable (7.1). By so doing, we shall have only integrals over a finite range for which the variable-order Gauss-Legendre code will be employed.

Further, we encounter certain integrals whose lower and upper limits are finite from the very beginning [see Eqs. (4.23) and (4.26)]. These integrals will also be computed by using the Gauss-Legendre rule. Finally, we have the integrals over the *symmetric* finite intervals, which are left after the "subtraction technique" [see Eqs. (3.54), (4.32), and (6.30)]. In this case, we use an *even-order* Gauss-Legendre quadrature rule which is symmetric about the singularity at $\tau\approx a$ or $\tau\approx b$ situated in the middle of the integration interval.[29]

The results of the computation of the differential cross sections for the symmetric resonant charge exchange

$$H^+ + H(1s)\rightarrow H(1s)+H^+\ , \tag{7.3}$$

are shown in Figs. 1–4. The present technique of obtaining the data of the CB2 theory automatically provides the corresponding results of the BK2 method, which includes only the contribution from matrix element $I_{if}(V_T,V_P)$. For completeness, we also quote the cross section of the first-order CB1 and BK1 approximations.

There is a common pattern seen in Figs. 1–4, when comparing these theories. Irrespective of incident energies, the CB1 approximation always exhibits an unphysical dip, which is due to cancellation of the contributions from potentials $V_P(r_P)$ and $W_P(R)$. Such an experimentally unobserved dip is absent from the angular distributions obtained in the CB2 method, at those impact energies for which second-order term $V_f G_{0e}^{+} V_i$ becomes important. The presence of the dip in the first-order term T_{if}^{CB1} is, nevertheless, strongly felt in the differential cross section $d^{CB2}\sigma/d\Omega$, through a clear change of the slope of the corresponding curves at 100 and 125 keV. In the dip area of the CB1 approximation at 60 keV, however, data $d^{CB2}\sigma/d\Omega$ exhibit a pronounced minimum. This is expected, since the role of propagator $V_f G_{0e}^{+} V_i$, which partially allows for continuum intermediate states, becomes less important with decreasing incident energy. Such an expectation is based upon the well-known evidence about the relative significance of charge exchange and ionization or excitation channels. Namely, the two latter channels are dominated by charge exchange at lower energies, and the pattern is just reversed in the high-energy region.

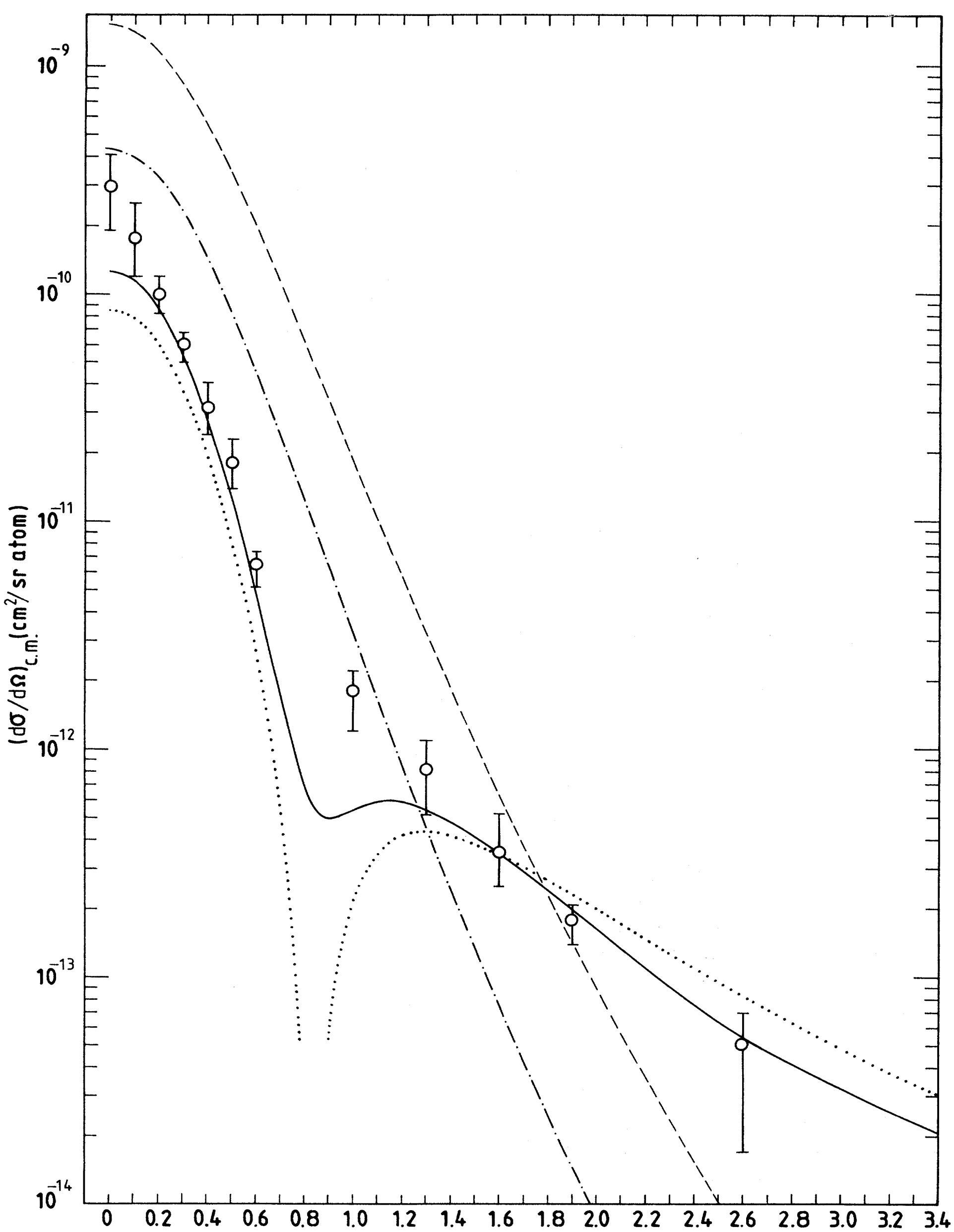

FIG. 1. Differential cross sections $(d\sigma/d\Omega)_{c.m.}$ for charge exchange $H^+ + H(1s) \rightarrow H(\Sigma) + H^+$, as a function of the scattering angle $\theta_{c.m.}$ at 60 keV laboratory energy of the incident proton. Displayed theoretical results for the formation of atomic hydrogen in any state (Σ) are obtained through multiplication of the ground-state capture cross section by the Oppenheimer scaling factor (1.202). Theory (present *exact* numerical computations): BK1, —·—·—, BK2, — — —, CB1, · · · ·; and CB2, ——. Experiment: ○, Martin *et al.* (Ref. 31).

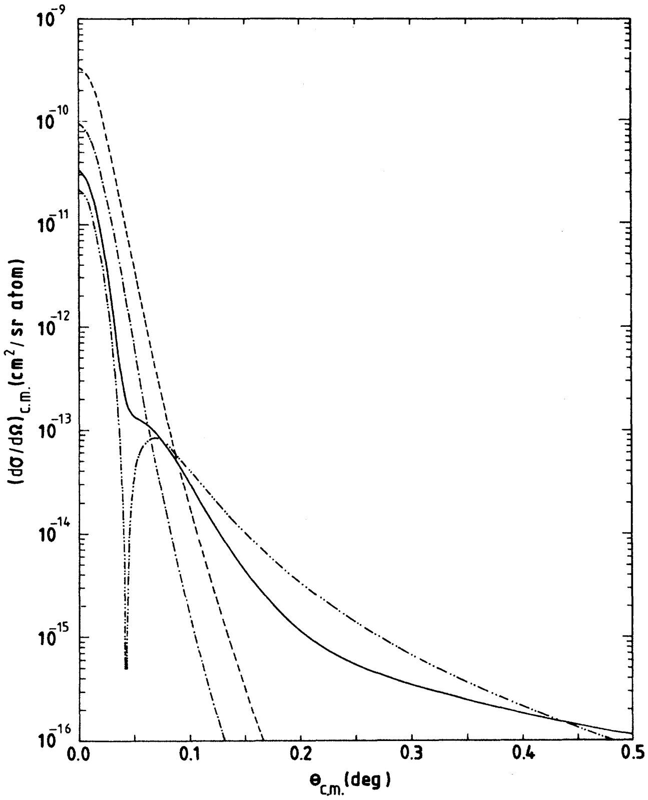

FIG. 2. Differential cross sections $(d\sigma/d\Omega)_{c.m.}$ for charge exchange (7.3) as a function of the scattering angle $\theta_{c.m.}$ at 100 keV laboratory energy of the incident proton. Only the transition $1s \rightarrow 1s$ is considered without allowance for the excited states of atomic hydrogen. All the cross sections are the theoretical results of the present *exact* numerical computations: BK1, —·—·—; BK2, — — —; CB1, —··—··—; and CB2, ——.

Hence, at lower energies, any failure of the CB1 method, e.g., the dip in the angular distributions, should be corrected by inclusion of discrete intermediate states of the electron in the Coulomb fields of the projectile and target nucleus. In this regard, the recently introduced method of Belkić and Taylor[16] is promising, since it variationally unifies the CB2 theory with an L^2-expansion method in terms of the Sturmian basis-set wave functions centered at both Coulomb centers. Naturally, a second-order perturbative approach, such as the CB2 method, is not expected to be fully adequate for charge exchange at energies as low as 60 keV. Nevertheless, this energy is included in the analysis, with the purpose of empirically assessing a low-energy limit of the validity of the CB2 theory. At still lower energies, such as 25 keV, we have verified that, in a narrow angular region around the dip, the CB1 and CB2 approximations yield nearly the same differential cross sections which, however, cannot be accepted, due to their unphysically vanishing values.

As for comparisons with the experimental data of Martin *et al.*,[31] it can be seen from Figs. 1 and 3 that the CB2 method is reasonably successful at 60 and 125 keV. Good agreement between the CB2 theory and the measurement in these cases is appealing, since the latter data relate to capture into all final bound states $(Z_P,e)_\Sigma$. Theoretical results are obtained by explicitly including only $1s \rightarrow 1s$ transition, whereas capture to any state is only roughly provided through multiplication of the cross sections by the well-known Oppenheimer n_f^{-3} scaling factor given by the Riemann ζ function $\zeta(3) \simeq 1.202$. Limitation of such a procedure is obvious, since application of this well-known scaling rule is justified provided that the incident energy and/or principal quantum number n_f is sufficiently high. Furthermore, the Oppenheimer law is originally established in the BK1 approximation for the *total* cross sections, which are determined by integration over all the scattering angles. It seems hardly possible that differential cross sections, however, which exhibit structures, would support any linear scaling throughout the scattering angle region of interest. As recently demonstrated by Belkić, Saini, and Taylor[3] in the CB1 approximation, many excited states are required by *explicit* computations to fill in the dip, away from which, however, the cross section $1.202 d^{\text{CB1}}/d\Omega$ would suffice. Nevertheless, a smaller number of excited states seems to be necessary in the CB2 method, since the dip is already removed by the contribution from second-order term $\langle \Phi_f | V_f G_{0e}^{+} V_i | \Phi_i \rangle$. Despite these limitations concerning comparisons in Figs. 1 and 3, the CB2 approximation can be considered as satisfactory at these relatively low impact energies for application of perturbative treatments. Equally important, however, is the conclusion which emerges from this analysis, that there is a distinct improvement in description of charge exchange, by going from the first (CB1)- to the second (CB2)-order perturbation theory.

The situation is just the opposite in the case of the other two models under study, i.e., the first (BK1)- and second (BK2)-order approximations, which do not obey the correct boundary conditions. Namely, it is observed in Figs. 1–3, that the results of the BK2 model largely overestimate the findings of the BK1 method throughout the angular interval under consideration. For example, we have obtained at 100 keV, that $d\sigma^{\text{BK2}}/d\Omega > d\sigma^{\text{BK1}}/d\Omega$ by a factor ranging from 3.6 ($\theta = 0.0°$) to 15.2 ($\theta = 2.0°$). At 1000 keV (not shown), this factor is still considerable, reaching values of 1.55 and 11.6 at $\theta = 0.0°$ and 0.1°, respectively. As documented in Figs. 1 and 3, both the BK1 and BK2 models are in profound disagreement with the experimental data of Martin *et al.*[31] Contrary to expectation, the BK2 method is even worse than the BK1 approach. Namely, from the physical point of view, the second-order BK2 approximation should be more adequate than its first-order counterpart (BK1), due to inclusion of intermediate-state propagator $V_T G_{0e}^{+} V_P$. The fact that this is not so indicates a disregard of certain principles, which are *more fundamental* than the inclusion of higher-order terms in the perturbation Born series. Specifically, this problem concerns the correct boundary conditions, which are the essential and distinct features of any scattering event, in comparison to purely bound-state problems (e.g., search of binding energies of an isolated atom, etc.) These conditions refer to a proper definition of perturbing potentials at infinitely large distances between the scattering particles. Here it is evidently wrong to introduce purely *Coulombic* potentials $V_P(r_P)$, $V_T(r_T)$ for the perturbation interactions, and associate them respectively with unperturbed channel states Φ_i, Φ_f in which the *plane waves* describe the relative motion of heavy aggregates. This is precisely the case in the BK2 model, whose flagrant inadequacy has previously been attributed merely to the use of the free-particle Green's function G_{0e}^{+}. The CB2 theory, however, provides a convincing counterexample, which also employs G_{0e}^{+} and yields reliable results. Hence, the failure of the BK2 approximation is not in the adoption of the free-particle Green's function, but rather in the violation of the correct boundary conditions.

In first-order theories, the electron scatters only once, and that single encounter occurs at either of the two Coulomb centers Z_P or Z_T, depending upon the choice of the "post" or "prior" transition amplitude. However, it has been recognized for a long time,[32] that in contrast to excitation, ionization or electron loss, charge exchange (2.1) represents a genuine three-body problem. Thus, more refined treatments are required, which would acknowledge the fact that the electron moves in the field of two Coulomb centers. Assuming that the ratio of the projectile to the electron velocity is very large, Thomas[33] developed a purely classical method, in which the three-

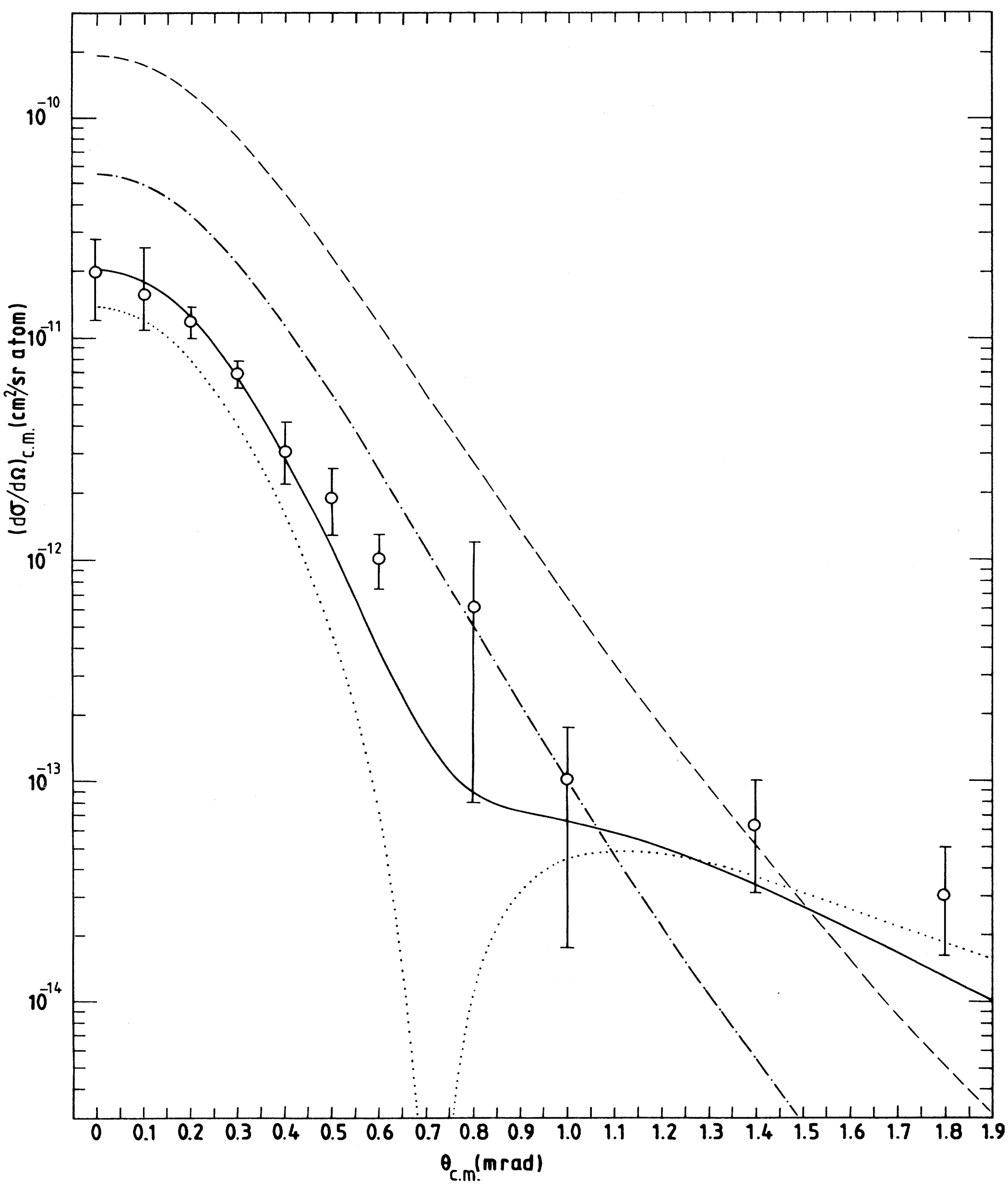

FIG. 3. Same as in Fig. 1, except for incident energy $E_{\mathrm{lab}} = 125$ keV.

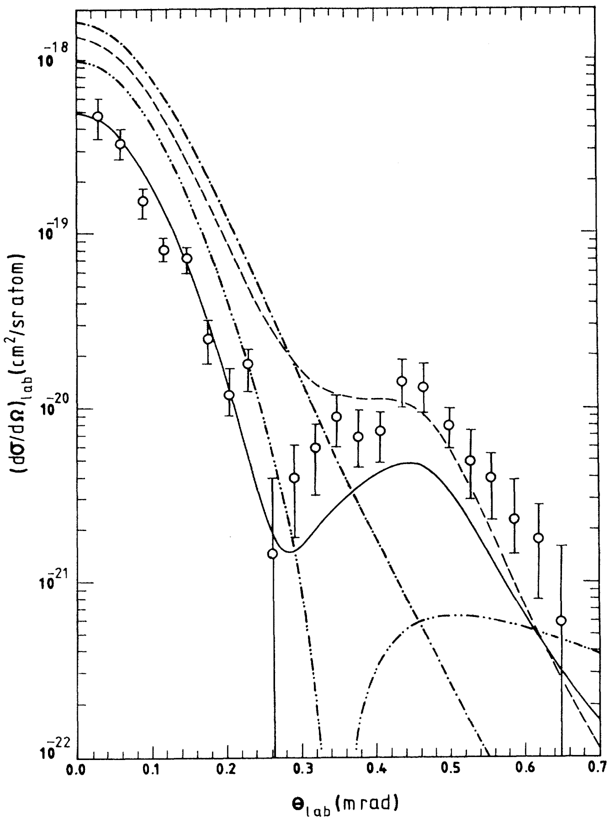

FIG. 4. Differential cross sections $(d\sigma/d\Omega)_{lab}$ for charge exchange $H^+ + H(1s) \rightarrow H(\Sigma) + H^+$, as a function of the scattering angle θ_{lab} at 5000 keV laboratory energy of the incident proton. Displayed theoretical results for the formation of atomic hydrogen in any state (Σ) are obtained through multiplication of the ground-state capture cross section by the Oppenheimer scaling factor (1.202). Theory (present *exact* numerical computations): BK1 —·—·—; BK2, — — —; CB1 —··—··— and CB2, ——. Experiment: ○, Vogt *et al.* (Ref. 35). Theoretical data are not folded over the experimental beam profile.

body collision is split into two successive binary encounters. First the electron, which is initially at rest, suffers a close scattering from projectile Z_P, and after being deflected through nearly 60° with respect to the incident direction, moves toward Z_T with velocity $\approx v$. Subsequently deflected by another $\approx 60°$, the electron exhibits through elastic scattering on its parent nucleus Z_T. After this sequence of two classical scattering events, projectile and electron escape the field of the target nucleus and continue to propagate in nearly parallel directions, with approximately the same velocity **v**. Such a circumstance is favorable to the capture of the electron by projectile Z_P, and action of the attractive potential $V_P(r_P)$ becomes sufficient for formation of the bound state (Z_P, e). Kinematics of this so-called Thomas double classical scattering is determined by the conservation laws of energy and momentum. As a net result, the projectile itself is deflected through an eikonal, critical Thomas angle $\theta_c = (1/m_P)\sqrt{3}/2$, where m_P is the projectile mass. In the particular case of proton impact, θ_c reaches the value ≈ 0.472 mrad in the laboratory frame.

Double scattering is also incorporated into the second-order quantum-mechanical CB2 approximation. In particular, the term $I_{if}(V_T, V_P) = \langle \Phi_f | V_I G_{0e}^+ V_P | \Phi_i \rangle$ describes the electron capture process in terms of two collisions mediated through the free-particle Green's function G_{0e}^+ as well as the Coulomb potentials $V_T(r_T)$ and $V_P(r_P)$. In the limit of very high impact velocities $(v \gg 1)$, the term $I_{if}(V_T, V_P)$ also exhibits a peak at a critical angle θ_c. Thomas double scattering, as the most prominent feature of high-energy charge exchange, has first been observed in measurements with proton impact on H_2 and He targets (Horsdal-Pedersen, Cocke, and Stockli[34]). More recently, Vogt *et al.*[35] provided the experimental data on differential cross sections for electron capture by protons from *atomic* hydrogen. These latter findings exhibit a clear structure around $\theta_{lab} = 0.45$ mrad, which is close to the Thomas critical value $\theta_c = 0.472$ mrad. This position of the experimentally observed Thomas peak at 5 MeV is seen in Fig. 4 to coincide with the prediction of the CB2 theory. On the other hand, the BK2 model displays only a shoulder around θ_c. Agreement between the magnitude of the cross sections in the CB2 method and the measurement is excellent, for scattering angles $\theta = 0.0$–0.3 mrad. Around θ_c, however, the results $d^{CB2}/d\Omega$ underestimate the experimental data. Here the situation could eventually improve by *explicitly* taking into account excited states and/or higher-order terms of the Born series. Experimental data exhibit a minimum around $\theta = 0.28$ mrad. The same structure, at nearly equal angle, is also obtained in the CB2 method, due to interference of the first- and second-order terms T_{if}^{CB1} and S_{if} in Eq. (2.4a). This interference is also responsible for a considerable reduction of $d^{CB2}/d\Omega$ in the forward direction, as compared to the sole contribution from the CB1 approximation. Comparison in Fig. 4 between the CB2 and BK2 methods reveals that the additional second-order terms of the former theory, i.e., $I_{if}(V_T, W_P)$, $I_{if}(W_T, V_P)$, and $I_{if}(W_T, W_P)$ are also of considerable importance even at this high-impact energy (5 MeV). It should be emphasized that the results of Vogt *et al.*[35] relate to capture into any state and this is, as already discussed, only roughly accounted for by displaying the corresponding theoretical results through $1.202 d\sigma/d\Omega$. Furthermore, the theoretical data shown in Fig. 4 are not folded with the experimental angular resolution.

VIII. CONCLUSION

We have studied the symmetric (homonuclear) charge exchange in fast collisions of completly stripped projectiles with hydrogenlike atoms. The second-order Born (CB2) approximation, in terms of free-particle Green's function G_{0e}^+, with the correct boundary conditions is employed and particular attention is paid to analytic properties of the quantum-mechanical transition amplitude T_{if}^{CB2}. Two typical singularities are encountered in the T matrix. These are the branch-point singularities coming from the spectrum of the three-particle resolvent

G_{0e}^{+} and poles due to the Coulomb potential in momentum space. They both render the numerical computation tremendously difficult at high incident energies. Because $T_{\rm if}^{\rm CB2}$ is initially defined through multidimensional integrals, the usefulness of the CB2 theory critically depends upon the regularization of the transition amplitude. The singularities are present throughout the computation, since they *move* from the innermost to the outermost integration axis. Nevertheless, by using an appropriate change of variable, together with the Cauchy "subtraction technique," it is shown that both of the singularities are integrable. In other words, these are only *apparent* singularities, which do not cause any divergence of the resulting transition amplitudes. The above twofold regularization, which simultaneously deals with branch points and poles, is carried out separately for each of the four matrix elements occurring in $T_{\rm if}^{\rm CB2}$. As a result, we obtain the transition amplitude of the CB2 approximation in terms of *two*-dimensional integrals over completely smooth functions. Certain parts of the matrix elements can even be reduced to *one*-dimensional integrals (see Sec. VI). Such a procedure is encoded into an algorithm, which is extremely expedient since small size samples of quadrature points suffice to obtain *exact* numerical results for the cross sections. The present analysis is illustrated in the case of the $1s \rightarrow 1s$ transition; however, no difficulties exist in extending the method to excited states. Such a generalization is particularly important for reliable comparisons with experimental data and will be reported shortly.

Nevertheless, as a preliminary test, we have used differential cross sections for capture into the ground state, in order to roughly assess the theory's validity for $H^{+}-H(1s)$ collision. In this case, the results of the BK2 model, also employing G_{0e}^{+} but with the incorrect boundary conditions, exhibit a flagrant inadequacy below 3 MeV, since they are even worse than the data of the first-order BK1 approximation, which itself largely overestimates measurements. In previous studies,[20] this failure has erroneously been attributed merely to the use of the free-particle Green's function. A counterexample is given by the CB2 theory also in terms of G_{0e}^{+} in which case, however, systematic and good agreement is found with the experimental data at 60, 125, and 5000 keV. Furthermore, we have obtained an *essential* improvement by going from the first (CB1) to the second (CB2) order in the perturbation Born series with the proper boundary conditions.

APPENDIX

Here we consider the following integral:

$$\mathcal{L}=\int du \frac{1}{(u+y)\sqrt{R(u)}} , \tag{A1}$$

where

$$R(u)=G+Fu+u^2 . \tag{A2}$$

We shall make the Euler substitution, i.e.,

$$\sqrt{R(u)}=z-u , \tag{A3}$$

which implies

$$\mathcal{L}=2\int dz \frac{1}{z^2+2yz+\Gamma} , \tag{A4}$$

where

$$\Gamma=Fy-G . \tag{A5}$$

Writing the denominator in (A4) in the form

$$z^2+2yz+\Gamma=(z-z_1)(z-z_2) , \tag{A6}$$

where

$$z_{1/2}=-y\pm\sqrt{R(-y)} , \tag{A7}$$

we obtain

$$\mathcal{L}=\frac{1}{\sqrt{R(-y)}}\ln\left[\frac{\sqrt{R(u)}+u+y-\sqrt{R(-y)}}{\sqrt{R(u)}+u+y+\sqrt{R(-y)}}\right]+\text{const} . \tag{A8}$$

In the main text, we encounter the integral of type (A1), i.e.,

$$\mathcal{L}_{k\beta j,x}^{(0,1)}(y)=\int_0^\infty du \frac{1}{(u+y)\sqrt{R_{k\beta j,x}(u)}} , \tag{A9}$$

with

$$R_{k\beta j,x}(u)=G_{k\beta j,x}+F_{k\beta j,x}u+u^2 , \tag{A10}$$

where the coefficients $G_{k\beta j,x}$ and $F_{k\beta j,x}$ are defined in Eq. (3.30b). It is now readily verified, from Eq. (A8) that

$$\mathcal{L}_{k\beta j,x}^{(0,1)}(y)=\frac{1}{\sqrt{R_{k\beta j,x}(-y)}} \times\ln\left[\frac{\sqrt{G_{k\beta j,x}}+y+\sqrt{R_{k\beta j,x}(-y)}}{\sqrt{G_{k\beta j,x}}+y-\sqrt{R_{k\beta j,x}(-y)}}\right] , \tag{A11}$$

which is the result quoted in Eq. (3.31a).

In the above calculation of integral (A1), it is assumed that

$$R(u)\geq 0 \tag{A12}$$

for all u belonging to a given interval. Consequently, in the Euler substitution (A3), we must also have

$$z-u\geq 0 . \tag{A13}$$

Clearly, these relations need to be verified in the case of the integral (A11). We first observe that the calculation of the integrals (2.9a)–(2.9d) is to be made by provisionally assuming that $\gamma>0$. By the argument of analytical continuation, the obtained results can be shown to be valid for γ arbitrary (real or complex), provided that $\text{Re}\gamma>0$. Hence, we are justified to let $\gamma^2\rightarrow\tau|\tau|-i\epsilon$ at the very end of the analysis. In this way, we shall be operating with real parameters $G_{k\beta j,x}$ and $F_{k\beta j,x}$, while proving the required inequalities of type (A12) and (A13) in the case of the integral (A11). Thus,

$$G_{k\beta j,x}=(xC_{k\beta j,x})^2\geq 0\ , \tag{A14}$$

since $x\geq 0$ and

$$C_{k\beta j,x}=\eta^2(\delta_{k,1}+t_0^2\delta_{k,2})+D_{k\beta j,x}\geq 0\ , \tag{A15}$$

where [see Eqs. (3.24a)–(3.24c)]

$$D_{k\beta j,x}=\delta_{k,1}\tau_{\beta j}^2+\delta_{k,2}\left[\left[t_\beta+\delta_j\frac{\tau^2}{2v}\right]^2+(\Delta+\gamma)^2\right]\geq 0\ . \tag{A16}$$

We first consider the equation $R_{k\beta j,x}(u)=0$, whose roots are given by

$$u_{1/2}=\frac{-F_{k\beta j,x}\pm iU_{k\beta j,x}}{2}\ , \tag{A17}$$

where

$$U_{k\beta j,x}=4x\eta[(\delta_{k,1}+t_0^2\delta_{k,2})D_{k\beta j,x}]^{1/2}\ . \tag{A18}$$

It is well known that, if the roots $x_{1/2}$ of the equation $ax^2+bx+c=0$ are complex numbers, then the sign of trinom ax^2+bx+c is the same as the sign of coefficient a. Since this is precisely the case in Eq. (A17), we conclude that

$$R_{k\beta j,x}(u)\geq 0,\quad \forall u\in[0,+\infty]\qquad (\text{Q.E.D.})\ . \tag{A19}$$

In the case of the integral (A9), transformation (A3) maps the original interval $u\in[0,+\infty]$ into $z\in[xC_{k\beta j,x},+\infty]$. Hence, the new integration variable z is positive, and it will be convenient, for the purpose of proving inequality (A13), to write

$$z=xC_{k\beta j,x}+r_{k\beta j,x},\quad \forall z\in[xC_{k\beta j,x},+\infty]\ , \tag{A20}$$

where $r_{k\beta j,x}\geq 0$ (here an explicit expression of the remainder $r_{k\beta j,x}$ is not required). It follows from Eq. (A3) that

$$u=\frac{z^2-G_{k\beta j,x}}{F_{k\beta j,x}+2z}\ , \tag{A21}$$

so that

$$z-u=\frac{R_{k\beta j,x}(z)}{F_{k\beta j,x}+2z}\ . \tag{A22}$$

Analogous to inequality (A19), it can be shown that

$$R_{k\beta j,x}(z)\geq 0,\quad \forall z\in[xC_{k\beta j,x},+\infty]\ . \tag{A23}$$

Hence, we see that inequality

$$z-u\geq 0,\quad \forall z\in[xC_{k\beta j,x},+\infty] \tag{A24}$$

will be satisfied if

$$F_{k\beta j,x}+2z\geq 0,\quad \forall z\in[xC_{k\beta j,x},+\infty]\ . \tag{A25}$$

At $z=xC_{k\beta j,x}$ we found from Eq. (A22) that $z-u=xC_{k\beta j,x}\geq 0$. Explicit calculation shows, using (A16) that

$$F_{k\beta j,x}+2z=4xD_{k\beta j,x}+2r_{k\beta j,x}\geq 0\ ,\qquad \forall z\in[xC_{k\beta j,x},+\infty]\ . \tag{A26}$$

since $r_{k\beta j,x}\geq 0$. This proves inequality (A24). A similar analysis is valid for the integral $\mathcal{L}_{\alpha j}^{(0,1)}(y)$ which is encountered in Eq. (4.15a).

[1]Dž. Belkić, R. Gayet, J. Hanssen, and A. Salin, J. Phys. B **19**, 2945 (1986).
[2]D. P. Dewangan and J. Eichler, J. Phys. B **19**, 2939 (1986).
[3]Dž. Belkić, S. Saini, and H. S. Taylor, Z. Phys. D **3**, 59 (1986).
[4]Dž. Belkić, S. Saini, and H. S. Taylor, Phys. Rev. A **36**, 1601 (1987).
[5]Dž. Belkić and H. S. Taylor, Phys. Rev. A **35**, 1991 (1987).
[6]N. Toshima, T. Jshihara, and J. Eichler, Phys. Rev. A **36**, 2659 (1987).
[7]Dž. Belkić, Phys. Rev. A **37**, 55 (1988).
[8]Dž. Belkić, Phys. Scr. **T28**, 106 (1988).
[9]Dž. Belkić, Phys. Scr. **40**, 610 (1989).
[10]F. Decker and J. Eichler, Phys. Rev. A **39**, 1530 (1989).
[11]Dž. Belkić and I. Mančev, Phys. Scr. **42**, 285 (1990).
[12]Dž. Belkić, R. Gayet, and A. Salin, Phys. Rep. **56**, 279 (1979).
[13]I. M. Cheshire, Proc. Phys. Soc. London **84**, 89 (1964).
[14]Dž. Belkic´, in *Abstracts of the Fifteenth International Conference on the Physics of Electronic and Atomic Collisions, Brighton, 1987,* edited by J. Geddes, H. B. Gilbody, A. E. Kingston, and C. J. Latimer (Queen's University, Belfast, 1987), p. 584.
[15]Dž. Belkić, Europhys. Lett. **7**, 323 (1988).
[16]Dž. Belkić and H. S. Taylor, Phys. Rev. A **39**, 6134 (1989).
[17]F. Decker and J. Eichler, J. Phys. B **22**, 3023 (1989).
[18]F. Decker and J. Eichler, J. Phys. B **22**, L95 (1989).
[19]J. E. Miraglia, R. D. Piacentini, R. D. Rivarola, and A. Salin, J. Phys. B **14**, L197 (1981).
[20]P. R. Simony and J. H. McGuire, J. Phys. B **14**, L737 (1981).
[21]P. J. Kramer, Phys. Rev. A **6**, 2125 (1972).
[22]J. Jackson and H. Schiff, Phys. Rev. **89**, 359 (1953).
[23]D. R. Bates and A. Dalgarno, Proc. Phys. Soc. London, Sect. A **66**, 972 (1953).
[24]Dž. Belkić, Z. Phys. **317**, 131 (1984).
[25]R. H. Dalitz, Proc. R. Soc. London, Ser. A **206**, 509 (1951).
[26]R. R. Lewis Jr., Phys. Rev. **102**, 537 (1956).
[27]J. M. Wadehra, R. Shakeshaft, and J. Macek, J. Phys. B **14**, L767 (1981).
[28]A. P. Prudnikov, Ju. Bričkov, and O. I. Maričev, *Integrali i Rjadi: Elementarnie funkcii* (Nauka, Moscow, 1981).
[29]I. H. Sloan, J. Comput. Phys. **3**, 332 (1968).
[30]I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Series and Products* (Academic, New York, 1980).
[31]P. J. Martin, D. M. Blankenship, T. J. Kvale, I. Redd, J. L. Peacher, and J. T. Park, Phys. Rev. A **23**, 3357 (1981).
[32]N. Bohr, K. Dan. Vidensk. Selsk. Mat.-Fys. Medd. **18**, 8 (1948).
[33]L. H. Thomas, Proc. R. Soc. London, Ser. A **114**, 561 (1927).
[34]E. Horsdal-Pedersen, C. L. Cocke, and M. Stockli, Phys. Rev. Lett. **50**, 1910 (1983).
[35]H. Vogt, R. Schuch, E. Justininao, M. Shulz, and W. Schwab, Phys. Rev. Lett. **57**, 2256 (1987).