Triangle amplitude with off-shell Coulomb *T* matrix for exchange reactions in atomic and nuclear physics

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The lowest-order rescattering contribution (triangle amplitude) in three-body models of exchange reactions with charged particles contains the off-shell two-body T matrix describing the intermediate-state Coulomb scattering of charged subsystems. General properties of the exact exchange triangle amplitude, when the incoming and outgoing particles are on the energy shell, are derived. This includes the analytic behavior, i.e., the positions and characters of its leading singularities, in the $\cos\vartheta$ plane, where ϑ is the scattering angle, in the vicinity of the forward- and backward-scattering directions. Since for computational reasons the Coulomb T matrix is usually replaced by the Coulomb potential, the effects of such an approximation on the analytic properties are investigated. The theoretically established behavior of the exact and the approximate exchange triangle amplitudes is then illustrated by numerical calculations, for both atomic and nuclear reactions, for energies below and above the corresponding three-body dissociation thresholds, for elastic and inelastic exchange. [S1050-2947(96)06111-2]

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I. INTRODUCTION

Exchange reactions in three-body systems with charged particles are conveniently described within the framework of the exact three-body theory either in terms of effective-two-body integral equations in momentum space [1–3], or in particular for applications at higher energies by means of the multiple-scattering representation of the relevant three-body transition operators (see, e.g., [4]). On the energy shell, there exists a close correspondence between the contributions to the effective potential occurring in the former approach, and the matrix elements between channel states of the multiple-scattering terms: in both formulations there occurs in lowest order the familiar one-particle exchange (OPE), followed by the single- and higher-rescattering contributions.

Up to now, in theoretical calculations of particle-exchange reactions, essentially only the single-rescattering contribution, the so-called triangle amplitude, has been taken into account, in addition to the OPE (however, there exist a few attempts to investigate—in some approximate way—also the influence of the double-scattering terms [5–7]; for a recent review of methods used in ion-atom scattering, see Ref. [8]). This restriction is justified in either one of the following situations: (i) one of the three particles is neutral because in that case the (multiple-scattering-type) expansion of the effective potential collapses to just these two terms (provided the additional short-range interaction has been represented as a sum of separable terms; see [2]), or (ii) the energies are sufficiently high so that the first two terms in the multiple-scattering representation of the effective potentials or even of the exchange amplitudes themselves suffice to provide a satisfactory description of the experimental data (but still below the asymptotic regime dominated by the double-rescattering contribution).

The general feature of (most of) the terms beyond the OPE, and in particular also of the triangle amplitude, is that they contain the off-shell two-particle T matrix describing intermediate-state Coulomb scattering of charged subsystems. As is evident, the complicated singularity structure of the latter in momentum space makes the calculation of such expressions rather difficult. Hence, in numerical applications (for a nuclear case, see, e.g., Ref. [9] and references therein; for atomic reactions, see e.g., Refs. [10,11]) the Coulomb T matrix is usually replaced by its Born approximation, namely, the Coulomb potential. In this way the analytic and numerical effort required for their computation is drastically reduced, but the quality of such an approximation, to be called the Coulomb-Born approximation in the following, is difficult to assess.

In fact, there exist only a few investigations in which the *exact* on-shell triangle amplitude has been investigated theoretically [12–16], and even fewer attempts to calculate it numerically [17,18]. In particular, in Ref. [17] the exact amplitude was evaluated for a few atomic electron-transfer processes, and compared with the corresponding Coulomb-Born approximation. The conclusion was that the latter was acceptable for none of the reactions examined (though, because of the use of analytical methods, it was restricted to hydrogenic 1*s* bound-state wave functions, in addition to being confined to such high energies that the zero-energy essential singularity of the Coulomb T matrix no longer gave rise to any numerical problems).

Studies of a certain off-shell continuation of the single-rescattering part of the effective potential, as it occurs in the integral equation approach, and its Coulomb-Born approximation have been performed in Refs. [19–23]. However, there the total three-body energy was restricted to values below the composite-particle breakup threshold, and only

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equal masses were considered. The finding was that at such low energies the ratio of exact to approximate rescattering contributions to the effective potential differs appreciably from the value 1, in most cases which are relevant for atomic exchange reactions, indicating that such a simplifying approximation is inappropriate. Only for parameter values pertaining to nuclear exchange processes was the Coulomb-Born approximation found to be reasonably accurate.

Recently, we exhaustively investigated [24] the behavior of the (numerically calculated) exact and approximate on-shell triangle amplitudes for nonrearrangement scattering, as functions of the energy (both below and above the bound-state dissociation threshold), the scattering angle, the masses, and the magnitudes of the charges of the particles involved. Bound-state excitation was also considered. For atomic reactions the quality of the approximation, consisting of the replacement of the intermediate-state Coulomb T matrix by the Coulomb potential (only the repulsive case was considered) turned out to be very poor in general over a wide range of the parameters mentioned. In contrast, for the nuclear cases studied, this approximation was found to be very satisfactory, making this substitution a reliable and simplifying tool for performing such nuclear charged-composite-particle reactions.

A similar investigation has now also been performed for the on-shell, single-rescattering exchange contribution (exchange triangle amplitude) to the effective potential in the integral-equation approach or to the multiple-scattering representation of the three-body scattering amplitude. We confine ourselves to the case where the particles that participate in the intermediate-state rescattering have charges of equal sign (this is, however, not a severe restriction, since most of the physically interesting reactions are included therein). Energies are considered from the reaction threshold up to very high energies, and scattering angles over the whole range. In addition, excitations of the incoming and/or outgoing bound state are allowed for. Thus the numerically calculated exact amplitude and its Coulomb-Born approximation can be compared, and the quality of the latter be estimated.

We also study the analytic properties of the exchange triangle amplitude in the $\cos\vartheta$-plane, where ϑ is the scattering angle. Comparison with the analogous singularity structure of the Coulomb-Born approximation suggests another, more appropriate approximation for the original amplitude, valid for medium to high energies (tests of its quality and range of validity for atomic reactions have already been communicated in Ref. [25]). Whenever applicable, the latter should greatly simplify the calculation of exchange processes.

The plan of our paper is as follows. In Sec. II we introduce some notation and, in particular, the triangle amplitude relevant to exchange reactions. In Sec. III general properties of this amplitude are discussed, both in its exact form as well as when the intermediate-state Coulomb T matrix is replaced by the Coulomb potential. We first describe a rigorous bound on the exact amplitude which involves its Coulomb-Born approximation, and discuss the behavior at high energies. In a next step the analysis of the singularity structure of the triangle amplitude as a function of the cosine of the scattering angle near both the physical forward- and backward-scattering regions is presented. The positions and characters of the leading singularities are determined. We then discuss under what circumstances the latter will be located so close as to influence the amplitude behavior strongly even within the physical region, and therefore be detectable experimentally. As a further result we derive an approximation for the exact amplitude. In Sec. IV, these theoretical properties of the triangle amplitude are illustrated by numerical calculations. A first part contains tests of the accuracy of the Coulomb-Born approximation for some selected atomic and nuclear exchange reactions, both for energies below and above the corresponding bound-state dissociation thresholds. In a second part, the influence of the above-mentioned singularities on the angle behavior in the physical region of the triangle amplitude is illustrated by means of the processes $\mathrm{H}(n\ell m)(p,p')\mathrm{H}(n'\ell'm')$ and $\mathrm{H}(n\ell m)(e,e')\mathrm{H}(n'\ell'm')$ for $(n\ell m,n'\ell'm')\in(1s,2s)$. A summary is given in Sec. V.

Natural units $\hbar=c=1$ are chosen. Furthermore, a conventional notation for two-body quantities; $A_\alpha \equiv A_{\beta\gamma}$, with $\alpha\neq\beta\neq\gamma$, is adopted. Finally, unit vectors are denoted by a hat, i.e., $\hat{\mathbf{p}}=\mathbf{p}/p$.

II. THREE-PARTICLE MODEL OF EXCHANGE SCATTERING

Let m_ν and e_ν, $\nu=1,2,3$, be the masses and charges of the three particles, respectively. We are interested in the reaction $\alpha+(\beta\gamma)_m\rightarrow\beta+(\gamma\alpha)_n$, leading from an initial state where particle α, having a center-of-mass momentum $\mathbf{q}_\alpha$, impinges on the bound state of particles β and γ characterized by the set of quantum numbers m, to a final state where now particles γ and α are bound in a state with quantum numbers n, and particle β, with the center-of-mass momentum $\mathbf{q}'_\beta$ is free. The wave function of the bound system $(\beta\gamma)_m$ belonging to the binding energy $\hat{E}_{\alpha m}$ is denoted by $|\psi_{\alpha m}\rangle$, and similarly for the outgoing bound state.

The lowest-order contribution containing intermediate-state Coulomb rescattering, as it results either in the integral-equation [1,2] or the multiple-scattering approach (see, e.g., Ref. [17]), to the exchange reaction amplitude is given on the energy shell, i.e., for

$$E=\frac{q_\alpha^2}{2M_\alpha}+\hat{E}_{\alpha m}=\frac{q_\beta'^2}{2M_\beta}+\hat{E}_{\beta n}, \tag{1}$$

by

$$\mathcal{M}^{T^C}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)=\langle\mathbf{q}'_\beta|\langle\psi_{\beta n}|T^C_\gamma(E_+)|\psi_{\alpha m}\rangle|\mathbf{q}_\alpha\rangle. \tag{2}$$

Here and in the following we always assume $\alpha\neq\beta\neq\gamma\neq\alpha$. The quantity T^C_γ denotes the transition operator describing Coulomb scattering of particles α and β; $M_\alpha=m_\alpha(m_\beta+m_\gamma)/(m_\alpha+m_\beta+m_\gamma)$ is the α-channel reduced mass, and $E_+=E+i0$.

Let us explicitly write expression (2) in momentum-space representation,

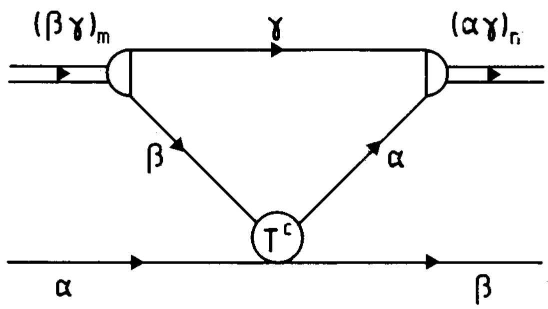

FIG. 1. Graphical representation of the exchange triangle amplitude (3). Semicircles represent the bound-state form factors. T^C denotes the two-body Coulomb T matrix.

$$\mathcal{M}^{T^C}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha) = \int \frac{d^3k}{(2\pi)^3}\psi^*_{\beta n}(\mathbf{p}''_\beta)\hat{T}^C_\gamma\left(\mathbf{p}'_\gamma,\mathbf{p}_\gamma;E_+-\frac{k^2}{2M_\gamma}\right)\psi_{\alpha m}(\mathbf{p}'_\alpha). \tag{3}$$

The various subsystem momenta are defined as

$$\mathbf{p}'_\alpha=\epsilon_{\beta\alpha}\left(\mathbf{k}+\frac{\mu_\alpha}{m_\beta}\mathbf{q}_\alpha\right),\quad \mathbf{p}''_\beta=\epsilon_{\alpha\beta}\left(\mathbf{k}+\frac{\mu_\beta}{m_\alpha}\mathbf{q}'_\beta\right),$$

$$\mathbf{p}_\gamma=\epsilon_{\gamma\alpha}\left(\mathbf{q}_\alpha+\frac{\mu_\gamma}{m_\beta}\mathbf{k}\right),\quad \mathbf{p}'_\gamma=\epsilon_{\alpha\gamma}\left(\mathbf{q}'_\beta+\frac{\mu_\gamma}{m_\alpha}\mathbf{k}\right). \tag{4}$$

Here $\mu_\alpha=m_\beta m_\gamma/(m_\beta+m_\gamma)$ is the reduced mass of the pair $(\beta\gamma)$, and analogous expressions hold for μ_β and μ_γ. For convenience, the antisymmetric symbol $\epsilon_{\beta\alpha}=-\epsilon_{\alpha\beta}$, with $\epsilon_{\alpha\beta}=+1$ if (α,β) is a cyclic ordering of (1,2,3), is used. Moreover, the Coulomb T matrix when read in the two-particle space is characterized by a hat, $\hat{T}^C$. The diagrammatical representation of $\mathcal{M}^{T^C}_{\beta n,\alpha m}$ is shown in Fig. 1. From its form the name (exchange) triangle amplitude becomes obvious.

Similarly we define the quantity $\mathcal{M}^{V^C}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)$ which follows from Eq. (3) by the replacement $\hat{T}^C_\gamma\to V^C_\gamma$:

$$\mathcal{M}^{V^C}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)=\int\frac{d^3k}{(2\pi)^3}\psi^*_{\beta n}(\mathbf{p}''_\beta)V^C_\gamma(\mathbf{p}'_\gamma,\mathbf{p}_\gamma)\psi_{\alpha m}(\mathbf{p}'_\alpha). \tag{5}$$

This will be referred to as the Coulomb-Born approximation of Eq. (3). As is well known, for simple bound-state wave functions, $\mathcal{M}^{V^C}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)$ can be calculated analytically [26]. A useful quantity is the ratio of the exact amplitude to its Coulomb-Born approximation

$$\mathcal{R}_{\beta n,\alpha m}=\frac{\mathcal{M}^{T^C}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)}{\mathcal{M}^{V^C}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)} \tag{6}$$

because it provides us with a measure of the quality of approximating the Coulomb T matrix by the Coulomb potential in the triangle amplitude.

III. PROPERTIES OF THE TRIANGLE AMPLITUDES $\mathcal{M}^{T^C}_{\beta n,\alpha m}$ AND $\mathcal{M}^{V^C}_{\beta n,\alpha m}$

A. Bounds on the ratio $\mathcal{M}^{T^C}_{\beta n,\alpha m}/\mathcal{M}^{V^C}_{\beta n,\alpha m}$

Among the simplest properties are bounds on the ratio (6). They are similar to those described in Ref. [24] for the corresponding non-rearrangement scattering amplitude.

(i) For a repulsive Coulomb interaction, $V^C_\gamma(\mathbf{p}',\mathbf{p})=4\pi e_\alpha e_\beta/(\mathbf{p}'-\mathbf{p})^2$, with $e_\alpha e_\beta>0$, which is the only one we are considering presently; the two-body T matrix is bounded by the potential as follows [21]:

$$0\leqslant\hat{T}^C_\gamma(\mathbf{p}',\mathbf{p};\hat{E}_\gamma+i0)\leqslant V^C_\gamma(\mathbf{p}',\mathbf{p}),$$
$$\forall\quad p,p',\hat{\mathbf{p}}'\cdot\hat{\mathbf{p}}\quad\text{for}\quad \hat{E}_\gamma<0, \tag{7}$$

$$0\leqslant|\hat{T}^C_\gamma(\mathbf{p}',\mathbf{p};\hat{E}_\gamma+i0)|\leqslant V^C_\gamma(\mathbf{p}',\mathbf{p}),$$
$$\forall\quad p,p',\hat{\mathbf{p}}'\cdot\hat{\mathbf{p}}\quad\text{for}\quad \hat{E}_\gamma>0. \tag{8}$$

From this one easily derives the following bounds for the elastic exchange ratio $\mathcal{R}_{\beta 0,\alpha 0}$, where the index 0 denotes a state whose wave function has no nodes,

$$0<\mathcal{R}_{\beta 0,\alpha 0}\leqslant 1,\quad \forall\cos\vartheta,\quad\text{for}\quad E<0, \tag{9}$$

$$0<|\mathcal{R}_{\beta 0,\alpha 0}|\leqslant 1,\quad \forall\cos\vartheta,\quad\text{for}\quad E>0. \tag{10}$$

Here $\cos\vartheta=\hat{\mathbf{q}}_\alpha\cdot\hat{\mathbf{q}}'_\beta$ is the cosine of the scattering angle. The implication is that for elastic exchange scattering off a target in a nodeless S state, the Coulomb-Born approximation always *overestimates* the exact amplitude. In other words, the error made by approximating the two-body Coulomb T matrix in Eq. (3) by the Coulomb potential is of known sign. Note that no analogous bounds result if either one or both bound pairs are in states whose wave functions have nodes.

(ii) Since for large two-body subsystem energies, $\hat{T}^C_\gamma$ approaches the Born approximation V^C_γ, for elastic and inelastic exchange scattering we expect

$$\mathcal{R}_{\beta n,\alpha m}\xrightarrow{E\to\infty}1. \tag{11}$$

However, it is obvious that for $\mathcal{R}_{\beta n,\alpha m}$ to reach the value 1, the energy E must be higher than that for which, on the two-body level, we have $T^C_\gamma(\hat{E}_{\gamma+})\approx V^C_\gamma$. In $\mathcal{M}^{T^C}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)$ the Coulomb T matrix enters for all γ-subsystem energies from E down to minus infinity, for $E\geqslant\hat{E}_\gamma=E-k^2/2M_\gamma>-\infty$. Thus a behavior like Eq. (11) can result only as a combined effect of $\hat{T}^C_\gamma(E_+-k^2/2M_\gamma)$ being approximately equal to V^C_γ over the whole range of momenta $\mathbf{k}$ for which the product of the momentum-space bound-state wave functions differs appreciably from zero.

B. Analytic behavior of $\mathcal{M}^{T^C}_{\beta n,\alpha m}$ near the forward-scattering direction

In this subsection we investigate the singularity structure of the exchange triangle amplitude $\mathcal{M}^{T^C}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)$, Eq. (3), in the z plane, where $z=\cos\vartheta$ is the cosine of the scattering angle, in the vicinity of the forward-scattering direction, using the techniques developed in Ref. [27]. Forward scattering (fs) is defined such that in the center-of-mass system particle β, which is free in the final state, leaves the collision point in the direction of incidence of the projectile α. With our notation for the momenta this is equivalent to $\hat{\mathbf{q}}'_\beta=\hat{\mathbf{q}}_\alpha$. Below, it will be shown that $\mathcal{M}^{T^C}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)$ possesses a singularity at

$$\left(\frac{\mu_\beta}{m_\alpha}\mathbf{q}'_\beta-\frac{\mu_\alpha}{m_\beta}\mathbf{q}_\alpha\right)^2+(\kappa_{\alpha m}+\kappa_{\beta n})^2=0, \tag{12}$$

or equivalently at $z=\zeta_{(\mathrm{fs})}$ with

$$\zeta_{(\mathrm{fs})}=\frac{\left(\frac{\mu_\alpha}{m_\beta}q_\alpha\right)^2+\left(\frac{\mu_\beta}{m_\alpha}q'_\beta\right)^2+(\kappa_{\alpha m}+\kappa_{\beta n})^2}{2\frac{\mu_\alpha}{m_\beta}\frac{\mu_\beta}{m_\alpha}q_\alpha q'_\beta}>1. \tag{13}$$

Here we have introduced $\kappa_{\alpha m}=\sqrt{2\mu_\alpha|\hat{E}_{\alpha m}|}$ and $\kappa_{\beta n}=\sqrt{2\mu_\beta|\hat{E}_{\beta n}|}$. It is apparent that this singular point lies outside of the physical region. But, as will be discussed below under certain circumstances it can be located so close to its border that observable effects on forward differential cross sections may result.

Quite generally we can write the bound-state wave function as

$$\psi_{\alpha m}(\mathbf{p}'_\alpha)=\frac{G_{\alpha m}(\mathbf{p}'_\alpha)}{[p'^2_\alpha+\kappa^2_{\alpha m}]^{1-\eta_{\alpha m}}}, \tag{14}$$

where

$$\eta_{\alpha m}=\frac{e_\beta e_\gamma \mu_\alpha}{\kappa_{\alpha m}} \tag{15}$$

is the Coulomb parameter for the bound state $(\beta\gamma)_m$. $G_{\alpha m}(\mathbf{p}'_\alpha)$ is the so-called reduced form factor which is nonsingular at $p'^2_\alpha=-\kappa^2_{\alpha m}$. Introducing Eq. (14) into Eq. (3) yields

$$\mathcal{M}^{T^C}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)=\int\frac{d^3k}{(2\pi)^3}\frac{G^*_{\beta n}(\mathbf{p}''_\beta)}{[p''^2_\beta+\kappa^2_{\beta n}]^{1-\eta_{\beta n}}}\times\hat{T}^C_\gamma\left(\mathbf{p}'_\gamma,\mathbf{p}_\gamma;E_+-\frac{k^2}{2M_\gamma}\right)\times\frac{G_{\alpha m}(\mathbf{p}'_\alpha)}{[p'^2_\alpha+\kappa^2_{\alpha m}]^{1-\eta_{\alpha m}}}. \tag{16}$$

The singularity of interest of the integral in Eq. (16) results from the coincidence of the singularities of the integrand at

$$p'^2_\alpha+\kappa^2_{\alpha m}=\left(\mathbf{k}+\frac{\mu_\alpha}{m_\beta}\mathbf{q}_\alpha\right)^2+\kappa^2_{\alpha m}=0 \tag{17}$$

and

$$p''^2_\beta+\kappa^2_{\beta n}=\left(\mathbf{k}+\frac{\mu_\beta}{m_\alpha}\mathbf{q}'_\beta\right)^2+\kappa^2_{\beta n}=0, \tag{18}$$

while the momentum transfer in the intermediate-state Coulomb scattering amplitude remains different from zero:

$$\mathbf{p}'_\gamma-\mathbf{p}_\gamma=\epsilon_{\alpha\gamma}(\mathbf{k}+\mathbf{q}_\alpha+\mathbf{q}'_\beta)\neq 0. \tag{19}$$

In Sec. III C it is shown that, if Eqs. (17) and (18) are satisfied and simultaneously the momentum transfer (19) vanishes, $\mathcal{M}^{T^C}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)$ develops another singularity which governs its behavior in the backward direction, i.e., for $\hat{\mathbf{q}}'_\beta\to-\hat{\mathbf{q}}_\alpha$.

Recall that the two-body Coulomb T matrix $\hat{T}^C_\gamma(\mathbf{p}'_\gamma,\mathbf{p}_\gamma;E_+-k^2/2M_\gamma)$ becomes singular if the relative kinetic energy of the particles in the initial ($p^2_\gamma/2\mu_\gamma$) and/or the final ($p'^2_\gamma/2\mu_\gamma$) state approaches the energy variable (here $E_+-k^2/2M_\gamma$) [28]. Taking into account the identities $p'^2_\gamma/2\mu_\gamma-(E_+-k^2/2M_\gamma)=(p''^2_\beta+\kappa^2_{\beta n})/2\mu_\beta$ and $p^2_\gamma/2\mu_\gamma-(E_+-k^2/2M_\gamma)=(p'^2_\alpha+\kappa^2_{\alpha m})/2\mu_\alpha$, which follow from definitions (4) with the help of Eq. (1), we can write this near- (subsystem) energy-shell behavior as

$$\hat{T}^C_\gamma\left(\mathbf{p}'_\gamma,\mathbf{p}_\gamma;E_+-\frac{k^2}{2M_\gamma}\right)\approx[p''^2_\beta+\kappa^2_{\beta n}]^{i\eta_\gamma}[p'^2_\alpha+\kappa^2_{\alpha m}]^{i\eta_\gamma}\widetilde{T}^C_\gamma, \tag{20}$$

with

$$\widetilde{T}^C_\gamma:=\frac{4\pi e_\alpha e_\beta}{(\mathbf{k}+\mathbf{q}_\alpha+\mathbf{q}'_\beta)^{2+2i\eta_\gamma}}\times\left(\frac{\mu^2_\gamma}{\mu_\alpha\mu_\beta}\right)^{i\eta_\gamma}\frac{e^{-\pi\eta_\gamma}|\Gamma(1+i\eta_\gamma)|^2}{[8\mu_\gamma(E_+-k^2/2M_\gamma)]^{i\eta_\gamma}} \tag{21}$$

being nonsingular at the positions (17) and (18). Here

$$\eta_\gamma=\frac{e_\alpha e_\beta \mu_\gamma}{\sqrt{2\mu_\gamma(E_+-k^2/2M_\gamma)}} \tag{22}$$

is the relevant Coulomb parameter. Consequently, in the neighborhood of these singular points we have

$$\mathcal{M}^{T^C}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)\approx\mathcal{M}^{T^C(\mathrm{fs})}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha):=\int\frac{d^3k}{(2\pi)^3}\frac{G^*_{\beta n}(\mathbf{p}''_\beta)}{[p''^2_\beta+\kappa^2_{\beta n}]^{1-\eta_{\beta n}-i\eta_\gamma}}\widetilde{T}^C_\gamma\frac{G_{\alpha m}(\mathbf{p}'_\alpha)}{[p'^2_\alpha+\kappa^2_{\alpha m}]^{1-\eta_{\alpha m}-i\eta_\gamma}}$$
$$\approx G^*_{\beta n}(i\kappa_{\beta n})G_{\alpha m}(i\kappa_{\alpha m})\int\frac{d^3k}{(2\pi)^3}\frac{\widetilde{T}^C_\gamma}{\left[\left(\mathbf{k}+\frac{\mu_\beta}{m_\alpha}\mathbf{q}'_\beta\right)^2+\kappa^2_{\beta n}\right]^{1-\eta_{\beta n}-i\eta_\gamma}\left[\left(\mathbf{k}+\frac{\mu_\alpha}{m_\beta}\mathbf{q}_\alpha\right)^2+\kappa^2_{\alpha m}\right]^{1-\eta_{\alpha m}-i\eta_\gamma}}. \tag{23}$$

In order to simplify the discussion we have in the last equality in Eq. (23) assumed orbital angular momentum zero for both bound states $(\beta\gamma)_m$ and $(\gamma\alpha)_n$; thus the form factors could be taken out from under the integral at the singular points. Otherwise, only their radial parts can be taken out, and the appropriate angular functions have to be retained in the integrand.

The proof that $\mathcal{M}^{T^C(\mathrm{fs})}_{\beta n,\alpha m}$ becomes singular at position (12) is based on the close relation between the singularity of the amplitude which is nearest to the physical region in the z plane and the asymptotic behavior of its partial-wave projection for $\ell\to\infty$ (see, e.g., [29]). It has, e.g., been used in [30] to extract the leading singularity of the two-particle Coulomb amplitude as the momentum transfer goes to zero.

The asymptotic evaluation of the partial-wave projection of $\mathcal{M}^{T^C(\mathrm{fs})}_{\beta n,\alpha m}$ makes use of saddle-point integration methods. Before applying them, however, we simplify expression (23) by taking out from under the integral the term $\widetilde{T}^C_\gamma$ with the momenta fixed at their saddle-point values. This does not alter the final result, since $\widetilde{T}^C_\gamma$ is nonsingular at, and smooth in the neighborhood of, this point. In detail, we first note that $\widetilde{T}^C_\gamma$ depends on k^2 via the kinetic energy $k^2/2M_\gamma$ of particle γ, cf. Eqs. (21) and (22). Hence k^2 is to be taken equal to its saddle-point value $k^2_{(\mathrm{sp})}$ (see below)

$$k^2_{(\mathrm{sp})}=\frac{\left(\frac{\mu_\alpha}{m_\beta}q_\alpha\right)^2\kappa_{\beta n}+\left(\frac{\mu_\beta}{m_\alpha}q'_\beta\right)^2\kappa_{\alpha m}+\kappa_{\beta n}\kappa_{\alpha m}(\kappa_{\beta n}+\kappa_{\alpha m})}{(\kappa_{\beta n}+\kappa_{\alpha m})}, \tag{24}$$

and thus η_γ is equal to

$$\eta^{(\mathrm{sp})}_\gamma:=\eta_\gamma(k_{(\mathrm{sp})})=\frac{e_\alpha e_\beta\mu_\gamma}{\sqrt{2\mu_\gamma(E_+-k^2_{(\mathrm{sp})}/2M_\gamma)}}. \tag{25}$$

Here we have to assume that the three-body c.m. energy is such that $E\neq k^2_{(\mathrm{sp})}/2M_\gamma$. The corresponding dependence of $\widetilde{T}^C_\gamma$ on the integration variable k is eliminated thereupon. But $\widetilde{T}^C_\gamma$ also depends on $\hat{\mathbf{k}}$ via $1/(\mathbf{k}+\mathbf{q}_\alpha+\mathbf{q}'_\beta)^{2+2i\eta^{(\mathrm{sp})}_\gamma}$. On account of condition (19) this latter factor is regular at that point in the k plane where the singular points (17) and (18) coincide, thereby pinching the integration contour. Hence it too can be taken out from under the integral over $\mathbf{k}$. In order to find the position where this can be done, different methods can be employed. For instance, we can evaluate $(\mathbf{k}+\mathbf{q}_\alpha+\mathbf{q}'_\beta)^2$ by substituting for $\mathbf{k}\cdot\mathbf{q}_\alpha$ and $\mathbf{k}\cdot\mathbf{q}'_\beta$ the corresponding expressions following from the conditions (17) and (18), respectively, and finally replacing k by $k_{(\mathrm{sp})}$. Alternatively we can proceed as follows. Rewrite Eq. (23) by introducing the integration variable $\mathbf{p}=\epsilon_{\alpha\gamma}(\mathbf{k}+\mathbf{q}_\alpha+\mathbf{q}'_\beta)$, and the abbreviations

$$\mathbf{p}_\alpha=\epsilon_{\alpha\beta}\left(\mathbf{q}'_\beta+\frac{\mu_\alpha}{m_\gamma}\mathbf{q}_\alpha\right),\quad \mathbf{p}'_\beta=\epsilon_{\beta\alpha}\left(\mathbf{q}_\alpha+\frac{\mu_\beta}{m_\gamma}\mathbf{q}'_\beta\right). \tag{26}$$

For later use we point out that taking into account the on-shell condition (1) results in the identity

$$(p^2_\alpha+\kappa^2_{\alpha m})/2\mu_\alpha=(p'^2_\beta+\kappa^2_{\beta n})/2\mu_\beta. \tag{27}$$

Equation (23) then assumes the form

$$\mathcal{M}^{T^C(\mathrm{fs})}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)\approx G^*_{\beta n}(i\kappa_{\beta n})G_{\alpha m}(i\kappa_{\alpha m})\int\frac{d^3p}{(2\pi)^3}\frac{\widetilde{T}^C_\gamma}{[(\mathbf{p}-\mathbf{p}'_\beta)^2+\kappa^2_{\beta n}]^{1-\eta_{\beta n}-i\eta_\gamma}[(\mathbf{p}+\mathbf{p}_\alpha)^2+\kappa^2_{\alpha m}]^{1-\eta_{\alpha m}-i\eta_\gamma}}, \tag{28}$$

with $\widetilde{T}^C_\gamma$ being now proportional to $1/p^{2+2i\eta^{(sp)}_\gamma}$. Thus it is the coincidence of the singularities of the integrand of Eq. (28) at

$$(\mathbf{p}-\mathbf{p}'_\beta)^2+\kappa^2_{\beta n}=0 \tag{29}$$

and at

$$(\mathbf{p}+\mathbf{p}_\alpha)^2+\kappa^2_{\alpha m}=0, \tag{30}$$

which eventually leads to a singularity of the exchange amplitude at position (12) [note that condition (19) is equivalent to $p^2\neq0$]. By an argumentation which is similar to the one leading to the expression (24) for $k^2_{(\mathrm{sp})}$ and will therefore not be given, it follows from representation (28) that the term $1/p^{2+2i\eta^{(\mathrm{sp})}_\gamma}$ can be taken out from the integral at the saddle point

$$p^2_{(\mathrm{sp})}=\frac{\left(\mathbf{q}'_\beta+\frac{\mu_\alpha}{m_\gamma}\mathbf{q}_\alpha\right)^2\kappa_{\beta n}+\left(\mathbf{q}_\alpha+\frac{\mu_\beta}{m_\gamma}\mathbf{q}'_\beta\right)^2\kappa_{\alpha m}+\kappa_{\beta n}\kappa_{\alpha m}(\kappa_{\beta n}+\kappa_{\alpha m})}{(\kappa_{\beta n}+\kappa_{\alpha m})}. \tag{31}$$

Note that here the quantity $\mathbf{q}_\alpha\cdot\mathbf{q}'_\beta$ still has to be replaced by the corresponding expression $q_\alpha q'_\beta\zeta_{(\mathrm{sp})}$ following from condition (12), or equivalently Eq. (13). As a consequence, the whole function $\widetilde{T}^C_\gamma$ can be taken out of the integral with the momenta fixed at their saddle-point values. The resulting quantity will simply be denoted by $\widetilde{T}^C_{\gamma(\mathrm{sp})}$.

Thus, when attempting to derive the behavior of $\mathcal{M}^{T^C(\mathrm{fs})}_{\beta n,\alpha m}$ at the coincidence of singularities of the integrand at positions (17) and (18), it suffices to consider

$$\mathcal{M}^{T^{C}(\mathrm{fs})}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)\approx G^*_{\beta n}(i\kappa_{\beta n})G_{\alpha m}(i\kappa_{\alpha m})\widetilde{T}^C_{\gamma(\mathrm{sp})}\int\frac{d^3k}{(2\pi)^3}\frac{1}{\left[\left(\mathbf{k}+\frac{\mu_\beta}{m_\alpha}\mathbf{q}'_\beta\right)^2+\kappa^2_{\beta n}\right]^{1-\eta_{\beta n}-i\eta_\gamma}}\frac{1}{\left[\left(\mathbf{k}+\frac{\mu_\alpha}{m_\beta}\mathbf{q}_\alpha\right)^2+\kappa^2_{\alpha m}\right]^{1-\eta_{\alpha m}-i\eta_\gamma}}. \tag{32}$$

Denote the integral in Eq. (32) by

$$J:=\int\frac{d^3k}{(2\pi)^3}\frac{1}{[(\mathbf{k}+\overline{\mathbf{q}'_\beta})^2+\kappa^2_{\beta n}]^{\lambda_f}[(\mathbf{k}+\overline{\mathbf{q}_\alpha})^2+\kappa^2_{\alpha m}]^{\lambda_i}}, \tag{33}$$

where the short-hand notations

$$\lambda_i=1-\eta_{\alpha m}-i\eta_\gamma,\quad \lambda_f=1-\eta_{\beta n}-i\eta_\gamma, \tag{34}$$

$$\overline{\mathbf{q}_\alpha}=\frac{\mu_\alpha}{m_\beta}\mathbf{q}_\alpha,\quad \overline{\mathbf{q}'_\beta}=\frac{\mu_\beta}{m_\alpha}\mathbf{q}'_\beta, \tag{35}$$

have been introduced. Next we apply the expansions

$$\frac{1}{[(\mathbf{k}+\overline{\mathbf{q}_\alpha})^2+\kappa^2_{\alpha m}]^{\lambda_i}}=\frac{1}{(2k\overline{q_\alpha})^{\lambda_i}}\frac{1}{(\zeta_\alpha+z_\alpha)^{\lambda_i}}=\frac{1}{(2k\overline{q_\alpha})^{\lambda_i}}\sum_{\ell=0}^{\infty}(2\ell+1)\times P_\ell(-z_\alpha)a_\ell(\zeta_\alpha), \tag{36}$$

with (see Ref. [31], or Ref. [32], Eq. 7.229)

$$a_\ell(\zeta_\alpha)=\tfrac{1}{2}\int_{-1}^{+1}\frac{dz_\alpha P_\ell(z_\alpha)}{(\zeta_\alpha-z_\alpha)^{\lambda_i}}=\frac{i}{2\pi}(1-e^{2\pi i(1-\lambda_i)})\Gamma(1-\lambda_i)\times(\zeta_\alpha^2-1)^{(1-\lambda_i)/2}Q_\ell^{-1+\lambda_i}(\zeta_\alpha), \tag{37}$$

and similarly

$$\frac{1}{[(\mathbf{k}+\overline{\mathbf{q}'_\beta})^2+\kappa^2_{\beta n}]^{\lambda_f}}=\frac{1}{(2k\overline{q'_\beta})^{\lambda_f}}\sum_{\ell=0}^{\infty}(2\ell+1)\times P_\ell(-z_\beta)b_\ell(\zeta_\beta), \tag{38}$$

with

$$b_\ell(\zeta_\beta)=\frac{i}{2\pi}(1-e^{2\pi i(1-\lambda_f)})\Gamma(1-\lambda_f)\times(\zeta_\beta^2-1)^{(1-\lambda_f)/2}Q_\ell^{-1+\lambda_f}(\zeta_\beta). \tag{39}$$

$P_\ell(z)$ are the Legendre polynomials, and $Q_\ell^\lambda(\zeta)$ the associated Legendre functions of the second kind. Furthermore,

$$\zeta_\alpha=\frac{k^2+\overline{q_\alpha^2}+\kappa^2_{\alpha m}}{2k\overline{q_\alpha}},\quad \zeta_\beta=\frac{k^2+\overline{q'^2_\beta}+\kappa^2_{\beta n}}{2k\overline{q'_\beta}}, \tag{40}$$

and $z_\alpha(z_\beta)$ is the cosine of the angle between $\mathbf{k}$ and $\overline{\mathbf{q}_\alpha}(\overline{\mathbf{q}'_\beta})$. Introducing expansions (36) and (38) into Eq. (33), one obtains

$$J=\sum_{\ell=0}^{\infty}(2\ell+1)P_\ell(z)J_\ell,\quad z=\hat{\mathbf{q}}_\alpha\cdot\hat{\mathbf{q}}'_\beta, \tag{41}$$

with

$$J_\ell=\frac{1}{2\pi^2}\int_0^\infty dk\frac{k^2}{(2k\overline{q'_\beta})^{\lambda_f}(2k\overline{q_\alpha})^{\lambda_i}}b_\ell(\zeta_\beta)a_\ell(\zeta_\alpha). \tag{42}$$

In order to find the large-ℓ behavior of J_ℓ, we make use of the asymptotic formulas [33]

$$Q_\ell^{-1+\lambda}(\zeta)\overset{\ell\to\infty}{\approx}e^{i\pi(-1+\lambda)}\ell^{-1+\lambda}Q_\ell(\zeta), \tag{43}$$

$$Q_\ell(\zeta)\overset{\ell\to\infty}{=}\left(\frac{\pi}{\ell}\right)^{1/2}\frac{e^{-\ell\ln\tau}}{\sqrt{\tau^2-1}}+o\left(\frac{1}{\sqrt{\ell}}\right), \tag{44}$$

$$\tau=\tau(\zeta)=\zeta+\sqrt{\zeta^2-1}. \tag{45}$$

Here $Q_\ell(\zeta)$ are the Legendre functions of the second kind. The order relation has the usual meaning: $f(x)=o(g(x))$ for $x\to x_0$, if $\lim_{x\to x_0}f(x)/g(x)=0$ $(g(x_0)\neq 0)$. The intimate connection between the position $(-\zeta_\alpha)$ of the singularity of $1/(\zeta_\alpha+z_\alpha)^{\lambda_i}$ and the large-ℓ behavior of the partial-wave projection $a_\ell(\zeta_\alpha)$ is made explicit by applying these asymptotic relations to Eq. (37):

$$a_\ell(\zeta_\alpha)\overset{\ell\to\infty}{\approx}\frac{\sqrt{\pi}}{\ell^{3/2-\lambda_i}}\frac{(\zeta_\alpha^2-1)^{(1-\lambda_i)/2}}{\Gamma(\lambda_i)}\frac{e^{-\ell\ln\tau_\alpha}}{\sqrt{\tau_\alpha^2-1}}. \tag{46}$$

As is apparent, ζ_α can be read off, e.g., from the quantity $\tau_\alpha:=\tau(\zeta_\alpha)$, which occurs in the exponent on the right-hand side of Eq. (46), as $\zeta_\alpha=(\tau_\alpha+\tau_\alpha^{-1})/2$. Also the character λ_i of the singularity can be extracted directly, e.g., from the corresponding power of ℓ.

Introducing Eq. (46), and a similar expression for b_ℓ, into Eq. (42) leads to

$$J_\ell \overset{\ell\to\infty}{\approx} \int_0^\infty dk\, A(k)\, \ell^{\lambda_i+\lambda_f-3} k^{2-\lambda_i-\lambda_f} \frac{(\zeta_\alpha^2-1)^{(1-\lambda_i)/2}(\zeta_\beta^2-1)^{(1-\lambda_f)/2}}{\sqrt{(\tau_\alpha^2-1)(\tau_\beta^2-1)}} e^{-\ell \ln(\tau_\alpha\tau_\beta)}, \tag{47}$$

with

$$A^{-1}(k) := \pi\, 2^{\lambda_i+\lambda_f+1}\, \overline{q}_\alpha^{\lambda_i} \overline{q'_\beta}^{\lambda_f} \Gamma(\lambda_i)\Gamma(\lambda_f) \tag{48}$$

and $\tau_\beta := \tau(\zeta_\beta)$. Note that $\zeta_\alpha > 1$, which also entails $\tau_\alpha > 1$. The same holds true for ζ_β and τ_β.

Since the dominant ℓ dependence of the integrand of Eq. (47) resides in the exponential, for $\ell\to\infty$ the contribution to the integral comes from the region around the saddle point, which can be found from the equation

$$\frac{d}{dk}\ln(\tau_\alpha\tau_\beta) = 0. \tag{49}$$

Its solution $k^2 = k^2_{(\mathrm{sp})}$, Eq. (24), the derivation of which is somewhat tedious but straightforward, was given in [27] (for the case of two charged and one neutral particles; see also Ref. [35]). Thus, when attempting to calculate this integral, all k-dependent factors which are nonsingular at the saddle point can be taken out from under the integral at $k = k_{(\mathrm{sp})}$. The remaining integration can be performed, and yields

$$J_\ell \overset{\ell\to\infty}{\approx} \sqrt{2\pi} \frac{A(k_{(\mathrm{sp})})}{\ell^{(3/2-\Lambda)} k^\Lambda_{(\mathrm{sp})}} \times \frac{(\zeta_\alpha^{(\mathrm{sp})2}-1)^{(1-\lambda_i^{(\mathrm{sp})})/2}(\zeta_\beta^{(\mathrm{sp})2}-1)^{(1-\lambda_f^{(\mathrm{sp})})/2}}{\sqrt{(\tau_\alpha^{(\mathrm{sp})2}-1)(\tau_\beta^{(\mathrm{sp})2}-1)}} \times \frac{e^{-\ell \ln(\tau_\alpha^{(\mathrm{sp})}\tau_\beta^{(\mathrm{sp})})}}{\sqrt{(\ln\tau_\alpha\tau_\beta)''|_{k=k_{(\mathrm{sp})}}}}. \tag{50}$$

The double prime means a second derivative. Here quantities $\zeta_\alpha^{(\mathrm{sp})}$ and $\zeta_\beta^{(\mathrm{sp})}$ defined as in Eq. (40) occur, but with k replaced by $k_{(\mathrm{sp})}$:

$$\zeta_\alpha^{(\mathrm{sp})} = \frac{k^2_{(\mathrm{sp})} + \overline{q}^2_\alpha + \kappa^2_{\alpha m}}{2k_{(\mathrm{sp})}\overline{q}_\alpha}, \quad \zeta_\beta^{(\mathrm{sp})} = \frac{k^2_{(\mathrm{sp})} + \overline{q'_\beta}^2 + \kappa^2_{\beta n}}{2k_{(\mathrm{sp})}\overline{q'_\beta}}. \tag{51}$$

Similarly, $\tau_\alpha^{(\mathrm{sp})}$ and $\tau_\beta^{(\mathrm{sp})}$ are given in terms of $\zeta_\alpha^{(\mathrm{sp})}$ and $\zeta_\beta^{(\mathrm{sp})}$, respectively, as in Eq. (45). Furthermore,

$$\lambda_i^{(\mathrm{sp})} := \lambda_i(k = k_{(\mathrm{sp})}) = 1 - \eta_{\alpha m} - i\,\eta_\gamma^{(\mathrm{sp})}, \tag{52}$$

with an analogous definition for $\lambda_f^{(\mathrm{sp})}$. Finally, the abbreviation

$$\Lambda := \lambda_i^{(\mathrm{sp})} + \lambda_f^{(\mathrm{sp})} - 2 = -\eta_{\alpha m} - \eta_{\beta n} - 2i\,\eta_\gamma^{(\mathrm{sp})}, \tag{53}$$

has been introduced.

Our goal is to deduce, from such a high-ℓ behavior of the partial-wave projection J_ℓ, the singularity of the integral J in the z plane which is nearest to the physical region. For this purpose we define a quantity

$$\tau_{(\mathrm{sp})} := \tau_\alpha^{(\mathrm{sp})}\tau_\beta^{(\mathrm{sp})}, \tag{54}$$

and a corresponding $\zeta_{(fs)} = (\tau_{(\mathrm{sp})} + \tau^{-1}_{(\mathrm{sp})})/2$ [cf. Eq. (45)]. The latter has already been given explicitly in Eq. (13). Herewith we rewrite Eq. (50) as (in the following we assume $\Lambda \neq -n,\ n = 0,1,2,\ldots$)

$$J_\ell \overset{\ell\to\infty}{\approx} B\left\{ \frac{\sqrt{\pi}}{\ell^{(3/2-\Lambda)}} \frac{(\zeta^2_{(fs)}-1)^{(1-\Lambda)/2}}{\Gamma(\Lambda)} \frac{e^{-\ell \ln\tau_{(\mathrm{sp})}}}{\sqrt{\tau^2_{(\mathrm{sp})}-1}} \right\}, \tag{55}$$

with the abbreviation

$$B = \frac{\sqrt{2}A(k_{(\mathrm{sp})})\Gamma(\Lambda)}{k^\Lambda_{(\mathrm{sp})}\sqrt{(\ln\tau_\alpha\tau_\beta)''|_{k=k_{(\mathrm{sp})}}}} \times \frac{(\zeta_\alpha^{(\mathrm{sp})2}-1)^{(1-\lambda_i^{(\mathrm{sp})})/2}(\zeta_\beta^{(\mathrm{sp})2}-1)^{(1-\lambda_f^{(\mathrm{sp})})/2}}{(\zeta^2_{(\mathrm{fs})}-1)^{(1-\Lambda)/2}} \times \frac{\sqrt{\tau^2_{(\mathrm{sp})}-1}}{\sqrt{(\tau_\alpha^{(\mathrm{sp})2}-1)(\tau_\beta^{(\mathrm{sp})2}-1)}}. \tag{56}$$

In the wavy brackets we have combined all terms containing ℓ in such a form that, when inserted into Eq. (41), the partial-wave summation can be performed, thereby yielding essentially the singular factor $1/(\zeta_{(\mathrm{fs})}-z)^\Lambda$ [cf. Eqs. (46) and (36)]. Hence we arrive at the following behavior of the integral J:

$$J \approx \frac{B}{(\zeta_{(fs)}-z)^\Lambda} = \frac{(2\overline{q_\alpha q'_\beta})^\Lambda B}{[(\overline{\mathbf{q}'_\beta} - \overline{\mathbf{q}_\alpha})^2 + (\kappa_{\beta n}+\kappa_{\alpha m})^2]^\Lambda}. \tag{57}$$

Now inserting Eq. (57) into expression (32) and taking into account Eqs. (21), (31), and (56), we have the final result that in the vicinity of the singular point (12), which is nearest to the physical forward-scattering region, the leading singular part of the exact amplitude (3) behaves as

$$\mathcal{M}^{T^C(\mathrm{fs})}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha) \approx \frac{N^{T^C}_{(\mathrm{fs})}}{\left[\left(\dfrac{\mu_\beta}{m_\alpha}\mathbf{q}'_\beta - \dfrac{\mu_\alpha}{m_\beta}\mathbf{q}_\alpha\right)^2 + (\kappa_{\beta n}+\kappa_{\alpha m})^2\right]^{-\eta_{\alpha m}-\eta_{\beta n}-2i\,\eta_\gamma^{(\mathrm{sp})}}}, \tag{58}$$

with

$$N_{(\mathrm{fs})}^{T^C}:=\frac{e_\alpha e_\beta}{\sqrt{2}p_{(\mathrm{sp})}^{2+2i\eta_\gamma^{(\mathrm{sp})}}}e^{-\pi\eta_\gamma^{(\mathrm{sp})}}|\Gamma(1+i\eta_\gamma^{(\mathrm{sp})})|^2\left(\frac{\mu_\gamma^2}{\mu_\alpha\mu_\beta}\right)^{i\eta_\gamma^{(\mathrm{sp})}}\left(\frac{m_\beta}{\mu_\alpha}\right)^{(1+\eta_{\beta n}+i\eta_\gamma^{(\mathrm{sp})})}$$
$$\times\left(\frac{m_\alpha}{\mu_\beta}\right)^{(1+\eta_{\alpha m}+i\eta_\gamma^{(\mathrm{sp})})}\frac{G^*_{\beta n}(i\kappa_{\beta n})G_{\alpha m}(i\kappa_{\alpha m})}{[8\mu_\gamma(E_+-k_{(\mathrm{sp})}^2/2M_\gamma)]^{i\eta_\gamma^{(\mathrm{sp})}}}\frac{1}{\sqrt{(\ln\tau_\alpha\tau_\beta)''|_{k=k_{(\mathrm{sp})}}}}\frac{k_{(\mathrm{sp})}^{(\eta_{\alpha m}+\eta_{\beta n}+2i\eta_\gamma^{(\mathrm{sp})})}}{q_\alpha^{(1+\eta_{\beta n}+i\eta_\gamma^{(\mathrm{sp})})}q_\beta'^{(1+\eta_{\alpha m}+i\eta_\gamma^{(\mathrm{sp})})}}$$
$$\times\frac{\Gamma(-\eta_{\alpha m}-\eta_{\beta n}-2i\eta_\gamma^{(\mathrm{sp})})}{\Gamma(1-\eta_{\alpha m}-i\eta_\gamma^{(\mathrm{sp})})\Gamma(1-\eta_{\beta n}-i\eta_\gamma^{(\mathrm{sp})})}\frac{\sqrt{\tau_{(\mathrm{sp})}^2-1}}{\sqrt{(\tau_\alpha^{(\mathrm{sp})2}-1)(\tau_\beta^{(\mathrm{sp})2}-1)}}\frac{(\zeta_\alpha^{(\mathrm{sp})2}-1)^{(\eta_{\alpha m}+i\eta_\gamma^{(\mathrm{sp})})/2}(\zeta_\beta^{(\mathrm{sp})2}-1)^{(\eta_{\beta n}+i\eta_\gamma^{(\mathrm{sp})})/2}}{(\zeta_{(\mathrm{fs})}^2-1)^{(1+\eta_{\alpha m}+\eta_{\beta n}+2i\eta_\gamma^{(\mathrm{sp})})/2}} \quad (59)$$

measuring the strength of the triangle amplitude at the singularity. Hence we have the important result that in the neighborhood of the singular point (12), the leading angular behavior of $\mathcal{M}_{\beta n,\alpha m}^{T^C(\mathrm{fs})}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)$ is defined by the denominator in Eq. (58).

The leading behavior of the approximate amplitude $\mathcal{M}_{\beta n,\alpha m}^{V^C(\mathrm{fs})}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)$, which in the intermediate state contains the Coulomb potential instead of the off-shell Coulomb amplitude, is obtained from Eqs. (58) and (59) by setting $\eta_\gamma^{(\mathrm{sp})}$ equal to zero everywhere [provided that neither $\eta_{\alpha m}$ nor $\eta_{\beta n}$ equals a positive integer nor both vanish simultaneously. The latter happens, e.g., in deuteron-induced nuclear reactions of the type $A(d,p)B$, with B being a bound state of $A+n$; see below.] Then for $\eta_\gamma^{(\mathrm{sp})}$ real, i.e., for $E-k_{(\mathrm{sp})}^2/2M_\alpha>0$, for the magnitude of ratio (6) at singularity (12) we find the simple result

$$|\mathcal{R}_{\beta n,\alpha m}|\approx|\mathcal{R}_{\beta n,\alpha m}^{(\mathrm{fs})}|:=C_0^2\left|\frac{\Gamma(-\eta_{\alpha m}-\eta_{\beta n}-2i\eta_\gamma^{(\mathrm{sp})})}{\Gamma(-\eta_{\alpha m}-\eta_{\beta n})}\times\frac{\Gamma(1-\eta_{\alpha m})}{\Gamma(1-\eta_{\alpha m}-i\eta_\gamma^{(\mathrm{sp})})}\frac{\Gamma(1-\eta_{\beta n})}{\Gamma(1-\eta_{\beta n}-i\eta_\gamma^{(\mathrm{sp})})}\right|, \quad (60)$$

with $C_0^2=2\pi\eta_\gamma^{(\mathrm{sp})}/(e^{2\pi\eta_\gamma^{(\mathrm{sp})}}-1)$ being the Coulomb penetration factor. For atomic reactions with hydrogenic bound states, one has

$$\eta_{\alpha m}=-n_{\alpha m}, \quad \eta_{\beta n}=-n_{\beta n}, \quad (61)$$

where $n_{\alpha m}$ and $n_{\beta n}$ are the principal quantum numbers of the incoming and outgoing bound states, respectively. Hence this ratio specializes to

$$|\mathcal{R}_{\beta n,\alpha m}^{(\mathrm{fs})}|=C_0^2\left|\frac{\Gamma(n_{\alpha m}+n_{\beta n}-2i\eta_\gamma^{(\mathrm{sp})})}{\Gamma(n_{\alpha m}+n_{\beta n})}\times\frac{\Gamma(1+n_{\alpha m})}{\Gamma(1+n_{\alpha m}-i\eta_\gamma^{(\mathrm{sp})})}\frac{\Gamma(1+n_{\beta n})}{\Gamma(1+n_{\beta n}-i\eta_\gamma^{(\mathrm{sp})})}\right|. \quad (62)$$

We point out that for lower energies when $\eta_\gamma^{(\mathrm{sp})}$ is purely imaginary, $|\mathcal{R}_{\beta n,\alpha m}^{(\mathrm{fs})}|$ is a more complicated function. Several comments are fitting.

(i) The results derived above are, in fact, valid for attractive and repulsive Coulomb scattering in the intermediate state.

(ii) From Eq. (25) it can be seen that only for sufficiently large energies, $\eta_\gamma^{(\mathrm{sp})}$ becomes so small that $|\mathcal{R}_{\beta n,\alpha m}^{(\mathrm{fs})}|$ approaches the value 1, implying that the Coulomb-Born approximation be reliable in the immediate vicinity of the singular point $\zeta_{(\mathrm{sp})}$. This supplements result (11) derived for physical values of $z=\cos\vartheta$.

(iii) Near the singular point (12), the dependence on the scattering angle of the leading nonregular parts of the magnitudes $|\mathcal{M}_{\beta n,\alpha m}^{T^C(\mathrm{fs})}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)|$ and $|\mathcal{M}_{\beta n,\alpha m}^{V^C(\mathrm{fs})}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)|$ are the same (with one exception to be discussed below). However, as mentioned above, their strengths at $z=\zeta_{(\mathrm{sp})}$, $N_{(\mathrm{fs})}^{T^C}$ and

$$N_{(\mathrm{fs})}^{V^C}=N_{(\mathrm{fs})}^{T^C}|_{\eta_\gamma^{(\mathrm{sp})}=0}, \quad (63)$$

are different. Hence, in some region around that point one has the following relation between the exact amplitude and the Coulomb-Born approximation:

$$|\mathcal{M}_{\beta n,\alpha m}^{T^C(\mathrm{fs})}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)|\approx|\mathcal{R}_{\beta n,\alpha m}^{(\mathrm{fs})}|\cdot|\mathcal{M}_{\beta n,\alpha m}^{V^C(\mathrm{fs})}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)|. \quad (64)$$

This holds true for $E-k_{(\mathrm{sp})}^2/2M_\gamma>0$ when $\eta_\gamma^{(\mathrm{sp})}$ is purely real. In contrast, for lower energies, and in particular for $E<0$, i.e., below the bound-state dissociation threshold, their angular behavior is different, and Eq. (64) has to be modified.

(iv) Relation (64) has been derived for ζ in the vicinity of $\zeta_{(\mathrm{sp})}$. However, provided the latter is located not too far from the physical region, we may expect the same proportionality to hold between the moduli of the physical amplitudes $\mathcal{M}_{\beta n,\alpha m}^{T^C}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)$ and $\mathcal{M}_{\beta n,\alpha m}^{V^C}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)$, viz.

$$|\mathcal{M}_{\beta n,\alpha m}^{T^C}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)|\approx|\mathcal{R}_{\beta n,\alpha m}^{(\mathrm{fs})}|\cdot|\mathcal{M}_{\beta n,\alpha m}^{V^C}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)|. \quad (65)$$

In fact, the range of the validity of Eq. (65) has already been explored for atomic reactions in Ref. [25]. As was shown there, for elastic exchange scattering of electrons and protons off hydrogen atoms (not necessarily in their ground states), the right-hand side of Eq. (65) represents an excellent approximation for the exchange amplitude over a wide range of (medium to high) energies and scattering angles (including the forward-scattering direction).

(v) Taking into account the slight difference in the scattering-angle dependence of $\mathcal{M}^{T^C(\mathrm{fs})}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)$ and $\mathcal{M}^{V^C(\mathrm{fs})}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)$, as can be derived from Eq. (58), a relation of type (65) even between the original amplitudes themselves (and not only between their moduli) suggests itself:

$$\mathcal{M}^{T^C}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha) \approx \frac{N^{T^C}_{(\mathrm{fs})}/N^{V^C}_{(\mathrm{fs})}}{\left[\left(\frac{\mu_\beta}{m_\alpha}\mathbf{q}'_\beta-\frac{\mu_\alpha}{m_\beta}\mathbf{q}_\alpha\right)^2+(\kappa_{\beta n}+\kappa_{\alpha m})^2\right]^{-2i\eta^{(\mathrm{sp})}_\gamma}} \times \mathcal{M}^{V^C}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha). \tag{66}$$

Although the Coulomb-Born approximation $\mathcal{M}^{V^C}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)$ is purely real, the right-hand side of relation (66) could be shown in Ref. [25] to represent a very good and easy-to-calculate approximation to the exact exchange amplitude, for sufficiently high energies and out to rather large scattering angles. Hence, whenever applicable, its use should greatly simplify the calculation of exchange cross sections.

(vi) For atomic processes, the bound-state Coulomb parameters are negative, i.e., $\eta_{\alpha m}<0$ and $\eta_{\beta n}<0$; hence, near Eq. (12), the angular dependence will become divergent. In particular, in reactions with hydrogenic bound states the singularity is very strong. For example, for elastic exchange scattering from the ground state, i.e., for $n_{\alpha 0}=n_{\beta 0}=1$, taking into account Eq. (61) one has

$$|\mathcal{M}^{T^C(\mathrm{fs})}_{\beta 0,\alpha 0}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)|\sim\frac{1}{\left[\left(\frac{\mu_\beta}{m_\alpha}\mathbf{q}'_\beta-\frac{\mu_\alpha}{m_\beta}\mathbf{q}_\alpha\right)^2+(\kappa_{\beta 0}+\kappa_{\alpha 0})^2\right]^2}, \tag{67}$$

and thus the cross section has a pole of fourth order,

$$\sigma^{(\mathrm{fs})}_{\mathrm{ex}}(1s\to 1s)\sim\frac{1}{\left[\left(\frac{\mu_\beta}{m_\alpha}\mathbf{q}'_\beta-\frac{\mu_\alpha}{m_\beta}\mathbf{q}_\alpha\right)^2+(\kappa_{\beta 0}+\kappa_{\alpha 0})^2\right]^4}. \tag{68}$$

For inelastic exchange scattering the singularity becomes more and more pronounced as $n_{\beta n}$ increases. For instance, for excitation from an $n_{\alpha 0}=1s$ to an $n_{\beta 1}=2s$ level, one obtains a cross-section pole behavior of the type

$$\sigma^{(\mathrm{fs})}_{\mathrm{ex}}(1s\to 2s)\sim\frac{1}{\left[\left(\frac{\mu_\beta}{m_\alpha}\mathbf{q}'_\beta-\frac{\mu_\alpha}{m_\beta}\mathbf{q}_\alpha\right)^2+(\kappa_{\beta 1}+\kappa_{\alpha 0})^2\right]^6}. \tag{69}$$

However, in a genuine calculation of excitation cross sections it must be expected that such a singular power behavior will partly be counterbalanced by the orthogonality of the initial and the final bound-state wave functions, which, in the full amplitude Eq. (3) tends to suppress the forward-scattering region. This orthogonality effect is lost in the derivation of expression (58) for z near the singular point.

(vii) For nuclear reactions where all particles either have charges of equal sign or are neutral, both bound-state Coulomb parameters are positive or zero. In this case the angular part of $|\mathcal{M}^{T^C(\mathrm{fs})}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)|$ will not diverge at all, for $\eta^{(\mathrm{sp})}_\gamma$ real; on the contrary, it even goes to zero when approaching Eq. (12). If, in particular, particle γ is neutral (e.g., the neutron in deuteron-proton, or more generally in deuteron-nucleus, exchange scattering), the initial- and final-state Coulomb parameters are zero, $\eta_{\alpha m}=\eta_{\beta n}=0$. Thus, in the vicinity of Eq. (12) the angular behavior (58) simplifies to

$$\mathcal{M}^{T^C(\mathrm{fs})}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)\sim\left[\left(\frac{\mu_\beta}{m_\alpha}\mathbf{q}'_\beta-\frac{\mu_\alpha}{m_\beta}\mathbf{q}_\alpha\right)^2+(\kappa_{\beta n}+\kappa_{\alpha m})^2\right]^{2i\eta^{(\mathrm{sp})}_\gamma}. \tag{70}$$

That is, in the main order $|\mathcal{M}^{T^C(\mathrm{fs})}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)|$ is independent of the scattering angle for $E>k^2_{(\mathrm{sp})}/2M_\gamma$ and even vanishes for smaller energies. As has been mentioned above, in this case the behavior of the Coulomb-Born approximation $\mathcal{M}^{V^C(\mathrm{fs})}_{\beta n,\alpha m}$ cannot be extracted from Eqs. (58) or (70) by simply setting $\eta^{(\mathrm{sp})}_\gamma$ equal to zero. However, an explicit consideration of the integral (33) (with $\eta_\gamma=0$) reveals that $\mathcal{M}^{V^C(\mathrm{fs})}_{\beta n,\alpha m}$ diverges logarithmically as point (12) is approached.

The decisive question is whether the angular behavior of the triangle amplitude, derived for the cosine of the scattering angle outside the physical region [cf. Eq. (13)], has observable consequences in the form of a (more or less sharp) rise of the differential cross section in the forward direction. The above discussion has made it evident that no noteworthy experimental signatures are to be expected for nuclear reactions. For atomic reactions the situation can be different, depending on the distance of the singular point (13) to the physical region, which for its part depends on the process considered.

We confine our discussion to the important special case that the masses of the particles which are unbound both in the initial and in the final state are equal, i.e., $m_\alpha=m_\beta$. Then expression (13) for the singular point simplifies to

$$\zeta_{(\mathrm{fs})}=\frac{q_\alpha^2+q'^2_\beta+(1+m_\alpha/m_\gamma)^2(\kappa_{\alpha m}+\kappa_{\beta n})^2}{2q_\alpha q'_\beta}=\frac{E+\left(1+\frac{m_\alpha}{m_\gamma}\right)(|\hat{E}_{\alpha m}|+|\hat{E}_{\beta n}|)+\left(1+2\frac{m_\alpha}{m_\gamma}\right)\sqrt{|\hat{E}_{\alpha m}\hat{E}_{\beta n}|}}{\sqrt{(E+|\hat{E}_{\alpha m}|)(E+|\hat{E}_{\beta n}|)}}, \tag{71}$$

where the on-shell condition (1) has been used. It is apparent that for asymptotic energies E or momenta q_α and q'_β, $\zeta_{(\mathrm{fs})}$ approaches the value 1, independent of the masses of the particles and of the binding energies, and hence a forward-scattering peak should occur (although our nonrelativistic theory is certainly no longer valid in this case). For non-asymptotic energies, if the mass of particle γ, which does not participate in the intermediate-state Coulomb scattering, is much smaller than the other mass, i.e., if $m_\gamma \ll m_\alpha$, $\zeta_{(\mathrm{fs})}$ is located rather far from the border of the physical region; thus the singularity will not manifest itself in a striking angular behavior. This situation prevails, e.g., in (p,p') reactions off hydrogen atoms with $m_\alpha = m_p$ and $m_\gamma = m_e$ where $m_p(m_e)$ is the proton (electron) mass. In the opposite case, i.e. for $m_\gamma \gg m_\alpha$, as realized, e.g., in (e,e') exchange scattering off hydrogen atoms with $m_\alpha = m_e$ and $m_\gamma = m_p$, the singular point lies close to the physical region, provided that the energy, and hence the on-shell momentum, is not very small. Thus, the chances for distinct observable effects at intermediate energies are much more favorable. Analogous comments also apply to the region of validity of the approximate relations (65) and (66).

For elastic exchange, i.e., for $q'_\beta = q_\alpha$, $n = m$, and $\kappa_{\beta m} = \kappa_{\alpha m}$, we find

$$\zeta_{(\mathrm{fs})} = 1 + 2\left(1 + \frac{m_\alpha}{m_\gamma}\right)^2 \frac{\kappa_{\alpha m}^2}{q_\alpha^2} = 1 + 2\left(1 + 2\frac{m_\alpha}{m_\gamma}\right)\frac{|\hat{E}_{\alpha m}|}{E + |\hat{E}_{\alpha m}|}. \tag{72}$$

Clearly, for fixed energy and fixed mass ratio m_α/m_γ, the singular point is located more closely to the physical region the smaller $|\hat{E}_{\alpha m}|$ is, i.e., the looser bound the composite particle is, enhancing the prospects for strong experimental signatures. This has, in fact, been verified in Ref. [25] for the elastic (p,p') and (e,e') exchange reactions with hydrogen atoms in the $2s$-state as compared to hydrogen atoms in the $1s$ state.

We mention that, e.g., for elastic exchange

$$\eta_\gamma^{(\mathrm{sp})} = \frac{e_\alpha^2}{2}\sqrt{\left(\frac{m_\alpha}{(2m_\alpha + m_\gamma)E/2(m_\alpha + m_\gamma) + \hat{E}_{\alpha m}}\right)^{1/2}}. \tag{73}$$

Thus, energies E of the order of the incoming mass m_α [but always much larger than $2(m_\alpha + m_\gamma)|\hat{E}_{\alpha m}|/(2m_\alpha + m_\gamma)$ so that $\eta_\gamma^{(\mathrm{sp})}$ be real] are sufficient to make $\eta_\gamma^{(\mathrm{sp})}$ rather small, practically independent of m_γ, leading to values of $\mathcal{R}^{(\mathrm{fs})}_{\beta m,\alpha m}$ close to 1. Since for $m_\alpha \ll m_\gamma$ the singular point $\zeta_{(\mathrm{fs})}$ lies close to the physical forward-scattering region, we can expect also $\mathcal{R}_{\beta m,\alpha m}|_{\cos\vartheta\approx 1} \approx 1$; in other words, for small scattering angles and for such energies, one expects $\mathcal{M}^{T^C}_{\beta m,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha) \approx \mathcal{M}^{V^C}_{\beta m,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)$.

Let us finally look at this situation in the Δ plane, with $\boldsymbol{\Delta}_\alpha = \mathbf{q}'_\beta - \mathbf{q}_\alpha$. From Eq. (58), with $m_\alpha = m_\beta$, we conclude that here the singularity is located at $\Delta^2 \approx \Delta_s^2$ with

$$\Delta_s^2 = -(1 + m_\alpha/m_\gamma)^2(\kappa_{\alpha m} + \kappa_{\beta n})^2. \tag{74}$$

It is evident that for pp-intermediate-state scattering in the reaction $H(p,p')H$ ($m_\alpha/m_\gamma = m_p/m_e$) this is very far from the physical region (for which $\Delta^2 \geq 0$). However, for intermediate-state ee scattering in $H(e,e')H$, it is located closer to its border. In fact, in the latter reaction for elastic exchange, where $\kappa_{\alpha m} = \kappa_{\beta n}$ and $m_\alpha/m_\gamma = m_e/m_p \ll 1$, we have

$$\Delta_s^2 \approx -4\kappa_{\alpha m}^2, \tag{75}$$

while, for inelastic exchange with $\kappa_{\beta n} < \kappa_{\alpha m}$,

$$\Delta_s^2 \approx -(\kappa_{\alpha m} + \kappa_{\beta n})^2. \tag{76}$$

That is, for inelastic exchange the singularity lies even closer to the physical region than for elastic exchange.

C. Analytic behavior of $\mathcal{M}^{T^C}_{\beta n,\alpha m}$ near the backward direction

In this subsection we derive the analytic behavior of the triangle amplitude (16) in the $z(=\cos\vartheta)$ plane in the vicinity of the backward-scattering (bs) direction. It represents a generalization of the results obtained in Ref. [34] (see also Ref. [35]), where it had been assumed that one of the three particles is neutral. Similar techniques will now be used to show that $\mathcal{M}^{T^C}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)$ possesses a further singularity which lies at

$$\left(\mathbf{q}'_\beta + \frac{\mu_\alpha}{m_\gamma}\mathbf{q}_\alpha\right)^2 + \kappa_{\alpha m}^2 = \left(\mathbf{q}_\alpha + \frac{\mu_\beta}{m_\gamma}\mathbf{q}'_\beta\right)^2 + \kappa_{\beta n}^2 = 0, \tag{77}$$

or equivalently at $z = \zeta_{(\mathrm{bs})}$ with

$$\zeta_{(\mathrm{bs})} = -\frac{\left(\frac{\mu_\alpha}{m_\gamma}q_\alpha\right)^2 + q'^2_\beta + \kappa_{\alpha m}^2}{2\frac{\mu_\alpha}{m_\gamma}q_\alpha q'_\beta} < -1 \tag{78}$$

outside of the physical backward-scattering region. This results from the coincidence of the singularities of the integrand at Eqs. (17) and (18), and at the forward-scattering singularity of the intermediate-state Coulomb T matrix which occurs at

$$\mathbf{p}'_\gamma - \mathbf{p}_\gamma = \epsilon_{\alpha\gamma}(\mathbf{k} + \mathbf{q}_\alpha + \mathbf{q}'_\beta) = \mathbf{0}. \tag{79}$$

Equivalently, if the integration variable $\mathbf{p} = \epsilon_{\alpha\gamma}(\mathbf{k} + \mathbf{q}_\alpha + \mathbf{q}'_\beta)$ is introduced, it is the coincidence of the singularities at Eqs. (29) and (30), and at

$$\mathbf{p} = \mathbf{0} \tag{80}$$

which gives rise to the singularity of $\mathcal{M}^{T^C}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)$ considered presently. Making use of condition (80) and recalling Eq. (27), we can rewrite Eqs. (29) and (30) for the positions of the singularities of the integrand of Eq. (16) as

$$p_\alpha^2 + \kappa_{\alpha m}^2 = p'^2_\beta + \kappa_{\beta n}^2 = 0, \tag{81}$$

which coincides with Eq. (77) [recall definitions (26)].

The following observation is instructive. Consider the pole diagram of Fig. 2, which describes the one-particle-exchange (OPE) contribution to the full exchange amplitude. Note that the momenta $\mathbf{p}_\alpha$ and $\mathbf{p}'_\beta$ introduced in Eq. (26) are

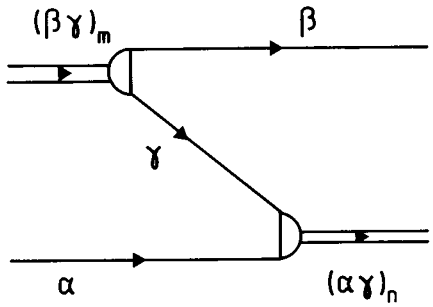

FIG. 2. Graphical representation of the one-particle-exchange amplitude (82). Semicircles represent the bound state form factors.

nothing but the on-shell relative momenta at the initial and the final bound state vertex, respectively. It is easily seen that Eq. (81) describes the locus of the singularity of the corresponding amplitude; that is, for $p_\alpha^2+\kappa_{\alpha m}^2\to 0$, or equivalently for $z\to\zeta_{(bs)}$, it behaves like

$$\mathcal{M}^{\mathrm{OPE}}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)\approx\mathcal{M}^{\mathrm{OPE(bs)}}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)$$

$$:=\frac{N^{\mathrm{OPE}}_{(\mathrm{bs})}}{(p_\alpha^2+\kappa_{\alpha m}^2)^{1-\eta_{\alpha m}-\eta_{\beta n}}},\tag{82}$$

with $N^{\mathrm{OPE}}_{(\mathrm{bs})}=-2\mu_\alpha G^*_{\beta n}(\hat{\mathbf{p}}'_\beta,i\kappa_{\beta n})G_{\alpha m}(\hat{\mathbf{p}}_\alpha,i\kappa_{\alpha m})$ [recall Eq. (14)]. Thus the assertion is that the near-backward-scattering singularity of the triangle amplitude $\mathcal{M}^{T^C}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)$ is located at exactly the same position as the singularity of the pole amplitude. In fact, not only the location but also the character (pole, cut, etc.) of these singularities of the two amplitudes coincide.

This can be seen as follows. Similarly to what was found in Sec. III B for the forward-scattering singularity, the location of the backward-scattering singularity can also be extracted from the (much simpler) Coulomb-Born approximation (5), and in the present case even its type; see Ref. [27]. In order to simplify the discussion we again assume that both bound states $(\beta\gamma)_m$ and $(\gamma\alpha)_n$ have a zero internal orbital angular momentum. Thus the corresponding bound-state form factors can be taken out from under the integral at the singular points $p'_\alpha=i\kappa_{\alpha m}$ and $p''_\beta=i\kappa_{\beta n}$, respectively. Using the integration variable $\mathbf{p}$ introduced above, in the vicinity of Eq. (81) the amplitude (5) becomes

$$\mathcal{M}^{V^C(bs)}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha):=4\pi e_\alpha e_\beta G^*_{\beta n}(i\kappa_{\beta n})G_{\alpha m}(i\kappa_{\alpha m})J',\tag{83}$$

with

$$J'=\int\frac{d^3p}{(2\pi)^3}\frac{1}{p^2}\frac{1}{[(\mathbf{p}-\ \mathbf{p}'_\beta)^2+\kappa_{\beta n}^2]^{1-\eta_{\beta n}}}\times\frac{1}{[(\mathbf{p}+\mathbf{p}_\alpha)^2+\kappa_{\alpha m}^2]^{1-\eta_{\alpha m}}}.\tag{84}$$

If Eq. (81) is satisfied, the integrand of Eq. (84) is singular at the origin $p=0$, which gives rise to a singularity of the whole integral. In fact, substituting $\mathbf{p}=(p_\alpha^2+\kappa_{\alpha m}^2)\mathbf{v}/2\mu_\alpha=(p'^2_\beta+\kappa_{\beta n}^2)\mathbf{v}/2\mu_\beta$ [recall Eq. (27)], one can read off the behavior of J' directly, and accordingly also that of $\mathcal{M}^{V^C(\mathrm{bs})}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)$, in the vicinity of Eq. (81):

$$\mathcal{M}^{V^C(\mathrm{bs})}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)\approx\frac{N^{V^C}_{(\mathrm{bs})}}{(p_\alpha^2+\kappa_{\alpha m}^2)^{1-\eta_{\alpha m}-\eta_{\beta n}}}=\frac{N^{V^C}_{(\mathrm{bs})}}{\left[\left(\mathbf{q}'_\beta+\frac{\mu_\alpha}{m_\gamma}\mathbf{q}_\alpha\right)^2+\kappa_{\alpha m}^2\right]^{1-\eta_{\alpha m}-\eta_{\beta n}}}.\tag{85}$$

Consequently, for the full triangle amplitude we arrive at

$$\mathcal{M}^{T^C(\mathrm{bs})}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)\approx\frac{N^{T^C}_{(\mathrm{bs})}}{\left[\left(\mathbf{q}_{\boldsymbol{\beta}}'+\frac{\mu_\alpha}{m_\gamma}\mathbf{q}_{\boldsymbol{\alpha}}\right)^2+\kappa_{\alpha m}^2\right]^{1-\eta_{\alpha m}-\eta_{\beta n}}},\tag{86}$$

where, of course, the residual strength factor $N^{T^C}_{(\mathrm{bs})}$ differs from the corresponding factor $N^{V^C}_{(\mathrm{bs})}$ of the Coulomb-Born approximation. This singular behavior, indeed, coincides with that of the pole amplitude, Eq. (82). Let us add the following remarks.

(i) This derivation is valid for attractive as well as repulsive Coulomb interactions between the particles experiencing intermediate-state scattering.

(ii) For nuclear reactions, where the bound-state Coulomb parameters $\eta_{\alpha m}$ and $\eta_{\beta n}$ are positive semidefinite, the backward-scattering singularity will either be very weak or even lead to the vanishing of the triangle (and of course also of the OPE) amplitude at this point. This is to be contrasted with the situation pertaining to atomic reactions, where $\eta_{\alpha m}<0$ and $\eta_{\beta n}<0$. Here the singularity will in general be rather strong. In fact, if the initial and final bound states are described by hydrogenic wave functions, the amplitude behavior looks like

$$\mathcal{M}^{T^C(\mathrm{bs})}_{\beta n,\alpha m}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)\sim\frac{1}{\left[\left(\mathbf{q}'_\beta+\frac{\mu_\alpha}{m_\gamma}\mathbf{q}_\alpha\right)^2+\kappa_{\alpha m}^2\right]^{1+n_{\alpha m}+n_{\beta n}}},\tag{87}$$

where $n_{\alpha m}$ and $n_{\beta n}$ are the corresponding principal quantum numbers. However, whether an experimentally detectable cross section peak in the backward direction will result from such a pole behavior of Eq. (87) depends on the distance of this singularity to the physical region [and, of course, of Eq. (82)].

As is well known and can be inferred from Eq. (78), the backward-scattering exchange singularity quite generally lies closer to the physical region the smaller the mass m_γ of the exchanged particle which is noninteracting in the intermediate state is, for sufficiently high energies. However, in order to simplify the discussion, we again consider in more detail only the case when the masses of the particles α and β, which are unbound in initial and final states, respectively, are equal, i.e., $m_\alpha=m_\beta$. Expression (78) for the locus of the singularity reduces to

$$\zeta_{(\mathrm{bs})} = -\frac{1}{2}\,\frac{\left(1+\dfrac{m_\gamma}{m_\alpha}+\dfrac{1}{1+m_\gamma/m_\alpha}\right)E-\left(1+\dfrac{m_\gamma}{m_\alpha}\right)(\hat{E}_{\alpha m}+\hat{E}_{\beta n})}{\sqrt{(E-\hat{E}_{\alpha m})(E-\hat{E}_{\beta n})}}, \tag{88}$$

where the on-shell condition (1) has been used. Several limiting cases are of interest.

(i) For a fixed ratio m_γ/m_α of the mass of the particle γ which is bound in initial and finals state to the other mass, if the energy becomes very large the location of the singular point is at

$$\zeta_{(\mathrm{bs})} \overset{E\to\infty}{=} -\left(1+\frac{m_\gamma^2}{2m_\alpha(m_\alpha+m_\gamma)}\right)+O(E^{-1}). \tag{89}$$

That is, even asymptotically the backward-scattering singularity never reaches the border of the physical region (for $m_\gamma\neq 0$), although the smaller the mass ratio is, the closer it will come to it.

(ii) For fixed energy, if $m_\gamma \gg m_\alpha$ one has $\zeta_{(\mathrm{bs})}\sim -m_\gamma/m_\alpha \ll -1$; thus the singularity lies very far from the physical region, and hence will not result in a noticeably peaking of the backward-scattering cross section. For instance, for electron elastic exchange scattering off hydrogen atoms in the state with quantum numbers $\{n\ell m\}$, $e+\mathrm{H}(n\ell m)\to e'+\mathrm{H}(n\ell m)$, where the heavy proton is the exchanged particle γ, Eq. (88) specializes up to terms of the order $O(m_e/m_p)$ to

$$\zeta_{(\mathrm{bs})} \approx -\frac{m_p}{2m_e}\left(1+\frac{|\hat{E}_n|}{E_i}\right) \ll -1. \tag{90}$$

Here $\hat{E}_n$ is the binding energy in the state with the principal quantum number n, and E_i is the projectile bombarding energy in the center of mass. Thus the position of the singularity depends only weakly on the energy, and for all energies including very large ones lies far off the physical region; hence it will not exert any influence on physical scattering observables.

(iii) For a light exchanged mass $m_\gamma(\ll m_\alpha)$, one finds

$$\zeta_{(\mathrm{bs})} = -\frac{E-\hat{E}_{\alpha m}-\hat{E}_{\beta n}}{\sqrt{(E-\hat{E}_{\alpha m})(E-\hat{E}_{\beta n})}}+O\left(\frac{m_\gamma}{m_\alpha}\right), \tag{91}$$

which, for sufficiently large energy, can come close to 1, i.e., to the border of the physical region [although according to Eq. (89) it will never reach it]. Consequently, the triangle amplitude will contribute to the OPE in yielding a striking backward-scattering peaking of differential cross sections. Consider as an example proton elastic exchange scattering with hydrogen atoms in the state $\{n\ell m\}$, $p+\mathrm{H}(n\ell m)\to p'+\mathrm{H}(n\ell m)$. Up to terms of higher order in m_e/m_p, one finds

$$\zeta_{(\mathrm{bs})} = -1-\frac{m_e}{m_p}\,\frac{|\hat{E}_n|}{E_i}+O\left(\frac{m_e^2}{m_p^2}\right). \tag{92}$$

Hence the singularity is located in the immediate vicinity of the physical region, in fact, the closer it is, the higher the projectile energy and/or the smaller the binding energy are.

IV. NUMERICAL RESULTS

The various theoretical results derived in Sec. III will now be illustrated by means of several examples from atomic and nuclear physics. To begin with, we investigate under what circumstances the Coulomb-Born approximation might be a good approximation for the exact exchange triangle amplitude, a question of considerable practical relevance. For this purpose we numerically calculated both amplitudes as functions of the center-of-mass kinetic energy of the projectile and the scattering angle (for some numerical details we refer to [24]). Figure 3 contains the absolute value of their ratio (6) for the elastic exchange reaction $e+\mathrm{H}(1s)\to e' +\mathrm{H}(1s)$, with the two electrons undergoing Coulomb scattering in the intermediate state. It obviously satisfies the general bounds (9) and (10). Furthermore, it approaches the value 1 at about 100 keV for all angles, in accordance with Eq. (11). An angle-independent value, albeit clearly smaller than 1, is also reached when approaching the reaction threshold. For energies less than, say, 10 keV, the Coulomb-Born approximation considerably overestimates the exact amplitude, in particular in the forward-scattering hemisphere for some intermediate-energy region. This situation resembles the one for the nonrearrangement triangle amplitude considered in [24], except that there the overestimation was most pronounced for backward scattering but practically absent at threshold. Furthermore, in the physical region for backward scattering the magnitude of the ratio depends on the energy and differs markedly from 1.

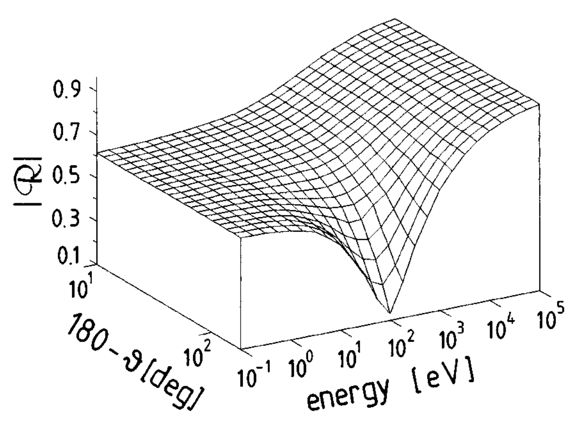

FIG. 3. Absolute value of the ratio of the exact triangle amplitude to the Coulomb-Born approximation, Eq. (6), for the elastic exchange reaction $\mathrm{H}(1s)(e,e')\mathrm{H}(1s)$, as function of the c.m. projectile kinetic energy and of the scattering angle.

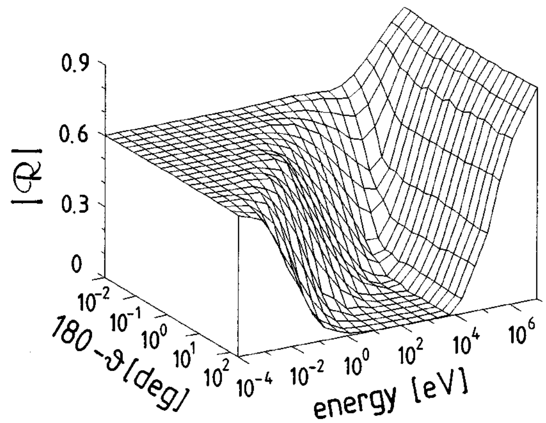

FIG. 4. Same as in Fig. 3, but for the reaction $H(1s)(p,p')H(1s)$.

The mass effect in the intermediate-state Coulomb scattering strongly influences the quality of the Coulomb-Born approximation. This can, e.g., be verified by looking at Fig. 4, which contains the results for the magnitude of ratio (6) for the elastic exchange reaction $p+H(1s)\rightarrow p'+H(1s)$, with the two heavy particles undergoing intermediate-state Coulomb scattering. The Coulomb-Born approximation fails completely except, of course, at very high energies which are, however, not shown in this figure. On the whole, the situation is rather similar to the nonrearrangement case studied in Ref. [24], except that again forward- and backward-scattering regions exchange their roles. Finally, we draw attention to the remarkable fact that the threshold value of $\mathcal{R}_{p'p}(1s)$ is very close to the one for electron-hydrogen exchange scattering discussed above.

An interesting, somewhat intermediate example is provided by the positronium-formation reaction $e^{+}+H(1s)\rightarrow Ps(1s)+H^{+}$, since here the masses of the two particles (positron and proton) scattering in the intermediate state lie on different scales, in contrast to the previous cases. For this case the magnitude of the ratio (6) is depicted in Fig. 5. As is apparent, the region where the Coulomb-Born approximation fails has become rather large but remains still smaller than for the proton-reaction discussed above.

The situation is, however, much more favorable for the

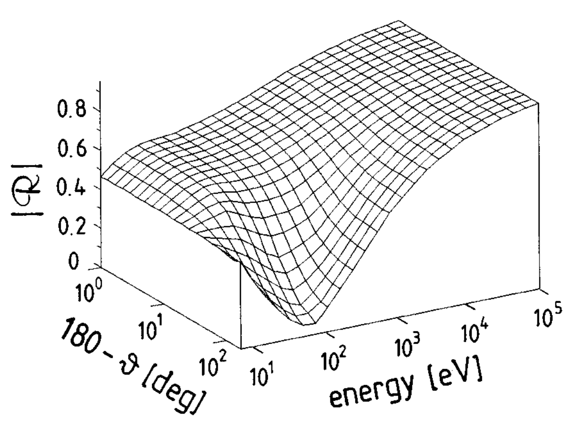

FIG. 5. Same as in Fig. 3, but for the reaction $e^{+}+H(1s)\rightarrow Ps(1s)+H^{+}$.

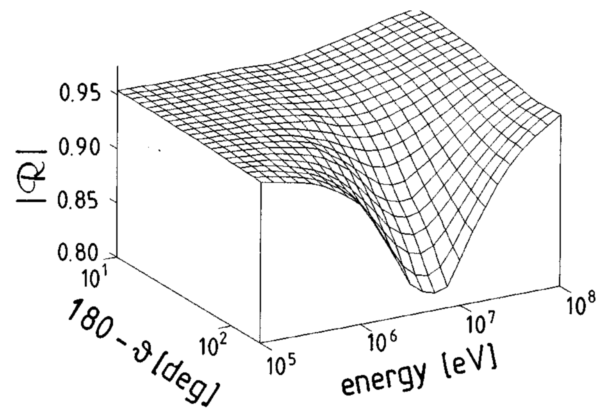

FIG. 6. Same as in Fig. 3, but for the nuclear reaction $d+p\rightarrow p'+d$.

nuclear reaction $d+p\rightarrow p'+d$, shown in Fig. 6. Except for projectile energies between 1 and 10 MeV for fairly small scattering angles, the Coulomb-Born approximation is found to be good to within 5%, similarly to the nonexchange case (cf. Ref. [24]). Hence for this reaction the latter provides a reliable approximation for taking into account the particle exchange rescattering.

The effect of the presence of the forward- and backward-scattering singularities on the exact exchange triangle amplitude is shown in Fig. 7 for the reactions $e+H(n\ell m)\rightarrow e'+H(n'\ell'm')$, for $(n\ell m,n'\ell'm')\in(1s,2s)$, at 100-keV electron kinetic energy. Obviously, the former completely dominates the forward-scattering region, the smaller the magnitudes of the binding energies in the initial and final states are, in accordance with the discussion at the end of Sec. III B. For excitation, the forward-scattering peak is, however, somewhat suppressed by the near orthogonality of the initial and final bound-state wave functions for small (but nonzero) momentum transfer. Nevertheless, at such a high-energy scattering for all three reac-

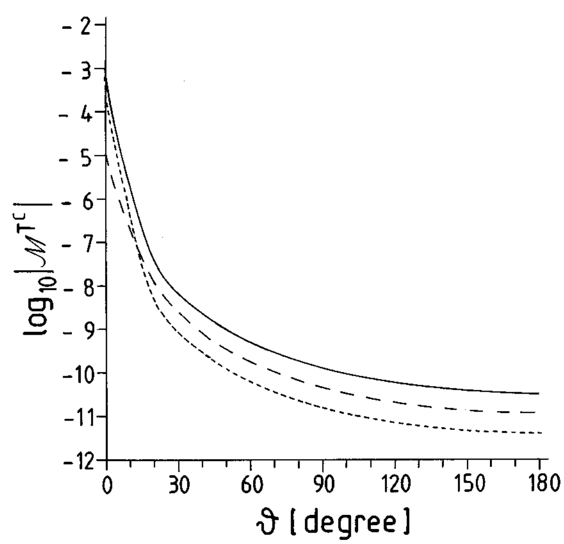

FIG. 7. Exact triangle amplitude (3) (in a.u.) for the reaction $H(n\ell m)(e,e')H(n'\ell'm')$ at 100-keV projectile energy, as a function of the scattering angle. Solid line: elastic exchange $1s\rightarrow 1s$; long-dashed line: target excitation $1s\rightarrow 2s$; short-dashed line: elastic exchange $2s\rightarrow 2s$.

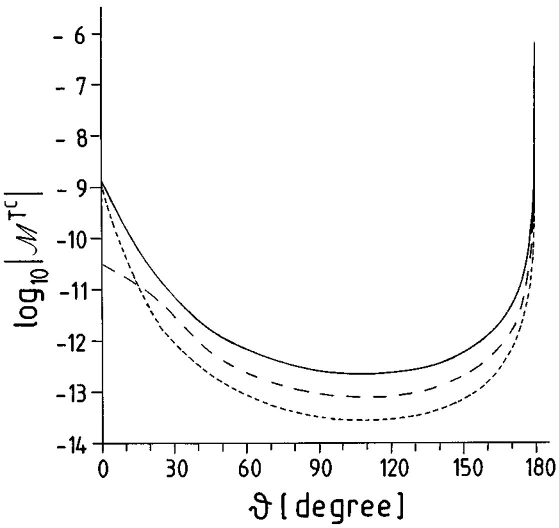

FIG. 8. Same as in Fig. 7, but for the reaction $\mathrm{H}(n\ell m)(p,p')\mathrm{H}(n'\ell'm')$.

tions is confined to rather small angles. Furthermore, because the exchanged particle is the heavy proton, there is no backward-scattering peak: as discussed in Sec. III C the corresponding backward-scattering singularity is too far away from the physical region to have any influence on the differential cross sections.

The situation is rather different in the case of the reactions $p+\mathrm{H}(n\ell m)\rightarrow p'+\mathrm{H}(n'\ell'm')$, for $(n\ell m,n'\ell'm')\in(1s,2s)$, depicted in Fig. 8. Though there exists a forward-scattering peak in all three amplitudes considered, that is in fact again larger for elastic exchange scattering off hydrogen atoms in the $2s$ state than in the $1s$ state, with the amplitude for excitation from $1s$ to $2s$ being reduced by the orthogonality effect described above. But the peak is generally reduced in comparison with the electron reaction. This is understandable since for (p,p') the forward-scattering singularity is farther away from the physical region than for (e,e'). In contrast to the latter, however, we have a very pronounced and sharp backward-scattering peaking of all three amplitudes. As discussed in Sec. III C, this is a consequence of the closeness of the backward-scattering singularity resulting from the small mass of the exchanged electron. This corroborates the well-known fact that for small exchanged mass the triangle amplitude contributes essentially to backward scattering only.

V. SUMMARY

We investigated theoretically and numerically the (on-shell) rescattering contribution which appears in the effective potential in the integral-equation approach and in the multiple-scattering representation of the reaction amplitude, pertaining to exchange processes in three-charged-particle systems. We have found the following interesting results.

(i) If in the exact exchange triangle amplitude the Coulomb T matrix describing the intermediate-state rescattering of the particles of a given pair is replaced by the Coulomb potential, the resulting approximate triangle amplitude in general fails dramatically for the atomic reactions investigated; for the nuclear reaction considered, however, this approximation is very good for practically all energies from reaction threshold to infinity, for nearly all scattering angles.

(ii) By investigating the analytic properties in the vicinity of the forward-scattering region, we extracted the leading singularity of the exact triangle amplitude. This enabled us first to identify the conditions under which the latter will induce a forward-scattering peak in the physical amplitudes and thus be observable. Second, it suggested another approximate triangle amplitude which is not much more difficult to calculate than the Coulomb-Born approximation, but is vastly superior to the latter for atomic processes for medium to high energies, in a wide range of scattering angles including the forward direction.

(iii) An analogous investigation of the leading backward-scattering singularity clarified the conditions under which the latter will result in a backward-scattering peak of the exact triangle amplitude.

(iv) These theoretical results have been illustrated by means of typical exchange reactions from the fields of atomic and nuclear physics.

We finally note that similar approximation formulas can also be derived for direct triangle amplitudes, as will be shown in a forthcoming paper. Both these results are presently being applied to the calculation of cross sections for electron and proton scattering off hydrogen atoms by solving three-body integral equations where, as mentioned in Sec. I, the various triangle amplitudes occur as contributions to the effective potentials. This fact makes it clear that such calculations will include all iterations of the triangle amplitudes, and thus not be confined to terms of first order in the Coulomb amplitude, in constrast to their use in the multiple-scattering representation of the exchange amplitude.

ACKNOWLEDGMENTS

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