Triangle Diagram with Off-Shell Coulomb T-Matrix for (In-)Elastic Atomic and Nuclear Three-Body Processes

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Abstract

The driving terms in three-body theories of elastic and inelastic scattering of a charged particle off a bound state of two other charged particles contain the fully off-shell two-body Coulomb T-matrix describing the intermediate-state Coulomb scattering of the projectile with each of the charged target particles. Up to now the latter is usually replaced by the Coulomb potential, either when using the multiple-scattering approach or when solving three-body integral equations. General properties of the exact and the approximate on-shell driving terms are discussed, and the accuracy of this approximation is investigated numerically, both for atomic and nuclear processes including bound-state excitation, for energies below and above the corresponding three-body dissociation threshold, over the whole range of scattering angles.

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I. INTRODUCTION

Elastic and inelastic scattering of a particle off a two-particle cluster is conveniently formulated in terms of the exact three-body integral equations in momentum space (Faddeev 1960) which, after suitable manipulations, can be given the practical form of multichannel equations of the two-body Lippmann-Schwinger type (Alt et al 1967). If the impinging, and one or both of the target particles, are charged, modifications of this theory are required (Veselova 1971, 1978, Alt 1978, Alt et al 1978, 1980). Nevertheless, the basic, effective-two-body, multi-channel structure of the equations can be preserved.

An alternative approach for calculating the (in-)elastic scattering amplitude, which is well-suited especially for high energies, is based on the multiple-scattering expansion of the corresponding three-body transition operator. Obviously, there exists a close correspondence between the terms occurring here and the various contributions to the effective potential of the integral equations approach.

In applications of either formalism to charged-particle scattering, terms occur which contain the fully off-shell two-particle Coulomb T-matrix, describing the intermediate-state Coulomb scattering of various charged two-body subsystems. It is evident that the singularity structure of the latter in momentum space renders the calculation of such terms a rather difficult task. Hence, in numerical work (see, e.g., Alt et al 1985, Alt et al 1994, and references therein) the Coulomb T-matrix is frequently replaced by its Born approximation, namely the Coulomb potential, which drastically reduces the analytical and numerical effort required. But the reliability of such an approximation, in the following called ‘Coulomb-Born approximation’, is difficult to estimate.

The first numerical studies of the quality of such a Coulomb-Born approximation appear to have been performed by Sinfailam and Chen (1972), who calculated the lowest-order multiple-scattering contributions to the elastic scattering amplitude for various atomic three-body processes, with the full two-body Coulomb T-matrix and with the latter replaced by the Coulomb potential. It turned out that, for most of the three-body systems studied, and for the energy and angular ranges considered, the Coulomb-Born approximation failed rather dramatically, the more in fact the lower the energy was. Of
course, if the latter is sufficiently high, both the exact and the approximate expression are expected to eventually yield the same answer; this was, indeed, found although at an energy larger than expected. This investigation, however, concerned only a limited variation of the scattering angle and the (altogether rather high) three-body energy. In particular, energies in the neighbourhood of the dissociation threshold, which represent critical tests of the reliability of the calculational procedures since the essential singularity of the two-body Coulomb T-matrix at zero subsystem energy plays a particularly important role there, were not considered at all.

Theoretical and numerical studies of the lowest-order (off-shell) driving terms, which occur in the three-body approach, have been performed by van Haeringen (1979), and Kok et al (1979,1980,1981,1982). However, the investigations were restricted to negative total three-body energies, i.e., to energies below the composite-particle breakup threshold (and to the case that the masses of all three particles are equal, and the charges of the two particles involved in the intermediate-state Coulomb scattering are of equal sign). In some situations, which relate more to nuclear reactions with light nuclei, the Coulomb-Born approximation was found to be reasonably accurate. But in other cases, which are more typical for the situation prevalent in atomic physics, its lack of accuracy considerably diminishes its usefulness, similarly to the situation found at high energies.

In this paper we address ourselves to a systematic investigation of the quality of the Coulomb-Born approximation, by comparing the exact with the corresponding approximate on-shell driving terms for elastic and inelastic scattering in three-body systems. In particular, we study the dependence on several important parameters. Namely, energies are considered from the reaction threshold up to such high values that the Coulomb-Born approximation practically yields the exact result. Scattering angles are varied over the whole angle regime, with particular emphasis on very small angles which are favoured in higher-energy scattering. Furthermore, different masses of the two particles which experience the intermediate-state Coulomb scattering, are allowed for: two light, one light and one heavy, and two heavy particles. Also the case that the magnitude of the charge of one of these two particles is larger than one is considered. And, finally, we also study the collisional excitation of the bound system. However, in the present investigation we
restrict ourselves to repulsive intermediate-state Coulomb interactions.

In Sect. II we briefly sketch the three-body approach to elastic and inelastic scattering and, in particular, introduce the relevant driving terms. Some known results for the two-particle off-shell Coulomb amplitude which are used in the subsequent investigations are collected in Section III. In Sect. IV, general properties of these elastic and inelastic driving terms are discussed, both in their exact form as well as if the intermediate-state Coulomb T-matrix is replaced by the Coulomb potential. Numerical tests of the accuracy of this approximation are presented for several typical atomic and nuclear three-body systems in Sect. V, both for energies below and above the corresponding bound state dissociation thresholds. The results obtained are summarized in Sect. VI.

Natural units $\hbar = c = 1$ are chosen. Furthermore, the conventional notation for two-body quantities: $A_\alpha \equiv A_{\beta\gamma}$, with $\alpha \neq \beta \neq \gamma \neq \alpha$, is adopted.
II. THREE-PARTICLE MODEL OF ELASTIC AND INELASTIC SCATTERING

Consider three particles with masses \( m_\nu \) and charges \( e_\nu, \nu = 1, 2, 3 \). We are interested in the reaction \( \alpha + (\beta\gamma)_m \rightarrow \alpha + (\beta\gamma)_n \), where particle \( \alpha \), having center-of-mass momentum \( q_\alpha \), impinges on the bound state of particles \( \beta \) and \( \gamma \); the bound state wave function, belonging to the binding energy \( \hat{E}_{am} \) (with quantum numbers \( m \)), is denoted by \( |\psi_{am}\rangle \).

In the final state, the bound state quantum numbers are characterized by the index \( n \), and the center-of-mass momentum of particle \( \alpha \) is \( q'_\alpha \).

The corresponding (in-)elastic scattering amplitude \( T_{\alpha n,am}(q'_\alpha, q_\alpha; E) \) can be written as matrix element of an effective-two-body operator \( T_{\alpha n,am}(E + i0) \) between the plane wave states describing the free asymptotic motion of the clusters,

\[
T_{\alpha n,am}(q'_\alpha, q_\alpha; E) = \langle q'_\alpha | T_{\alpha n,am}(E + i0) | q_\alpha \rangle,
\]

with the total three-body energy \( E \) being connected with the incoming and outgoing momenta by the on-shell condition

\[
E = \frac{q'^2_\alpha}{2M_\alpha} + \hat{E}_{am} = \frac{q'^2_\alpha}{2M_\alpha} + \hat{E}_{an}.
\]

Here, \( M_\alpha = m_\alpha (m_\beta + m_\gamma) / (m_\alpha + m_\beta + m_\gamma) \) is the \( \alpha \)-channel reduced mass.

According to the effective-two-body formulation of the three-body scattering theory (Alt et al 1967), the operators \( T_{\beta n,am}(z) \), together with the corresponding operators \( T_{\beta n,am}(z) \) appropriate for rearrangement scattering, are given as solutions of the following set of coupled Lippmann-Schwinger-type equations

\[
T_{\beta n,am}(z) = V_{\beta n,am}(z) + \sum_{\gamma=1}^{3} \sum_{rs} V_{\beta n,\gamma r}(z) G_{0;\gamma rs}(z) T_{\gamma s,am}(z).
\]

The sums over \( r \) and \( s \) extends at least over all bound states of subsystem \( \gamma \), consisting of particles \( \alpha \) and \( \beta \). Thus, the solution of (3) yields simultaneously the transition amplitudes for all two-fragment reactions. We note in parentheses that in the presence of Coulomb forces, the standard methods of integral equations theory can not be applied directly to (3) to obtain the physical reaction amplitudes, due to lack of compactness of their kernel (for a proper procedure in this case see Alt (1978), Alt et al (1978,1980)).
In leading order in an iterative solution of eq. (3), the on-shell amplitudes describing elastic and inelastic processes are given by the on-shell ‘diagonal’ effective potential

\[ T_{\alpha n, \alpha m}(q'_\alpha, q_\alpha; E) \approx V_{\alpha n, \alpha m}(q'_\alpha, q_\alpha; E) \]

\[ = \langle q'_\alpha|\langle \psi_{\alpha n}|U_{\alpha \alpha}'(E + i0)|\psi_{\alpha m}\rangle|q_\alpha\rangle. \]  

(4)

The auxiliary three-body operators \( U'_{\beta \alpha} \) satisfy the equations

\[ U'_{\beta \alpha}(z) = \bar{\delta}_{\beta \alpha} G_0^{-1}(z) + \sum_{\gamma=1}^{3} \bar{\delta}_{\beta \gamma} T'_\gamma(z) G_0(z) U'_{\gamma \alpha}(z). \]  

(5)

Here, \( G_0(z) = (z - H_0)^{-1} \) denotes the free three-body resolvent, and \( \bar{\delta}_{\beta \alpha} = 1 - \delta_{\beta \alpha} \) the anti-Kronecker symbol. \( T'_\gamma(z) \) is the sum of the two-particle off-shell Coulomb transition operator \( T^C_\gamma(z) \) plus a ‘remainder short-range transition operator’ in subsystem \( \gamma \). For the definition of the effective free Green function \( G_{0;\gamma,rs}(z) \) and further details we refer to Alt (1978), Alt et al (1978). We only mention that the nondiagonal effective-potential parts \( V_{\beta n, \alpha m}(z) \) with \( \beta \neq \alpha \), which are the driving terms relevant for rearrangement scattering, are defined similarly to (4) in terms of the operators \( U'_{\beta \alpha}(z) \). They are, however, not considered in the present investigation.

A Neumann series expansion of (5) leads to the following representation of the ‘diagonal’ on-shell effective potentials

\[ V_{\alpha n, \alpha m}(q'_\alpha, q_\alpha; E) = \sum_{\gamma=1}^{3} \bar{\delta}_{\gamma \alpha} \langle q'_\alpha|\langle \psi_{\alpha n}|T^C_\gamma(E + i0)|\psi_{\alpha m}\rangle|q_\alpha\rangle + \cdots. \]  

(6)

Explicitly shown are here only the leading Coulomb contributions due to (Coulomb) single-scattering in the intermediate state, which will be dealt with in the following investigation. The dots indicate single-scattering contributions from the remainder short-range transition operator as well as higher-order rescattering terms. We note in parentheses that, if only two of the three particles are charged, and if the shorter-ranged interactions are represented in purely separable form, the infinite series for \( V_{\alpha n, \alpha m}(q'_\alpha, q_\alpha; E) \) collapses exactly to just the terms written down explicitly in (3). Furthermore, the terms (3) would occur as the Coulomb single-rescattering contributions to the (in-)elastic scattering amplitude in a multiple-scattering approach.

Let us introduce for the terms on the right-hand side of (3) the notation...
\[
V_{\gamma, \nu}^{TC}(q'_{\alpha}, q_{\alpha}; E) = \langle q'_{\alpha} | \langle \psi_{\alpha n} | T_{\gamma}^{C} (E + i0) | \psi_{\alpha m} \rangle | q_{\alpha} \rangle \\
= \int \frac{d^{3}k}{(2\pi)^{3}} \psi_{\alpha n}^{*}(p'_{\alpha}) \hat{T}_{\gamma}^{C}(p'_{\gamma}, p_{\gamma}; E + i0 - \frac{k^{2}}{2M_{\gamma}}) \psi_{\alpha m}(p_{\alpha}). \quad (7)
\]

The various subsystem momenta are defined as

\[
p_{\alpha} = \epsilon_{\alpha \gamma} \left(k + \frac{\mu_{\alpha}}{m_{\beta}} q_{\alpha}\right), \quad p'_{\alpha} = \epsilon_{\alpha \gamma} \left(k + \frac{\mu_{\alpha}}{m_{\beta}} q'_{\alpha}\right),\\
p_{\gamma} = \epsilon_{\gamma \alpha} \left(q_{\alpha} + \frac{\mu_{\gamma}}{m_{\beta}} k\right), \quad p'_{\gamma} = \epsilon_{\gamma \alpha} \left(q'_{\alpha} + \frac{\mu_{\gamma}}{m_{\beta}} k\right). \quad (8)
\]

Here, \(\mu_{\alpha} = m_{\beta} m_{\gamma} / (m_{\beta} + m_{\gamma})\) is the reduced mass of the pair \((\beta \gamma)\). For convenience, the antisymmetric symbol \(\epsilon_{\beta \alpha} = -\epsilon_{\alpha \beta}\), with \(\epsilon_{\alpha \beta} = +1\) if \((\alpha, \beta)\) 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 graphical representation of \(V_{\gamma, \nu}^{TC}\) is given in Fig. 1.

Similarly we define the quantities \(V_{\gamma, \nu}^{VC}(q'_{\alpha}, q_{\alpha})\) by the expression (7) but with the Coulomb T-matrix \(T_{\gamma}^{C}\) replaced by the Coulomb potential \(V_{\gamma}^{C}\). They will be referred to as the ‘Coulomb-Born approximation’. We mention that for simple types of bound state wave functions \(V_{\gamma, \nu}^{VC}(q'_{\alpha}, q_{\alpha})\) can be calculated analytically (Lewis 1956).
III. THE TWO-PARTICLE COULOMB T-MATRIX

In the literature there exist several equivalent expressions for the fully off-shell two-body Coulomb T-matrix in momentum space. A fairly complete account of results concerning two-body Coulomb scattering can be found in van Haeringen (1985). We will take the relevant formulae from van Haeringen (1979), and Kok and van Haeringen (1980) (see also van Haeringen and van Wageningen (1975), Chen and Chen (1972)), which were developed there with regard to their applicability for the evaluation of expressions like the effective potential (7). Recall that we confine ourselves in the present investigation to case that the two particles participating in the intermediate-state rescattering have charges of equal sign.

The following T-matrix representation is used,

\[ \hat{T}_\gamma^C(p',p;\hat{E}_\gamma + i0) = V_\gamma^C(\Delta) \left\{ 1 + \frac{I(y)}{x} \right\}, \]  

(9)

with

\[ V_\gamma^C(\Delta) = \frac{4\pi e_\alpha e_\beta}{\Delta^2}, \]  

(10)

\[ I(y) = F_{in_\eta}(y) - F_{in_\eta}(y^{-1}). \]  

(11)

Here, \( \Delta = p' - p \) is the momentum transfer; \( \hat{E}_\gamma \) is the center-of-mass energy of the interacting pair of particles \( \alpha \) and \( \beta \), and \( \eta_\gamma = e_\alpha e_\beta \sqrt{\mu_\gamma/2\hat{E}_\gamma} \) the appropriate Coulomb parameter. Moreover, we have introduced the abbreviations

\[ x^2 = 1 + \frac{(p'^2 - 2\mu_\gamma \hat{E}_\gamma)(p^2 - 2\mu_\gamma \hat{E}_\gamma)}{2\mu_\gamma \hat{E}_\gamma \Delta^2}, \]  

(12)

\[ y = \frac{x + 1}{x - 1}, \]  

(13)

\[ F_{in_\eta}(y) \equiv 2F_1(1, in_\eta; 1 + in_\eta; y), \]  

(14)

with \( 2F_1(a,b;c;y) \) being the hypergeometric function. Note that in writing down the formulae of this section we always assume \( \hat{E}_\gamma \neq 0 \) (formulae suitable for \( \hat{E}_\gamma \) in the vicinity of zero can be found in van Haeringen (1979)). For \( \Re in_\eta > 0 \) the integral representation for the hypergeometric function is particularly useful.
\[ F_{\eta\gamma}(y) = i\eta_{\gamma} \int_{0}^{1} dt \, t^{i\eta_{\gamma} - 1} (1 - yt)^{-1}, \quad \Re i\eta_{\gamma} > 0. \] (15)

It leads to the following expression for the Coulomb T-matrix

\[ \hat{T}_{\gamma}^{C}(p', p; \hat{E}_{\gamma} + i0) = V_{\gamma}^{C}(\Delta) \left\{ 1 - 4i\eta_{\gamma} \int_{0}^{1} dt \, \frac{t^{i\eta_{\gamma}}}{4t - (x^{2} - 1)(1 - t)^{2}} \right\}, \quad \Re i\eta_{\gamma} > 0. \] (16)

Furthermore, for \( \Re x < 0 \), which implies \( |y| < 1 \), one has the series representation for the function \( I(y) \):

\[ I(y) = 1 - (-y)^{i\eta_{\gamma}} \frac{\pi \eta_{\gamma}}{\sinh \pi \eta_{\gamma}} + 2\eta_{\gamma}^{2} \sum_{n=1}^{\infty} \frac{y^{n}}{n^{2} + \eta_{\gamma}^{2}}. \] (17)

We mention that off the energy shell, in the limit of vanishing momentum transfer, the following behaviour is easily derived:

\[ \frac{I(y)}{x} \overset{\Delta \to 0}{\sim} \Delta \left\{ c_{1} + c_{2} \ln \Delta + c_{3}\Delta + o(\Delta) \right\}, \] (18)

that is, the most singular part of the repulsive Coulomb T-matrix is given by the potential, for all (off-shell) subsystem energies \( \hat{E}_{\gamma} \). This leads for the ratio \( R = \hat{T}_{\gamma}^{C}(p', p; \hat{E}_{\gamma} + i0)/V_{\gamma}^{C}(\Delta) \) to the well-known result

\[ |R| \overset{\Delta \to 0}{=} 1 + O(\Delta) \quad \forall \quad E_{\gamma}. \] (19)

Of course, on the energy shell one has \( |R| = 1 \) for all scattering angles and energies.

Kok and van Haeringen (1980) (see also van Haeringen and Kok (1984), van Haeringen (1985)) have derived useful general bounds on \( R \). Introduce the notation \( \cos \vartheta = p' \cdot p / pp' \).

For instance, they have proved the following inequalities valid for a repulsive Coulomb interaction:

\[ 0 \leq R \leq 1, \quad \forall \quad p, p', \cos \vartheta \quad \text{for} \quad \hat{E}_{\gamma} < 0, \quad e_{\alpha}e_{\beta} > 0, \] (20)

\[ 0 \leq |R| \leq 1, \quad \forall \quad p, p', \cos \vartheta \quad \text{for} \quad \hat{E}_{\gamma} > 0, \quad e_{\alpha}e_{\beta} > 0, \] (21)

which contain (19) as special case. Illustrative graphical representations for the ratio \( R \) are given in Kok and van Haeringen (1980).
IV. GENERAL PROPERTIES OF $V^{TC}_{\gamma,nm}$ AND $V^{VC}_{\gamma,nm}$

In this section we will discuss some general properties of the lowest-order contributions to the elastic effective potential, graphically represented by Fig. 1, and investigate the effects which arise from the replacement of the Coulomb T-matrix by the Coulomb potential.

Introducing the Coulomb T-matrix representation (9) into expression (7) one sees that the Coulomb potential can be taken out of the integral. Hence we can write

$$V^{TC}_{\gamma,nm}(q'_\alpha, q_\alpha; E) = V^C_{\gamma}(\Delta_\alpha) F^{TC}_{\gamma,nm}(q'_\alpha, q_\alpha; E),$$

(22)

where

$$F^{TC}_{\gamma,nm}(q'_\alpha, q_\alpha; E) = \int \frac{d^3k}{(2\pi)^3} \psi^*_{\alpha n}(p'_\alpha) \left\{ 1 + \frac{I(y)}{x} \right\} \psi_{\alpha m}(p_\alpha),$$

(23)

with

$$x^2 = 1 + \frac{[(p^2_\gamma - 2\mu_\gamma(E + i0 - k^2/2M_\gamma)) \left[ p^2_\gamma - 2\mu_\gamma(E + i0 - k^2/2M_\gamma) \right]}{2\mu_\gamma(E + i0 - k^2/2M_\gamma) \Delta^2_\alpha},$$

(24)

$$\Delta_\alpha = \epsilon_{\gamma\alpha}(q'_\alpha - q_\alpha).$$

(25)

$y$ is defined as before, cf. eq. (13), and $V^C_{\gamma}$ by (11). Similarly, $V^{VC}_{\gamma,nm}$ can be written as

$$V^{VC}_{\gamma,nm}(q'_\alpha, q_\alpha) = V^C_{\gamma}(\Delta_\alpha) F^{VC}_{\gamma,nm}(q'_\alpha, q_\alpha),$$

(26)

with

$$F^{VC}_{\gamma,nm}(q'_\alpha, q_\alpha) = \int \frac{d^3k}{(2\pi)^3} \psi^*_{\alpha n}(p'_\alpha) \psi_{\alpha m}(p_\alpha)$$

$$= \int \frac{d^3k}{(2\pi)^3} \psi^*_{\alpha n}(k) \psi_{\alpha m}(k + \mu_\alpha \Delta_\alpha/m_\beta)$$

(27)

for $m = n$ being called bound state form factor, and for $m \neq n$ transition form factor. In the following investigation we will mainly be concerned with the ratio

$$R_{\gamma,nm}(q'_\alpha, q_\alpha; E) := \frac{V^{TC}_{\gamma,nm}(q'_\alpha, q_\alpha; E)}{V^{VC}_{\gamma,nm}(q'_\alpha, q_\alpha)} = \frac{F^{TC}_{\gamma,nm}(q'_\alpha, q_\alpha; E)}{F^{VC}_{\gamma,nm}(q'_\alpha, q_\alpha)}.$$

(28)

Let us state some general results for $R_{\gamma,nm}$. 

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(i) For elastic scattering, both $V_{\gamma,mm}^{TC}$ and $V_{\gamma,mm}^{VC}$ diverge for $q'_{\alpha} - q_{\alpha} \to 0$ because of (9) and (11); however, as eq. (4) with (18) implies, their ratio tends in magnitude towards the value one,

$$|R_{\gamma,mm}(q'_{\alpha}, q_{\alpha}; E)| \to 1 \quad \text{for} \quad q'_{\alpha} \to q_{\alpha} \quad \forall \ E.$$  \hspace{1cm} (29)

(ii) The inequalities (20) and (21) result in the following inequalities for the elastic ratio $R_{\gamma,00}$, where the index 0 denotes the ground state:

$$0 < R_{\gamma,00}(q'_{\alpha}, q_{\alpha}; E) \leq 1, \quad \text{for} \quad E < 0,$$

$$0 < |R_{\gamma,00}(q'_{\alpha}, q_{\alpha}; E)| \leq 1, \quad \text{for} \quad E > 0.$$  \hspace{1cm} (30) (31)

That is, for elastic scattering off a target in the ground state the Coulomb-Born approximation always overestimates the exact driving term. Or, in other words, the error made by approximating in (7) the two-body Coulomb T-matrix by the Coulomb potential is of known sign. Note that no analogous bounds result if either one or both bound state wave functions have nodes.

(iii) Since for large two-body subsystem energies $T_{\gamma}^{C}$ approaches the Born approximation $V_{\gamma}^{C}$, we expect for elastic and inelastic scattering

$$R_{\gamma,nm}(q'_{\alpha}, q_{\alpha}; E) \xrightarrow{E \to \infty} 1.$$  \hspace{1cm} (32)

However, it is obvious that for (32) to hold the energy $E$ must be higher than that for which on the two-body level we have $T_{\gamma}^{C}(\hat{E}_{\gamma}) \approx V_{\gamma}^{C}$. For, in $V_{\gamma,mm}^{TC}(q'_{\alpha}, q_{\alpha}; E)$ the Coulomb T-matrix enters for all $\gamma$-subsystem energies from $E$ down to minus infinity, $-\infty < \hat{E}_{\gamma} = E - k^2/2M_{\gamma} \leq E$. Thus a behaviour like (32) can result only as a combined effect of $\hat{T}_{\gamma}^{C}(E - k^2/2M_{\gamma})$ being approximately equal to $V_{\gamma}^{C}$ over the whole range of momenta $k$ for which the momentum-space bound state wave functions differ appreciably from zero.

(iv) For excitation we deduce from (27)

$$\lim_{q'_{\alpha} \to q_{\alpha}} F_{\gamma,mm}^{VC}(q'_{\alpha}, q_{\alpha}) = 0 \quad \text{for} \quad n \neq m.$$  \hspace{1cm} (33)
because of the orthogonality of the bound state wave functions. Of course, on the energy shell \( (2) \) the momentum transfer can never vanish. However, in forward direction its magnitude, though remaining non-zero, can become small, thereby making \( R_{\gamma,nm}(q'_{\alpha}, q_{\alpha}; E) \) rather large. Furthermore, since the inequalities \((20)\) and \((21)\) do not result in inequalities like \((30)\) or \((31)\) for the ratio \( R_{\gamma,nm} \), values smaller and larger than one are possible.
V. NUMERICAL RESULTS

When performing the integration over the magnitude of the momentum $k$ of the non-interacting particle $\gamma$ in the exact driving term \([\text{7}]\) we must, for a given three-body energy $E > 0$, treat the two regions $2M, E < k^2 < \infty$ (region I) and $k^2 < 2M, E$ (region II) which correspond to negative and positive subsystem energy $\hat{E}_\gamma = E - k^2/2M$, differently. In region II, choosing $\Re x < 0$, the representation \([\text{17}]\) for the two-body Coulomb T-matrix can be used. In order to select an expression suitable for region I we first note that the Coulomb parameter $\eta_\gamma$ occurring in $\hat{T}^C_\gamma$ depends on the integration variable $k$ via

$$\eta_\gamma = e_\alpha e_\beta \mu / \sqrt{2\mu_\gamma (E + i0 - k^2/2M)}.$$  \hspace{1cm} (34)

Thus, $\eta_\gamma$ is imaginary. Since, as mentioned at the beginning, we restrict ourselves to that part of the elastic effective potential which contains Coulomb rescattering between the projectile and the target particle whose charge is of equal sign, i.e., $e_\alpha e_\beta > 0$, in region I the condition $\Re i\eta_\gamma > 0$ is always fulfilled so that the representation \([\text{16}]\) is applicable. Of course, if expression \([\text{7}]\) is calculated for a negative three-body energy $E < 0$, only region I is relevant.

In order to show that the numerical quadratures can be performed reliably even for positive three-body energies (where the integration contour touches the essential singularity of the Coulomb T-matrix at zero subsystem energy), we present in Fig. 2 as a typical example the real and the imaginary part of \([\text{7}]\), with all integrations except the one over the magnitude of $k$ having been performed, as function of $k$. We choose the elastic reaction $H(e, e)\bar{H}$ to be discussed below, for a center-of-mass projectile energy of 100 eV and a scattering angle of 20 degree. Inspection reveals that the real part of this integrand and its first derivative are very smooth in the neighbourhood of that momentum for which the subsystem energy $E - k^2/2M = 0$, in spite of the fact that, as discussed above, on either side of this point a completely different expression for the two-body Coulomb T-matrix is used. A similarly smooth behaviour is observed for the imaginary part. For other energies and scattering angles, and for other projectiles, qualitatively similar results are obtained (or course, if the projectile energy is smaller than the magnitude of the binding energy.
of the incoming bound state, which corresponds to negative total three-body energy, the imaginary part of the integrand is identically zero). For comparison we also include the analogous (real) integrand of the Coulomb-Born approximation (26) which, as is to be expected from (21), is so much larger in magnitude than the real part of the exact expression that the absolute value of the ratio (28) is smaller than one, in accordance with (31). We furthermore mention that it was carefully checked that the driving term (7) behaved smoothly and yielded the same value when the ionisation threshold was approached from below and from above.

A. Atomic reactions

For definiteness we consider only reactions where the bound states in the initial and in the final state are described by hydrogen-like wave functions. Let us begin by assuming the bound states to be in their ground states before and after the collision, i.e., we take \( m = n = \{100\} \) (with the usual notation \( \{n\ell m\} \) for the set of hydrogenic quantum numbers). Thus

\[
\psi_{\alpha m}(p) \equiv \psi_{100}(p) = \frac{8\pi^{1/2}\kappa_{\alpha 0}^{5/2}}{(p^2 + \kappa_{\alpha 0}^2)^2},
\]

and the same expression for the outgoing bound state. Here, \( \kappa_{\alpha 0}^2 = -2\mu_\alpha \tilde{E}_{\alpha 0} = (\mu_\alpha e_\beta e_\gamma)^2 \), \( \tilde{E}_{\alpha 0} \) being the Coulomb ground state energy of the bound pair \((\beta\gamma)\). Introducing the wave functions (35) into expressions (7) and (26) for the exact and the approximate driving terms, we can integrate analytically over the azimuthal angular integration variable. The remaining three-dimensional integrals have to be done numerically. It is to noted that for a few selected cases we have verified that our results coincide with those of Sinfailam and Chen (1972) within the accuracy with which the numbers can be extracted from their figures.

In Fig. 3 we present the ratio \( |R_{ee,00}(q'_\alpha, q_\alpha; E)| \) for elastic scattering of electrons off hydrogen atoms in their ground state, as function of the center-of-mass scattering angle \( \vartheta \) (with \( \cos \vartheta = q_\alpha \cdot q'_\alpha / q_\alpha q'_\alpha \)) and of the center-of-mass projectile energy, starting at the elastic threshold. Here and in the following, the notation is such that the two particles,
which undergo Coulomb scattering in the intermediate state and which are denoted by the subsystem index \( \gamma \) in (28), are explicitly indicated. Furthermore, the ground state quantum numbers \( \{100\} \) in the initial and the final state are abbreviated by the index ‘0’. As is apparent, for each energy \( |R_{ee,00}(q'_\alpha, q_\alpha; E)| \) starts in the forward direction at the value one, thus satisfying the condition (29). For energies beyond 100 keV the ratio becomes practically equal to one again, in accordance with (32). Away from these regions this figure allows us to estimate the error made when using the Born approximation for the Coulomb T-matrix in the driving term (7). Inspection reveals that over a wide range of angles and energies the Coulomb-Born approximation dramatically overestimates the exact rescattering contribution. It is interesting to note that the minimum value of \( |R_{ee,00}(q'_\alpha, q_\alpha; E)| \) of approximately 0.27 is reached not in the backward direction but at an angle of about 60 degree (for a projectile energy of around 70 eV).

The effect of increasing the mass of one of the particles undergoing intermediate-state Coulomb scattering can be inferred from Fig. 4. There we show the ratio \( |R_{pe+,00}(q'_\alpha, q_\alpha; E)| \) for positron-hydrogen scattering, with the positron scattering off the proton. It is apparent that the picture is similar to the previous case, but minimum has deepened (to about 0.054 around 60 eV) and occurs in backward direction.

The case of two heavy particles experiencing Coulomb scattering in the intermediate state is presented in Fig. 5, which contains the ratio \( |R_{pp,00}(q'_\alpha, q_\alpha; E)| \) for proton-hydrogen scattering. Evidently, the mass effect is very pronounced, the Coulomb-Born approximation failing completely nearly everywhere, even at extremely small scattering angles for higher energies. The inadequacy of the Coulomb-Born approximation becomes still more pronounced if one of the heavy particles has a charge of magnitude greater than one. This can be inferred from \( |R_{p+C^{6+},00}(q'_\alpha, q_\alpha; E)| \) for the elastic reaction \( C^{6+} + H(1s) \), with \( C^{6+} \) considered as a structureless particle, which is displayed in Fig. 6. In both cases the minimum (of the order \( 10^{-6} \) or less) occurs at 180 degree.

In order to study the quality of the Coulomb-Born approximation for excitation we calculated the exact and the approximate driving terms (7) and (26) by assuming that the outgoing bound state is in a 2s-state, characterized by a wave function
\[
\psi_{\alpha n}(p) \equiv \psi_{200}(p) = 64(2\pi\kappa_{\alpha 0}^5)^{1/2} \frac{4p^2 - \kappa_{\alpha 0}^2}{(4p^2 + \kappa_{\alpha 0}^2)^3}.
\] (36)

To simplify the notation, the bound state quantum numbers \{200\} will be abbreviated by the index ‘1’. We have already pointed out in Sect. [X] that for excitation the magnitude of the ratio (28) is no longer bounded from above by the value one. In fact, the Coulomb-Born approximation becomes very small in forward direction, thereby giving rise to large values of the ratio. This situation is exemplified in Fig. 7 where we have plotted \(|R_{ee,01}(\mathbf{q}_\alpha', \mathbf{q}_\alpha; E)|\) for excitation of hydrogen atoms from the 1s- to the 2s-state by electron impact. It is seen to take on values larger and smaller than one. The value one is again reached at higher energies similar to those for elastic scattering shown in Fig. 3. Furthermore, although barely visible in the figure, \(|R_{ee,01}(\mathbf{q}_\alpha', \mathbf{q}_\alpha; E)|\) develops a minimum of 0.27 at 45 eV projectile energy and 90 degree. Interestingly, this minimum value coincides with that for the elastic ratio and, as was the case there, occurs at non-backward angles. Since, when approaching the forward direction, \(|R_{ee,01}(\mathbf{q}_\alpha', \mathbf{q}_\alpha; E)|\) increases sharply, this figure has been cut off at a scattering angle of 1 degree. It is clear that the larger the energy is, the relatively smaller values of the momentum transfer are accessible and thus the smaller the Coulomb-Born approximation becomes (cf. eq. (33)). Of course, for sufficiently high energy the near-vanishing of \(V^{ec}_{ee,01}(\mathbf{q}_\alpha, \mathbf{q}_\alpha; E)\) in the forward direction has to be counterbalanced by a corresponding near-vanishing of \(V^{ec}_{ee,01}(\mathbf{q}_\alpha', \mathbf{q}_\alpha; E)\), in order that their ratio eventually approaches the value one. We only mention that a similar picture is obtained for the ratio \(|R_{pp,01}(\mathbf{q}_\alpha', \mathbf{q}_\alpha; E)|\) for excitation of hydrogen atoms from their ground to the same excited state by proton impact.

Since due to these kinematic effects the ratio (28) is no longer an appropriate quantity to visualize the quality of the Coulomb-Born approximation (except for scattering angles larger than, say, 90 degree), we plot in Fig. 8 only the absolute value of the exact driving term \(|V^{TC}_{ee,01}(\mathbf{q}_\alpha', \mathbf{q}_\alpha; E)|\) for excitation of hydrogen atoms by electron impact, as function of the scattering angle and the projectile energy. It is a very smooth quantity, however ranging over 14 orders of magnitude in the range of parameters considered. The mass effect is again illustrated by considering the exact driving term \(|V^{TC}_{pp,01}(\mathbf{q}_\alpha', \mathbf{q}_\alpha; E)|\) for excitation of hydrogen atoms by proton impact, displayed in Fig. 9. Not only is the
range of accessible values smaller than in the previous case; but there appears also to be more structure in the amplitude. We point out that, at small scattering angles, the exact driving terms for both reactions increase in magnitude with increasing the energy, and decrease only at rather high energies; the energy where the maximum is reached lies the higher the smaller the angle is.

B. Nuclear reactions

In order to investigate whether these rather large deviations from the value one of $|R_{\gamma,00}|$ do hold also for other systems, we considered two examples of elastic deuteron-nucleus scattering, i.e., one of the three particles is a neutron. The nuclear interactions are assumed to be given in separable form. Recall that under such conditions, the expression (7), with $\gamma$ denoting the proton-nucleus subsystem, represents the exact ‘diagonal’ contribution to the on-shell effective potential. The deuteron bound state wave function used here is the same as that considered, e. g., by Alt et al (1985) in their calculation of elastic proton-deuteron scattering observables. That is, the deuteron is assumed to be in an pure S state, with a momentum space wave function

$$\psi_0(p) = \frac{N}{(p^2 + \kappa_d^2)(p^2 + \beta^2)}.$$ (37)

Here, $\kappa_d = \sqrt{-m_N \hat{E}_d}$, with $\hat{E}_d = -2.226$ MeV being the deuteron binding energy and $m_N$ the nucleon mass; $N$ is a normalisation constant, and $\beta$ a parameter fitted to the low energy neutron-proton scattering parameters in the $^3S_1$-state.

First we look at proton-deuteron scattering. With this bound state wave function we have calculated the ratio $|R_{pp,00}(q'_\alpha, q_\alpha; E)|$ with proton-proton intermediate-state Coulomb scattering, again as function of the center-of-mass scattering angle and proton bombarding energy. Note that the threshold for the deuteron breakup is at a center-of-mass proton kinetic energy of $2.226$ MeV. The results are shown in Fig. 10. Clearly, $|R_{pp,00}(q'_\alpha, q_\alpha; E)|$ satisfies the general constraints (29), (30), (31) and (32). But, as is apparent, it differs only very little from the value one, the maximal deviation of 12 percent occurring at energies between 6 and 7 MeV, in backward direction. The conclusion
is that for such a reaction the use of the approximation $T^C_\gamma \rightarrow V^C_\gamma$ in (7) appears to be well justified.

Similarly to the atomic case, the Coulomb-Born approximation quickly ceases to be acceptable if the charge of one of the charged particles is increased. This is illustrated in Fig. 11, where we show the ratio $|R_{p,C^{6+},00}(q'_\alpha, q_\alpha; E)|$ for the reaction of $C^{6+}$ colliding with deuterons (again, $C^{6+}$ is considered a structureless nucleus). Here, the ratio drops to 0.47 (at 12 MeV and a scattering angle of 67 degree).
VI. DISCUSSION

We have investigated the quality of the replacement of the two-particle Coulomb amplitude by the Coulomb potential in the driving term for elastic and inelastic scattering, both for atomic and nuclear three-body reactions. We have found the following interesting results.

(i) For the atomic reactions studied, the Coulomb-Born approximation quite generally turns out to be completely unsatisfactory. Its failure becomes the more striking the heavier the masses of the particles involved in the intermediate-state Coulomb scattering are, and - not surprisingly - the higher their charge is.

(ii) In the nuclear cases considered the situation is much more favourable. At least for proton-deuteron scattering the Coulomb-Born approximation, which on the energy shell has been shown to be generally accurate to better than 10 per cent, is fully justified (this is particularly so, since the effective-potential part itself represents only a correction to the dominant driving term, which is induced by the nuclear interaction; in fact, its Coulomb-Born approximation is known to contribute something of the order of 10 per cent to the final proton-deuteron observables, cf. Alt et al 1985). Of course, also here its quality is diminished if the charge of one of the particles is increased, but the effect is not so dramatic as for the analogous atomic system.

(iii) For atomic as well as nuclear elastic scattering processes it has been found that the exact driving term becomes equal to the approximate one, eq. (26), not only in forward direction and for higher energies, but also if the projectile energy goes to zero or, in other words, if the elastic threshold is approached, for arbitrary scattering angle. We have not yet succeeded in developing a convincing argument for this unexpected fact. A first suggestion, however, is based on the known invariance of the ratio \( \tilde{T}^C(\mathbf{p}', \mathbf{p}; \tilde{E}_\gamma + i0)/V^C(\mathbf{p}', \mathbf{p}) \) under the transformations \( p/k \rightarrow k/p, \quad p'/k \rightarrow k/p' \), with \( k = \sqrt{2m_\gamma \tilde{E}_\gamma} \) (cf, e.g., Kok and van Haeringen 1980), which correlate high-energy \( (k \rightarrow \infty) \) with low-energy properties \( (k \rightarrow 0) \). This speculation is supported by the fact that the value one of the ratio is reached for the larger and the smaller projectile energies, respectively, the larger the scattering angle becomes.
(iv) The minimum of the elastic ratio \( \text{28} \) is in all cases attained for energies above the dissociation threshold, frequently but not always in the backward direction.

(v) For excitation the Coulomb-Born approximation is of similar quality as for the corresponding elastic reaction, except for the additional failure in the near-forward direction. Moreover, in this case the ratio \( \text{28} \) does not approach the value one at the reaction threshold.

(vi) In all reactions considered the ratio \( \text{28} \), and hence also the exact driving term \( \text{7} \), behave smoothly when the bound state dissociation threshold is crossed.

(vii) In general, the imaginary part of the exact driving term \( \text{7} \) is much smaller than its real part (the Coulomb-Born approximation \( \text{26} \) is real everywhere), except in the region of parameters where the ratio approaches its minimum value. There they become comparable in magnitude.

From the numerical point of view it may be of interest to note that the use of the Coulomb T-matrix in the calculation at least of the on-shell driving term \( \text{7} \) for particles with charges of equal sign, does not present any problem with modern computers. Whether this holds true also for the calculation of similar expressions but with oppositely charged particles, or for the corresponding off-shell quantities (which would be needed as input in the three-body integral equations approach) remains to be seen.

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Figure Captions

Fig. 1. Graphical representation of the elastic and inelastic driving term $V_{T^C}^{\gamma, nm}$.

Fig. 2. The integrand of $V_{ee,00}^{T^C}(q'_\alpha, q_\alpha; E)$ (cf. eq. (7)) for $e + H(1s) \rightarrow e + H(1s)$ as a function of the magnitude of the momentum $k$ of the proton (the integrations over all other variables are already performed) at incident c.m. energy of 100 eV and at c.m. scattering angle 20 deg. Upper curve is the real part, and lower curve the imaginary part of the integrand. Also shown is the analogous integrand for the Coulomb-Born approximation $V_{ee,00}^{V^C}(q'_\alpha, q_\alpha; E)$, reduced by a factor of 5. The arrow indicates the point where the ee-subsystem energy is zero. The integrand and $k$ are in a.u.

Fig. 3. The ratio $|R_{ee,00}(q'_\alpha, q_\alpha; E)|$ as a function of c.m. incident energy and c.m. scattering angle for elastic electron + $H(1s)$ scattering.

Fig. 4. The ratio $|R_{p,e^+,00}(q'_\alpha, q_\alpha; E)|$ as a function of c.m. incident energy and c.m. scattering angle for elastic positron + $H(1s)$ scattering.

Fig. 5. The ratio $|R_{pp,00}(q'_\alpha, q_\alpha; E)|$ as a function of c.m. incident energy and c.m. scattering angle for elastic proton + $H(1s)$ scattering.

Fig. 6. The ratio $|R_{p,C^6+,00}(q'_\alpha, q_\alpha; E)|$ as a function of c.m. incident energy and c.m. scattering angle for elastic scattering of $C^6+$ off $H(1s)$.

Fig. 7. The ratio $|R_{ee,01}(q'_\alpha, q_\alpha; E)|$ as a function of c.m. incident energy and c.m. scattering angle for the inelastic reaction $e + H(1s) \rightarrow e + H(2s)$.

Fig. 8. The amplitude $V_{ee,01}^{T^C}$ as a function of c.m. incident energy and c.m. scattering angle for the inelastic reaction $e + H(1s) \rightarrow e + H(2s)$.

Fig. 9. The amplitude $V_{pp,01}^{T^C}$ as a function of c.m. incident energy and c.m. scattering angle for the inelastic reaction $p + H(1s) \rightarrow p + H(2s)$.

Fig. 10. The ratio $|R_{pp,00}(q'_\alpha, q_\alpha; E)|$ as a function of c.m. incident energy and c.m. scattering angle for elastic proton-deuteron scattering.

Fig. 11. The ratio $|R_{p,C^6+,00}(q'_\alpha, q_\alpha; E)|$ as a function of c.m. incident energy and c.m. scattering angle for elastic $C^6+ - d$ scattering.