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Multiple-Scattering Expansions for Nonrelativistic Three-Body Collision Problems. V. An Off-Shell Approach to the Faddeev-Watson Expansions*

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Explicit relations between the on-shell and off-shell three-body scattering and rearrangement-collision amplitudes are given. It is shown that the off-shell approach to the determination of the on-shell amplitudes is equivalent to the conventional method of taking on-shell matrix elements. As an example, the bare-potential term of the Faddeev-Watson multiple-scattering expansion for rearrangement collisions is evaluated using the two alternative approaches.

I. INTRODUCTION

In a series of papers,[1-4] we have recently reviewed and investigated the application of the Faddeev-Watson multiple-scattering expansions to high-energy three-body atomic scattering and rearrangement collisions. In these papers, the three-body collision amplitudes are determined by evaluating the appropriate on-shell matrix elements. In another series of papers[5-8] concerning the application of the Faddeev equations to low-energy three-body scattering and rearrangement collisions, the collision amplitudes are determined by taking the limit of the off-shell three-body amplitude on the energy shell. These two alternative methods of determining the collision amplitudes are, of course, equivalent. However, a recent paper by Shastry and Rajagopal[9] has questioned this equivalence. The purpose of this paper is to make this equivalence more explicit. Since the difficulty in seeing the equivalence of the off-shell method with the conventional method of taking matrix elements appears to have come from the bare-potential term in the expansion for rearrangement collisions, we demonstrate the equivalence of the two methods by obtaining the result of this bare-potential term from the corresponding term in the Faddeev-Watson expansion for the off-shell three-

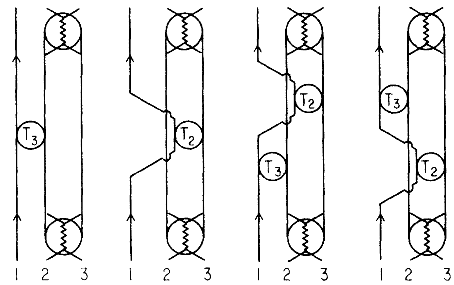

FIG. 1. Diagrams for the successive terms in the Faddeev-Watson multiple-scattering expansion for the off-shell scatterings amplitude. The bubbles are the two-body scattering matrices.

body rearrangement-collision amplitude. It perhaps is worthwhile to note that the claim of Shastry and Rajagopal[9] that the two-body Coulomb T matrix in the plane-wave representation is zero on the energy shell has been shown[3,10] to be erroneous.

II. MULTIPLE-SCATTERING EXPANSION FOR OFF-SHELL THREE-BODY AMPLITUDES

The off-shell three-body collision amplitudes may be denoted by $\mathcal{T}(\vec{p}_j\vec{q}_j,\vec{p}_i\vec{q}_i;E)$, where E is an energy argument and the momentum pairs $(\vec{p}_i,\vec{q}_i)$ have the significance that $\vec{p}_i$ represents the relative momentum between particles j and k and $\vec{q}_i$ represents the relative momentum between particle i and the two-body subsystem (j,k). We found it is convenient to take for $\vec{p}_i$ and $\vec{q}_i$ the mass-scaled momentum variables defined in a cyclic order as

$$\vec{p}_i=\frac{m_k\vec{k}_j-m_j\vec{k}_k}{[2m_jm_k(m_j+m_k)]^{1/2}}\,,$$
$$\vec{q}_i=\frac{m_i(\vec{k}_j+\vec{k}_k)-(m_j+m_k)\vec{k}_i}{[2m_i(m_j+m_k)(m_i+m_j+m_k)]^{1/2}}\,, \tag{2.1}$$

where m_1, m_2, and m_3 and $\vec{k}_1$, $\vec{k}_2$, and $\vec{k}_3$ are the masses and asymptotic momenta of the three particles. These mass-scaled momentum variables are linearly dependent on each other with the relations (in a cyclic order)

$$\vec{p}_i=-\alpha_{ij}\vec{p}_j-\beta_{ij}\vec{q}_j=-\alpha_{ki}\vec{p}_k+\beta_{ki}\vec{q}_k\,,$$
$$\vec{q}_i=-\alpha_{ij}\vec{q}_j+\beta_{ij}\vec{p}_j=-\alpha_{ki}\vec{q}_k-\beta_{ki}\vec{p}_k\,, \tag{2.2}$$

where the mass coefficients are defined as

$$\alpha_{ij}=\left(\frac{m_im_j}{(m_i+m_k)(m_j+m_k)}\right)^{1/2},\quad \beta_{ij}=(1-\alpha_{ij}^2)^{1/2}\,. \tag{2.3}$$

The on-shell three-body collision amplitude $\mathcal{T}$ can be obtained from the off-shell amplitude $\mathcal{T}(\vec{p}_j\vec{q}_j,\vec{p}_i\vec{q}_i;E)$ by requiring its arguments to satisfy the energy-conservation relation

$$E=\kappa_f^2+\epsilon_f^{(j)}=\kappa_i^2+\epsilon_i^{(i)}\,, \tag{2.4}$$

where $\vec{\kappa}_i$ and $\vec{\kappa}_f$ are the mass-scaled asymptotic momenta of the incident and outgoing particles with respect to their corresponding two-body subsystems in the energy states $\epsilon_i^{(i)}$ and $\epsilon_f^{(j)}$, respectively. This can be accomplished by approaching the energy shell in the following manner:

$$p_i^2\to\epsilon_i^{(i)},\quad p_j^2\to\epsilon_f^{(j)}\,,$$
$$q_i^2\to E-\epsilon_i^{(i)},\quad q_j^2\to E-\epsilon_f^{(j)}\,. \tag{2.5}$$

Here E is the total energy of the three-body system.

To obtain the Faddeev-Watson multiple-scattering expansion for the off-shell three-body collision amplitudes, we construct all possible connected diagrams in terms of bubbles. Each of these bubbles represents a two-body interaction to all orders. We then group these connected bubble diagrams according to their initial- and final-state interactions.

Consider, for example, the scattering process

$$1+(2,3)\to1+(2,3)\,, \tag{2.6}$$

where for convenience we have taken pair 1 (i.e., particles 2 and 3) to be the two-body bound subsystem before and after the interaction. To obtain the multiple-scattering expansion for the scattering process given by Eq. (2.6), we collect all the possible connected bubble diagrams which begin with a bubble involving the interaction of particles 2 and 3 and ending with a bubble involving also the interaction of particles 2 and 3. Such diagrams which are shown in Fig. 1 can be summed up to give the series

$$\tilde{T}_s=T_1G_0T_2G_0T_1+T_1G_0T_3G_0T_1+T_1G_0T_2G_0T_3G_0T_1$$
$$+T_1G_0T_3G_0T_2G_0T_1+\cdots\,, \tag{2.7}$$

with

$$T_i=V_1+V_iG_0T_i\,, \tag{2.8}$$

where V_i is the two-body Coulomb potential V_{jk}, G_0 is the Green's functions for the three-body system in the absence of interaction, and T_i is the two-body T matrix in the presence of a spectator particle "i." The multiple-scattering expansion for the off-shell three-body scattering amplitude then takes the form

$$\mathcal{T}_s(\vec{p}_1'\vec{q}_1',\vec{p}_1\vec{q}_1;E)=\langle\vec{p}_1'\vec{q}_1'|\tilde{T}_s|\vec{p}_1\vec{q}_1\rangle\,. \tag{2.9}$$

Similarly, for rearrangement collisions we have

$$1+(2,3)\to(1,2)+3\,. \tag{2.10}$$

We collect all the possible connected bubble diagrams which begin with a bubble involving the interaction of particles 2 and 3 and end with a bubble involving the interaction of particles 1 and 2. These

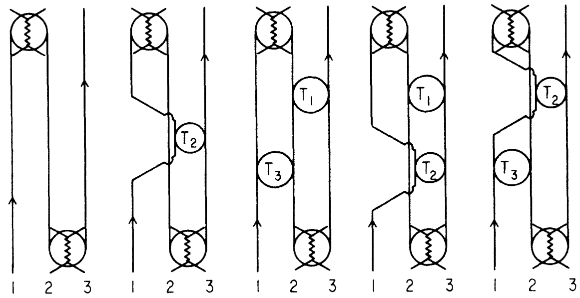

FIG. 2. Diagrams for the successive terms in the Faddeev-Watson multiple-scattering expansion for the off-shell rearrangement-collision amplitude. The bubbles are the two-body scattering matrices.

diagrams which are shown in Fig. 2 can be summed up to give the series

$$\tilde{T}_r = T_3 G_0 T_1 + T_3 G_0 T_2 G_0 T_1 + T_3 G_0 T_1 G_0 T_2 G_0 T_1 + T_3 G_0 T_1 G_0 T_3 G_0 T_1 + T_3 G_0 T_2 G_0 T_3 G_0 T_1 + \cdots \; . \tag{2.11}$$

The multiple-scattering expansion for the off-shell three-body rearrangement-collision amplitude takes the form

$$\mathcal{T}_r(\vec{p}_3\vec{q}_3, \vec{p}_1\vec{q}_1; E) = \langle \vec{p}_3\vec{q}_3 | \tilde{T}_r | \vec{p}_1\vec{q}_1 \rangle \; , \tag{2.12}$$

with $\tilde{T}_r$ given by Eq. (2.11).

III. RELATIONS BETWEEN ON-SHELL AND OFF-SHELL MULTIPLE-SCATTERING EXPANSIONS

The Faddeev-Watson multiple-scattering expansions for nonrelativistic three-body processes have recently attracted considerable enthusiasm in applications to three-body atomic and molecular scattering problems.[1–4,11,12] In all these applications, the on-shell version of the multiple-scattering expansion was used. In the on-shell approach, the transition amplitudes for scatterings and rearrangement collisions are given in terms of matrix elements.

Following the notations of Paper I, we have for the scattering amplitude the matrix element

$$\mathcal{T}_s = \langle \psi_b^{(1)} | T_s | \psi_a^{(1)} \rangle \tag{3.1}$$

and for the rearrangement-collision amplitude the matrix element

$$\mathcal{T}_r = \langle \psi_b^{(3)} | T_r | \psi_a^{(1)} \rangle \; , \tag{3.2}$$

where $\psi_a^{(\alpha)}$ are the asymptotic scattering states with α denoting the channels and a denoting the additional information to complete the description of a given channel. The Faddeev-Watson multiple-scattering expansion for the scattering transition operator T_s is

$$T_s = T_2 + T_3 + T_2 G_0 T_3 + T_3 G_0 T_2 + \cdots \; , \tag{3.3}$$

and for the rearrangement-collision transition operator T_r

$$T_r = V_1 + T_2 + T_1 G_0 T_2 + T_1 G_0 T_3 + T_2 G_0 T_3 + \cdots \; . \tag{3.4}$$

In this section, we exhibit the explicit relations between the on-shell expansions given by Eqs. (3.1)–(3.4) and the off-shell expansions given by Eqs. (2.7)–(2.12).

From Eqs. (3.1) and (3.3), we obtain the multiple-scattering expansion for the on-shell scattering amplitude

$$\mathcal{T}_s = \langle \psi_b^{(1)} | T_2 | \psi_a^{(1)} \rangle + \langle \psi_b^{(1)} | T_3 | \psi_a^{(1)} \rangle + \langle \psi_b^{(1)} | T_2 G_0 T_3 | \psi_a^{(1)} \rangle + \langle \psi_b^{(1)} | T_3 G_0 T_2 | \psi_a^{(1)} \rangle + \cdots \; . \tag{3.5}$$

The counterpart multiple-scattering expansion for the off-shell scattering amplitude can be obtained from Eqs. (2.7) and (2.9),

$$\mathcal{T}_s(\vec{p}_1'\vec{q}_1', \vec{p}_1\vec{q}_1; E) = \langle \vec{p}_1'\vec{q}_1' | T_1 G_0 T_2 G_0 T_1 | \vec{p}_1\vec{q}_1 \rangle + \langle \vec{p}_1'\vec{q}_1' | T_1 G_0 T_3 G_0 T_1 | \vec{p}_1\vec{q}_1 \rangle + \langle \vec{p}_1'\vec{q}_1' | T_1 G_0 T_2 G_0 T_3 G_0 T_1 | \vec{p}_1\vec{q}_1 \rangle + \langle \vec{p}_1'\vec{q}_1' | T_1 G_0 T_3 G_0 T_2 G_0 T_1 | \vec{p}_1\vec{q}_1 \rangle + \cdots \; . \tag{3.6}$$

Similarly, from Eqs. (3.2) and (3.4) we obtain the multiple-scattering expansion for the on-shell rearrangement-collision amplitude,

$$\mathcal{T}_r = \langle \psi_b^{(3)} | V_1 | \psi_a^{(1)} \rangle + \langle \psi_b^{(3)} | T_2 | \psi_a^{(1)} \rangle + \langle \psi_b^{(3)} | T_1 G_0 T_2 | \psi_a^{(1)} \rangle + \langle \psi_b^{(3)} | T_1 G_0 T_3 | \psi_a^{(1)} \rangle + \langle \psi_b^{(3)} | T_2 G_0 T_3 | \psi_a^{(1)} \rangle + \cdots \; , \tag{3.7}$$

The expansion for the off-shell rearrangement-collision amplitude is obtained from Eqs. (2.11) and (2.12),

$$\mathcal{T}_r(\vec{p}_3\vec{q}_3, \vec{p}_1\vec{q}_1; E) = \langle \vec{p}_3\vec{q}_3 | T_3 G_0 T_1 | \vec{p}_1\vec{q}_1 \rangle + \langle \vec{p}_3\vec{q}_3 | T_3 G_0 T_2 G_0 T_1 | \vec{p}_1\vec{q}_1 \rangle + \langle \vec{p}_3\vec{q}_3 | T_3 G_0 T_1 G_0 T_2 G_0 T_1 | \vec{p}_1\vec{q}_1 \rangle + \langle \vec{p}_3\vec{q}_3 | T_3 G_0 T_1 G_0 T_3 G_0 T_1 | \vec{p}_1\vec{q}_1 \rangle + \langle \vec{p}_3\vec{q}_3 | T_3 G_0 T_2 G_0 T_3 G_0 T_1 | \vec{p}_1\vec{q}_1 \rangle + \cdots \; . \tag{3.8}$$

As remarked in Sec. II, the on-shell amplitudes $\mathcal{T}_s$ and $\mathcal{T}_r$ for scattering and rearrangement collisions can be obtained from the corresponding off-shell amplitudes $\mathcal{T}_s(\vec{p}_1'\vec{q}_1', \vec{p}_1\vec{q}_1; E)$ and $\mathcal{T}_r(\vec{p}_3\vec{q}_3, \vec{p}_1\vec{q}_1; E)$ for scattering and rearrangement collisions by requiring their arguments to satisfy the appropriate energy-conservation relations. In addition to the energy conservation, we must also specify the initial and final quantum states.

The angular momentum states of the initial and final two-body bound subsystems $l_i m_i$ and $l_f m_f$ can be easily specified by projection. We have from Eq. (3.6)

$$\mathcal{T}_s(p_1' l_1' m_1' \vec{q}_1', p_1 l_1 m_1 \vec{q}_1; E) = \langle Y_{l_1'}^{m_1'}(\hat{p}_1') | \mathcal{T}_s(\vec{p}_1' \vec{q}_1', \vec{p}_1 \vec{q}_1; E) | Y_{l_1}^{m_1}(\hat{p}_1) \rangle$$

$$= \langle p_1' l_1' m_1' \vec{q}_1' | T_1 G_0 T_2 G_0 T_1 | p_1 l_1 m_1 \vec{q}_1 \rangle + \langle p_1' l_1' m_1' \vec{q}_1' | T_1 G_0 T_3 G_0 T_1 | p_1 l_1 m_1 \vec{q}_1 \rangle + \cdots \tag{3.9}$$

and similarly from Eq. (3.8)

$$\mathcal{T}_r(p_3 l_3 m_3 \vec{q}_3, p_1 l_1 m_1 \vec{q}_1; E) = \langle Y_{l_3}^{m_3}(\hat{p}_3) | \mathcal{T}_r(\vec{p}_3 \vec{q}_3, \vec{p}_1 \vec{q}_1; E) | Y_{l_1}^{m_1}(\hat{p}_1) \rangle$$

$$= \langle p_3 l_3 m_3 \vec{q}_3 | T_3 G_0 T_1 | p_1 l_1 m_1 \vec{q}_1 \rangle + \langle p_3 l_3 m_3 \vec{q}_3 | T_3 G_0 T_2 G_0 T_1 | p_1 l_1 m_1 \vec{q}_1 \rangle + \cdots , \tag{3.10}$$

where we have made use of the notation

$$\langle p_j l_j m_j \vec{q}_j | \mathcal{O} | p_i l_i m_i \vec{q}_i \rangle = \langle Y_{l_j}^{m_j}(\hat{p}_j) | \langle \vec{p}_j \vec{q}_j | \mathcal{O} | \vec{p}_i \vec{q}_i \rangle | Y_{l_i}^{m_i}(\hat{p}_i) \rangle , \tag{3.11}$$

with $\mathcal{O}$ denoting the appropriate operators.

For the specification of the principal states of the initial and final two-body bound subsystems, two alternative representations[13] for the off-shell two-body partial-wave Coulomb amplitude $t_l^{(i)}(p_1, p_i'; E')$ have been found to be suitable.[5,6] We have $t_l^{(i)}(p_i, p_i'; E')$ in the Sturmian-function representation

$$t_l^{(i)}(p_i, p_i'; E') = \sum_\lambda [1 - \gamma_{\lambda l}^{(i)}(E')]^{-1} \phi_{\lambda l}^{(i)}(p_i, E') \phi_{\lambda l}^{(i)}(p_i', E') , \tag{3.12}$$

with

$$\phi_{\lambda l}^{(i)}(p_i, E') = \left(\frac{2^{4l+3} \lambda (\lambda - l - 1)!}{(\lambda + l)!} \right)^{1/2} (-E')^{(2l+3)/4} \frac{l! p_i^l}{(p_i^2 - E')^{l+1}} C_{\lambda - l - 1}^{l+1} \left(\frac{p_i^2 + E'}{p_i^2 - E'} \right) \tag{3.13}$$

and in the Coulomb-function representation

$$t_l^{(i)}(p_i, p_i'; E') = \frac{1}{2} \pi \sum_n{}' \frac{(p_i^2 - \epsilon_n^{(i)}(p_i'^2 - E')}{E' - \epsilon_n^{(i)}} \chi_{nl}^{(i)}(p_i) \chi_{nl}^{(i)*}(p_i') , \tag{3.14}$$

with bound states

$$\chi_{nl}^{(i)}(p_i) = \left(\frac{2^{4l+5} n (n - l - 1)!}{\pi (n + l)!} \right)^{1/2} [-\epsilon_n^{(i)}]^{(2l+5)/4} \frac{l! p_i^l}{(p_i^2 - \epsilon_n^{(i)})^{l+2}} C_{n-l-1}^{l+1} \left(\frac{p_i^2 + \epsilon_n}{p_i^2 - \epsilon_n} \right) , \tag{3.15}$$

where the C's are the Gegenbauer polynomials and the prime on the sum over n for the Coulomb functions indicates a sum over the discrete states and an integration over the continuum states.

The Sturmian functions which satisfy the orthonormality property

$$\pi^{-1} \int_0^\infty dp\, ^2 p \frac{\phi_{\lambda' l}^{(i)}(p, E') \phi_{\lambda l}^{(i)}(p, E')}{p^2 - E'} = \delta_{\lambda\lambda'} \tag{3.16}$$

are solutions of the homogeneous Lippmann-Schwinger equations with eigenvalues $[\gamma_{\lambda l}^{(i)}]^{-1}$

$$\gamma_{\lambda l}^{(i)}(E') = -\frac{\lambda (-2E'/\mu_{jk})^{1/2}}{Z_i} . \tag{3.17}$$

The Coulomb functions which satisfy the orthonormality property

$$\int_0^\infty \chi_{nl}^{(i)}(p) \chi_{n'l}^{(i)}(p) p^2 dp = \delta_{nn'} \tag{3.18}$$

are solutions of the Schrödinger equations with eigenvalues $\epsilon_n^{(i)}$

$$\epsilon_n^{(i)} = -\tfrac{1}{2} |Z_i|^2 \mu_{jk} / n^2 . \tag{3.19}$$

In terms of the Sturmian functions, the on-shell scattering amplitude can then be obtained from the off-shell scattering amplitude given by Eq. (3.9) by following the limiting procedure given in Ref. 6. We have

$$\mathcal{T}_s = N_s \lim_{\substack{q_1^2 \to E - \epsilon_{n_i}^{(1)} \\ q_1'^2 \to E - \epsilon_{n_f}^{(1)}}} \left(\frac{(E - q_1'^2 - \epsilon_{n_f}^{(1)})(E - q_1^2 - \epsilon_{n_i}^{(1)})}{[-\epsilon_{n_f}^{(1)}]^{1/2} \phi_{n_f l_f}^{(1)}(p_1', E - q_1'^2)[-\epsilon_{n_i}^{(1)}]^{1/2} \phi_{n_i l_i}^{(1)}(p_1, E - q_1^2)} \mathcal{T}_s(p_1' l_f m_f \vec{q}_1', p_1 l_i m_i \vec{q}_1; E) \right) . \quad (3.20)$$

Similarly from Eq. (3.10), we have for the rearrangement-collision amplitude

$$\mathcal{T}_r = N_s \lim_{\substack{q_1^2 \to E - \epsilon_{n_i}^{(1)} \\ q_3^2 \to E - \epsilon_{n_f}^{(3)}}} \left(\frac{(E - q_3^2 - \epsilon_{n_f}^{(3)})(E - q_1^2 - \epsilon_{n_i}^{(1)})}{[-\epsilon_{n_f}^{(3)}]^{1/2} \phi_{n_f l_f}^{(3)}(p_3, E - q_3^2)[-\epsilon_{n_i}^{(1)}]^{1/2} \phi_{n_i l_i}^{(1)}(p_1, E - q_1^2)} \mathcal{T}_r(p_3 l_f m_f \vec{q}_3, p_1 l_i m_i \vec{q}_1; E) \right) , \quad (3.21)$$

where

$$N_s = 2\pi^4 \quad (3.22)$$

is the normalization constant for the three-body amplitudes.

The on-shell amplitudes can also be obtained from the off-shell scattering amplitude in terms of Coulomb functions. We have from Eqs. (3.9) and (3.10)

$$\mathcal{T}_s = N_c \lim_{\substack{q_1^2 \to E - \epsilon_{n_i}^{(1)} \\ q_1'^2 \to E - \epsilon_{n_f}^{(1)}}} \left(\frac{(E - q_1'^2 - \epsilon_{n_f}^{(1)})(E - q_1^2 - \epsilon_{n_i}^{(1)})}{(p_1'^2 - \epsilon_{n_f}^{(1)}) \chi_{n_f l_f}^{(1)}(p_1')(p_1^2 - \epsilon_{n_i}^{(1)}) \chi_{n_i l_i}^{(1)}(p_1)} \mathcal{T}_s(p_1' l_f m_f \vec{q}_1', p_1 l_i m_i \vec{q}_1; E) \right) , \quad (3.23)$$

$$\mathcal{T}_r = N_c \lim_{\substack{q_1^2 \to E - \epsilon_{n_i}^{(1)} \\ q_3^2 \to E - \epsilon_{n_f}^{(3)}}} \left(\frac{(E - q_3^2 - \epsilon_{n_f}^{(3)})(E - q_1^2 - \epsilon_{n_i}^{(1)})}{(p_3^2 - \epsilon_{n_f}^{(3)}) \chi_{n_f l_f}^{(3)}(p_3)(p_1^2 - \epsilon_{n_i}^{(1)}) \chi_{n_i l_i}^{(1)}(p_1)} \mathcal{T}_r(p_3 l_f m_f \vec{q}_3, p_1 l_i m_i \vec{q}_1; E) \right) , \quad (3.24)$$

where the normalization constant is

$$N_c = 8\pi^3 . \quad (3.25)$$

The normalization constants N_s and N_c were not explicitly given in Ref. 6 since there the initial-state representation was not specified. {We take this occasion to point out an error in Ref. 6, that a factor of $[-\epsilon_{n_f}^{(j)}]^{-1/2}[-\epsilon_{n_i}^{(i)}]^{-1/2}$ was missing in putting the amplitude in the Sturmian-function representation on the energy shell, see, for example, Eq. (3.6) of Ref. 6.}

From Eqs. (3.20) to (3.25) the on-shell amplitudes may be calculated from the off-shell amplitude to all orders in the Faddeev-Watson multiple-scattering expansions. We illustrate these by calculating the bare-potential term for rearrangement collisions since it is this term which gives rise to the difficulties[9] in seeing the equivalence of the two approaches.

IV. DETERMINATION OF AMPLITUDE BY OFF-SHELL METHOD

In this section we demonstrate the equivalence of the off-shell method with the conventional method of taking matrix elements by evaluating the bare-potential term in the expansion for rearrangement collisions using both methods.

The bare-potential term in the multiple-scattering for the on-shell rearrangement-collision amplitude given by Eq. (3.7) canbe written as[2]

$$\langle \psi_f^{(3)} | V_1 | \psi_i^{(1)} \rangle = \frac{(2\pi)^3}{\beta_{31}^3} \int d\vec{p}_1 \, \chi_f^{(3)*}(-\vec{\kappa}_5) \chi_i^{(1)}(\vec{p}_1) V_1(\vec{\kappa}_4, \vec{p}_1) , \quad (4.1)$$

with

$$V_1(\vec{\kappa}_4, \vec{p}_1) = (Z_1 e^2 / 2\pi^2)(1/|\vec{\kappa}_4 - \vec{p}_1|^2) , \quad (4.2)$$

$$\vec{\kappa}_4 = (\alpha_{31} \vec{\kappa}_i + \vec{\kappa}_f)/\beta_{31}, \quad \vec{\kappa}_5 = (\vec{\kappa}_i + \alpha_{31} \vec{\kappa}_f)/\beta_{31} . \quad (4.3)$$

For simplicity, we consider the case where the initial two-body bound subsystem is in the ground state. We then have[2]

$$\langle \psi_f^{(3)} | V_1 | \psi_{1s}^{(1)} \rangle = \frac{16\pi Z_1 e^2}{\sqrt{2}\, \beta_{31}^3} [-\epsilon_1^{(1)}]^{5/4} \left[\frac{1}{\kappa_4} \int_0^\infty \frac{dp_1' p_1'}{(p_1'^2 - \epsilon_1^{(1)})^2} \ln \left(\frac{p_1' + \kappa_4}{p_1' - \kappa_4} \right)^2 \right] \chi_f^{(3)*}(-\vec{\kappa}_5)$$

$$= \frac{8\sqrt{2}\,\pi^2 Z_1 e^2(-)^{l_f}[-\epsilon_1^{(1)}]^{3/4}}{\beta_{31}^3(\kappa_4^2-\epsilon_1^{(1)})}\, Y_{l_f}^{m_f *}(\hat{\kappa}_5)\,\chi_{n_f l_f}(\kappa_5)\ . \tag{4.4}$$

This is the bare-potential approximation for the three-body rearrengement-collision amplitude between the ground state and $(n_f l_f m_f)$ state.

From Eqs. (3.21) and (3.24) together with the on-shell expansion [Eq. (3.7)] and the off-shell expansion [Eqs. (3.8) and (3.10)], it is seen that the on-shell bare-potential term is related to the off-shell bare-potential by the limiting relations:

$$\langle \psi_f^{(3)} | V_1 | \psi_i^{(1)} \rangle = \frac{N_s}{(2\mu_{23})^{1/2}} \lim_{\substack{q_1^2 \to E-\epsilon_{n_i}^{(1)} \\ q_3^2 \to E-\epsilon_{n_f}^{(3)}}} \left(\frac{(E-q_3^2-\epsilon_{nf}^{(3)})(E-q_1^2-\epsilon_{n_i}^{(1)})\langle p_3 l_f m_f \vec{q}_3 | T_3 G_0 T_1 | p_1 l_i m_i \vec{q}_1\rangle}{[-\epsilon_{n_f}^{(3)}]^{1/2}\phi_{n_f l_f}^{(3)}(p_3, E-q_3^2)[-\epsilon_{n_i}^{(1)}]^{1/2}\phi_{n_i l_i}^{(1)}(p_1, E-q_1^2)} \right), \tag{4.5}$$

$$\langle \psi_f^{(3)} | V_1 | \psi_i^{(1)} \rangle = \frac{N_c}{(2\mu_{23})^{1/2}} \lim_{\substack{q_1^2 \to E-\epsilon_{n_i}^{(1)} \\ q_3^2 \to E-\epsilon_{n_f}^{(3)}}} \left(\frac{(E-q_3^2-\epsilon_{nf}^{(3)})(E-q_1^2-\epsilon_{n_i}^{(1)})\langle p_3 l_f m_f \vec{q}_3 | T_3 G_0 T_1 | p_1 l_i m_i \vec{q}_1\rangle}{(p_3^2-\epsilon_{nf}^{(3)})\,\chi_{n_f l_f}^{(3)}(p_3)(p_1^2-\epsilon_{n_i}^{(1)})\chi_{n_i l_i}^{(1)}(p_i)} \right), \tag{4.6}$$

with

$$\langle p_3 l_f m_f \vec{q}_3 | T_3 G_0 T_1 | p_1 l_i m_i \vec{q}_1\rangle = \langle Y_{l_f}^{m_f}(\hat{p}_3) | \langle \vec{p}_3 \vec{q}_3 | T_3 G_0 T_1 | \vec{p}_1 \vec{q}_1 \rangle | Y_{l_i}^{m_i}(\hat{p}_1)\rangle\ . \tag{4.7}$$

The $(2\mu_{23})^{-1/2}$ mass factor in Eqs. (4.5) and (4.6) accounts for the appropriate normalization of the Coulomb potential which is given by Eq. (4.2) in terms of the mass-scaled momentum variables.

The operator $T_3 G_0 T_1$ in the momentum representation can be written as

$$\langle \vec{p}_3 \vec{q}_3 | T_3 G_0 T_1 | \vec{p}_1 \vec{q}_1 \rangle = -\int d\vec{p}_1' d\vec{q}_1' \frac{\delta(\vec{q}_3-\vec{q}_3')\delta(\vec{q}_1-\vec{q}_1')}{p_1'^2+q_1'^2-E} T_3(\vec{p}_3, \vec{p}_3'; E-q_3^2) T_1(\vec{p}_1', \vec{p}_1; E-q_1^2)$$

$$= -\frac{T_3(\vec{p}_3, -\vec{\kappa}_5, E-q_3^2)T_1(\vec{\kappa}_4, \vec{p}_1, E-q_1^2)}{\beta_{31}^3(\kappa_4^2+q_1^2-E)}\ . \tag{4.8}$$

Making use of the partial-wave expansion for the off-shell two-body Coulomb amplitude

$$T_i(\vec{p}_i, \vec{p}_i'; E-q_i^2) = \frac{1}{2\pi^2}\sum_l (2l+1) P_l(\hat{p}_i\cdot\hat{p}_i')\, t_l^{(i)}(p_i, p_i'; E-q_i^2) \tag{4.9}$$

and Eq. (4.8) for $\langle \vec{p}_3 \vec{q}_3 | T_3 G_0 T_1 | \vec{p}_1 \vec{q}_1\rangle$, we obtain from Eq. (4.7)

$$\langle p_3 l_f m_f \vec{q}_3 | T_3 G_0 T_1 | p_1 l_i m_i \vec{q}_1 \rangle = -\frac{4(-)^{l_f}}{\pi^2 \beta_{31}^3} Y_{l_f}^{m_f *}(\hat{\kappa}_5) Y_{l_i}^{m_i}(\hat{\kappa}_4) \frac{t_{l_f}^{(3)}(p_3, \kappa_5; E-q_3^2)\, t_{l_i}^{(1)}(\kappa_4, p_1; E-q_1^2)}{\kappa_4^2+q_1^2-E}\ . \tag{4.10}$$

Now we are in position to evaluate Eq. (4.5) and Eq. (4.6) for $\langle \psi_f^{(3)} | V_1 | \psi_i^{(1)}\rangle$ by making use of either the Sturmian-function or the Coulomb-function representations for the off-shell partial-wave Coulomb amplitude given by Eqs. (3.12) and (3.14), respectively.

We first consider the case with the Sturmian-function representation for $t_l^{(i)}$. Substitution of Eq. (4.10) into Eq. (4.5) yields, with the help of Eqs. (3.12), (3.17), and (3.22), the bare-potential result

$$\langle \psi_f^{(3)} | V_1 | \psi_i^{(1)} \rangle = \frac{-16\pi^2 |Z_1| e^2 (-)^{l_f}[-\epsilon_{nf}^{(3)}]^{1/2}}{n_i \beta_{31}^3(\kappa_4^2-\epsilon_{n_i}^{(1)})} Y_{l_f}^{m_f *}(\hat{\kappa}_5) Y_{l_i}^{m_i}(\hat{\kappa}_4)\, \phi_{n_f l_f}^{(3)}(\kappa_5, \epsilon_{n_f}^{(3)})\phi_{n_i l_i}^{(1)}(\kappa_4, \epsilon_{n_i}^{(1)})\ . \tag{4.11}$$

For the case where the initial two-body bound subsystem is in the ground state, Eq. (4.11) reduces to

$$\langle \psi_f^{(3)} | V_1 | \psi_{1s}^{(1)} \rangle = \frac{8\sqrt{2}\,\pi^2 Z_1 e^2(-)^{l_f}[-\epsilon_1^{(1)}]^{3/4}}{\beta_{31}^3(\kappa_4^2-\epsilon_1^{(1)})} Y_{l_f}^{m_f *}(\hat{\kappa}_5)\left(\frac{2[-\epsilon_{nf}^{(3)}]^{1/2}}{\pi^{1/2}(\kappa_4^2-\epsilon_1^{(1)})}\, \phi_{n_f l_f}^{(3)}(\kappa_5, \epsilon_{n_f}^{(3)}) \right)$$

$$= \frac{8\sqrt{2}\,\pi^2 Z_1 e^2(-)^{l_f}[-\epsilon_1^{(1)}]^{3/4}}{\beta_{31}^3(\kappa_4^2-\epsilon_1^{(1)})} Y_{l_f}^{m_f *}(\hat{\kappa}_5)\,\chi_{n_f l_f}^{(3)}(\kappa_5)\ , \tag{4.12}$$

where, in the second writing, we have made use of the relation

$$\kappa_4^{(2)} - \epsilon_{n_i}^{(1)} = \kappa_5^{(2)} - \epsilon_{n_f}^{(3)} \tag{4.13}$$

and Eqs. (3.13) and (3.15). Similarly in terms of the Coulomb functions, we obtain from Eq. (4.6), with the help of Eqs. (4.10), (3.14), and (3.25), the result

$$\langle \psi_f^{(3)} | V_1 | \psi_i^{(1)} \rangle = -\frac{8\pi^3(-)^{l_f}}{\beta_{31}^3(2\mu_{23})^{1/2}} (\kappa_5^2 - \epsilon_{n_f}^{(3)}) Y_{l_f}^{m_f *}(\hat{\kappa}_5) Y_{l_i}^{m_i}(\hat{\kappa}_4) \chi_{n_f l_f}^{(3)}(\kappa_5) \chi_{n_i l_i}^{(1)}(\kappa_4), \tag{4.14}$$

which for the $i = 1s$ case reduces again to Eqs. (4.4) and (4.12).

This then concludes the demonstration of the equivalence of the two alternative methods for the determination of on-shell amplitudes. It is of interest to note that for this bare-potential case, the off-shell approach is actually more simple and has no integrals to be evaluated.

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