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A New Approach to the 3D Faddeev Equation for Three-body Scattering

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Abstract A novel approach to solve the Faddeev equation for three-body scattering at arbitrary energies is proposed. This approach disentangles the complicated singularity structure of the free three-nucleon propagator leading to the moving and logarithmic singularities in standard treatments. The Faddeev equation is formulated in momentum space and directly solved in terms of momentum vectors without employing a partial wave decomposition. In its simplest form the Faddeev equation for identical bosons, which we are using, is an integral equation in five variables, magnitudes of relative momenta and angles. The singularities of the free propagator and the deuteron propagator are now both simple poles in two different momentum variables, and thus can both be integrated with standard techniques.

1 Introduction

In 1960 L.D. Faddeev formulated his mathematically rigorous scattering theory for three particles by proposing a set of three coupled integral equations, which do have a unique solution [1–3]. In the first numerical realizations of this approach, separable interactions were introduced, reducing the three-body equations to a set of one-dimensional coupled integral equations, whose numerical solutions was feasible at the time [4,5]. Despite a simplification due to the choice of the two-body interaction, the standard formulation of the momentum space Faddeev equations in the continuum contains for the free three-body propagator a complicated singularity structure within the integral kernel [6–8]. These complications arise because the position of the propagator cut does not only depend on the total energy of the system but also on external momentum variables on a grid (thus the term moving singularities). In addition branch points occur leading to logarithmic singularities.

It is possible to carry out the integration along a path in the complex plane, thus avoiding to directly deal with these singularities, but indirectly imposing conditions on the analytical properties of the two-body force. This method of contour deformation was introduced for separable potentials by Hetherington and Schick [9] and perfected by Cahill and Sloan [10]. The need to use realistic forces, which are predominantly local, led to methods integrating the singularities on the real momentum axis [11]. It took until the 1980s until the Faddeev equations were solved in the continuum with a realistic nucleon–nucleon (NN) force as input [12,13].

During the last two decades calculations of nucleon–deuteron scattering experienced large improvements and refinements. It is fair to say that below about the pion production projectile energy the momentum space

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Faddeev equations for three-nucleon scattering can now be solved with high accuracy for the most modern two- and three-nucleon forces. A summary of these achievements can be found in [14–18]. The approach described there is based on using angular momentum eigenstates for the two- and three-body systems. This partial wave decomposition replaces the continuous angle variables by discrete orbital angular momentum quantum numbers, and thus reduces the number of continuous variables to be discretized in a numerical treatment to two. For low projectile energies the procedure of considering orbital angular momentum components appears physically justified due to arguments related to the centrifugal barrier and the short range of the nuclear force. However, when considering three nucleon scattering at higher energies, it appears natural to avoid a partial wave representation completely and work directly with vector variables. Only recently exact Faddeev calculations for three-body scattering in the intermediate energy regime became available. The formulation and numerical realization based on vector variables for the nonrelativistic Faddeev equations [19,20] as well as fully Poincaré invariant ones [21,22] have been carried out for scalar interactions up to projectile energies of 2 GeV.

Despite the technical sophistication with which the Faddeev equations in the continuum are solved today, the treatment of the singularity structure of the free three-nucleon propagator experienced only minor modifications from the original suggestion [13], e.g. in [19] the logarithmic singularities are integrated semi-analytically with splines in contrast to the earlier subtraction techniques. However, it would be most desirable to have a kernel without any logarithmic singularities. In [23] a solution to this long lasting technical challenge is proposed and successfully carried out in the context of the partial wave decomposed Faddeev equations. It is the purpose of this paper to examine this suggestion in the context of a three-dimensional treatment of the Faddeev equation and introduce a kernel in which only simple poles in one variable occur. Those poles can then be integrated by standard subtraction techniques.

In Sect. 2, we briefly revisit the form of the nonrelativistic Faddeev equation used in previous work [19] to allow an easy comparison of the differences in our new approach. In Sect. 3, we describe in detail the simplification of the singularity structure of the free three-body propagator, and in Sect. 4 we complete the calculation with the remaining angular integrations and connect to previous work in calculating the operators for elastic and breakup scattering. We conclude in Sect. 5.

2 The Faddeev Equation for Three Identical Bosons

There are various presentations of three-body scattering in the Faddeev scheme [1–3] presented in the literature [8,14,24]. We consider here the Faddeev equation for identical particles in the form

$$T|\phi\rangle = tP|\phi\rangle + tPG_0T|\phi\rangle. \quad (1)$$

The driving term of this integral equation consists of a two-body t -matrix t , the sum P of a cyclic and anticyclic permutation of three identical particles, and the initial state $|\phi\rangle = |\varphi_d\mathbf{q}_0\rangle$, composed of a two-body bound state and the momentum eigenstate of the projectile particle. The kernel of Eq. (1) contains the free three-body propagator, $G_0 = (E - H_0 + i\epsilon)^{-1}$, where E is the total energy in the center-of-momentum (c.m.) frame. The operator T determines both the full breakup amplitude

$$U_0 = (1 + P)T \quad (2)$$

and the amplitude for elastic scattering

$$U = PG_0^{-1} + PT. \quad (3)$$

For the explicit solution of Eq. (1) the standard Jacobi momenta \mathbf{p} , the relative momentum in the subsystem, and \mathbf{q} , the relative momentum of the spectator to the subsystem are introduced. The momentum states are normalized according to $\langle\mathbf{p}'\mathbf{q}'|\mathbf{p}\mathbf{q}\rangle = \delta^3(\mathbf{p}' - \mathbf{p}) \delta^3(\mathbf{q}' - \mathbf{q})$. Projecting Eq. (1) onto these basis states leads to

$$T(\mathbf{p}, \mathbf{q}; \mathbf{q}_0) = T_0(\mathbf{p}, \mathbf{q}; \mathbf{q}_0) + \int d^3p' d^3p'' d^3q'' t(\mathbf{p}, \mathbf{p}'; \varepsilon) \langle\mathbf{p}'\mathbf{q}|P|\mathbf{p}''\mathbf{q}''\rangle \frac{1}{E + i\epsilon - E''} T(\mathbf{p}'', \mathbf{q}''; \mathbf{q}_0). \quad (4)$$

Here we abbreviate $\langle\mathbf{p}\mathbf{q}|T|\varphi_d\mathbf{q}_0\rangle \equiv T(\mathbf{p}, \mathbf{q}; \mathbf{q}_0)$ and the driving term as $\langle\mathbf{p}\mathbf{q}|tP|\varphi_d\mathbf{q}_0\rangle \equiv T_0(\mathbf{p}, \mathbf{q}; \mathbf{q}_0)$. Under the integral we take advantage of the fact that the two-body t -matrix only depends on the relative momenta \mathbf{p}

and \mathbf{p}' of the subsystem, and the thus the t -matrix is evaluated at the energy $\varepsilon = E - \frac{3}{4m}q^2$. The energy E'' of the free three-body propagator is given by

$$E'' = \frac{1}{m} \left(p''^2 + \frac{3}{4}q''^2 \right). \quad (5)$$

The permutation operator is explicitly given as

$$\langle \mathbf{p}' \mathbf{q} | P | \mathbf{p}'' \mathbf{q}'' \rangle = \delta(\mathbf{p}' + \boldsymbol{\pi}_1) \delta(\mathbf{p}'' - \boldsymbol{\pi}_2) + \delta(\mathbf{p}' - \boldsymbol{\pi}_1) \delta(\mathbf{p}'' + \boldsymbol{\pi}_2), \quad (6)$$

with the ‘shifted’ momenta

$$\begin{aligned} \boldsymbol{\pi}_1 &= \frac{1}{2} \mathbf{q} + \mathbf{q}'', \\ \boldsymbol{\pi}_2 &= \mathbf{q} + \frac{1}{2} \mathbf{q}''. \end{aligned} \quad (7)$$

Inserting Eqs. (5)–(7) into Eq. (4) leads to

$$\begin{aligned} T(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= T_0(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) + \int d^3 p' d^3 p'' d^3 q'' t(\mathbf{p}, \mathbf{p}'; \varepsilon) \\ &\quad \times [\delta(\mathbf{p}' + \boldsymbol{\pi}_1) \delta(\mathbf{p}'' - \boldsymbol{\pi}_2) + \delta(\mathbf{p}' - \boldsymbol{\pi}_1) \delta(\mathbf{p}'' + \boldsymbol{\pi}_2)] \\ &\quad \times \frac{1}{E + i\epsilon - E''} T(\mathbf{p}'', \mathbf{q}'', \mathbf{q}_0). \end{aligned} \quad (8)$$

The direct evaluation of the matrix elements of the permutation operator gives

$$\begin{aligned} T(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= T_0(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) + \int d^3 q'' \\ &\quad \times \left[t(\mathbf{p}, -\boldsymbol{\pi}_1; \varepsilon) \frac{1}{E + i\epsilon - E''} T(\boldsymbol{\pi}_2, \mathbf{q}'', \mathbf{q}_0) \right. \\ &\quad \left. + t(\mathbf{p}, \boldsymbol{\pi}_1; \varepsilon) \frac{1}{E + i\epsilon - E''} T(-\boldsymbol{\pi}_2, \mathbf{q}'', \mathbf{q}_0) \right]. \end{aligned} \quad (9)$$

Defining a symmetrized t -matrix

$$t_s(\mathbf{p}, \boldsymbol{\pi}_1; \varepsilon) = t(\mathbf{p}, \boldsymbol{\pi}_1; \varepsilon) + t(\mathbf{p}, -\boldsymbol{\pi}_1; \varepsilon) \quad (10)$$

and realizing that for identical bosons $T(\boldsymbol{\pi}_2, \mathbf{q}''; \mathbf{q}_0) = T(-\boldsymbol{\pi}_2, \mathbf{q}''; \mathbf{q}_0)$ one arrives at the expression

$$T(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) = T_0(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) + \int d^3 q'' t_s(\mathbf{p}, \boldsymbol{\pi}_1; \varepsilon) \frac{1}{E + i\epsilon - \frac{1}{m}(q^2 + q''^2 + \mathbf{q} \cdot \mathbf{q}'')} T(\boldsymbol{\pi}_2, \mathbf{q}'', \mathbf{q}_0), \quad (11)$$

which is the starting point for the numerical calculations presented in [19]. The free propagator in Eq. (11) clearly displays the difficulties inherent in numerically solving the three-body scattering problem in this form. The propagator depends on the magnitude of q'' and through the scalar product $\mathbf{q} \cdot \mathbf{q}''$ on the angle between \mathbf{q}'' and a fixed axis given by \mathbf{q} . The integration over $d^3 q''$ leads to singularities with respect to that angle for each fixed value of q'' and q . These singularities are integrable, but lead to logarithmic singularities in the variable q'' . However, despite being integrable, they pose numerical challenges. For scattering calculations in a three-dimensional approach these challenges were met in [19,20] for the nonrelativistic Faddeev equation and in [21,22] for Poincaré invariant Faddeev equation. Nonetheless, three-body scattering calculations would be less challenging, if these singularities in the angles could be extricated from the ones in the momenta. A suggestion for accomplishing this task is made in Sect. 3, following [23].

3 A New Look at the Singularity Structure of the Free Three-body Propagator

As demonstrated in the previous section, using the vector variables in the evaluation of the matrix elements of the permutation operator of Eq. (6) leads to the representation of the free three-body propagator of Eq. (11), containing both integration variables q'' and $\hat{\mathbf{q}} \cdot \hat{\mathbf{q}}''$. If we want to disentangle those two variables, we should start by separating the angular piece of the delta functions from the piece containing magnitudes of momenta and write

$$\begin{aligned}\delta(\mathbf{p}' + \boldsymbol{\pi}_1) \delta(\mathbf{p}'' - \boldsymbol{\pi}_2) &= \frac{\delta(p' - \pi_1)}{p'^2} \frac{\delta(p'' - \pi_2)}{p''^2} \delta(\hat{\mathbf{p}}' + \hat{\boldsymbol{\pi}}_1) \delta(\hat{\mathbf{p}}'' - \hat{\boldsymbol{\pi}}_2), \\ \delta(\mathbf{p}' - \boldsymbol{\pi}_1) \delta(\mathbf{p}'' + \boldsymbol{\pi}_2) &= \frac{\delta(p' - \pi_1)}{p'^2} \frac{\delta(p'' - \pi_2)}{p''^2} \delta(\hat{\mathbf{p}}' - \hat{\boldsymbol{\pi}}_1) \delta(\hat{\mathbf{p}}'' + \hat{\boldsymbol{\pi}}_2).\end{aligned}\quad (12)$$

This leads to

$$\begin{aligned}T(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= T_0(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) + \int dp' p'^2 d\hat{\mathbf{p}}' dp'' p''^2 d\hat{\mathbf{p}}'' d^3 q'' t(\mathbf{p}, \mathbf{p}', \varepsilon) \\ &\quad \times [\delta(\hat{\mathbf{p}}' + \hat{\boldsymbol{\pi}}_1) \delta(\hat{\mathbf{p}}'' - \hat{\boldsymbol{\pi}}_2) + \delta(\hat{\mathbf{p}}' - \hat{\boldsymbol{\pi}}_1) \delta(\hat{\mathbf{p}}'' + \hat{\boldsymbol{\pi}}_2)] \\ &\quad \times \frac{\delta(p' - \pi_1)}{p'^2} \frac{\delta(p'' - \pi_2)}{p''^2} \frac{1}{E + i\epsilon - E''} T(\mathbf{p}'', \mathbf{q}'', \mathbf{q}_0) \\ &= T_0(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) + \int d^3 q'' dp' dp'' \delta(p' - \pi_1) \delta(p'' - \pi_2) \\ &\quad \times \frac{1}{E + i\epsilon - \frac{1}{m}(p'^2 + \frac{3}{4}q''^2)} (t_s(\mathbf{p}, p' \hat{\boldsymbol{\pi}}_1; \varepsilon) T(p'' \hat{\boldsymbol{\pi}}_2, \mathbf{q}'', \mathbf{q}_0).\end{aligned}\quad (13)$$

We arrived at the last expression by integrating over the angles and taking into account the symmetrized two-body t -matrix from Eq. (10). The magnitudes of the two vectors $\boldsymbol{\pi}_1$ and $\boldsymbol{\pi}_2$ are given by

$$|\boldsymbol{\pi}_1| = \sqrt{\frac{1}{4}q^2 + q'^2 + qq''x''}, \quad (14)$$

$$|\boldsymbol{\pi}_2| = \sqrt{q^2 + \frac{1}{4}q''^2 + qq''x''},$$

where $x'' = \hat{\mathbf{q}} \cdot \hat{\mathbf{q}}''$. The above relations can be used to rewrite the two delta functions of Eq. (13) in a form better suited for our further considerations. We rewrite

$$\delta(p' - \pi_1) = \frac{2p'}{qq''} \delta(x'' - x_0) \Theta(1 - |x_0|), \quad (15)$$

where

$$x_0 = \frac{1}{qq''} \left(p'^2 - \frac{1}{4}q^2 - q'^2 \right) = \frac{1}{qq''} \left(p''^2 - \frac{1}{4}q''^2 - q^2 \right), \quad (16)$$

and

$$\delta(p' - \pi_2) = \delta \left(p'' - \sqrt{p'^2 + \frac{3}{4}q^2 - \frac{3}{4}q'^2} \right) \Theta \left(p'' - \sqrt{p'^2 + \frac{3}{4}q^2 - \frac{3}{4}q'^2} \right). \quad (17)$$

Inserting these expressions into Eq. (13) gives

$$\begin{aligned}T(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= T_0(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) \\ &\quad + \int d^3 q'' dp' dp'' \frac{2p'}{qq''} \delta(x'' - x_0) \Theta(1 - |x_0|) \\ &\quad \times \delta \left(p'' - \sqrt{p'^2 + \frac{3}{4}q^2 - \frac{3}{4}q'^2} \right) \Theta \left(p'^2 + \frac{3}{4}q^2 - \frac{3}{4}q'^2 \right) \\ &\quad \times \frac{1}{E + i\epsilon - \frac{1}{m}(p'^2 + \frac{3}{4}q''^2)} t_s(\mathbf{p}, p' \hat{\boldsymbol{\pi}}_1; \varepsilon) T(p'' \hat{\boldsymbol{\pi}}_2, \mathbf{q}'', \mathbf{q}_0).\end{aligned}\quad (18)$$

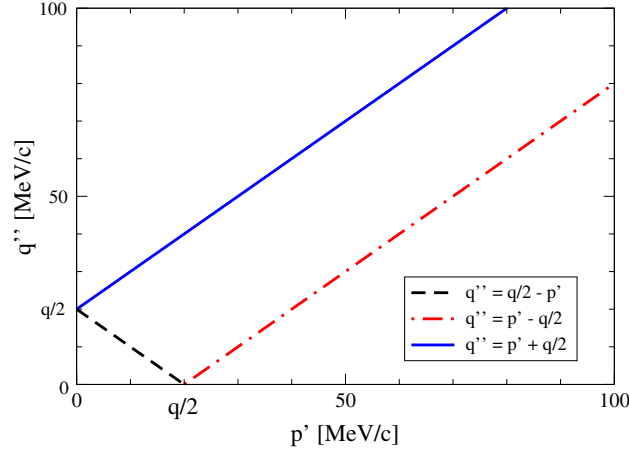


Fig. 1 The domain for the integration over the momenta p' and q'' as function of the external momentum q . Here $q = 40$ MeV/c is chosen. The area of integration is the rectangle enclosed by the three lines

Before we continue, we remember that the underlying two-body force supports one bound state with energy E_d . This means, that $t_s(\mathbf{p}, \mathbf{p}'; z)$ has a pole at $z = E_d$. Because the transition operator T of Eq. (18) is needed for all values of \mathbf{q} , one will encounter this pole of t_s . Extracting the residue explicitly by defining

$$t_s(\mathbf{p}, \mathbf{p}'; z) \equiv \frac{\hat{t}_s(\mathbf{p}, \mathbf{p}'; z)}{z - E_d} \quad (19)$$

and similarly for T and T_0 one can rewrite Eq. (18) as

$$\begin{aligned} \hat{T}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= \hat{T}_0(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) \\ &+ \int d^3 q'' dp' dp'' \frac{2p'}{qq''} \delta(x'' - x_0) \Theta(1 - |x_0|) \\ &\times \delta\left(p'' - \sqrt{p'^2 + \frac{3}{4}q^2 - \frac{3}{4}q''^2}\right) \Theta\left(p'^2 + \frac{3}{4}q^2 - \frac{3}{4}q''^2\right) \\ &\times \frac{1}{E + i\epsilon - \frac{1}{m}(p''^2 + \frac{3}{4}q''^2)} \hat{t}_s(\mathbf{p}, p' \hat{\boldsymbol{\pi}}_1; \varepsilon) \frac{\hat{T}(p'' \hat{\boldsymbol{\pi}}_2, \mathbf{q}'', \mathbf{q}_0)}{E + i\epsilon - E_d - \frac{3}{4m}q''^2}. \end{aligned} \quad (20)$$

Now we carry out the integration in p'' and arrive at

$$\begin{aligned} \hat{T}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= \hat{T}_0(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) \\ &+ \frac{2}{q} \int d\hat{\mathbf{q}}'' dq'' dp' \delta(x'' - x_0) \Theta(1 - |x_0|) \Theta\left(p'^2 + \frac{3}{4}q^2 - \frac{3}{4}q''^2\right) \\ &\times \frac{p'q''}{E + i\epsilon - \frac{1}{m}(p'^2 + \frac{3}{4}q^2)} \hat{t}_s(\mathbf{p}, p' \hat{\boldsymbol{\pi}}_1; \varepsilon) \frac{\hat{T}(p'' \hat{\boldsymbol{\pi}}_2, \mathbf{q}'', \mathbf{q}_0)}{E + i\epsilon - E_d - \frac{3}{4m}q''^2}, \end{aligned} \quad (21)$$

where $p'' \equiv \sqrt{p'^2 + \frac{3}{4}q^2 - \frac{3}{4}q''^2}$. The two theta-functions in Eq. (21) restrict the integration in the magnitudes of q'' and p' into an area whose size depends on the magnitude of the spectator momentum q . An example of this area is indicated in Fig. 1 for the choice of $q = 40$ MeV/c.

Next we consider the product of propagators in Eq. (21) and separate this product as in [23]

$$\begin{aligned} \frac{1}{E + i\epsilon - \frac{1}{m}(p'^2 + \frac{3}{4}q^2)} \frac{1}{E + i\epsilon - E_d - \frac{3}{4m}q''^2} &= \left[\frac{1}{E + i\epsilon - \frac{1}{m}(p'^2 + \frac{3}{4}q^2)} - \frac{1}{E + i\epsilon - E_d - \frac{3}{4m}q''^2} \right] \\ &\times \frac{1}{-E_d - \frac{3}{4m}q''^2 + \frac{1}{m}(p'^2 + \frac{3}{4}q^2)}. \end{aligned}$$

The new denominator function,

$$\bar{G}(q, q'', p') = \frac{1}{-E_d - \frac{3}{4m}q''^2 + \frac{1}{m}(p'^2 + \frac{3}{4}q^2)} \quad (22)$$

cannot become singular inside the integration domain $p' - q''$. Using the relation from Eq. (17) we see that

$$\bar{G}(q, q'', p') = \frac{1}{-E_d + \frac{1}{m}p''^2} = \frac{1}{|E_d| + \frac{1}{m}p''^2} > 0. \quad (23)$$

With this separation of propagators the three-body transition amplitude from Eq. (21) consists now of two integrals and can be written as

$$\begin{aligned} \hat{T}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= \hat{T}_0(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) \\ &+ \frac{2}{q} \int_0^\infty dp' p' \frac{1}{E + i\epsilon - \frac{1}{m}(p'^2 + \frac{3}{4}q^2)} \int_{|q/2-p'|}^{q/2+p'} dq'' q'' \bar{G}(q, q'', p') \\ &\times \int d\hat{\mathbf{q}}'' \delta(x'' - x_0) \hat{t}_s(\mathbf{p}, p' \hat{\boldsymbol{\pi}}_1; \varepsilon) \hat{T}(p'' \hat{\boldsymbol{\pi}}_2, \mathbf{q}'', \mathbf{q}_0) \\ &- \frac{2}{q} \int_0^\infty dq'' q'' \frac{1}{E + i\epsilon - E_d - \frac{3}{4m}q''^2} \int_{|q/2-q''|}^{q/2+q''} dp' p' \bar{G}(q, q'', p') \\ &\times \int d\hat{\mathbf{q}}'' \delta(x'' - x_0) \hat{t}_s(\mathbf{p}, p' \hat{\boldsymbol{\pi}}_1; \varepsilon) \hat{T}(p'' \hat{\boldsymbol{\pi}}_2, \mathbf{q}'', \mathbf{q}_0). \end{aligned} \quad (24)$$

In the second part of the kernel we changed the sequence of integrations over p' and q'' .

This new form of the kernel now exhibits only simple poles in the p' and q'' integration, and the angle integration does **not** contain any singularity any more. As a remark, the simultaneous occurrence of poles in the angle and momentum integration when solving Eq. (11) leads to the logarithmic singularities, which are not present in Eq. (24). The poles of the free propagator occur in the variable p' and the deuteron pole in the variable q'' .

4 The Angle Integration

Since we ignore spin and isospin dependencies, the matrix element $T(\mathbf{p}, \mathbf{q}, \mathbf{q}_0)$ is a scalar function of the variables \mathbf{p} and \mathbf{q} for a given projectile momentum \mathbf{q}_0 . As was shown in [19], one needs five variables to uniquely specify the geometry of those three vectors. For the clarity of presentation we repeat some of the arguments here. Having in mind that with three vectors one can span two planes, i.e. the $\mathbf{p} - \mathbf{q}_0$ -plane and the $\mathbf{q} - \mathbf{q}_0$ -plane, a natural choice of independent variables is

$$p = |\mathbf{p}|, \quad q = |\mathbf{q}|, \quad x_p = \hat{\mathbf{p}} \cdot \hat{\mathbf{q}}_0, \quad x_q = \hat{\mathbf{q}} \cdot \hat{\mathbf{q}}_0, \quad x_{pq}^{q_0} = (\widehat{\mathbf{q}_0 \times \mathbf{q}}) \cdot (\widehat{\mathbf{q}_0 \times \mathbf{p}}). \quad (25)$$

The last variable, $x_{pq}^{q_0}$, is the angle between the two normal vectors of the $\mathbf{p} - \mathbf{q}_0$ -plane and the $\mathbf{q} - \mathbf{q}_0$ -plane. It should further be pointed out, that the angle between the vectors \mathbf{p} and \mathbf{q} , $y_{pq} = \hat{\mathbf{p}} \cdot \hat{\mathbf{q}}$ is not an independent variable, but can be related to the ones given above as

$$y_{pq} = x_p x_q + \sqrt{1 - x_p^2} \sqrt{1 - x_q^2} x_{pq}^{q_0}. \quad (26)$$

For the special case where $\hat{\mathbf{q}}_0$ is parallel to the z -axis (q_0 -system) one can write

$$y_{pq} = x_p x_q + \sqrt{1 - x_p^2} \sqrt{1 - x_q^2} \cos \varphi_{pq}, \quad (27)$$

where the angle φ_{pq} is the difference of the azimuthal angles of $\hat{\mathbf{p}}$ and $\hat{\mathbf{q}}$ related to the specified z -axis.

The δ -function in the angle integration of Eq. (24), $\delta(x'' - x_0) = \delta(\hat{\mathbf{q}} \cdot \hat{\mathbf{q}}'' - x_0)$ suggests to choose for the $\hat{\mathbf{q}}''$ integration the z -axis parallel to the vector \mathbf{q} (q -system). The angle dependence of the two-body t -matrix is then explicitly given as

$$\hat{t}_s(\mathbf{p}, p' \hat{\boldsymbol{\pi}}_1; E(q)) \equiv \hat{t}_s(p, p', \hat{\mathbf{p}} \cdot \hat{\boldsymbol{\pi}}_1; \varepsilon), \quad (28)$$

where

$$\hat{\mathbf{p}} \cdot \hat{\boldsymbol{\pi}}_1 = \frac{\frac{1}{2}qy_{pq} + y_{pq}x''}{\sqrt{\frac{1}{4}q^2 + q''^2 + qq''x''}} \quad (29)$$

and

$$y_{pq}x'' = \hat{\mathbf{p}} \cdot \hat{\mathbf{q}}'' = y_{pq}x'' + \sqrt{1 - y_{pq}^2} \sqrt{1 - x''^2} \cos(\varphi_p - \varphi''). \quad (30)$$

The angle φ_p is the azimuthal angle of $\hat{\mathbf{p}}$ in the q -system. As mentioned before, $x'' = \hat{\mathbf{q}} \cdot \hat{\mathbf{q}}''$ and $q'' = |\mathbf{q}''|$. The angle dependence of the three-body transition amplitude is more intricate and can be written as

$$\hat{T}(p'' \hat{\boldsymbol{\pi}}_2, \mathbf{q}'', \mathbf{q}_0) \equiv \hat{T}(p'', x_{\pi_2}, x_{\pi_2}^{q_0}, y_{q_0 q''}, q''; q_0). \quad (31)$$

Explicitly these angles are given as

$$\begin{aligned} \hat{\boldsymbol{\pi}}_2 \cdot \mathbf{q}_0 &\equiv x_{\pi_2} = \frac{qx_q + \frac{1}{2}q''y_{q_0 q''}}{\sqrt{q^2 + \frac{1}{4}q''^2 + qq''x''}}, \\ \hat{\mathbf{q}}'' \cdot \mathbf{q}_0 &\equiv y_{q_0 q''} = x_q x'' + \sqrt{1 - x_q^2} \sqrt{1 - x''^2} \cos(\varphi_{q_0} - \varphi''), \\ x_{\pi_2}^{q_0} y_{q_0 q''} &\equiv \frac{\hat{\boldsymbol{\pi}}_2 \cdot \hat{\mathbf{q}}'' - (\hat{\boldsymbol{\pi}}_2 \cdot \hat{\mathbf{q}}_0)(\hat{\mathbf{q}}'' \cdot \hat{\mathbf{q}}_0)}{\sqrt{1 - (\hat{\boldsymbol{\pi}}_2 \cdot \hat{\mathbf{q}}_0)^2} \sqrt{1 - (\hat{\mathbf{q}}'' \cdot \hat{\mathbf{q}}_0)^2}} \\ &= \frac{\frac{qx'' - \frac{1}{2}q''}{\sqrt{q^2 + \frac{1}{4}q''^2 + qq''x''}} - x_{\pi_2} y_{q_0 q''}}{\sqrt{1 - x_{\pi_2}^2} \sqrt{1 - y_{q_0 q''}^2}}. \end{aligned} \quad (32)$$

Like φ_p in Eq. (30) the angle φ_{q_0} is the azimuthal angle of $\hat{\mathbf{q}}_0$ in the q -system. It was shown in [19] that because of the φ'' integration, only the knowledge of $\cos(\varphi_{q_0} - \varphi_p)$ is required. This difference can be explicitly represented as

$$\cos(\varphi_{q_0} - \varphi_p) = \frac{\hat{\mathbf{q}}_0 \cdot \hat{\mathbf{p}} - (\hat{\mathbf{q}} \cdot \hat{\mathbf{q}}_0)(\hat{\mathbf{q}} \cdot \hat{\mathbf{p}})}{\sqrt{1 - (\hat{\mathbf{q}} \cdot \hat{\mathbf{q}}_0)^2} \sqrt{1 - (\hat{\mathbf{p}} \cdot \hat{\mathbf{q}})^2}} = \frac{x_p - y_{pq}x_q}{\sqrt{1 - y_{pq}^2} \sqrt{1 - x_q^2}}. \quad (33)$$

Since only difference of the angles enters, one can choose φ_{q_0} arbitrarily, e.g. $\varphi_{q_0} = 0$. Furthermore, $\cos \varphi_p$ and $\sin \varphi_p$ required in Eq. (30) are then also uniquely given [19].

With these preparations we are ready to carry out the angle integration $\int d\hat{\mathbf{q}}'' = \int_{-1}^1 dx'' \int_0^{2\pi} d\varphi''$ of Eq. (24) explicitly. The x'' integration is fixed by the δ -function in terms of $x_0 = x_0(q, p', q'')$ from Eq. (16), leaving only an integration over φ'' . Explicitly, the variables of Eqs. (30) and (32) need only be evaluated at a

fixed $x'' = x_0(q, p', q'')$. Thus, the explicit representation for the transition amplitude \hat{T} reads

$$\begin{aligned}
\hat{T}(p, x_p, x_{pq}^{q_0}, x_q, q; q_0) &= \hat{T}_0(p, x_p, x_{pq}^{q_0}, x_q, q; q_0) \\
&+ \frac{2}{q} \int_0^\infty dp' p' \frac{1}{E + i\epsilon - \frac{1}{m}(p'^2 + \frac{3}{4}q^2)} \int_{|q/2-p'|}^{q/2+p'} dq'' q'' \bar{G}(q, q'', p') \\
&\times \int_0^{2\pi} d\varphi'' \hat{t}_s \left(p, p', \frac{\frac{1}{2}q y_{pq} + y_{pq''}(x_0)}{\sqrt{\frac{1}{2}q^2 + q'^2 + qq''x_0}}; \varepsilon \right) \\
&\times \hat{T} \left(p'', \frac{qx_q + \frac{1}{2}q'' y_{q_0q''}(x_0)}{\sqrt{q^2 + \frac{1}{4}q'^2 + qq_0x_0}}, x_{\pi_2 y_{q_0q''}}^{q_0}(x_0), y_{q_0q''}(x_0), q''; q_0 \right) \\
&- \frac{2}{q} \int_0^\infty dq'' q'' \frac{1}{E + i\epsilon - E_d - \frac{3}{4m}q'^2} \int_{|q/2-q''|}^{q/2+q''} dp' p' \bar{G}(q, q'', p') \\
&\times \int_0^{2\pi} d\varphi'' \hat{t}_s \left(p, p', \frac{\frac{1}{2}q y_{pq} + y_{pq''}(x_0)}{\sqrt{\frac{1}{2}q^2 + q'^2 + qq''x_0}}; \varepsilon \right) \\
&\times \hat{T} \left(p'', \frac{qx_q + \frac{1}{2}q'' y_{q_0q''}(x_0)}{\sqrt{q^2 + \frac{1}{4}q'^2 + qq_0x_0}}, x_{\pi_2 y_{q_0q''}}^{q_0}(x_0), y_{q_0q''}(x_0), q''; q_0 \right), \quad (34)
\end{aligned}$$

where $p'' = \sqrt{p'^2 + \frac{3}{4}q^2 - \frac{3}{4}q'^2}$ is fixed.

The only remaining detail is to provide an explicit expression for the Born term,

$$T(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) \equiv \langle \mathbf{p}\mathbf{q} | tP | \varphi_d \mathbf{q}_0 \rangle, \quad (35)$$

where φ_d stands for the deuteron bound state. Projecting on Jacobi momenta and evaluating the permutation operator leads to

$$T(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) = \varphi_d \left(\mathbf{q} + \frac{1}{2}\mathbf{q}_0 \right) t_s \left(\mathbf{p}, \frac{1}{2}\mathbf{q} + \mathbf{q}_0, \varepsilon \right). \quad (36)$$

Using the invariant variables of Eq. (25) one arrives at

$$\begin{aligned}
\hat{T}_0(p, x_p, x_{pq}^{q_0}, x_q, q; q_0) &= \varphi_d \left(\sqrt{q^2 + \frac{1}{4}q_0^2 + qq_0x_q} \right) \\
&\times \hat{t}_s \left(p, \sqrt{\frac{1}{4}q^2 + q_0^2 + qq_0x_q}, \frac{\frac{1}{2}q y_{pq} + q_0x_p}{\sqrt{\frac{1}{4}q^2 + q_0^2 + qq_0x_q}}; \varepsilon \right). \quad (37)
\end{aligned}$$

The transition amplitude of Eq. (34) together with the Born term given above has as far as the angle integration is concerned a structure very similar to the one given in Eq. (2.19) of [19]. Even in the case where logarithmic singularities have to be integrated, they are independent of the angle φ'' . Thus, in the numerical realization demonstrated in [19] the φ'' -integration of the kernel is carried out for each fixed value x'' and q'' on their respective grids. Then the singularity structure depending only on the x'' and q'' variables is explicitly dealt with. In Eq. (34) the φ'' -integration needs to be carried out for each fixed value q'' and p' given on their respective grids. These grids also fix $x_0(q, p', q'')$. Since the functional dependence on φ'' is the same in both integrals over φ'' as is the area of integration in the $p' - q''$ -plane, the integral over φ'' in the kernel needs to be evaluated only once if both integrals of Eq. (34) are calculated on the same $p' - q''$ -grid. Under these conditions the numerical effort as far as the angle integration is concerned is similar to the one of [19].

Once the transition operator $T(\mathbf{p}, \mathbf{q}, \mathbf{q}_0)$ is explicitly calculated as function of the five independent variables, the amplitude for elastic scattering is obtained by calculating the matrix elements of the operator U given in Eq. (2) as

$$\begin{aligned} \langle \mathbf{q}\varphi_d | U | \mathbf{q}_0\varphi_d \rangle &= 2\varphi_d \left(\frac{1}{2}\mathbf{q} + \mathbf{q}_0 \right) \left(E - \frac{1}{m}(q^2 + \mathbf{q} \cdot \mathbf{q}_0 + q_0^2) \right) \varphi_d \left(\mathbf{q} + \frac{1}{2}\mathbf{q}_0 \right) \\ &+ 2 \int d^3q'' \varphi_d \left(\frac{1}{2}\mathbf{q} + \mathbf{q}'' \right) \frac{\langle \mathbf{q} + \frac{1}{2}\mathbf{q}'', \mathbf{q}'' | \hat{T} | \mathbf{q}_0\varphi_d \rangle}{E - \frac{3}{4m}q''^2 - E_d + i\varepsilon}. \end{aligned} \quad (38)$$

The amplitude for the full breakup process is given according to Eq. (3) by

$$\begin{aligned} \langle \mathbf{p}\mathbf{q} | U_0 | \mathbf{q}_0\varphi_d \rangle &= \frac{\langle \mathbf{p}\mathbf{q} | \hat{T} | \mathbf{q}_0\varphi_d \rangle}{E - \frac{3}{4m}\mathbf{q}^2 - E_d} \\ &+ \frac{\langle -\frac{1}{2}\mathbf{p} + \frac{3}{4}\mathbf{q}, -\mathbf{p} - \frac{1}{2}\mathbf{q} | \hat{T} | \mathbf{q}_0\varphi_d \rangle}{E - \frac{3}{4m}(-\mathbf{p} - \frac{1}{2}\mathbf{q})^2 - E_d} + \frac{\langle -\frac{1}{2}\mathbf{p} - \frac{3}{4}\mathbf{q}, +\mathbf{p} - \frac{1}{2}\mathbf{q} | \hat{T} | \mathbf{q}_0\varphi_d \rangle}{E - \frac{3}{4m}(+\mathbf{p} - \frac{1}{2}\mathbf{q})^2 - E_d}. \end{aligned} \quad (39)$$

Both operators are explicitly given in [19] using the independent variables of Eq. (25), and can be directly applied with the expression of Eq. (34).

5 Summary and Conclusions

In [19] the formulation of the nonrelativistic Faddeev equation for three identical bosons as function of vector variables was introduced and successfully solved for laboratory projectile energies up to the GeV regime. The key point allowing the calculation at those higher energies is to neglect the partial-wave decomposition generally used at lower energies and to work directly with momentum vectors, thus including all partial waves automatically. In the formulation of the Faddeev integral equation in the continuum which is most widely used, the singularities of the free three-body propagator occur simultaneously in an angle and momentum integration, leading to the so-called logarithmic singularities. They require special care in numerical applications. Although sophisticated algorithms have been developed to integrate those singularities along the real axis, it still is desirable to have a formulation of the Faddeev kernel, in which the singularity structure is simpler.

Starting from the formulation given in [19,23] we propose a new formulation of the Faddeev kernel which does not contain this technical obstacle of logarithmic singularities. Instead, the singularities of the free three-nucleon propagator appear as poles in a single variable. Those kind of poles can be integrated with standard techniques as, e.g. used in integrating the two-body Lippmann–Schwinger equation. The singularity given by the deuteron pole is a simple pole (as before), but is now cleanly separated in a separate integration. The integration over the angle variable not affected by the pole structure remains very similar. This simplification in handling the singularities of the three-body continuum in a similar fashion as the two-body continuum should ease applications of the Faddeev integral equations in different areas of physics.

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