

Numerical Implementation of a 3D Faddeev Formalism without Moving Singularities

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Numerical Implementation of a 3D Faddeev Formalism without Moving Singularities

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Abstract The three-dimensional (3D) momentum space treatment of three-body scattering above the breakup threshold is numerically challenging because of the moving logarithmic singularities in the kernel of Faddeev integral equation arising from the three-body free propagator. Elster et al. proposed a reformulation of the 3D Faddeev equation in which these moving logarithmic singularities are eliminated, leaving only simple pole singularities. In the present work, we numerically implement this formulation and assess its numerical behavior over a range of incident energies spanning the breakup threshold. The calculation is performed in two steps: first, the fully off-shell two-body transition matrix is obtained by solving the Lippmann–Schwinger equation using the Malfliet–Tjon potential. The matrix elements are then used as input for the three-body Faddeev integral equation. The latter is solved using Padé summation, while the remaining simple pole singularities are treated by evaluating the corresponding principal value integrals with a standard subtraction method. Numerical convergence is investigated with respect to the angular discretization while the momentum grids are kept fixed, following the momentum-grid choice of Liu et al. Elastic, breakup, and total cross sections are calculated, and the optical theorem is used as an additional numerical consistency check. The results show very good agreement with the corresponding Liu et al. calculation below the three-body breakup threshold, whereas noticeable differences emerge above the threshold. The optical theorem deviations obtained in the present calculation are smaller than those reported by Liu et al., indicating better internal consistency between the two independent evaluations of the total cross section. The comparison provides a numerical assessment of the Elster et al. formulation and demonstrates that the moving logarithmic singularities can be avoided in the numerical solution of the 3D Faddeev equation.

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1 Introduction

The three-body scattering problem is a fundamental problem in few-body nuclear physics. The Faddeev equations provide a framework for describing three-body scattering in terms of coupled integral equations [1]. Momentum space Faddeev calculations have traditionally been performed using a partial wave decomposition. Although this approach has been successfully applied to a wide range of three-nucleon scattering problems [2], the number of partial waves required for convergence generally increases with increasing projectile energy. At intermediate and higher energies, the increasing number of angular momentum channels can therefore make calculations computationally demanding. These limitations have motivated the development of direct three-dimensional (3D) approaches in which momentum vectors are used explicitly without introducing a partial wave expansion.

The development of 3D momentum space approach has covered both two- and three-nucleon scattering [3]-[14]. An important development in this direction was presented by Liu, Elster, and Glöckle, who formulated the Faddeev equation for three-body scattering in momentum space and solved it numerically at intermediate energies [6]. Using a Malfliet-Tjon (MT) interaction, they demonstrated the numerical feasibility and stability of the approach and calculated elastic and breakup cross sections at incident energies extending to approximately 1 GeV [6, 7]. These calculations provide an important numerical benchmark for 3D treatments of three-body scattering above the breakup threshold. A major numerical difficulty in the 3D solution of the Faddeev equation arises from the singular structure of the free three-body propagator. Above the three-body breakup threshold, the kernel contains moving logarithmic singularities whose locations depend on the integration variables. Their treatment requires special numerical procedures and can substantially complicate the solution of the integral equation [6, 7]. Consequently, an alternative formulation that simplifies the singularity structure can be advantageous for numerical calculations.

Elster, Glöckle, and Witała proposed a reformulation of the 3D Faddeev equation in which the complicated singularity structure associated with the free three-body propagator is disentangled. In their formulation, the moving logarithmic singularities are eliminated, while the remaining singularities of the propagators appear as simple poles in different momentum variables. The formulation retains the direct momentum space character of the 3D approach and avoids the explicit treatment of moving logarithmic singularities [15].

In the present work, we perform a numerical implementation of the 3D Faddeev formulation of Elster et al. and systematically investigate its numerical behavior. The MT interaction is used as a benchmark potential, allowing direct comparison with the earlier calculations of Liu et al. [6]. The numerical

procedure includes the calculation of the fully off-shell two-body transition matrix, discretization of the momentum and angular variables, treatment of the remaining simple pole singularities, and solution of the resulting Faddeev equation using Padé summation. Convergence with respect to the numerical grids is examined at several incident energies. Elastic and breakup cross sections are calculated, and the optical theorem is used as an independent consistency check. Finally, the calculated observables are compared with the corresponding results of Liu et al. [6].

This paper is organized as follows. In Section 2, we present the final momentum space representations of the 3D Faddeev equations given by Liu et al. and Elster et al., with particular emphasis on their different singularity structures. Section 3 introduces the elastic and breakup transition amplitudes and the corresponding cross sections, including the optical theorem relation used for consistency checks. Section 4 presents the numerical implementation and the present results. The MT interaction is used as a benchmark, and the present results, their convergence with respect to the angular discretization, and their comparison with the results of Liu et al. are discussed. Finally, the conclusions are summarized in Section 5.

2 Three-Body Scattering in the Faddeev Scheme

For a system of three interacting particles, the scattering dynamics can be formulated in terms of the transition operator T , which satisfies the Faddeev integral equation [1]

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

where t denotes the two-body transition operator and $P = P_{12}P_{23} + P_{13}P_{23}$ is the permutation operator defined as the sum of the cyclic and anticyclic permutations of the three particles. The initial state $|\phi\rangle = |\varphi_d \mathbf{q}_0\rangle$ consists of a two-body bound state $|\varphi_d\rangle$, with binding energy E_d , and the momentum state of the spectator particle with initial momentum $|\mathbf{q}_0\rangle$. The free three-body propagator is given by $G_0 = (E - H_0 + i\varepsilon)^{-1}$, where H_0 is the free Hamiltonian and E denotes the total energy in the center of mass frame. The total energy can be expressed in terms of the initial spectator momentum and the incident laboratory energy according to

$$E = E_d + \frac{3}{4m}q_0^2 = E_d + \frac{2}{3}E_{lab}. \quad (2)$$

A momentum space representation of Eq. (1), following the formulation of Liu et al. leads to [6]

$$\begin{aligned} \hat{T}(\mathbf{p}, \mathbf{q}; \mathbf{q}_0) &= \hat{t}_s(\mathbf{p}, \boldsymbol{\pi}, \varepsilon) \varphi_d(\boldsymbol{\pi}') \\ &+ \int d\mathbf{q}'' \frac{\hat{t}_s(\mathbf{p}, \tilde{\boldsymbol{\pi}}; \varepsilon)}{E - \frac{1}{m}(q^2 + \mathbf{q} \cdot \mathbf{q}'' + q''^2) + i\varepsilon} \frac{\hat{T}(\tilde{\boldsymbol{\pi}}', \mathbf{q}'', \mathbf{q}_0)}{\frac{3}{4m}(q_0^2 - q''^2) + i\varepsilon}, \end{aligned} \quad (3)$$

where the momentum variables are related through

$$\boldsymbol{\pi} = \frac{1}{2}\mathbf{q} + \mathbf{q}_0, \quad \boldsymbol{\pi}' = \mathbf{q} + \frac{1}{2}\mathbf{q}_0, \quad \tilde{\boldsymbol{\pi}} = \frac{1}{2}\mathbf{q} + \mathbf{q}'', \quad \tilde{\boldsymbol{\pi}}' = \mathbf{q} + \frac{1}{2}\mathbf{q}''. \quad (4)$$

Here, $\mathbf{p}$ denotes the relative momentum of the interacting two-body subsystem, while $\mathbf{q}$ is the relative momentum of the spectator particle with respect to this subsystem. The energy of the two-body subsystem is given by $\varepsilon = E - 3q^2/4m$.

For energies below the three-body breakup threshold, $E < 0$, the singular structure of the kernel is relatively simple. Above the breakup threshold, $E > 0$, the second denominator in Eq. (3) contains a simple pole that can be treated using a standard subtraction procedure. More importantly, the first denominator develops moving logarithmic singularities as a consequence of the angular integration. These singularities depend on the integration variables and therefore require special numerical treatment in the formulation of Liu et al. [6]. To overcome this difficulty, Elster et al. introduced an alternative formulation of the 3D Faddeev equation [15]. Their approach reorganizes the integral equation such that the moving logarithmic singularities are removed from the kernel. In this formulation, Eq. (1) can be expressed as

$$\begin{aligned} \hat{T}(\mathbf{p}, \mathbf{q}; \mathbf{q}_0) &= \hat{t}_s(\mathbf{p}, \boldsymbol{\pi}, \varepsilon) \varphi_d(\boldsymbol{\pi}') \\ &+ \frac{2}{q} \int_0^\infty dp' p' \int_{|q/2-p'|}^{q/2+p'} dq'' q'' \int d\hat{\mathbf{q}}'' \delta(x_{q''} - x_0) \frac{\hat{t}_s(\mathbf{p}, p' \hat{\boldsymbol{\pi}}; \varepsilon)}{|E_d| + p''^2/m} \frac{\hat{T}(p'' \hat{\boldsymbol{\pi}}', \mathbf{q}''; \mathbf{q}_0)}{\varepsilon - p'^2/m + i\epsilon} \\ &- \frac{2}{q} \int_0^\infty dq'' q'' \int_{|q/2-q''|}^{q/2+q''} dp' p' \int d\hat{\mathbf{q}}'' \delta(x_{q''} - x_0) \frac{\hat{t}_s(\mathbf{p}, p' \hat{\boldsymbol{\pi}}; \varepsilon)}{|E_d| + p''^2/m} \frac{\hat{T}(p'' \hat{\boldsymbol{\pi}}', \mathbf{q}''; \mathbf{q}_0)}{\frac{3}{4m}(q_0^2 - q''^2) + i\epsilon}, \end{aligned} \quad (5)$$

where

$$x_0 = \frac{1}{qq''}(p''^2 - \frac{1}{4}q''^2 - q^2), \quad p'' = (p'^2 + \frac{3}{4}q^2 - \frac{3}{4}q''^2)^{1/2}. \quad (6)$$

The new representation separates the singular behavior in a way that avoids the moving logarithmic singularity encountered in the kernels of Faddeev integral equation. The remaining singularities occur as simple poles in the momentum integrations and can therefore be handled by evaluating the corresponding principal value integrals using a subtraction technique.

Since the incident momentum q_0 specifies the initial state, its magnitude can be regarded as fixed. To represent the transition operator $\hat{T}$ as a scalar function, five independent variables are sufficient. These variables are chosen as

$$p = |\mathbf{p}|, \quad q = |\mathbf{q}|, \quad x_p = \hat{\mathbf{p}} \cdot \hat{\mathbf{q}}_0, \quad x_q = \hat{\mathbf{q}} \cdot \hat{\mathbf{q}}_0,$$

$$x_{pq}^{q_0} = (\widehat{\mathbf{q}_0 \times \mathbf{p}}) \cdot (\widehat{\mathbf{q}_0 \times \mathbf{q}}) = \frac{\hat{\mathbf{p}} \cdot \hat{\mathbf{q}} - (\hat{\mathbf{q}}_0 \cdot \hat{\mathbf{p}})(\hat{\mathbf{q}}_0 \cdot \hat{\mathbf{q}})}{\sqrt{1 - (\hat{\mathbf{q}}_0 \cdot \hat{\mathbf{p}})^2} \sqrt{1 - (\hat{\mathbf{q}}_0 \cdot \hat{\mathbf{q}})^2}} = \frac{x_{pq} - x_p x_q}{\sqrt{1 - x_p^2} \sqrt{1 - x_q^2}}. \quad (7)$$

where $p = |\mathbf{p}|$ and $q = |\mathbf{q}|$ are the magnitudes of the Jacobi momenta, while the remaining variables describe the angular dependence of the momenta with respect to the incident momentum direction. For the numerical treatment of Eq. (5), it is convenient to introduce a coordinate system in which the z -axis is chosen parallel to the vector $\mathbf{q}$. We refer to this coordinate system as the q -system. With this choice, the 3D Faddeev equation can be written explicitly in terms of the five scalar variables introduced above:

$$\begin{aligned} \hat{T}(p, x_p, x_{pq}^{q_0}, x_q, q) &= \hat{t}_s(p, \pi, x_{p\pi}; \varepsilon) \varphi_d(\pi') \\ &+ \frac{2}{q} \int_0^\infty dp' p' \int_{|q/2-p'|}^{q/2+p'} dq'' q'' \int_0^{2\pi} d\varphi'' \frac{\hat{t}_s(p, p', x_{p\tilde{\pi}}; \varepsilon) \hat{T}(p'', x_{\tilde{\pi}'}, x_{\tilde{\pi}'q''}^{q_0}, x_{q''q_0}, q'')}{|E_d| + p'^2/m} \frac{\hat{T}(p'', x_{\tilde{\pi}'}, x_{\tilde{\pi}'q''}^{q_0}, x_{q''q_0}, q'')}{\varepsilon - p'^2/m + i\epsilon} \\ &- \frac{2}{q} \int_0^\infty dq'' q'' \int_{|q/2-q''|}^{q/2+q''} dp' p' \int_0^{2\pi} d\varphi'' \frac{\hat{t}_s(p, p', x_{p\tilde{\pi}}; \varepsilon) \hat{T}(p'', x_{\tilde{\pi}'}, x_{\tilde{\pi}'q''}^{q_0}, x_{q''q_0}, q'')}{|E_d| + p'^2/m} \frac{\hat{T}(p'', x_{\tilde{\pi}'}, x_{\tilde{\pi}'q''}^{q_0}, x_{q''q_0}, q'')}{\frac{3}{4m}(q_0^2 - q''^2) + i\epsilon}, \end{aligned} \quad (8)$$

The angular and momentum variables appearing in Eq. (8) are related through the following expressions:

$$\begin{aligned} x_{q''} &= \hat{\mathbf{q}} \cdot \hat{\mathbf{q}}'' = x_0 \\ \pi &= \sqrt{\frac{1}{4}q^2 + qq_0x_q + q_0^2}, \\ \pi' &= \sqrt{q^2 + qq_0x_q + \frac{1}{4}q_0^2}, \\ x_{p\pi} &= \hat{\mathbf{p}} \cdot \hat{\boldsymbol{\pi}} = \frac{\frac{1}{2}qx_{pq} + q_0x_p}{\pi}, \\ x_{p\tilde{\pi}} &= \hat{\mathbf{p}} \cdot \hat{\boldsymbol{\pi}} = \frac{\frac{1}{2}qx_{pq} + q''x_{pq''}}{\tilde{\pi}}, \\ x_{\tilde{\pi}'} &= \hat{\boldsymbol{\pi}}' \cdot \hat{\mathbf{q}}_0 = \frac{qx_q + \frac{1}{2}q''x_{q_0q''}}{\tilde{\pi}'}, \\ x_{\tilde{\pi}'q''} &= \hat{\boldsymbol{\pi}}' \cdot \hat{\mathbf{q}}'' = \frac{qx_{qq''} + \frac{1}{2}q''}{\tilde{\pi}'}, \\ x_{pq} &= \hat{\mathbf{p}} \cdot \hat{\mathbf{q}} = x_px_q + \sqrt{1-x_p^2}\sqrt{1-x_q^2}x_{pq_0}^{q_0}, \\ x_{q''q_0} &= \hat{\mathbf{q}}'' \cdot \hat{\mathbf{q}}_0 = x_0x_q + \sqrt{1-x_0^2}\sqrt{1-x_q^2}\cos\varphi'', \\ x_{pq''} &= \hat{\mathbf{p}} \cdot \hat{\mathbf{q}}'' = x_{pq}x_0 + \sqrt{1-x_{pq}^2}\sqrt{1-x_0^2}\cos(\varphi_{pq_0} - \varphi''), \\ \cos\varphi_{pq_0} &= \frac{x_p - x_{pq}x_q}{\sqrt{1-x_{pq}^2}\sqrt{1-x_q^2}}, \sin\varphi_{pq_0} = \pm\sqrt{1-\cos^2\varphi_{pq_0}}, \\ x_{\tilde{\pi}'q''}^{q_0} &= \frac{\hat{\boldsymbol{\pi}}' \cdot \hat{\mathbf{q}}'' - (\hat{\mathbf{q}}_0 \cdot \hat{\boldsymbol{\pi}}')(\hat{\mathbf{q}}_0 \cdot \hat{\mathbf{q}}'')}{\sqrt{1-(\hat{\mathbf{q}}_0 \cdot \hat{\boldsymbol{\pi}}')^2}\sqrt{1-(\hat{\mathbf{q}}_0 \cdot \hat{\mathbf{q}}'')^2}} = \frac{x_{\tilde{\pi}'q''} - x_{\tilde{\pi}'}x_{q_0q''}}{\sqrt{1-x_{\tilde{\pi}}^2}\sqrt{1-x_{q_0q''}^2}}. \end{aligned} \quad (9)$$

An important feature of this formulation is the resulting singularity structure of the kernel. In contrast to Eq. (3), the kernels in Eq. (8) contain only simple pole singularities in the p' and q'' integrations. The remaining simple pole singularities lead to principal value integrals, which are evaluated using the standard subtraction method. The remaining angular integrations are free of moving logarithmic singularities.

3 Elastic and breakup scattering amplitudes

The elastic scattering operator U is obtained from the three-body transition operator T through the relation

$$U = PG_0^{-1} + PT. \quad (10)$$

A momentum space representation of Eq. (10), following Ref. [10], is given by

$$\begin{aligned} \langle \mathbf{q}\varphi_d|U|\mathbf{q}_0\varphi_d\rangle &= 2\varphi_d(\boldsymbol{\pi}) \left(E - \frac{1}{m}(q^2 + \mathbf{q} \cdot \mathbf{q}_0 + q_0^2)\right) \varphi_d(\boldsymbol{\pi}') \\ &+ 2 \int d^3\mathbf{q}'' \varphi_d(\tilde{\boldsymbol{\pi}}) \frac{\hat{T}(\tilde{\boldsymbol{\pi}}', \mathbf{q}''; \mathbf{q}_0)}{\frac{3}{4m}(q_0^2 - q''^2) + i\epsilon}. \end{aligned} \quad (11)$$

To obtain a form suitable for numerical calculations, Eq. (11) can be expressed in the q -system introduced in the previous section as:

$$\begin{aligned} U(q_0, x_q) &= 2\varphi_d^2(\pi) \left(E - \frac{q_0^2}{m}(2 + x_q)\right) \\ &+ 2 \int_0^\infty dq'' q''^2 \int_{-1}^1 dx'' \int_0^{2\pi} d\varphi'' \varphi_d(\tilde{\pi}) \frac{\hat{T}(\tilde{\pi}', x_{\tilde{\pi}'}, x_{\tilde{\pi}'q''}^{q_0}, x_{q_0q''}, q'')}{\frac{3}{4m}(q_0^2 - q''^2) + i\epsilon}. \end{aligned} \quad (12)$$

The momentum and angular variables in Eq. (12) are determined from the relations given in Eqs. (9), with the specific substitutions $q=q_0$ and $x_0=x''$.

For the breakup process, the corresponding transition operator is defined by

$$U_0 = (1 + P)T. \quad (13)$$

A momentum space representation of the breakup transition operator is then obtained as

$$\langle \mathbf{p}\mathbf{q}|U_0|\mathbf{q}_0\varphi_d\rangle = \frac{\hat{T}(\mathbf{p}, \mathbf{q}; \mathbf{q}_0)}{E - \frac{3}{4m}q^2 - E_d} + \frac{\hat{T}(\mathbf{p}_2, \mathbf{q}_2; \mathbf{q}_0)}{E - \frac{3}{4m}q_2^2 - E_d} + \frac{\hat{T}(\mathbf{p}_3, \mathbf{q}_3; \mathbf{q}_0)}{E - \frac{3}{4m}q_3^2 - E_d}. \quad (14)$$

where the transformed Jacobi momenta are given by

$$\mathbf{p}_2 = -\frac{1}{2}\mathbf{p} + \frac{3}{4}\mathbf{q}, \quad \mathbf{q}_2 = -\mathbf{p} - \frac{1}{2}\mathbf{q}, \quad \mathbf{p}_3 = -\frac{1}{2}\mathbf{p} - \frac{3}{4}\mathbf{q}, \quad \mathbf{q}_3 = \mathbf{p} - \frac{1}{2}\mathbf{q}, \quad (15)$$

Using the scalar representation of the three-body transition matrix introduced in Section 2, Eq. (14) can be written in terms of the independent momentum and angular variables as

$$U_0(p, x_p, x_{pq}^{q_0}, x_q, q) = \frac{\hat{T}(p, x_p, x_{pq}^{q_0}, x_q, q)}{E - \frac{3}{4m}q^2 - E_d} + \frac{\hat{T}(p_2, x_{p_2}, x_{p_2q_2}^{q_0}, x_{q_2}, q_2)}{E - \frac{3}{4m}q_2^2 - E_d} + \frac{\hat{T}(p_3, x_{p_3}, x_{p_3q_3}^{q_0}, x_{q_3}, q_3)}{E - \frac{3}{4m}q_3^2 - E_d}. \quad (16)$$

The magnitudes and angular variables associated with the transformed Jacobi momenta are given by

$$\begin{aligned} p_2 &= \frac{1}{2}\sqrt{p^2 + \frac{9}{4}q^2 - 3pqx_{pq}}, \\ p_3 &= \frac{1}{2}\sqrt{p^2 + \frac{9}{4}q^2 + 3pqx_{pq}}, \\ q_2 &= \sqrt{p^2 + \frac{1}{4}q^2 + pqx_{pq}}, \\ q_3 &= \sqrt{p^2 + \frac{1}{4}q^2 - pqx_{pq}}, \\ x_{p_2} &= \hat{\mathbf{p}}_2 \cdot \hat{\mathbf{q}}_0 = \frac{-\frac{1}{2}px_q + \frac{3}{4}qx_p}{p_2}, \\ x_{p_3} &= \hat{\mathbf{p}}_3 \cdot \hat{\mathbf{q}}_0 = \frac{-\frac{1}{2}px_q - \frac{3}{4}qx_p}{p_3}, \\ x_{q_2} &= \hat{\mathbf{q}}_2 \cdot \hat{\mathbf{q}}_0 = \frac{-px_p - \frac{1}{2}qx_q}{q_2}, \\ x_{q_3} &= \hat{\mathbf{q}}_3 \cdot \hat{\mathbf{q}}_0 = \frac{px_p - \frac{1}{2}qx_q}{q_3}, \\ x_{p_2q_2}^{q_0} &= \frac{\hat{\mathbf{p}}_2 \cdot \hat{\mathbf{q}}_2 - (\hat{\mathbf{q}}_0 \cdot \hat{\mathbf{p}}_2)(\hat{\mathbf{q}}_0 \cdot \hat{\mathbf{q}}_2)}{\sqrt{1 - (\hat{\mathbf{q}}_0 \cdot \hat{\mathbf{p}}_2)^2}\sqrt{1 - (\hat{\mathbf{q}}_0 \cdot \hat{\mathbf{q}}_2)^2}} = \frac{x_{p_2q_2} - x_{p_2}x_{q_2}}{\sqrt{1 - x_{p_2}^2}\sqrt{1 - x_{q_2}^2}}, \\ x_{p_3q_3}^{q_0} &= \frac{\hat{\mathbf{p}}_3 \cdot \hat{\mathbf{q}}_3 - (\hat{\mathbf{q}}_0 \cdot \hat{\mathbf{p}}_3)(\hat{\mathbf{q}}_0 \cdot \hat{\mathbf{q}}_3)}{\sqrt{1 - (\hat{\mathbf{q}}_0 \cdot \hat{\mathbf{p}}_3)^2}\sqrt{1 - (\hat{\mathbf{q}}_0 \cdot \hat{\mathbf{q}}_3)^2}} = \frac{x_{p_3q_3} - x_{p_3}x_{q_3}}{\sqrt{1 - x_{p_3}^2}\sqrt{1 - x_{q_3}^2}}, \end{aligned} \quad (17)$$

The differential elastic scattering cross section in the center of mass frame is obtained from the elastic transition operator according to

$$\frac{d\sigma_{el}}{d\Omega} = \left(\frac{2m}{3}\right)^2 (2\pi)^4 |U(q_0, x_q)|^2. \quad (18)$$

Integration over the scattering angle gives the total elastic cross section,

$$\sigma_{el} = \left(\frac{2m}{3}\right)^2 (2\pi)^5 \int_{-1}^1 dx_q |U(q_0, x_q)|^2, \quad (19)$$

while the total breakup cross section is calculated from the breakup transition operator as

$$\sigma_{br} = \frac{1}{3} \frac{(2\pi)^5 m^2}{3q_0} \int_0^{\sqrt{\frac{4mE}{3}}} dq q^2 p \int_{-1}^1 dx_p \int_{-1}^1 dx_q \int_0^{2\pi} d\varphi |U_0(p, x_p, \cos \varphi, x_q, q)|^2, \quad (20)$$

where the momenta p and q are constrained by the available three-body energy through the relation

$$E = E_d + \frac{3}{4m} q_0^2 = \frac{p^2}{m} + \frac{3q^2}{4m}. \quad (21)$$

The optical theorem can be used to calculate the total cross section directly from the forward elastic scattering amplitude as

$$\sigma_{opt} = -\frac{(2\pi)^3 4m}{3q_0} \text{Im } U(q_0, x_q = 1). \quad (22)$$

According to the unitarity relation between U and U_0 , the total cross section satisfies $\sigma_{opt} = \sigma_{el} + \sigma_{br}$. Their difference provides a useful numerical consistency test of the calculated scattering amplitudes and cross sections.

4 Numerical Calculations and Results

The numerical calculations are performed using the MT potential. The parameters of the potential are chosen to reproduce the deuteron bound state energy and are listed in Table 1. The momentum space representation of this interaction is [16],

$$V(\mathbf{p}', \mathbf{p}) = \frac{1}{2\pi^2} \left(\frac{V_R}{(\mathbf{p}' - \mathbf{p})^2 + \mu_R^2} - \frac{V_A}{(\mathbf{p}' - \mathbf{p})^2 + \mu_A^2} \right). \quad (23)$$

The numerical calculation is carried out in two successive steps. First, the Lippmann–Schwinger equation is solved to obtain the fully off-shell two-body transition matrix for each value of the two-body subsystem energy, $\varepsilon = E - 3q^2/4m$. These matrix elements are then used as input for the three-body Faddeev equation, which is subsequently solved using Padé summation. The integrations appearing in the equations are evaluated using Gauss–Legendre quadrature. The remaining simple pole singularities are treated by evaluating the corresponding principal value integrals using the standard subtraction method.

For the momentum variables, the Gauss–Legendre points are mapped from the interval $[-1, 1]$ to the required momentum intervals using a combination of hyperbolic and linear transformations as

$$k = \frac{1+x}{1/k_1 + (2/\bar{k} - 1/k_1)x}, \quad k = \frac{k_{max} - \bar{k}}{2}x + \frac{k_{max} + \bar{k}}{2}, \quad (24)$$

Table 1 Parameters of the Malfliet–Tjon potential and the corresponding deuteron bound state energy. We use units such that $\hbar c = 197.3286 \text{ MeV fm} = 1$.

$V_A [\text{MeV fm}]$	$\mu_A [\text{fm}^{-1}]$	$V_R [\text{MeV fm}]$	$\mu_R [\text{fm}^{-1}]$	$E_d [\text{MeV}]$
626.8932	1.550	1438.7228	3.11	-2.2307

Table 2 Calculated elastic, breakup, and total cross sections at selected incident energies. The last column gives the relative deviation from the optical theorem.

$E_{lab} [\text{GeV}]$	$\sigma_{el} [\text{mb}]$	$\sigma_{br} [\text{mb}]$	$\sigma_{opt} [\text{mb}]$	$(\sigma_{el}^q + \sigma_{br}) [\text{mb}]$	$\delta_{opt} [\%]$
0.003	2561.61	0.00	2560.41	2561.61	0.05
0.1	250.06	70.60	320.96	320.66	0.09
0.2	142.46	33.71	178.53	176.17	1.32
0.5	59.58	31.98	93.62	91.56	2.20
1.0	29.31	22.93	51.19	52.24	2.05

where $x \in [-1, 1]$ is the Gauss–Legendre variable. The parameters of these mappings are chosen separately for the different momentum integrations. For the two-body Lippmann–Schwinger equation, the momentum variables are mapped using $k_1 = 3 \text{ fm}^{-1}$, $\bar{k} = 10 \text{ fm}^{-1}$, and $k_{max} = 60 \text{ fm}^{-1}$. The equation is solved using 60 and 40 grid points for the momentum and the angle variables. For the three-body Faddeev integral equation, the momentum variables are mapped using $\bar{k} = \sqrt{4mE/3}$ and $k_1 = \bar{k}/3$. The upper cutoff is taken as $k_{max} = 20 \text{ fm}^{-1}$ for p and p' while $k_{max} = 30 \text{ fm}^{-1}$ is used for q and q'' momenta. In the Faddeev calculation, 49 grid points are used for the momentum variables p , q , p' and q'' , following the momentum-grid choice of Liu et al. [6]. These momentum grids are kept fixed in the convergence study, and only the angular discretization is varied. The calculated elastic and breakup cross sections are presented in Table 2. The total cross section is evaluated independently in two ways: from the sum of the elastic and breakup contributions and from the optical theorem. To quantify the consistency between these two evaluations, we define the relative optical theorem deviation as

$$\delta_{opt} = \frac{|\sigma_{opt} - (\sigma_{el} + \sigma_{br})|}{\sigma_{opt}} \times 100\%. \quad (25)$$

The values of δ_{opt} are also listed in Table 2.

At the lowest incident energy, $E_{lab} = 0.003 \text{ GeV}$, which lies below the three-body breakup threshold, the calculated elastic cross section is in very close agreement with the total cross section obtained from the optical theorem, with a relative deviation of only 0.05%. Above the breakup threshold, the breakup contribution becomes nonzero and increasingly important, while the elastic cross section decreases with increasing incident energy. The agreement between the two independent evaluations of the total cross section gradually becomes less accurate, with δ_{opt} increasing from less than 0.09% at 0.1 GeV to about 2% at the highest energies considered. Overall, the results show a decreasing elastic contribution, a significant breakup contribution at higher

Table 3 Numerical convergence of the calculated cross sections with respect to the angular discretization. The momentum grids are fixed at 49 points following Liu et al. [6].

E_{lab}	$N_{p,p'}$	N_x	$N_{q,q''}$	$N_{\varphi''}$	σ_{el} [mb]	σ_{br} [mb]	σ_{opt} [mb]	$(\sigma_{el} + \sigma_{br})$ [mb]
0.003	49	12	49	12	2562.54	0.00	2561.61	2562.54
	49	16	49	16	2561.90	0.00	2560.76	2561.90
	49	20	49	20	2561.68	0.00	2560.51	2561.68
	49	24	49	20	2561.61	0.00	2560.41	2561.61
0.1	49	12	49	12	249.92	69.92	318.76	319.84
	49	16	49	16	249.99	70.38	320.44	320.37
	49	20	49	20	250.03	70.57	320.80	320.60
	49	24	49	20	250.06	70.60	320.96	320.66
0.5	49	12	49	12	52.84	35.26	76.31	88.10
	49	16	49	16	57.13	31.82	87.98	88.95
	49	20	49	20	58.51	31.64	91.64	90.15
	49	24	49	20	59.58	31.98	93.62	91.56

energies, and a reasonably small deviation from the optical theorem over the entire energy range investigated.

The numerical convergence of the calculated cross sections is investigated with respect to the angular discretization. The momentum grids are kept fixed at 49 points, following the momentum-grid choice of Liu et al. [6], while the number of angular mesh points is varied. As shown in Table 3, the numbers of points used for the three angular cosine variables x_p , x_{pq} , and x_q are varied simultaneously and are denoted by N_x , while the azimuthal variable φ'' is discretized independently with $N_{\varphi''}$ points.

At $E_{lab} = 0.003$ GeV, the elastic cross section changes only slightly from 2562.54 mb at $N_x = 12$, $N_{\varphi} = 12$ to 2561.61 mb at $N_x = 24$, $N_{\varphi} = 20$. Similarly, at $E_{lab} = 0.1$ GeV, the elastic cross section changes from 249.92 to 250.06 mb, while the breakup cross section changes from 69.92 to 70.60 mb. These small variations indicate good angular convergence at the lower incident energies. A stronger dependence on the angular resolution is observed at higher energies. At $E_{lab} = 0.5$ GeV, the elastic cross section changes from 52.84 to 59.58 mb as the angular grid is refined, while the breakup contribution changes from 35.26 to 31.98 mb. These results show that the angular resolution becomes increasingly important at higher incident energies.

The results obtained with the present implementation of the Elster et al. formulation are compared with the corresponding results of Liu et al. [6] in Table 4. For the comparison presented in Table 4, the final numerical grid is chosen to reproduce the number of quadrature points used by Liu et al. for each individual momentum and angular variable. At the lowest incident energy considered, $E_{lab} = 0.003$ GeV, which is below the three-body breakup threshold, the present results are in very good agreement with those of Liu et al. The elastic cross sections obtained in the two calculations differ only slightly. Above the breakup threshold, however, noticeable differences between the two calculations are observed. The deviations are relatively moderate at

Table 4 Comparison of the present results obtained with the Elster et al. formulation with the corresponding results of Liu et al. [6]. For this comparison, the number of mesh points used for each individual momentum and angular variable is chosen exactly as in the calculation of Liu et al.

E_{lab} [GeV]	Formalism	σ_{el} [mb]	σ_{br} [mb]	σ_{opt} [mb]	$(\sigma_{el} + \sigma_{br})$ [mb]	δ_{opt}
0.003	Elster et al.	2561.61	0.00	2560.41	2561.61	0.05
	Liu et al.	2561.14	0.00	2562.65	2561.14	0.06
0.1	Elster et al.	250.06	70.60	320.96	320.66	0.09
	Liu et al.	272.20	75.18	346.16	347.38	0.35
0.2	Elster et al.	142.46	33.71	178.53	176.17	1.32
	Liu et al.	204.30	53.93	245.57	258.23	5.15
0.5	Elster et al.	59.58	31.98	93.62	91.56	2.20
	Liu et al.	64.61	36.39	110.35	101.00	8.47
1.0	Elster et al.	29.31	22.93	51.19	52.24	2.05
	Liu et al.	21.90	23.46	49.59	45.36	8.53

$E_{lab} = 0.1$ GeV, but become more pronounced at higher incident energies. In particular, differences are observed in both the elastic and breakup cross sections, and the corresponding total cross sections also show a clear deviation from the results of Liu et al.

An additional comparison is provided by the optical theorem consistency. The values of δ_{opt} obtained in the present calculation are smaller than those reported by Liu et al. at all common incident energies listed in Table 4. For example, at $E_{lab} = 0.2$ GeV, the values are 1.32% and 5.15%, respectively; at 0.5 GeV, they are 2.20% and 8.47%; and at 1.0 GeV, they are 2.05% and 8.53% respectively. Thus, according to this internal consistency criterion, the present calculation satisfies the optical theorem closely than the corresponding calculation of Liu et al.

The origin of the differences in the calculated cross sections cannot be identified unambiguously from the present calculations. It is important to note, however, that the comparison is performed using the same MT interaction and the same momentum and angular mesh resolutions as those adopted by Liu et al. Therefore, the observed differences cannot simply be attributed to a different number of momentum or angular grid points. Moreover, the discrepancies become apparent mainly above the three-body breakup threshold, where the moving logarithmic singularities of the standard three-body propagator play an important role. In the Liu et al. formulation, these singularities require a dedicated numerical treatment, whereas in the Elster et al. formulation they are eliminated and replaced by simple poles. Consequently, differences in the treatment of the singular structures, together with the associated interpolation and quadrature procedures, may contribute to the observed differences.

5 Conclusion

In this work, we have numerically implemented the 3D Faddeev formulation proposed by Elster et al. for three-body scattering. The main numerical advantage of this formulation is that the moving logarithmic singularities of the standard three-body propagator are eliminated, leaving only simple pole singularities. The calculated elastic, breakup, and total cross sections were examined at several incident energies below and above the three-body breakup threshold. A convergence study was carried out by varying the angular discretization while keeping the momentum grids fixed at 49 points, following the momentum-grid choice of Liu et al. The results show weak sensitivity to the angular resolution at lower energies, whereas the dependence becomes more pronounced as the incident energy increases. This behavior indicates that a finer angular resolution is required for the higher energy calculations. The calculated total cross section was also evaluated independently using the optical theorem. The resulting values of δ_{opt} remain small over the energy range considered, providing an additional check of the numerical consistency of the calculated scattering amplitudes and cross sections.

The present results were compared with the established 3D calculations of Liu et al. At the energy below the three-body breakup threshold, the elastic cross sections are in very good agreement. Above the breakup threshold, noticeable differences appear in the elastic, breakup, and total cross sections. The values of δ_{opt} obtained in the present calculation are smaller than those reported by Liu et al. at the common energies, indicating better internal consistency between the two independent evaluations of the total cross section. This comparison should be interpreted as a numerical consistency test rather than as a direct measure of the absolute accuracy of either calculation.

The origin of the differences between the two calculations cannot be established from the present results alone. For the comparison in Table 4, the same MT interaction is used, and the number of mesh points for each individual momentum and angular variable is chosen as in the calculation of Liu et al. Therefore, the observed differences cannot simply be attributed to a different number of momentum or angular mesh points. Since the discrepancies become apparent mainly above the three-body breakup threshold, the different numerical treatment of the singular structures may play a role. In the Liu et al. formulation, the moving logarithmic singularities require a dedicated numerical treatment, whereas in the Elster et al. formulation they are eliminated, leaving only simple-pole singularities. Differences in the associated numerical treatment, including interpolation and quadrature procedures, may therefore contribute to the observed discrepancies, although their individual contributions cannot be isolated from the present calculations.

Finally, it is emphasized that the present work does not introduce a new Faddeev formalism. The theoretical formulation is that developed by Elster et al.; the contribution of the present study is its numerical implementation and systematic assessment through angular convergence studies, treatment of the remaining simple pole singularities, optical theorem consistency checks,

and comparison with established 3D results. The results demonstrate that the Elster et al. formulation provides a practical route to numerical three-body scattering calculations without the explicit treatment of moving logarithmic singularities.

Declarations

Ethics approval and consent to participate

Not applicable.

Consent for publication

Not applicable.

Availability of data and materials

The datasets generated and analyzed during the current study are available from the corresponding author on reasonable request.

Competing interests

The authors declare that they have no competing interests.

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Authors' contributions

M.R. designed and directed the project; M.R. and A. A. developed the Numerical calculations, discussed the results and contributed to the final manuscript.

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