Few-Body Syst (2025) 66:24
https://doi.org/10.1007/s00601-025-01991-z

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Three-Dimensional Integral Faddeev Equations without a Certain Symmetry

Received: 20 September 2024 / Accepted: 16 April 2025

Abstract A method for the direct integration of the three-dimensional Faddeev equations with respect to the breakup T-matrix in momentum space for three-body systems with differing masses is presented. The Faddeev equations are explicitly formulated without imposing symmetry or antisymmetry requirements on the two-body t-matrices, thus accounting for mass differences between the three interacting particles. An algorithm for the algebraic determination of non-relativistic wave functions for three-body systems with arbitrary masses is given. Furthermore, it is directly demonstrated how the domain of logarithmic singularities in the integral kernels of the Faddeev equations is significantly altered by varying the masses of the interacting particles. The developed method for traversing logarithmic singularities is tested using the example of calculating the total cross sections for elastic neutron-deuteron scattering and breakup reaction.

1 Introduction

The solutions to the dynamic equations of Faddeev [1] and Faddeev-Yakubovsky [2], along with numerous generalizations and simplifications (see, e.g., [3–6] and also review of four-nucleon calculations [7]), provided a strong foundation for precise methods in the nonrelativistic theory of interacting three- and few-body systems, respectively. The Faddeev and Faddeev-Yakubovsky equations are best known in their separable form, also known as the AGS form [8], the applicability of which is ensured by the rapid convergence of the Hilbert-Schmidt norm with increasing scattering energy. Few-body dynamics in the AGS form have proven themselves well not only in the description of elastic scattering and nuclear reactions at low energies, but also in various types of eigenvalue problems with the search for binding energies in exotic meson-nuclear [9–11] and hyperon-nuclear [12–14] systems.

Methods for accurately accounting for the Coulomb interaction in the few-body dynamics of arbitrary charged, strongly interacting particles within the Faddeev approach in momentum space are also well-known [15–20]. Two-potential methods for treating the Coulomb interaction in three-body dynamics with Coulomb off shell effects have also been developed [21,22]. Calculations of Coulomb effects using the two-potential method are known to be independent on the choice of the screening region for the Coulomb potential and do not also require the use of regularization techniques.

One area of few-body physics that remains relatively undeveloped is the solution of the Faddeev equations in their integral form, without resorting to partial wave decomposition [23–25]. Direct numerical integration of the three-dimensional equations for the breakup T-matrix has remained underutilized, largely due to the

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Published online: 04 June 2025

computational demands on early computers and the traditional reliance on low-order partial wave expansions for the short-range potentials commonly used in few-body calculations (see, e.g., [26,27]). However, advances in computer technology and the growing application of precise few-body methods in atomic-molecular systems [28–31] are creating new demands. This includes both expanding the types of potentials used and requiring improvements in computational methods and the approximations employed, which were often specific to short-range interactions. Direct numerical integration of the Faddeev equations, without partial wave decomposition, has only been applied to scattering problems in the simplest, symmetrized case of nucleon scattering on a coupled system, namely the deuteron [25]. This work demonstrated the viability of the numerical methods and achieved good agreement between the results and experimental data.

When considering the complex energy plane to explore virtual and resonant three-body states, one encounters significant challenges in multichannel dynamics where the number of coupled dynamic equations increases with changes in the particle types. Given that two-body interactions must be analytically continued into the unphysical energy sheets for each partial wave, as done in Ref. [32], further increasing the number of coupled equations via partial wave expansions ceases to be a simplifying approach. Even without changing the topology of the energy surface, the inclusion of the Coulomb interaction necessitates addressing several fundamental issues, such as the overlap of singularities between the t-matrix and the resolvent, the satisfaction of asymptotic conditions for scattering functions, and the independence of the result from the choice of the potential's screening area. Consequently, direct numerical integration for the scattering matrix becomes an increasingly attractive method, both for solving scattering problems and for addressing spectral problems that involve analytical continuation of two-body potentials, as well as two- and three-body t-matrices, onto unphysical energy sheets [32,33].

This work focuses specifically on the influence of mass differences between interacting particles as they appear in the three-dimensional integral Faddeev equations, which results in eigenfunctions lacking specific symmetry properties. It is explicitly derived the matrix elements of all particle permutation operators in the vector basis, and their action on the momentum dependence of the two-body t-matrices and the three-body system eigenfunctions is also demonstrated. Once formulation of the integral Faddeev equations in vector form is used to provide expressions for the eigenvalue wave functions of three-body systems, the calculations of these functions for the ^{3}He system is also presented. One analyzes in detail how the domain of logarithmic singularities arising in the integral kernels of the inhomogeneous Faddeev equations changes as the masses of the interacting particles are varied over a wide range.

Since the appearance of the regions of logarithmic singularities is the same for both coordinate and momentum representations and does not depend on the use of partial-wave expansions, a similar analysis should be performed in each work devoted to the dynamics of three bodies of different masses. In particular, it is worth noting the works [34–40] in which either the incident particle or the target is considered as clustered within the framework of the Faddeev three-body equations. However, in most of these works, the focus is on discussing the inclusion of the Coulomb interaction, the method of solving the Faddeev equation, or comparing its solutions with the continuum discretized coupled channels method. The singularities have been fully taken into account in these calculations, but not described in detail for different particle masses, since the idea of their treatment is exactly the same as for identical particles, but with a larger number of intermediate steps (see also the review [41]). Present work us focused on writing explicitly such kinematic conditions for singularities proposing and testing a simple method for avoiding its in cross section calculation.

2 Equations for the three-body breakup T-matrix without certain symmetry

For three bodies of different masses, the Jacobi variables $\vec{p}_i, \vec{q}_i, i \in [1, 2, 3]$ where the index i-enumerates the particles for which $\vec{p}$ is the relative momentum in the interacting pair i, and $\vec{q}$-the spectator momentum of the particle i relative to this pair will have two equivalent representations expressing these momenta through each other

$$\vec{p}_1 = -\frac{m_2}{m_2+m_3}\vec{p}_2 + \frac{\vec{q}_2}{m_2+m_3}\left(m_3 + \frac{m_2 m_3}{m_3+m_1}\right); \vec{q}_1 = -\vec{p}_2 - \vec{q}_2\frac{m_1}{m_1+m_3};$$
$$\vec{p}_1 = -\frac{m_3}{m_2+m_3}\vec{p}_3 - \vec{q}_3\frac{m_2 M}{(m_2+m_3)(m_1+m_2)}; \vec{q}_1 = \vec{p}_3 - \vec{q}_3\frac{m_1}{m_1+m_2};$$
$$\vec{p}_2 = -\frac{m_1}{m_3+m_1}\vec{p}_1 - \frac{q_1}{m_3+m_1}\left(\frac{m_1 m_3}{m_2+m_3} + m_3\right); \vec{q}_2 = \vec{p}_1 - \vec{q}_1\frac{m_2}{m_2+m_3};$$

$$\vec{p}_2 = -\frac{m_3}{m_3+m_1}\vec{p}_3 + \frac{\vec{q}_3}{m_3+m_1}\Big(m_1 + \frac{m_1 m_3}{m_1+m_2}\Big); \vec{q}_2 = -\vec{p}_2 - \vec{q}_3\frac{m_2}{m_1+m_2};$$
$$\vec{p}_3 = -\frac{m_1}{m_1+m_2}\vec{p}_1 + \frac{\vec{q}_1}{m_1+m_2}\Big(m_2 + \frac{m_1 m_2}{m_2+m_3}\Big); \vec{q}_3 = -\vec{p}_1 - \vec{q}_1\frac{m_3}{m_2+m_3};$$
$$\vec{p}_3 = -\frac{m_2}{m_1+m_2}\vec{p}_2 - \frac{\vec{q}_2}{m_1+m_2}\Big(\frac{m_2 m_1}{m_1+m_3} + m_1\Big); \vec{q}_3 = \vec{p}_2 - \vec{q}_2\frac{m_3}{m_3+m_1}. \quad (1)$$

Here $M = m_1 + m_2 + m_3$ is the sum of the masses of the three particles.

Since spin observables are beyond the scope of this work, the subsequent formalism and calculations will be restricted to central potentials only.

Two-body t matrices are known enter the three-body phase space together with delta functions that exclude the dynamic presence of a third particle in two-body domain. In the $\vec{p}$, $\vec{q}$ representation for some vector $\mid \Psi'\rangle \equiv \mid tP\Psi\rangle$, where $\mid \Psi\rangle$ is a stationary state of a three-body system, one should has

$$\langle \vec{p}_i, \vec{q}_i \mid t_i P\Psi\rangle = \sum_k \int d^3q_i' d^3p_i' d^3q_k'' d^3p_k'' \langle \vec{p}_i, \vec{q}_i \mid t_i \mid \vec{p}_i', \vec{q}_i'\rangle\langle \vec{p}_i', \vec{q}_i' \mid P \mid \vec{p}_k'', \vec{q}_k''\rangle\cdot$$
$$\cdot\langle \vec{p}_k'', \vec{q}_k'' \mid \Psi\rangle = \sum_k \int d^3q_i' d^3p_i' d^3q_k'' d^3p_k'' \langle \vec{p}_i \mid t_i \mid \vec{p}_i'\rangle \delta^{(3)}(\vec{q}_i - \vec{q}_i') \quad (2)$$
$$\Big(\delta^{(3)}(\vec{p}_i' - \vec{p}_k'')\delta^{(3)}(\vec{q}_i' - \vec{q}_k'')\Big)\langle \vec{p}_k'', \vec{q}_k'' \mid \Psi\rangle.$$

Jacobi indices $i, j, k \in [1, 2, 3]$ in (2) denote a specific, native representation for the two-body t-matrix, the permutation operator P, and for the wave function Ψ. Summation over the representation indices effectively reflects the presence of three equivalent sets of Jacobi variables in the system.

The matrix elements of the permutation operator P, after performing the integration, change the momentum dependence of the t-matrix and the wave function Ψ, which is a characteristic feature of the dynamic manifestation of the third particle in previously defined objects, such as the two-body t-matrix and the bound two-body state. In what follows, the representation indices will be omitted, and the action of the permutation operators will be explicitly taken into account.

Removing six integrals in expressions (2) using kinematic relations (1) one leads to the following explicit representations for two-body t matrices

$$\langle \vec{p}, \vec{q} \mid t_1 P\Psi\rangle = \int d^3q'' \langle \vec{p} \mid t_1 \mid -\vec{q}\tfrac{m_1}{m_1+m_3} - \vec{q}''\rangle\langle \vec{q} + \vec{q}''\tfrac{m_2}{m_2+m_3}, \vec{q}'' \mid \Psi\rangle +$$
$$+\langle \vec{p} \mid t_1 \mid \vec{q}\tfrac{m_1}{m_1+m_2} + \vec{q}''\rangle\langle -\vec{q} - \vec{q}''\tfrac{m_3}{m_2+m_3}, \vec{q}'' \mid \Psi\rangle;$$
$$\langle \vec{p}, \vec{q} \mid t_2 P\Psi\rangle = \int d^3q'' \langle \vec{p} \mid t_2 \mid \vec{q}\tfrac{m_2}{m_2+m_3} + \vec{q}''\rangle\langle -\vec{q} - \vec{q}''\tfrac{m_1}{m_3+m_1}, \vec{q}'' \mid \Psi\rangle + \quad (3)$$
$$+\langle \vec{p} \mid t_2 \mid -\vec{q}\tfrac{m_2}{m_1+m_2} - \vec{q}''\rangle\langle \vec{q} + \vec{q}''\tfrac{m_3}{m_3+m_1}, \vec{q}'' \mid \Psi\rangle;$$
$$\langle \vec{p}, \vec{q} \mid t_3 P\Psi\rangle = \int d^3q'' \langle \vec{p} \mid t_3 \mid -\vec{q}\tfrac{m_3}{m_2+m_3} - \vec{q}''\rangle\langle \vec{q} + \vec{q}''\tfrac{m_1}{m_1+m_2}, \vec{q}'' \mid \Psi\rangle +$$
$$+\langle \vec{p} \mid t_3 \mid \vec{q}\tfrac{m_3}{m_3+m_1} + \vec{q}''\rangle\langle -\vec{q} - \vec{q}''\tfrac{m_2}{m_1+m_2}, \vec{q}'' \mid \Psi\rangle.$$

The system of coupled Faddeev equations for a three-body T_i matrix, where the index i-characterizes a spectator particle marked relative to an interacting pair, without introducing a certain symmetry with respect to the permutation of particles in places, is represented as

$$T_1 = t_1\Psi_2 + t_1\Psi_3 + t_1 R_0 T_2 + t_1 R_0 T_3;$$
$$T_2 = t_2\Psi_1 + t_2\Psi_3 + t_2 R_0 T_1 + t_2 R_0 T_3; \quad (4)$$
$$T_3 = t_3\Psi_1 + t_3\Psi_2 + t_3 R_0 T_1 + t_3 R_0 T_2,$$

where R_0 is an interaction-free three-body Green function.

Choosing a coordinate system according to work [25], in which the momentum $\vec{q}_0$ characterizes the relative momentum of a particle impinging on a bound system. Then in the selected $\vec{p}$, $\vec{q}$ representation, in which $\langle \vec{p}, \vec{q} \mid T\Psi\rangle \equiv T(p, x_p, x_{pq}^{q_0}, x_q, q; q_0)\langle \vec{p}, \vec{q} \mid \Psi\rangle$ and x_p, x_q are the cosines of the polar angles of the vectors $\vec{p}$ and $\vec{q}$, respectively, and $x_{pq}^{q_0}$ is the angle between the normals drawn for the planes $\vec{p}-\vec{q}_0$ and $\vec{q}-\vec{q}_0$, the system (4) takes the following final form

$$
\begin{aligned}
T_1(p, x_p, x_{pq}^{q_0}, x_q, q) &= t_1\Big(p, p'_{11}, \theta_{pp'_{11}}\Big)\langle \vec{q} + \vec{q}_0\tfrac{m_2}{m_2+m_3}, \vec{q}_0 \mid \Psi\rangle \\
&+ t_1\Big(p, p'_{12}, \theta_{pp'_{12}}\Big)\langle -\vec{q} - \vec{q}_0\tfrac{m_3}{m_2+m_3}, \vec{q}_0 \mid \Psi\rangle + \int d^3q''\Big[t_1\Big(p, f_{11}(q''), \theta_{f_{11}q''}\Big) \\
&\Big(E - \tfrac{q^2}{2\mu_{23}} - \tfrac{q''^2}{2\mu_{13}} - \tfrac{qq'' y_{qq''}}{m_3}\Big)^{-1} T_2\Big(g_{11}(q''), X_{g_{11}}, x_{g_{11}q''}^{q_0}, x_{q''}, q''\Big) \\
&+ t_1\Big(p, f_{12}(q''), \theta_{f_{12}q''}\Big)\Big(E - \tfrac{q^2}{2\mu_{23}} - \tfrac{q''^2}{2\mu_{12}} - \tfrac{qq'' y_{qq''}}{m_2}\Big)^{-1} \\
&T_3\Big(g_{12}(q''), X_{g_{12}}, x_{g_{12}q''}^{q_0}, x_{q''}, q''\Big)\Big]; \\
T_2(p, x_p, x_{pq}^{q_0}, x_q, q) &= t_2\Big(p, p'_{21}, \theta_{pp'_{21}}\Big)\langle -\vec{q} - \vec{q}_0\tfrac{m_1}{m_3+m_1}, \vec{q}_0 \mid \Psi\rangle \\
&+ t_2\Big(p, p'_{22}, \theta_{pp'_{22}}\Big)\langle \vec{q} + \vec{q}_0\tfrac{m_3}{m_3+m_1}, \vec{q}_0 \mid \Psi\rangle + \int d^3q''\Big[t_2\Big(p, f_{21}(q''), \theta_{f_{21}q''}\Big) \\
&\Big(E - \tfrac{q^2}{2\mu_{31}} - \tfrac{q''^2}{2\mu_{23}} - \tfrac{qq'' y_{qq''}}{m_3}\Big)^{-1} T_1\Big(g_{21}(q''), X_{g_{21}}, x_{g_{21}q''}^{q_0}, x_{q''}, q''\Big) \\
&+ t_2\Big(p, f_{22}(q''), \theta_{f_{22}q''}\Big)\Big(E - \tfrac{q^2}{2\mu_{31}} - \tfrac{q''^2}{2\mu_{12}} - \tfrac{qq'' y_{qq''}}{m_1}\Big)^{-1} \\
&T_3\Big(g_{22}(q''), X_{g_{22}}, x_{g_{22}q''}^{q_0}, x_{q''}, q''\Big)\Big]; \\
T_3(p, x_p, x_{pq}^{q_0}, x_q, q) &= t_3\Big(p, p'_{31}, \theta_{pp'_{31}}\Big)\langle \vec{q} + \vec{q}_0\tfrac{m_1}{m_1+m_2}, \vec{q}_0 \mid \Psi\rangle \\
&+ t_3\Big(p, p'_{32}, \theta_{pp'_{32}}\Big)\langle -\vec{q} - \vec{q}_0\tfrac{m_2}{m_1+m_2}, \vec{q}_0 \mid \Psi\rangle + \int d^3q''\Big[t_3\Big(p, f_{31}(q''), \theta_{f_{31}q''}\Big) \\
&\Big(E - \tfrac{q^2}{2\mu_{12}} - \tfrac{q''^2}{2\mu_{23}} - \tfrac{qq'' y_{qq''}}{m_2}\Big)^{-1} T_1\Big(g_{31}(q''), X_{g_{31}}, x_{g_{31}q''}^{q_0}, x_{q''}, q''\Big) \\
&+ t_3\Big(p, f_{32}(q''), \theta_{f_{32}q''}\Big)\Big(E - \tfrac{q^2}{2\mu_{12}} - \tfrac{q''^2}{2\mu_{31}} - \tfrac{qq'' y_{qq''}}{m_1}\Big)^{-1} \\
&T_2\Big(g_{32}(q''), X_{g_{32}}, x_{g_{32}q''}^{q_0}, x_{q''}, q''\Big)\Big];
\end{aligned}
\tag{5}
$$

where, for simplicity, the parametric dependence of all T matrices on the momentum q_0 was omitted, and the values $\mu_{i,j\neq i}$ are the usual reduced particle masses. The notation is introduced in (5) for convenience

$$
\begin{aligned}
f_{11}(q'') &= \sqrt{\Big(q\frac{m_1}{m_1+m_3}\Big)^2 + q''^2 + 2qq''\frac{m_1}{m_1+m_3}y_{qq''}}; \\
\theta_{f_{11}q''} &= -y_{pq}\frac{q}{f_{11}(q'')}\frac{m_1}{m_1+m_3} - y_{pq''}\frac{q''}{f_{11}(q'')}; \\
g_{11}(q'') &= \sqrt{q^2 + \Big(q''\frac{m_2}{m_2+m_3}\Big)^2 + 2qq''\frac{m_2}{m_2+m_3}y_{qq''}}; \\
X_{g_{11}} &= y_{qq_0}\frac{q}{g_{11}(q'')} + y_{q''q_0}\frac{q''}{g_{11}(q'')}\frac{m_2}{m_2+m_3}; \\
x_{g_{11}q''}^{q_0} &= \frac{y_{qq''}\frac{q}{g_{11}(q'')} + \frac{q''}{g_{11}(q'')}\frac{m_2}{m_2+m_3} - a_{qq''}x_{q''}}{\sqrt{1-a_{qq''}^2}\sqrt{1-x_{q''}^2}};
\end{aligned}
$$

$$
\begin{aligned}
a_{qq''} &= y_{qq_0}\frac{q}{g_{11}(q'')} + y_{q''q_0}\frac{q''}{g_{11}(q'')}\frac{m_2}{m_2+m_3};\\
f_{12}(q'') &= \sqrt{\left(q\frac{m_1}{m_1+m_2}\right)^2 + q''^2 + 2qq''\frac{m_1}{m_1+m_2}y_{qq''}};\\
\theta_{f_{12}q''} &= y_{pq}\frac{q}{f_{12}(q'')}\frac{m_1}{m_1+m_2} + y_{pq''}\frac{q''}{f_{12}(q'')};\\
g_{12}(q'') &= \sqrt{q^2 + \left(q''\frac{m_3}{m_2+m_3}\right)^2 + 2qq''\frac{m_3}{m_2+m_3}y_{qq''}};\\
X_{g_{12}} &= -y_{qq_0}\frac{q}{g_{12}(q'')} - y_{q''q_0}\frac{q''}{g_{12}(q'')}\frac{m_3}{m_2+m_3};\\
x^{q_0}_{g_{12}q''} &= \frac{-y_{qq''}\frac{q}{g_{12}(q'')} - \frac{q''}{g_{12}(q'')}\frac{m_3}{m_2+m_3} - b_{qq''}x_{q''}}{\sqrt{1-b^2_{qq''}}\sqrt{1-x^2_{q''}}};\\
b_{qq''} &= -y_{qq_0}\frac{q}{g_{12}(q'')} - y_{q''q_0}\frac{q''}{g_{12}(q'')}\frac{m_3}{m_2+m_3}.
\end{aligned}
\tag{6}
$$

and also

$$
\begin{aligned}
p'_{11} &= \sqrt{\left(q\frac{m_1}{m_1+m_3}\right)^2 + q_0^2 + 2qq_0\frac{m_1}{m_1+m_3}y_{qq_0}};\\
p'_{12} &= \sqrt{\left(q\frac{m_1}{m_1+m_2}\right)^2 + q_0^2 + 2qq_0\frac{m_1}{m_1+m_2}y_{qq_0}};\\
\theta_{pp'_{11}} &= -y_{pq}\frac{q}{p'_{11}}\frac{m_1}{m_1+m_3} - y_{pq_0}\frac{q_0}{p'_{11}},\ \theta_{pp'_{12}} = y_{pq}\frac{q}{p'_{12}}\frac{m_1}{m_1+m_2} + y_{pq_0}\frac{q_0}{p'_{12}};\\
y_{q''q_0} &= x''x_{q_0} + \sqrt{1-x''^2}\sqrt{1-x^2_{q_0}}\cos(\phi''-\phi_{q_0}),\ y_{qq_0} = x_q;\\
y_{pq''} &= y_{pq}x'' + \sqrt{1-x''^2}\sqrt{1-y^2_{pq}}\cos(\phi_p-\phi''),\ y_{pq_0} = x_p;\\
y_{pq} &= x_q x_p + \sqrt{1-x_q^2}\sqrt{1-x_p^2}\cos(\phi_q-\phi_p),\ y_{qq''} = x'';\\
x_{q''} &= x''x_{q_0} + \sqrt{1-x''^2}\sqrt{1-x^2_{q_0}}\cos(\phi''-\phi_{q_0}).
\end{aligned}
\tag{7}
$$

In addition to obtain the expressions p'_{21}, p'_{22}, $\theta_{pp'_{21}}$, $\theta_{pp'_{22}}$, $f_{21}(q'')$, $\theta_{f_{21}q''}$, $f_{22}(q'')$, $\theta_{f_{22}q''}$, $g_{21}(q'')$, $g_{22}(q'')$, $X_{g_{21}}$, $X_{g_{22}}$, $x^{q_0}_{g_{21}q''}$ and $x^{q_0}_{g_{22}q''}$ it is enough in the formulas (6,7) to replace the masses $m_1 \leftrightarrow m_2$ and change the signs at all angles $\theta_{pp'_{11}}$, $\theta_{pp'_{12}}$, $\theta_{f_{11}q''}$, $\theta_{f_{12}q''}$, $X_{g_{11}}$, $X_{g_{12}}$, $x^{q_0}_{g_{11}q''}$ and $x^{q_0}_{g_{12}q''}$ to the opposite. It can also be shown that the expressions for p'_{31}, p'_{32}, $\theta_{pp'_{31}}$, $\theta_{pp'_{32}}$, $f_{31}(q'')$, $\theta_{f_{31}q''}$, $f_{32}(q'')$, $\theta_{f_{32}q''}$, $g_{31}(q'')$, $g_{32}(q'')$, $X_{g_{31}}$, $X_{g_{32}}$, $x^{q_0}_{g_{31}q''}$ and $x^{q_0}_{g_{32}q''}$ are obtained from the formulas (6,7) by replacing the masses (m_1, m_2, m_3) with (m_3, m_1, m_2) with the same sign at all angles.

By setting the three-body scattering energy E and integrating the expression (6), which includes two-body t matrices defined on half off mass shell, one can obtain a solution of the three-body scattering problem relative to the breakup T-matrices T_1, T_2, and T_3. Subsequently, these T matrices can be used, as is known [23], in finding the amplitudes of elastic scattering and reactions.

Having fixed the initial state of the system in the form of $\Psi_{1(23)}$, where the pair (23) forms a coupled state, which is described by its eigenstate function $\phi_{(23)}(\vec{q})$, the transition operator will formally act according to the rule

$$
\begin{aligned}
U \mid \Psi_{1(23)}\rangle = (P_{12}P_{23} + P_{13}P_{23})\big(R_0^{-1} + T_1\big)\Psi_{1(23)} = \\
\big(R_0^{-1} + T_2\big)\Psi_{2(31)} + \big(R_0^{-1} + T_3\big)\Psi_{3(12)}.
\end{aligned}
\tag{8}
$$

The expression for the elastic scattering amplitude $\langle\Psi \mid U \mid \Psi\rangle$ is obtained from the matrix elements of the transition operator and has an explicit form for a system of three different masses

$$\begin{aligned}
&\langle\Psi_{1(23)} \mid U \mid \Psi_{1(23)}\rangle = \\
&= \phi_{(23)}\big(-\vec{q}\tfrac{m_1}{m_1+m_3} - \vec{q}_0\big)\big(E - \tfrac{q^2}{2\mu_{23}} - \tfrac{q_0^2}{2\mu_{13}} - \tfrac{q_0 q y_{qq_0}}{m_3}\big)\phi_{(31)}(\vec{q} + \vec{q}_0\tfrac{m_2}{m_2+m_3}) + \\
&+ \phi_{(23)}(\vec{q}\tfrac{m_1}{m_1+m_2} + \vec{q}_0)\big(E - \tfrac{q^2}{2\mu_{23}} - \tfrac{q_0^2}{2\mu_{12}} - \tfrac{q_0 q y_{qq_0}}{m_2}\big)\phi_{(12)}(-\vec{q} - \vec{q}_0\tfrac{m_3}{m_2+m_3}) + \\
&+ \int d^3q'\Big[\langle\Psi_{1(23)} \mid -\vec{q}\tfrac{m_1}{m_1+m_3} - \vec{q}\,', \vec{q}\,'\rangle\langle\vec{q} + \vec{q}\,'\tfrac{m_2}{m_2+m_3}, \vec{q}\,' \mid T_2 \mid \Psi_{2(31)}\rangle + \\
&+ \langle\Psi_{1(23)} \mid \vec{q}\tfrac{m_1}{m_1+m_2} + \vec{q}\,', \vec{q}\,'\rangle\langle-\vec{q} - \vec{q}\,'\tfrac{m_3}{m_2+m_3}, \vec{q}\,' \mid T_3 \mid \Psi_{3(12)}\rangle\Big]. \qquad (9)
\end{aligned}$$

It is important to note that in elastic scattering, the free motion of the spectator's particle (not coupled in the pair) is split off and the momentum of the bombarding particle $\vec{q}_0$ is preserved in magnitude, whereas for scattering with rearrangement, the momentum $\vec{q}_0$ is equal in modulus to the final particle momentum $\vec{q}$. Antisymmetrization of three-body states $\psi_{1(23)}$ for the case of three identical fermions directly leads equation (9) to a simple case given in the work [25].

The breakup amplitude $\langle\vec{p}, \vec{q} \mid U_0 \mid \Psi_{1(23)}\rangle$ is obtained by the action of the breakup operator $U_0 = (1 + P)T_1\Psi_{1(23)}$ and in accepted notation has the form

$$\begin{aligned}
\langle\vec{p}, \vec{q} \mid U_0 \mid \Psi_{1(23)}\rangle = T_1(p, x_p, x_{pq}^{q_0}, x_q, q) + T_2(p_2, x_{p_2}, x_{p_2q_2}^{q_0}, x_{q_2}, q_2) \\
+T_3(p_3, x_{p_3}, x_{p_3q_3}^{q_0}, x_{q_3}, q_3).
\end{aligned} \qquad (10)$$

In the selected frame of reference, when the Oz axis is aligned with the momentum $\vec{q}_0$, one has for independent variables of T matrices $\langle\vec{p}\,', \vec{q}\,' \mid T_k \mid \Psi_{k(ij)}\rangle \equiv T_k(p'_k, x_{p'_k}, x_{p'_kq'}^{q_0}, x', q')$ (9), where $k \in [2, 3]$ and $i \neq j \neq k$ the following explicit expressions

$$\begin{aligned}
p'_k &= \sqrt{q^2 + \Big(q'\frac{m_k}{m_2 + m_3}\Big)^2 + 2qq'\frac{m_k}{m_2 + m_3}y_{qq'}}; \\
x_{p'_k} &= (-1)^k x_q\frac{q}{p'_k} + (-1)^k x'\frac{q'}{p'_k}\frac{m_k}{m_2 + m_3}x'; \\
x_{p'_kq'}^{q_0} &= (-1)^k\frac{y_{qq'}\frac{q}{p'_k} + \frac{q'}{p'_k}\frac{m_k}{m_2+m_3} - c_{qq'}x'}{\sqrt{1 - x'^2}\sqrt{1 - c_{qq'}^2}}; \\
c_{qq'} &= (-1)^k x_q\frac{q}{p'_k} + (-1)^k x'\frac{q'}{p'_k}\frac{m_k}{m_2 + m_3}; \\
y_{qq'} &= x_q x' + \sqrt{1 - x_q^2}\sqrt{1 - x'^2}\cos(\phi_q - \phi').
\end{aligned} \qquad (11)$$

Kinematic variables for the breakup T-matrices of the breakup amplitude have a more complex form (10)

$$\begin{aligned}
p_k &= \sqrt{\Big(\frac{pm_k}{m_2 + m_3}\Big)^2 + \Big(\frac{qm_lM}{(m_2 + m_3)(m_1 + m_l)}\Big)^2 + (-1)^l 2pqy_{pq}\frac{m_2m_3M}{(m_2 + m_3)^2(m_1 + m_l)}}; \\
y_{pq} &= x_px_q + \sqrt{1 - x_p^2}\sqrt{1 - x_q^2}x_{pq}^{q_0}; \\
q_k &= \sqrt{p^2 + \Big(\frac{qm_1}{m_1 + m_l}\Big)^2 + 2pq\frac{m_1}{m_1 + m_l}y_{pq}}; \\
x_{p_k} &= -\frac{m_k}{m_2 + m_3}\frac{p}{p_k}x_p + (-1)^k\frac{q}{p_k}\frac{m_lM}{(m_2 + m_3)(m_1 + m_l)}x_q; \\
x_{q_k} &= -\frac{p}{q_k}x_p - \frac{q}{q_k}\frac{m_1}{m_1 + m_l}x_q;
\end{aligned}$$

$$x^{q0}_{p_k q_k} = \frac{\frac{(-1)^k m_k p^2}{p_k q_q (m_2+m_3)} + \frac{m_1 m_k - m_l M}{(m_2+m_3)(m_1+m_l)} \frac{pq}{p_k q_k} y_{pq} - \frac{(-1)^k m_1 m_l M}{(m_2+m_3)(m_1+m_l)^2} \frac{q^2}{p_k q_k} - x_{p_k} x_{q_k}}{\sqrt{1-x^2_{p_k}}\sqrt{1-x^2_{q_k}}}, \tag{12}$$

where the indices $k, l \in [2, 3]$ run through the same values and $k \neq l$.

3 Eigenstates of the system

It is natural to expect that, as in the case of three identical particles (fermions or bosons), the eigenfunction of the system (5) is also found as an eigenvector of a homogeneous algebraic system of equations for a given binding energy E_b of three-body system.

Let $a_{ij}, i \neq j, i, j \in [1, 2, 3]$ are the integral kernels of a homogeneous system of equations (5). Then the eigenvector of this system is found by a simple algebraic approximation of the integral equation to a numerical grid of nodes $N \times N$, where N is the number of grid nodes along the momentum $\vec{q}$ or $\vec{q}_0$

$$\left[\begin{pmatrix} 1_{N\times N} & 0 & 0 \\ 0 & 1_{N\times N} & 0 \\ 0 & 0 & 1_{N\times N} \end{pmatrix} - \begin{pmatrix} 0 & a_{12} & a_{13} \\ a_{21} & 0 & a_{23} \\ a_{31} & a_{32} & 0 \end{pmatrix}\right]_{E=E_b} \begin{pmatrix} \phi_{(1-N)} \\ \phi_{(N+1-2N)} \\ \phi_{(2N+1-3N)} \end{pmatrix} = 0 \tag{13}$$

In equation (13) $\phi_{(1-N)}, \phi_{(N+1-2N)}$, and $\phi_{(2N+1-3N)}$ are components of the algebraic wave function, projected for each partial component of two-body t matrices on a momentum grid $|\ \vec{q}\ |$. It is important to note that for eigenvalue problems, the independent variables of the integral kernels a_{ij} are q'',x'',ϕ'', and p, q, with only the last two variables being set the kinematic ones of the process and are approximated by grid momenta. That is why the solution of the system (13) allows one to obtain eigenstate functions projected for definite partial waves only.

The absence of a certain symmetry for the three-body wave function leads to another interesting consequence characteristic of solving systems of coupled equations. The system (5) couples different Faddeev components $\Psi_{1(23)}$, $\Psi_{2(31)}$, and $\Psi_{3(12)}$ of the total wave function between themselves. Therefore, the algebraic solutions (13) must also be linearly related with each others and with Faddeev's components, as follows from the system (5)

$$\begin{aligned} \phi_{(1-N)} &= a\big(\Psi_{2(31)} + \Psi_{3(12)}\big); \\ \phi_{(N+1-2N)} &= b\big(\Psi_{1(23)} + \Psi_{3(12)}\big); \\ \phi_{(2N+1-3N)} &= c\big(\Psi_{1(23)} + \Psi_{2(31)}\big), \end{aligned} \tag{14}$$

where a, b, c are some constants. Since the sum of the Faddeev's components is a total wave function, which on the other hand has an algebraic approximation in the form of $\phi_{(1-3N)}$, then one leads to the relation

$$\phi_{(1-N)} + \phi_{(N+1-2N)} + \phi_{(2N+1-3N)} = \Psi_{1(23)} + \Psi_{2(31)} + \Psi_{3(12)}, \tag{15}$$

from which it automatically follows that the constants $a = b = c = 1/2$. Using the relations (14), it is possible to express the Faddeev's components of the total wave function of the considered system through algebraic solutions (13).

The figure (1) shows the Faddeev's components $\Psi_{1(23)}$ as an example of the wave function of the proton-neutron-proton three-nucleon system (^{3}He) calculated at different masses $m_1 = 0.5m_p, m_p, 2m_p$ of the spectator nucleon. The separable Bonn parameterization of the fourth rank [43] was used as a model of NN interaction, which provides a reliable description of the phase shifts $^1S_0$, $^3S_1 -^3 D_1$, as well as the binding energy of the deuteron. For comparison, the partial $^1S_0 - S$ component of the parameterization of the three-nucleon function from the work [42] is presented in the same figure. As one can see, despite the similar magnitude of the wave function in the region of small momenta values of the $\vec{p}$-interacting pair and $\vec{q}$-nucleon spectator, the form of attenuation of the wave function in the calculations of this work is not symmetrical and steeper than in the parameterization of [42]. The decrease and smearing of the wave function $\Psi_{pnp}(p, q)$ in the region of small momenta values looks unexpected with both a decrease and an increase in the mass of the m_1 spectator particle.

Thus, the developed approach with direct integration of the Faddeev equations without an explicit requirement for symmetry or antisymmetry of the wave functions of interacting particles, as calculations have shown,

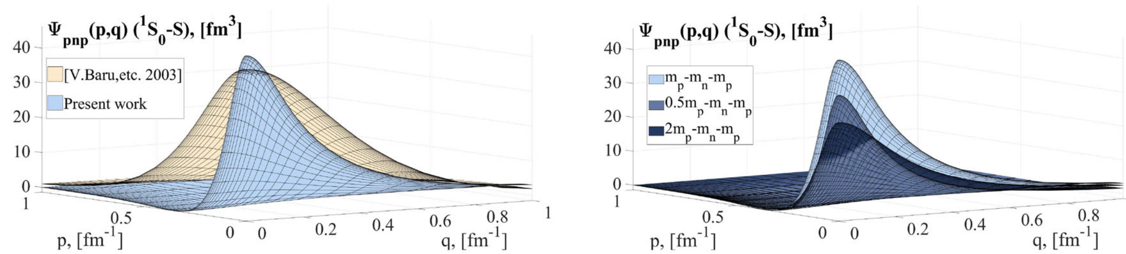

Fig. 1 Left: the partial $^1S_0 - S$ component of the wave function of the three-nucleon system (p-n-p), calculated on the basis of parameterization V.Baru [42] and in this work using a simple Bonn separable model of NN interaction [43]. Right: comparison of various calculations of the Faddeev's $\Psi_{1(23)}$ component in partial $^1S_0 - S$ wave with mass variation $m_1 = 0.5m_p, m_p, 2m_p$

gives not only an physically acceptable result for known three-nucleon systems with a description of their binding energies [44], but also allows one to arbitrarily change the masses of interacting particles with a corresponding change of two-body interactions.

4 Regions of logarithmic singularities for different particle masses

How the regions of the logarithmic singularities of the integral kernels a_{ij} (5) change depending on the masses of interacting particles? For to answer this item, one consider the interaction-free three-body Green function R_0:

$$\begin{aligned} R_0 &= \Big(E - \frac{q^2}{2\mu_{23}} - \frac{q''^2}{2\mu_{13}} - \frac{qq'' y_{qq''}}{m_3}\Big)^{-1}; \\ y_0 &= \frac{m_3}{qq''}\Big(E - \frac{q^2}{2\mu_{23}} - \frac{q''^2}{2\mu_{13}}\Big). \end{aligned} \tag{16}$$

The boundaries of the logarithmic singularities domain are known to be determined by the equality $y_0 = \pm 1$. From this simple equality, three ranges of values of the integration variable q'' follow, outlining the area of moving logarithmic singularities as a function of the spectator momentum $|\vec{q}|$:

$$\begin{cases} f_1 : \ q'' = -\frac{\mu_{13} q y_0}{m_3} + \sqrt{2\mu_{13}\Big(E + q^2\Big[\frac{\frac{m_1 m_2}{m_3}(y_0^2-1)-M}{2m_2(m_1+m_3)}\Big]\Big)}; \\ f_2 : \ q'' = \frac{\mu_{13} q y_0}{m_3} - \sqrt{2\mu_{13}\Big(E + q^2\Big[\frac{\frac{m_1 m_2}{m_3}(y_0^2-1)-M}{2m_2(m_1+m_3)}\Big]\Big)}; \\ f_3 : \ q'' = \frac{\mu_{13} q y_0}{m_3} + \sqrt{2\mu_{13}\Big(E + q^2\Big[\frac{\frac{m_1 m_2}{m_3}(y_0^2-1)-M}{2m_2(m_1+m_3)}\Big]\Big)}. \end{cases} \tag{17}$$

Moreover, the definition area of the functions f_1, f_2, and f_3 for $y_0 \geq 0$ are determined

$$f_1 \in [0, \sqrt{q_\vee^2}], \ f_2 \in [\sqrt{q_\vee^2}, \sqrt{q_\wedge^2}], \ f_3 \in [0, \sqrt{q_\wedge^2}], \tag{18}$$

where

$$\begin{aligned} q_\wedge^2 &= \frac{2m_2 E(m_1+m_3)}{M - \frac{m_1 m_2}{m_3}(y_0^2 - 1)}; \\ q_\vee^2 &= \frac{2m_2 m_3 E(m_1+m_3)}{m_1 m_2 + m_3 M}. \end{aligned} \tag{19}$$

In the case when $y_0 < 0$, the definition areas of the functions f_1 and f_3 (18) are swapped.

The figure (2) shows the regions of logarithmic singularities occurring in the proton-neutron-proton system ($m_p - m_n - m_p$ or ^{3}He) at the scattering energy $E = 1$ MeV. The boundaries of the integration regions (19) are marked with bold dots. Changes in these boundaries due to a ten times increase and one hundred times decrease in the mass of the m_1 component are marked with solid arrows with the number 1. Similarly, boundary

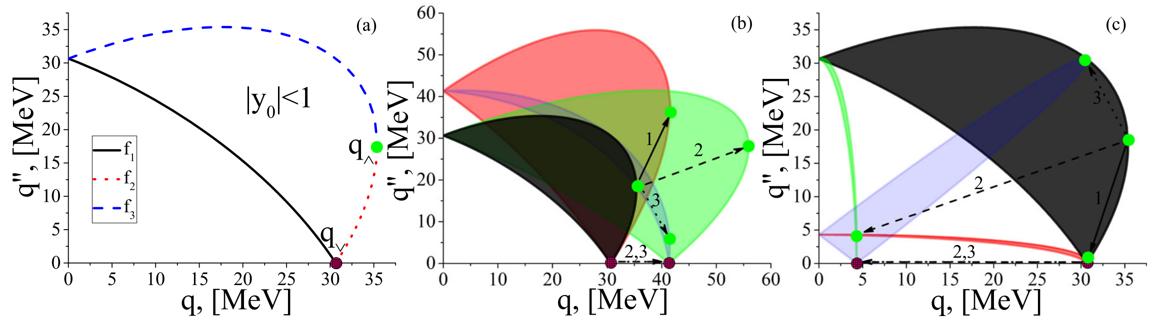

Fig. 2 Regions of logarithmic singularities at scattering energy $E = 1$ MeV (a): in the system $m_p - m_n - m_p$, (b): in the systems $10m_p - m_n - m_p$, $m_p - 10m_n - m_p$, $m_p - m_n - 10m_p$, (c): in the systems $m_p/100 - m_n - m_p$, $m_p - m_n/100 - m_p$, $m_p - m_n - m_p/100$. Circles mark the positions of the boundaries of $q_\vee$, $q_\wedge$, and arrows with numbers (1,2,3 - change in mass of m_1, m_2, m_3, respectively) mark the movement of these boundaries from one to another system due to changes in the masses of one of the components. Additionally, the area $|\ y_0\ | < 1$ is marked in Figure (a) inside the boundaries described by the functions f_1, f_2, and f_3 (17). The colors in Figures (b) and (c) indicate the areas of logarithmic singularities: the black system is $m_p - m_n - m_p$, the red system is $10m_p - m_n - m_p$, $m_p/100 - m_n - m_p$, the green system is $m_p - 10m_n - m_p$, $m_p - m_n/100 - m_p$ and the blue system is $m_p - m_n - 10m_p$, $m_p - m_n - m_p/100$

movements (19) are denoted due to a ten times increase and one hundred times decrease in the mass of the components m_2 (dash-dotted arrow) and m_3 (dotted arrow). The zones of logarithmic singularities visible in the figure, can vary markedly depending on the change in the masses of one or another component of the system. Increasing the energy E with constant masses of the components of the system, the regions of logarithmic singularities invariably grow, while with an increasing in the mass of one of the components, the zone can stretch along the momenta q'' and q, as shown in the figure (2)(b), and can also shrink into an arc as the mass of m_3 increases. A similar nontrivial behavior of the logarithmic singularities domain is seen with a sharp decrease in the mass of one of the components of the system by a factor of 100. In this case, the singularity area is transformed into an arc, and also stretches into a wedge in the case of a decrease in the mass of m_3 as shown in the figure (2)(c). Such behavior of the logarithmic singularities areas for systems without a certain symmetry, i.e. with a difference in particle masses, including with a strong difference of tens and hundreds of times, can play a useful role in the numerical solution of a system of inhomogeneous Faddeev equations (5). This simplification may consist in jumping over these logarithmic singularities areas in the direct numerical integration of the system (5) on irregular grids of momenta q and q'' due to its smallness.

One note how expressions for functions (17) will change for the remaining Green's functions (5). If one denote by the quantities $R_0^{[1]}$ and $R_0^{[2]}$ those Green functions that are included in the first line of the equation (5), and by the quantities $R_0^{[3]}$, $R_0^{[4]}$ and $R_0^{[5]}$, $R_0^{[6]}$ those Green functions that are included in the second and third lines, respectively, then similar (17) expressions can be obtained by changing the masses of particles according to the rule

$$
\begin{gathered}
R_0 \equiv R_0^{[1]}(m_1, m_2, m_3);\\
R_0^{[1]}(m_1, m_3, m_2) = R_0^{[2]}(m_1, m_2, m_3),\ R_0^{[1]}(m_2, m_1, m_3) = R_0^{[3]}(m_1, m_2, m_3);\\
R_0^{[3]}(m_3, m_2, m_1) = R_0^{[4]}(m_1, m_2, m_3),\ R_0^{[2]}(m_3, m_2, m_1) = R_0^{[5]}(m_1, m_2, m_3);\\
R_0^{[5]}(m_2, m_1, m_3) = R_0^{[6]}(m_1, m_2, m_3).
\end{gathered} \tag{20}
$$

To accurately traverse the region of logarithmic singularities, a numerical method was developed to control the indices of cycles corresponding to the variable q'' for an arbitrary numerical grid, depending on the form of the resolvent R_0 (16) and the sign of the cosine y_0. This fully automated numerical approach for locating the boundaries of the moon like region of singularities allows the determination of the boundaries of cycles of the variable q'' within which this zone resides for any relative momentum $q \equiv q_{i(jk)}$ of the spectator particle. Based on the identified indices of the q'' variables, the resolvent of the form (16) was approximated in the region of logarithmic singularities using linear or cubic functions. The form of the linear function was determined by

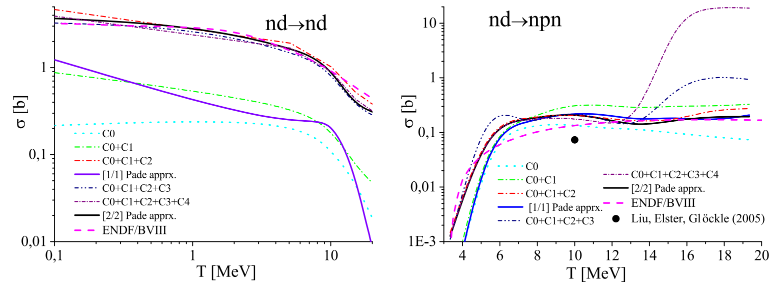

Fig. 3 Left: Contribution of individual approximations C_i (see formula (22)) and Padé approximants to the total nd elastic scattering cross section. Right: Similar contributions to the total breakup cross section. For comparison, data from the ENDF library [46] and a similar microscopic calculation [25] are shown

the following formula:

$$R_0^{-1} \Rightarrow \frac{\mid R_0^{-1} \mid_{i_{\leq}-1} + \mid R_0^{-1} \mid_{i_{\geq}+1}}{2} \cdot \frac{R_{0\,i_{\leq}-1}^{-1}}{\mid R_0^{-1} \mid_{i_{\leq}-1}} \tag{21}$$

This approximation method is referred to as linear. Points with indices $i_{\leq}$ correspond to the boundaries of the variable q'' defining the function f_1 or f_2. Similarly, points with indices $i_{\geq}$ define the boundaries of the running variable q'' for the function f_3.

The cubic approximation method refers to the use of a Hermite cubic one-dimensional spline, developed in [45] for the analogous purpose of traversing the region of logarithmic singularities. In this case, this cubic spline is applied only to replace the resolvent itself, using four points from the set $[i_{\leq-1}, i_{\leq}, i_{\geq}, i_{\geq+1}]$.

The validation of the chosen linear method for approximating the integrand resolvent in the region of logarithmic singularities in an automated manner for any predefined set of considered masses m_1, m_2, and m_3 of the three-body interacting system was performed using the examples of neutron-deuteron elastic scattering and the breakup process $nd \rightarrow npn$. The system of equations (5) was solved iteratively in a schematic form.

$$T_i \approx \sum_{\alpha=0}^{4} C_\alpha, \tag{22}$$

where C_α represents individual iterations of equation (5), C_0 is the inhomogeneous term, C_1 is the first iteration, and so on. From individual iterations of equation (5), rational functions - Padé approximants of the form [1/1] and [2/2] - were constructed, which were then used to find the elastic scattering amplitudes (9) and breakup amplitudes (10). A comparison of the obtained cross sections using the Bonn potential [43] with data from the ENDF evaluated nuclear data library [46] is presented in Figure (3).

As direct calculations show, constructing a [2/2] Padé approximant is sufficient to describe the cross sections of the processes under consideration. At the same time, the contributions of individual iterations of equation (5), in particular iterations C_3 and C_4, can give local spikes in the region of kinetic energies of the incident neutron $T > 12$ MeV. This cross-section calculation completes the validation of the developed numerical method for finding and localizing the regions of logarithmic singularities for a system of three interacting bodies of different masses and shows that, along with the traditional cubic spline, approximating the entire integrand in equations (5), a simple linear approximation of the resolvent in the region of logarithmic singularities can also lead to a physically acceptable result.

5 Conclusion

In this work, inhomogeneous Faddeev integral equations for three different bodies are explicitly written out without using the traditional partial wave decomposition for the resulting breakup T-matrix. Expressions for the amplitude of elastic scattering and reaction are also written out in the context of direct integration of the obtained equations in momentum space without using partial wave decomposition. An algebraic method for searching for eigenfunctions of stationary states of three-body systems with different masses based on homogeneous Faddeev equations is proposed and tested. The behavior of logarithmic singularities for a system of three bodies of different masses is also analyzed also in total cross sections calculations for neutron-deuteron elastic and breakup processes. It was found that at certain values of one of the masses of the three particles, logarithmic regions of singularities are compressed into an arc or elongated into a wedge-like region. Padé approximations for given Faddeev three-body equation and two methods for resolvent approximations in singularities zone are also tested and results are in a good agreement with data.

The results of this work can be directly used both for the direct solution (for example, using Padé approximants) of inhomogeneous Faddeev equations for a system of three bodies of different masses to search for the scattering cross section and the reaction cross section in the cluster model of the target nucleus, and for finding various non-relativistic wave functions of three-body systems.

Acknowledgements Egorov Mikhail gratefully acknowledges the financial support of the Foundation for the Advancement of Theoretical Physics and Mathematics "BASIS" (project No 23-1-3-3-1) and the research was carried out with the support of a grant from the Government of the Russian Federation (Agreement No. 075-15-2025-009 of 28 February 2025).

Author contributions Egorov M. wrote the main manuscript with figures and done all of the calculations.

Data Availability No datasets were generated or analysed during the current study.

Declarations

Competing interests The authors declare no competing interests.

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