

Operator form of the three-nucleon scattering amplitude

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(Received 21 March 2017; published 17 July 2017)

To extend the applications of the so-called “three-dimensional” formalism to the description of three-nucleon scattering within the Faddeev formalism, we develop a general form of the three-nucleon scattering amplitude. This form significantly decreases the numerical complexity of the “three-dimensional” calculations by reducing the scattering amplitude to a linear combination of momentum-dependent spin operators and scalar functions of momenta. The number and structure of the spin operators is fixed and the scalar functions can be represented numerically using standard methods such as multidimensional arrays. In this paper, we show that all orders of the iterated Faddeev equation can be written in this general form. We argue that calculations utilizing the three-nucleon force will also conform to the same general form. Additionally, we show how the general form of the scattering amplitude can be used to transform the Faddeev equation to make it suitable for numerical calculations using iterative methods.

DOI: [10.1103/PhysRevC.96.014611](https://doi.org/10.1103/PhysRevC.96.014611)

I. INTRODUCTION

The “three-dimensional” (3D) formalism is a framework for performing quantum mechanical calculations related to few-nucleon systems without resorting to partial wave decomposition. This approach uses the 3D vector degrees of freedom of the nucleons directly and was applied, in particular, to calculate the two-nucleon (2N) bound state and transition operator [1,2] and the ^3H bound state [3]. An introduction to the “three-dimensional” formalism can be found in Refs. [1–7]. Also, the Tehran group published a series of papers (see, e.g., Refs. [8–17]), where many investigations within the “three-dimensional” formalism, especially regarding three-body and four-body bound states are discussed in detail. For recent investigations on the “three-dimensional” approach using the low-momentum interaction or the relativistic interaction, see Refs. [15] and [16,17], respectively. The 3D approach is characterized by flexibility because it provides an easy way to exchange models of nuclear interactions since the potential does not need to undergo the partial wave decomposition procedure. The precision of these computations was compared to partial wave calculations in our recent paper [18], where we calculated observables related to neutron-deuteron (Nd) scattering in the first order of the iterated Faddeev equation. In spite of the fact that our results in this paper were obtained using the first-order terms only, they demonstrated the usefulness of the 3D approach for certain kinematical configurations of the breakup reaction where the convergence for partial wave results is slow.

Our motivation for the present work is the extension of the three-nucleon (3N) 3D scattering calculations [18] to all orders of the Faddeev equation. The hope is that avoiding partial wave expansion will facilitate the applicability of three- and many-body nuclear forces derived from chiral effective field theory [19–25].

Our framework to study the Nd scattering process is based on the Faddeev formalism [26]. The central element of this description is the Faddeev equation for the 3N transition operator \check{T} :

$$\check{T}|\phi\rangle = \check{t}\check{P}|\phi\rangle + \check{t}\check{G}_0\check{P}\check{T}|\phi\rangle, \quad (1)$$

where $\check{P} = \check{P}_{12}\check{P}_{23} + \check{P}_{13}\check{P}_{23}$ is an operator built from particle transpositions \check{P}_{ij} , \check{G}_0 is the free propagator, \check{t} is the 2N transition operator satisfying the Lippmann-Schwinger equation, and $|\phi\rangle$ is the initial product state composed from a deuteron and a free nucleon with momentum \mathbf{q}_0 in the 3N center of mass frame. Nd scattering observables can be calculated using two types of matrix elements. For the breakup channel observables can be calculated from

$$\langle\phi_0|(\check{1} + \check{P})\check{T}|\phi\rangle, \quad (2)$$

while for the elastic scattering channel from

$$\langle\phi'|\check{P}\check{G}_0^{-1} + \check{P}\check{T}|\phi\rangle. \quad (3)$$

In Eq. (2), $\langle\phi_0|$ is a final state containing three free nucleons and in (3) $\langle\phi'|$ is a final product state composed from a deuteron and a free nucleon with momentum \mathbf{q}'_0 .

Our attempt to use the 3D formalism to solve Eq. (1) begins with considerations related to numerical complexity. Since we do not use partial wave decomposition and work instead with the 3D degrees of freedom of the nucleons directly, we will focus on the matrix element $\langle\mathbf{p}'\mathbf{q}'|\check{T}|\mathbf{p}\mathbf{q}\rangle$, where $\mathbf{p}', \mathbf{q}', \mathbf{p}, \mathbf{q}$ are Jacobi momenta in the final and initial states. This matrix element is an operator in the isospin-spin space of the 3N system and can be represented using a $8 \times 8 = 64$ by 64 matrix (there are 8 possible spin states and 8 possible isospin states for the 3N system) for every momentum combination. Each element of this matrix is a complex-valued function of the $4 \times 3 = 12$ components of the four Jacobi momenta. It follows that our calculations would involve $64 \times 64 = 4,096$ complex-valued functions of 12 arguments. If each argument of these functions were discretized over a lattice of 32 points, then our code would have to handle arrays of $4,096 \times 32^{12} \approx 4.7 \times 10^{21}$ complex numbers to represent $\langle\mathbf{p}'\mathbf{q}'|\check{T}|\mathbf{p}\mathbf{q}\rangle$ numerically. This is equivalent to approximately 7.5×10^{13} GB of data for double precision numbers and is clearly not practical or even possible using modern computing resources.

Fortunately, from the form of Eq. (1) and the matrix elements Eqs. (2) and (3), it is clear that we only need to calculate the state $\check{T}|\phi\rangle$. This state can be projected onto a

Jacobi momentum eigenstate $\langle \mathbf{p}\mathbf{q}|\check{T}|\phi\rangle$ and represented by $8 \times 8 = 64$ functions for each momentum combination, thus significantly reducing the numerical complexity of the problem. We expect each of these functions to have nine arguments coming from the components of the Jacobi momenta \mathbf{p}, \mathbf{q} and the free nucleon momentum \mathbf{q}_0 in the initial state $|\phi\rangle$. Overall, if each argument of these functions were discretized over a lattice of 32 points, our code would have to handle arrays containing $64 \times 32^9 \approx 2.3 \times 10^{15}$ complex numbers to represent $\langle \mathbf{p}\mathbf{q}|\check{T}|\phi\rangle$. This is still a very large number and if we hope to create a practical numerical implementation of 3D Nd scattering calculations, we need to further reduce this figure.

In the following sections, we show how this large number can be additionally reduced to approximately $64 \times 8 \times 32^6 \approx 5.5 \times 10^{11}$ by using spatial rotation symmetry. Once this symmetry is taken into account, the 3N scattering amplitude $\langle \mathbf{p}\mathbf{q}|\check{T}|\phi\rangle$ can be represented by 64×8 (64 functions for each of the 8 possible isospin cases) complex-valued scalar functions of $\mathbf{p}, \mathbf{q}, \mathbf{q}_0$. The scalar nature of these functions means that each will only have six real arguments (number of vectors \times number of components for each vector – number of dimensions: $3 \times 3 - 3 = 6$), and thus the size of arrays representing these functions in numerical implementations is decreased by a couple orders of magnitude.

The paper is organized as follows. In Sec. II, we make a general argument about the form of the 3N scattering amplitude in the Faddeev equations. This argument is applicable not only to Eq. (1) but also to the Faddeev equation with the 3N force included (see, e.g., Ref. [26]). In Sec. III, we discuss the arguments of the scalar functions that determine the scattering amplitude, and in Sec. IV, we show how, using the general form, the Faddeev Eq. (1) can be transformed into an operator equation that can be solved iteratively using Krylov subspace methods. Finally, in Sec. IVC we discuss the singularities of the 3N scattering amplitude resulting from the 2N transition operator, and in Sec. V we summarize. Additionally Appendices A and B contain the most important result of this work, a set of operators and scalar functions necessary to represent the Nd scattering amplitude.

II. THE 3N SCATTERING AMPLITUDE

To make a general argument about the form of the 3N scattering amplitude $\langle \mathbf{p}\mathbf{q}|\check{T}|\phi\rangle$, we will express it more explicitly. In the first step, we insert the identity operator between the 3N transition operator \check{T} and $|\phi\rangle$, and use the Dirac δ function $\delta^3(\mathbf{q}' - \mathbf{q}_0)$ arising from the momentum state $|\mathbf{q}_0\rangle$ of the free nucleon in $|\phi\rangle$:

$$\begin{aligned} \langle \mathbf{p}\mathbf{q}|\check{T}|\phi\rangle &= \int d^3 p' d^3 q' \langle \mathbf{p}\mathbf{q}|\check{T}|\mathbf{p}'\mathbf{q}'\rangle \langle \mathbf{p}'\mathbf{q}'|\phi\rangle \\ &= \int d^3 p' \langle \mathbf{p}\mathbf{q}|\check{T}|\mathbf{p}'\mathbf{q}_0\rangle \langle \mathbf{p}'\mathbf{q}_0|\phi\rangle. \end{aligned} \quad (4)$$

We can further rewrite Eq. (4) using the operator form of the deuteron bound state [1]:

$$\langle \mathbf{p}|\phi_d\rangle = \sum_{l=1}^2 \phi_l(\mathbf{p}) \check{b}_l(\mathbf{p}) |1m_d\rangle, \quad (5)$$

where $|1m_d\rangle$ is the deuteron spin state, $\check{b}_l(\mathbf{p})$ are spin operators given in Ref. [1] and the bound state is determined by two scalar functions $\phi_l(\mathbf{p})$ of the 2N relative momentum that are directly related to the s - and d -wave components of the deuteron as given explicitly in Ref. [1]. The two operators $\check{b}_{l=1,2}(\mathbf{p})$ that make up the deuteron bound state in Ref. [1] will be capitalized in the following $\check{B}_l(\mathbf{p}')$ to mark that they act in the isospin-spin space of three particles. This results in

$$\begin{aligned} \langle \mathbf{p}\mathbf{q}|\check{T}|\phi\rangle &= \int d^3 p' \sum_{l=1}^2 \phi_l(\mathbf{p}') [\langle \mathbf{p}\mathbf{q}|\check{T}|\mathbf{p}'\mathbf{q}_0\rangle] [\check{B}_l(\mathbf{p}')]|s\rangle, \end{aligned} \quad (6)$$

where we use square brackets to denote operators in the isospin-spin space and

$$|s\rangle = \left(|\frac{1}{2} \pm \frac{1}{2}\rangle \otimes |00\rangle\right)^{3N \text{ isospin}} \otimes (|S_N\rangle \otimes |1m_d\rangle)^{3N \text{ spin}} \quad (7)$$

is a 3N isospin-spin state made up from the free neutron (proton) isospin $|\frac{1}{2} - \frac{1}{2}\rangle$ ($|\frac{1}{2} + \frac{1}{2}\rangle$), the deuteron isospin $|00\rangle$, the free nucleon spin $|S_N\rangle$, and the deuteron spin $|1m_d\rangle$ states.

Overall, apart from the implicit energy dependence, the right-hand side of Eq. (6) depends on the Jacobi momenta in the final state \mathbf{p}, \mathbf{q} and on the momentum of the free nucleon \mathbf{q}_0 , which is related to the 3N system energy $E^{3N} = \frac{3}{4m}\mathbf{q}_0^2 + E_d$, the deuteron bound state energy E_d , and the nucleon mass m . The isospin-spin operators, marked in Eq. (6) by using square brackets can be constructed from combinations of $\mathbf{p}, \mathbf{q}, \mathbf{q}_0$, and pure spin and isospin operators. Examples of pure isospin and pure spin operators might include the three isospin vector operators $\check{\tau}(i)$ and the three spin vector operators $\check{\sigma}(i)$ for each of the three nucleons $i = 1, 2, 3$ whose matrix representations are given in terms of the Pauli matrices.

Using these observations we deduce that $\langle \mathbf{p}\mathbf{q}|\check{T}|\phi\rangle$ must have the following general form:

$$\langle \mathbf{p}\mathbf{q}|\check{T}|\phi\rangle = [\check{X}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0)]|s\rangle, \quad (8)$$

where $\check{X}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0)$ is an operator acting in the isospin - spin space of the 3N system. Furthermore, symmetry considerations lead us to expect the $\check{X}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0)$ operator to have rotational symmetry, i.e.,

$$[R][\check{X}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0)] = [\check{X}(R(\mathbf{p}), R(\mathbf{q}), R(\mathbf{q}_0))][R],$$

where R is a spatial rotation and $[R]$ is the matrix representation of the rotation in isospin-spin space. We can therefore use the algorithm from Sec. 2 of Ref. [27], with minor adjustments, to find its general, rotation invariant, form. To do this we consider the spin and isospin parts of Eq. (8) separately,

$$\check{X}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) = \check{X}^{\text{isospin}} \otimes \check{X}^{\text{spin}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0),$$

and focus on the spin part since the isospin operator has no momentum dependence and does not change under spatial

rotations. $\check{X}^{\text{spin}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0)$ can be constructed from scalar combinations of the following set of vectors:

$$\{\check{\sigma}(1), \check{\sigma}(2), \check{\sigma}(3), \mathbf{p}, \mathbf{q}, \mathbf{q}_0\}, \quad (9)$$

and this set needs to be substituted for \mathbb{T} in the procedure from Ref. [27].

The final result of using the modified procedure [27] is the operator form,

$$\check{X}^{\text{spin}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) = \sum_{r=1}^{64} \tau_r(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) \check{O}_r(\mathbf{p}, \mathbf{q}, \mathbf{q}_0), \quad (10)$$

where the 3N spin operators $\check{O}_r(\mathbf{p}, \mathbf{q}, \mathbf{q}_0)$ are listed in Appendix A and $\tau_r(\mathbf{p}, \mathbf{q}, \mathbf{q}_0)$ are some scalar functions. The algorithm guarantees that any rotation invariant operator constructed from elements of Eq. (9) can be written in this form.

Using Eq. (10) we can finally write the general form of the scattering amplitude,

$$\langle \mathbf{p}\mathbf{q} | \check{T} | \phi \rangle = \sum_{\gamma^{3N}} \sum_{r=1}^{64} \tau_r^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) |\gamma^{3N}\rangle \otimes (\check{O}_r(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) |\alpha\rangle), \quad (11)$$

$$\pm \sqrt{-(\mathbf{p} \cdot \mathbf{q})^2 q_0^2 - (\mathbf{p} \cdot \mathbf{q}_0)^2 q^2 + 2(\mathbf{p} \cdot \mathbf{q})(\mathbf{p} \cdot \mathbf{q}_0)(\mathbf{q} \cdot \mathbf{q}_0) + p^2(q_0^2 q^2 - (\mathbf{q} \cdot \mathbf{q}_0))}.$$

This ambiguity is unacceptable, since we want to uniquely fix the angles between \mathbf{p}, \mathbf{q} and \mathbf{q}_0 .

There are many possible proper choices for the arguments that uniquely fix all the angles in the set of three vectors $\mathbf{p}, \mathbf{q}, \mathbf{q}_0$. One such choice is given in Ref. [29],

$$\tau_r^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) \equiv \tau_r^{\gamma^{3N}}(p^2, q^2, q_0^2, \widehat{(\mathbf{q}_0 \times \mathbf{q})} \cdot \widehat{(\mathbf{q}_0 \times \mathbf{p}), \mathbf{q} \cdot \mathbf{q}_0, \mathbf{q}_0 \cdot \mathbf{p}), \quad (12)$$

and we refer the reader to this paper where all relevant angles are worked out in terms of the scalar function arguments from Eq. (12).

IV. REMOVING SPIN AND ISOSPIN DEPENDENCIES

The 3N Faddeev Eq. (1) can now be rewritten using Eq. (11). After removing the spin and isospin dependencies, Eq. (1) will be transformed into a set of coupled equations for the scalar functions $\tau_r^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0)$. In the following subsections, we will consider each term of the Faddeev equation separately and form a simple linear equation with operators acting on the scalar functions τ (of vectors $\mathbf{p}, \mathbf{q}, \mathbf{q}_0$ and integer arguments r, γ^{3N}):

$$\tau = \tilde{\tau} + \check{Q}\tau. \quad (13)$$

where the first sum is over the eight possible isospin states $|\gamma^{3N}\rangle$ of the 3N system and $|\alpha\rangle$ is a 3N spin state that, in principle, does not have to be equal to the spin part of $|s\rangle$ from Eq. (7), making Eq. (11) more general than Eq. (6). In Eq. (11), the 3N scattering amplitude is fully determined by the 64×8 complex-valued scalar functions $\tau_r^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0)$ of momenta. It follows from the scalar nature of these functions that they have only six independent real arguments. This leads to a significant reduction of numerical complexity and makes 3D calculations of Nd scattering observables, which incorporate all orders of the Faddeev equation, feasible. There are multiple choices for the six arguments and the next section discusses two possible options. Since this section does not make direct references to the two- or three-nucleon potential, Eq. (11) can also be used in the version of the Faddeev equation that utilizes the three nucleon force.

III. SCALAR FUNCTION ARGUMENTS

We begin with a flawed example to demonstrate the importance of a proper choice for the arguments of the scalar functions. Let us assume that the scalar functions have the following arguments:

$$\tau_r^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) \equiv \tau_r^{\gamma^{3N}}(p^2, q^2, q_0^2, \mathbf{p} \cdot \mathbf{q}, \mathbf{q} \cdot \mathbf{q}_0, \mathbf{q}_0 \cdot \mathbf{p}).$$

Using this choice and trying to compute the value of $\mathbf{p} \times \mathbf{q} \cdot \mathbf{q}_0$, we encounter two possible answers:

The two terms $\check{i}\check{P}|\phi\rangle$ and $\check{i}\check{G}_0\check{P}\check{T}|\phi\rangle$ on the right-hand side of Eq. (1) will be transformed into $\tilde{\tau}$ (a scalar function of $\mathbf{p}, \mathbf{q}, \mathbf{q}_0$ and integer arguments r, γ^{3N}) and the operator \check{Q} acting on τ , respectively. The left-hand side will be transformed into an identity operator acting on τ .

Equation (13) can be rearranged by moving the unknown function τ to the left-hand side,

$$(\check{I} - \check{Q})\tau = \tilde{\tau}, \quad (14)$$

to form a more explicit linear equation for τ . The transformation of Eq. (1) into Eq. (14) makes it possible to apply iterative Krylov subspace methods, for example, the Arnoldi algorithm [28], to find the solution—the scalar functions τ that define $\check{T}|\phi\rangle$ in Eq. (11). Scalar functions $\tau, \tilde{\tau}$ in Eq. (14) can be represented as multidimensional complex arrays and the iterations can be constructed around the $(\check{I} - \check{Q})$ operator to produce its representation as a matrix with a relatively small size. Using this, Eq. (14) can be transformed to a small system of linear equations and solved using popular linear solvers (e.g., LAPACK).

A. Operator form of $\langle \mathbf{p}\mathbf{q} | \check{i}\check{P} | \phi \rangle$

Arguments similar to those that led to $\check{T}|\phi\rangle$ having the general form of Eq. (11) also lead to the conclusion that $\check{i}\check{P}|\phi\rangle$ and $\check{i}\check{G}_0\check{P}\check{T}|\phi\rangle$ can be written in the same way. Writing

$\langle \mathbf{p}q | \check{t} \check{P} | \phi \rangle$ in the general form of Eq. (11),

$$\langle \mathbf{p}q | \check{t} \check{P} | \phi \rangle = \sum_{\gamma^{3N}} \sum_{r=1}^{64} \check{\tau}_r^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) |\gamma^{3N}\rangle \otimes (\check{O}_r(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) |\alpha\rangle), \quad (15)$$

and removing the spin and isospin dependencies will result in a set of coupled linear equations for the scalar functions $\check{\tau}_r^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0)$. To show this, we begin by inserting the identity operator between the 2N transition operator \check{t} and the permutation operator \check{P} , and between the permutation operator and the initial state $|\phi\rangle$:

$$\langle \mathbf{p}q | \check{t} \check{P} | \phi \rangle = \int d^3 \mathbf{p}' d^3 \mathbf{q}' \int d^3 \mathbf{p}'' d^3 \mathbf{q}'' \langle \mathbf{p}q | \check{t} | \mathbf{p}' \mathbf{q}' \rangle \times \langle \mathbf{p}' \mathbf{q}' | \check{P} | \mathbf{p}'' \mathbf{q}'' \rangle \langle \mathbf{p}'' \mathbf{q}'' | \phi \rangle. \quad (16)$$

The three matrix elements in Eq. (16) will introduce four Dirac δ functions into the integrations, thus eliminating them completely.

Namely, the 2N transition operator \check{t} acts in a two-particle subsystem with the relative momenta of the two nucleons \mathbf{p}, \mathbf{p}' and cannot change the Jacobi momenta \mathbf{q}, \mathbf{q}' between the initial and final state. This results in the first element $\langle \mathbf{p}q | \check{t} | \mathbf{p}' \mathbf{q}' \rangle$ introducing $\delta^3(\mathbf{q} - \mathbf{q}')$. The initial state $|\phi\rangle$ is a product of $|\mathbf{q}_0\rangle$ and the deuteron wave function therefore the third element $\langle \mathbf{p}'' \mathbf{q}'' | \phi \rangle$ introduces $\delta^3(\mathbf{q}'' - \mathbf{q}_0)$. Using both these observations, the \mathbf{q}' and \mathbf{q}'' integrations can be eliminated and these vectors replaced by \mathbf{q} and \mathbf{q}_0 , respectively. The remaining matrix element $\langle \mathbf{p}' \mathbf{q}' | \check{P} | \mathbf{p}'' \mathbf{q}'' \rangle$ introduces two Dirac δ functions, and there are two cases to consider. Each case corresponds to one of the two terms in the permutation operator $\check{P} = \check{P}_{12} \check{P}_{23} + \check{P}_{13} \check{P}_{23}$. This leads to two different sets of momentum vectors that will be substituted for \mathbf{p} and \mathbf{p}'' after carrying out the integrations in Eq. (16). The first term, $\langle \mathbf{p}' \mathbf{q}' = \mathbf{q} | \check{P}_1 = \check{P}_{12} \check{P}_{23} | \mathbf{p}'' \mathbf{q}'' = \mathbf{q}_0 \rangle$, results in

$$\begin{aligned} \mathbf{p}' &= \mathbf{p}'_1 \equiv \frac{1}{2} \mathbf{q} + \mathbf{q}_0, \\ \mathbf{p}'' &= \mathbf{p}''_1 \equiv -\frac{1}{2} \mathbf{q}_0 - \mathbf{q}, \end{aligned} \quad (17)$$

and the second term, $\langle \mathbf{p}' \mathbf{q}' = \mathbf{q} | \check{P}_2 = \check{P}_{13} \check{P}_{23} | \mathbf{p}'' \mathbf{q}'' = \mathbf{q}_0 \rangle$, results in

$$\begin{aligned} \mathbf{p}' &= \mathbf{p}'_2 \equiv -\frac{1}{2} \mathbf{q} - \mathbf{q}_0, \\ \mathbf{p}'' &= \mathbf{p}''_2 \equiv \frac{1}{2} \mathbf{q}_0 + \mathbf{q}. \end{aligned} \quad (18)$$

Using relation Eqs. (17) and (18) together with the operator forms of the 2N transition operator $\langle \mathbf{p}q | \check{t} | \mathbf{p}'_u \mathbf{q} \rangle$ from Ref. [1] and initial state $\langle \mathbf{p}''_u \mathbf{q}_0 | \phi \rangle$ from Eq. (5), we can rewrite Eq. (16) as

$$\begin{aligned} \langle \mathbf{p}q | \check{t} \check{P} | \phi \rangle &= \sum_{u=1}^2 \sum_{\gamma^{2N}} \sum_{l=1}^2 \sum_{i=1}^6 \\ &\times t_i^{\gamma^{2N}} \left(E^{3N} - \frac{3}{4m} \mathbf{q}^2, p, p'_u, \hat{\mathbf{p}} \cdot \hat{\mathbf{p}}'_u \right) \phi_l(p''_u) \\ &\times [\check{I} \otimes |\gamma^{2N}\rangle \langle \gamma^{2N}|] \otimes [\check{I} \otimes \check{w}_i(\mathbf{p}, \mathbf{p}'_u)] \\ &\times [\check{P}_u^{is}] \otimes [\check{P}_u^s] \\ &\times [\check{I}] \otimes [\check{I} \otimes \check{b}_l(\mathbf{p}''_u)] |s\rangle, \end{aligned} \quad (19)$$

where m is the nucleon mass and the sum over u is related to the two terms in the permutation operator. The last three lines of Eq. (19) have the isospin and spin parts of operators separated. Square brackets on the left and right side of \otimes are used to mark the isospin and spin components with 8×8 matrix representations. These two separate components are additionally divided in line three and five to separate operators acting in the space of particles 2 and 3 (on the right-hand side of \otimes in [...]) from operators acting in the space of particle 1 (on the left-hand side of \otimes in [...]). Since the matrix representation of the permutation in the 3N isospin space $[\check{P}_u^{is}]$ and the 3N spin space $[\check{P}_u^s]$ is the same, in the following we will use $[\check{P}_u] \equiv [\check{P}_u^{is}] = [\check{P}_u^s]$. The deuteron bound state $|\phi_d\rangle$ in $|\phi\rangle$ has the form of Eq. (5), and in Eq. (19) the two capitalized (acting in the space of particles 2 and 3) spin operators from Eq. (6), $\check{B}_l(\mathbf{p}) = \check{I} \otimes \check{b}_l(\mathbf{p})$, are written explicitly. The six spin operators $\check{w}_i(\mathbf{p}, \mathbf{p}'_u)$ in Eq. (19) are part of the 2N transition operator,

$$\begin{aligned} &\langle \mathbf{p}' \gamma^{2N} | \check{t} | \mathbf{p} \gamma^{2N} \rangle \\ &= \delta_{\gamma^{2N}} \sum_{i=1}^6 t_i^{\gamma^{2N}}(E^{2N}, p', p, \hat{\mathbf{p}}' \cdot \hat{\mathbf{p}}) \check{w}_i(\mathbf{p}', \mathbf{p}), \end{aligned} \quad (20)$$

and are defined in Ref. [1]. In Eqs. (19) and (20), we write the energy argument E explicitly and mark the difference between the 3N and 2N energy $E^{2N} = E^{3N} - \frac{3}{4m} \mathbf{q}^2$. The transition operator is determined by the scalar functions $t_i^{\gamma^{2N}}(E^{2N}, p', p, \hat{\mathbf{p}}' \cdot \hat{\mathbf{p}})$ and the sum over γ^{2N} in Eq. (19) is over the four possible 2N isospin states. Since the 2N transition operator does not mix isospin states in the 2N subsystem [1], the isospin component in line three of Eq. (19) contains the $|\gamma^{2N}\rangle \langle \gamma^{2N}|$ operator acting in the subspace of particles 2 and 3.

Using the general form of Eq. (15) and splitting Eq. (7) into the isospin and spin components $|s\rangle = |\gamma\rangle \otimes |\alpha\rangle$, Eq. (19) can be written as

$$\begin{aligned} &\sum_{\gamma^{3N}} \sum_{r=1}^{64} \check{\tau}_r^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) |\gamma^{3N}\rangle \otimes (\check{O}_r(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) |\alpha\rangle) \\ &= \sum_{u=1}^2 \sum_{\gamma^{2N}} \sum_{l=1}^2 \sum_{i=1}^6 t_i^{\gamma^{2N}} \left(E^{3N} - \frac{3}{4m} \mathbf{q}^2, p, p'_u, \hat{\mathbf{p}} \cdot \hat{\mathbf{p}}'_u \right) \\ &\times \phi_l(p''_u) [\check{I} \otimes |\gamma^{2N}\rangle \langle \gamma^{2N}|] \\ &\otimes [\check{I} \otimes \check{w}_i(\mathbf{p}, \mathbf{p}'_u)] [\check{P}_u] \otimes [\check{P}_u] [\check{I}] \\ &\otimes [\check{I} \otimes \check{b}_l(\mathbf{p}''_u)] (|\gamma\rangle \otimes |\alpha\rangle). \end{aligned} \quad (21)$$

This equation holds for all spin states $|\alpha\rangle$, not only for the deuteron spin part of Eq. (7). The spin dependencies can, therefore, be removed by acting from the left, on both sides of Eq. (21), with

$$\langle \gamma^{3N} | \otimes \langle \alpha | \check{O}_w(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) \quad (22)$$

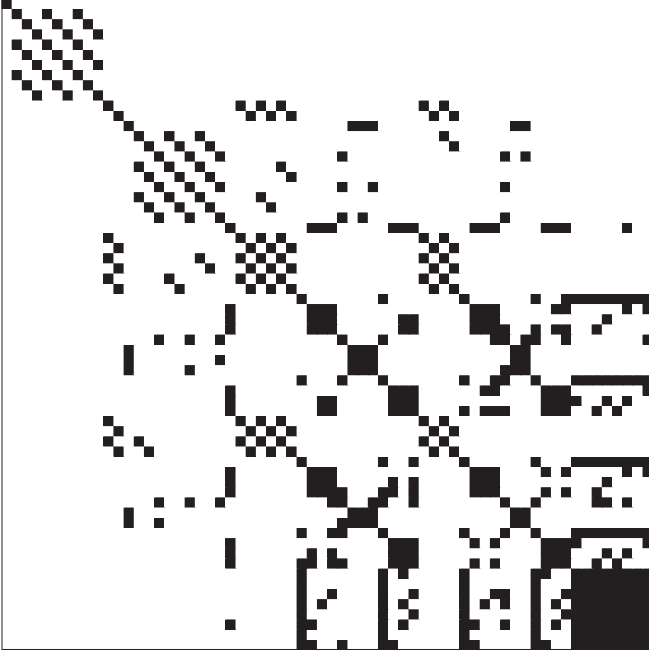


FIG. 1. Distribution of nonzero elements in the A_{rw} matrix. The nonzero elements of this sparse matrix are marked using black squares. Each row and column of squares corresponds to the appropriate row and column of A_{rw} .

and summing over all possible 3N spin states $|\alpha\rangle$. This procedure transforms the left-hand side of Eq. (21) into

$$\begin{aligned} & \sum_{r=1}^{64} A_{wr}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) \tilde{\tau}_r^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) \\ & \equiv \sum_{r=1}^{64} \sum_{\alpha} \langle \alpha | \check{O}_w(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) \check{O}_r(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) | \alpha \rangle \tilde{\tau}_r^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0), \end{aligned} \quad (23)$$

where we introduced the $64 \times 64 = 4096$ element A_{rw} matrix containing scalar coefficients. This matrix is symmetric, $A_{ij} = A_{ji}$, and the distribution of its nonzero elements is illustrated in Fig. 1. Appendix B contains a complete list of expressions for the nonzero elements of this matrix on and above the diagonal.

The right-hand side of Eq. (21) is more complicated. Applying Eq. (22) and summing over the spin states $|\alpha\rangle$ results in

$$\begin{aligned} & \sum_{u=1}^2 \sum_{l=1}^2 \sum_{i=1}^6 \\ & \times \sum_{\gamma^{2N}} t_i^{\gamma^{2N}} \left(E^{3N} - \frac{3}{4m} \mathbf{q}^2, p, p'_u, \hat{\mathbf{p}} \cdot \hat{\mathbf{p}}'_u \right) \\ & \times \phi_l(p'_u) \langle \gamma^{3N} | [\check{1} \otimes |\gamma^{2N}\rangle \langle \gamma^{2N} | [\check{P}_u] | \gamma \rangle \\ & \times \sum_{\alpha} \langle \alpha | [\check{O}_w(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) [\check{1} \otimes \check{w}_i(\mathbf{p}, \mathbf{p}'_u)] \\ & \times [\check{P}_u] [\check{1} \otimes \check{b}_l(p'_u)] | \alpha \rangle. \end{aligned} \quad (24)$$

Lines two and three of Eq. (24) constitute new scalar functions,

$$\begin{aligned} f_{uil}^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) & \equiv \sum_{\gamma^{2N}} t_i^{\gamma^{2N}} \left(E^{3N} - \frac{3}{4m} \mathbf{q}^2, p, p'_u, \hat{\mathbf{p}} \cdot \hat{\mathbf{p}}'_u \right) \phi_l(p'_u) \\ & \times \langle \gamma^{3N} | [\check{1} \otimes |\gamma^{2N}\rangle \langle \gamma^{2N} | [\check{P}_u] | \gamma \rangle, \end{aligned} \quad (25)$$

of momenta and indexes u, i, l, γ^{3N} that are related to the permutation, the transition operator scalar function, the deuteron scalar function, and the 3N isospin, respectively. Lines four and five of Eq. (24) define new coefficients that can be easily calculated using software for symbolic algebra [30]:

$$\begin{aligned} B_{wiul}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) & \equiv \sum_{\alpha} \langle \alpha | [\check{O}_w(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) [\check{1} \otimes \check{w}_i(\mathbf{p}, \mathbf{p}'_u)] [\check{P}_u] \\ & \times [\check{1} \otimes \check{b}_l(p'_u)] | \alpha \rangle. \end{aligned} \quad (26)$$

Using Eqs. (25) and (26) the right-hand side of Eq. (21) can be transformed to

$$\sum_{u=1}^2 \sum_{l=1}^2 \sum_{i=1}^6 f_{uil}^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) B_{wiul}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0). \quad (27)$$

Collecting the left- and right-hand sides from Eqs. (23) and (27), we get a simple matrix equation for the values of the scalar functions $\tilde{\tau}_r^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0)$:

$$\begin{aligned} & \sum_{r=1}^{64} A_{wr}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) \tilde{\tau}_r^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) \\ & = \sum_{u=1}^2 \sum_{l=1}^2 \sum_{i=1}^6 f_{uil}^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) B_{wiul}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0). \end{aligned} \quad (28)$$

Finding the solution requires the inversion of the A_{rw} matrix:

$$\begin{aligned} \tilde{\tau}_r^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) & = \sum_{u=1}^2 \sum_{l=1}^2 \sum_{i=1}^6 f_{uil}^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) \\ & \times \sum_{w=1}^{64} A_{rw}^{-1}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) B_{wiul}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0). \end{aligned} \quad (29)$$

Equation (29) allows the first part $\check{r}\check{P}|\phi\rangle$ of the Faddeev Eq. (1) to be written in the general operator form of Eq. (11). It is also a recipe for the $\tilde{\tau}$ function from Eq. (13). The successful application of this formula depends on the numerical properties of A ; these should be carefully investigated during the numerical realization.

B. Operator form of $\langle pq | \check{r}\check{G}_0 \check{P}\check{T} | \phi \rangle$

Writing $\langle pq | \check{r}\check{G}_0 \check{P}\check{T} | \phi \rangle$ in the general form of Eq. (11),

$$\begin{aligned} & \langle pq | \check{r}\check{G}_0 \check{P}\check{T} | \phi \rangle \\ & = \sum_{\gamma^{3N}} \sum_{r=1}^{64} \tilde{\tau}_r^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) |\gamma^{3N}\rangle \otimes (\check{O}_r(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) | \alpha \rangle), \end{aligned} \quad (30)$$

with new scalar functions $\tilde{\tau}_r^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0)$ and removing the spin and isospin dependencies will complete the reformulation of

the Faddeev Eq. (1) into Eq. (14). We begin by inserting two identity operators between \check{G}_0 and \check{P} and between \check{P} and \check{T} :

$$\begin{aligned} & \langle \mathbf{p}\mathbf{q} | \check{i}\check{G}_0 \check{P} \check{T} | \phi \rangle \\ &= \int d^3 \mathbf{p}' d^3 \mathbf{q}' \int d^3 \mathbf{p}'' d^3 \mathbf{q}'' \langle \mathbf{p}\mathbf{q} | \check{i}\check{G}_0 | \mathbf{p}'\mathbf{q}' \rangle \\ & \quad \times \langle \mathbf{p}'\mathbf{q}' | \check{P} | \mathbf{p}''\mathbf{q}'' \rangle \langle \mathbf{p}''\mathbf{q}'' | \check{T} | \phi \rangle. \end{aligned} \quad (31)$$

The first matrix element $\langle \mathbf{p}\mathbf{q} | \check{i}\check{G}_0 | \mathbf{p}'\mathbf{q}' \rangle$ will introduce $\delta^3(\mathbf{q} - \mathbf{q}')$ into the integrand. The second matrix element $\langle \mathbf{p}'\mathbf{q}' | \check{P} | \mathbf{p}''\mathbf{q}'' \rangle$ will introduce two Dirac δ functions into the integrations and, in analogy to the previous subsection, we will have to consider two cases corresponding to the two terms in $\check{P} = \check{P}_{12}\check{P}_{23} + \check{P}_{13}\check{P}_{23}$. The third matrix element $\langle \mathbf{p}''\mathbf{q}'' | \check{T} | \phi \rangle$ can be written in the general operator form of Eq. (11) but does not explicitly introduce any Dirac delta functions. Altogether, this results in one integration remaining in Eq. (31), and it is important to choose this integration smartly due to the singular nature of the integrand.

We expect \check{T} to have at least one singularity coming from the 2N transition operator \check{i} . The explicit energy dependence of \check{i} in Eq. (31) is $E^{3N} - \frac{3}{4m}\mathbf{q}^2$ and the singularity will occur when this value approaches the deuteron-bound state energy. This directly translates to a singularity of $\langle \mathbf{p}''\mathbf{q}'' | \check{T} | \phi \rangle$ in \mathbf{q}'' . Using this observation and following Ref. [29], we eliminate three integrals and leave only the \mathbf{q}'' integration in Eq. (31).

After eliminating the integrals, the first term in the permutation operator $\langle \mathbf{p}'\mathbf{q}' = \mathbf{q} | \check{P}_1 = \check{P}_{12}\check{P}_{23} | \mathbf{p}''\mathbf{q}'' \rangle$ results in

$$\begin{aligned} \mathbf{p}' &= \mathbf{k}'_1 \equiv \frac{1}{2}\mathbf{q} + \mathbf{q}'', \\ \mathbf{p}'' &= \mathbf{k}'_1 \equiv -\frac{1}{2}\mathbf{q}'' - \mathbf{q}, \end{aligned} \quad (32)$$

and the second part $\langle \mathbf{p}'\mathbf{q}' = \mathbf{q} | \check{P}_2 = \check{P}_{13}\check{P}_{23} | \mathbf{p}''\mathbf{q}'' \rangle$ results in

$$\begin{aligned} \mathbf{p}' &= \mathbf{k}'_1 \equiv -\frac{1}{2}\mathbf{q} - \mathbf{q}'', \\ \mathbf{p}'' &= \mathbf{k}'_1 \equiv \frac{1}{2}\mathbf{q}'' + \mathbf{q}. \end{aligned} \quad (33)$$

With this, Eq. (31) can be written using the general form of Eq. (30):

$$\begin{aligned} & \sum_{\gamma^{3N}} \sum_{r=1}^{64} \bar{\tau}_r^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) |\gamma^{3N}\rangle \otimes (\check{O}_r(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) |\alpha\rangle) \\ &= \sum_{u=1}^2 \int d^3 \mathbf{q}'' [\langle \mathbf{p}\mathbf{q} | \check{i} | \mathbf{k}'_u \mathbf{q} \rangle] \frac{[\check{P}_u] \otimes [\check{P}_u]}{E + i\epsilon - \frac{3}{4m}\mathbf{q}^2 - \frac{1}{m}\mathbf{k}'_u{}^2} \\ & \quad \times \sum_{\gamma^{3N}} \sum_{r=1}^{64} \tau_r^{\gamma^{3N}}(\mathbf{k}''_u, \mathbf{q}'', \mathbf{q}_0) |\gamma^{3N}\rangle \otimes (\check{O}_r(\mathbf{k}''_u, \mathbf{q}'', \mathbf{q}_0) |\alpha\rangle), \end{aligned} \quad (34)$$

with the scalar function $\bar{\tau}$ determining \check{T} after the application of $\check{i}\check{G}_0\check{P}$ and $|\alpha\rangle$ being a 3N spin state.

Removing the spin and isospin dependencies from Eq. (34) follows the same procedure as in Sec. IV A. For this reason, we will not delve into details and only write the final result:

$$\begin{aligned} & \bar{\tau}_r^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) \\ &= \int d^3 \mathbf{q}'' \sum_{u=1}^2 \sum_{i=1}^6 \sum_{w=1}^{64} \sum_{s=1}^{64} A_{rw}^{-1}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) C_{wsiu} \\ & \quad \times (\mathbf{p}, \mathbf{q}, \mathbf{q}_0, \mathbf{q}'') g_{\text{sui}}^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0, \mathbf{q}''). \end{aligned} \quad (35)$$

In Eq. (35), $C_{wsiu}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0, \mathbf{q}'')$ are new functions that can be easily calculated using software for symbolic algebra,

$$\begin{aligned} C_{wsiu}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0, \mathbf{q}'') &\equiv \sum_{\alpha} \langle \alpha | [\check{O}_w(\mathbf{p}, \mathbf{q}, \mathbf{q}_0)] [\check{I} \otimes \check{w}_i(\mathbf{p}, \mathbf{k}'_u)] \\ & \quad \times [\check{P}_u] [\check{O}_s(\mathbf{k}''_u, \mathbf{q}'', \mathbf{q}_0)] | \alpha \rangle, \end{aligned} \quad (36)$$

and the sum is over all possible spin states. The functions $g_{\text{sui}}^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0, \mathbf{q}'')$ are related to the scalar functions τ via

$$\begin{aligned} & g_{\text{sui}}^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0, \mathbf{q}'') \\ & \equiv \sum_{\gamma^{2N}} \sum_{\gamma^{3N}} t_i^{\gamma^{2N}} \left(E^{3N} - \frac{3}{4m}\mathbf{q}^2, p, k'_u, \hat{\mathbf{p}} \cdot \hat{\mathbf{k}}'_u \right) \\ & \quad \times \left(E + i\epsilon - \frac{3}{4m}\mathbf{q}^2 - \frac{1}{m}\mathbf{k}''_u{}^2 \right)^{-1} \tau_s^{\gamma^{3N}}(\mathbf{k}''_u, \mathbf{q}'', \mathbf{q}_0) \\ & \quad \times \langle \gamma^{3N} | [\check{I} \otimes |\gamma^{2N}\rangle \langle \gamma^{2N}|] [\check{P}_u] | \gamma^{3N} \rangle. \end{aligned} \quad (37)$$

With this we have a complete set of definitions that can be used to solve Eq. (1) using iterative Krylov subspace methods.

C. Collecting all terms

We mentioned above that a smart choice of integration variable is important due to the singular behavior of the 2N transition operator around the deuteron-bound state energy. The form of this singularity is well known and can be used in Eqs. (29) and (35) by explicitly writing the scalar functions that define the 2N transition operator in Eq. (20) as

$$t_i^{\gamma^{2N}}(E^{2N}, p', p, \hat{\mathbf{p}}' \cdot \hat{\mathbf{p}}) = \frac{t_i^s \gamma^{2N}(E^{2N}, p', p, \hat{\mathbf{p}}' \cdot \hat{\mathbf{p}})}{E^{2N} - E_d}. \quad (38)$$

This substitution is only necessary for the case of the deuteron isospin $|\gamma^{2N}\rangle = |00\rangle$ and results in nonsingular scalar functions t^s . In addition to the deuteron, also the free propagator contributes to the singular behavior of the integral form of the Faddeev equation; this results in the so-called ‘‘moving singularities.’’ In our scheme, these poles will be treated numerically as described in Refs. [6,29], where equations very similar to the ones presented in the current paper are considered. Additional information on the treatment of the deuteron pole can be found in Ref. [26].

With this in mind, all ingredients are in place to implement Eq. (14),

$$(\check{I} - \check{Q})\tau = \bar{\tau},$$

numerically. Equation (29) together with Eqs. (25) and (26) can be used to construct $\tilde{\tau}$,

$$\begin{aligned} \tilde{\tau}_r^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= \sum_{u=1}^2 \sum_{l=1}^2 \sum_{i=1}^6 f_{uil}^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) \\ &\quad \times \sum_{w=1}^{64} A_{rw}^{-1}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) B_{wiul}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0), \end{aligned}$$

while Eq. (35) together with Eqs. (36) and (37) define the \check{Q} operator:

$$\begin{aligned} (\check{Q}\tau)_r^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= \tilde{\tau}_r^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) \\ &= \int d^3\mathbf{q}'' \sum_{u=1}^2 \sum_{i=1}^6 \sum_{w,s=1}^{64} A_{rw}^{-1}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) \\ &\quad \times C_{wsiu}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0, \mathbf{q}'') g_{sui}^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0, \mathbf{q}''). \end{aligned}$$

We managed to significantly reduce the numerical complexity of the problem by utilizing rotational symmetry; however, the numerical size of the problem is still significant. This poses a serious challenge for the future implementation, which we, nonetheless, regard to be feasible since even more simplifications are immediately apparent. For instance, looking at the final expressions, each free nucleon relative momentum magnitude q_0 case produces an independent equation and can be treated separately, thus further reducing the numerical complexity of the calculations.

V. SUMMARY

In Sec. II, we showed that the 3N scattering amplitude can be written in a general form,

$$\begin{aligned} \langle \mathbf{p}\mathbf{q} | \check{T} | \phi \rangle &= \sum_{\gamma^{3N}} \sum_{r=1}^{64} \tilde{\tau}_r^{\gamma^{3N}}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) |\gamma^{3N}\rangle \otimes (\check{O}_r(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) |\alpha\rangle), \end{aligned}$$

and the arguments we presented are applicable also in the case when a 3N force is taken into consideration. Next, we used this general form to rewrite the Faddeev equation as

$$(\check{I} - \check{Q})\tau = \tilde{\tau},$$

where \check{Q} is a linear operator acting on the scalar functions τ (depending on momenta $\mathbf{p}, \mathbf{q}, \mathbf{q}_0$ and integer arguments r and γ^{3N}) that define the scattering amplitude and $\tilde{\tau}$ is a given set of scalar functions calculated using the 2N transition operator. This simple linear equation can be solved iteratively for τ . These scalar functions can be represented numerically using only approximately 5.5×10^{11} complex numbers if they are discretized over a lattice of 32 points for each momentum magnitude and angular argument.

This is a significant reduction of numerical complexity with respect to approaches that do not utilize rotational symmetry, and we hope that it will allow us to construct a numerical scheme that accounts for all orders of the iterated Faddeev equation. We also hope that using the general form of the scattering amplitude will make it possible to include 3N forces

into the description of three nucleon scattering without using partial waves. However, to achieve this goal we will have to work out the general operator form of the 3N force. For first steps in this direction by H. Krebs *et al.*, see Ref. [25].

It should be mentioned that a further reduction of numerical complexity can be achieved by utilizing discrete symmetries. Utilizing symmetry properties under parity, time reversal and particle exchange might reduce the total number of scalar functions. We estimate that this is a much smaller gain than the one obtained by utilizing rotation symmetry; however, every simplification of the problem should be considered.

ACKNOWLEDGMENTS

This work was supported by the National Science Center of Poland under Grants No. DEC-2013/11/N/ST2/03733, No. DEC-2016/21/D/ST2/01120, and No. DEC-2013/10/M/ST2/00420. The character of the work presented here is theoretical; however, we acknowledge the support of the Jülich Supercomputing Center, which was important in works leading up to this paper.

APPENDIX A: SPIN OPERATORS IN THE GENERAL FORM OF THE 3N SCATTERING AMPLITUDE

$$\begin{aligned} \check{O}_1(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= 1 \\ \check{O}_2(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= \mathbf{p} \cdot \check{\sigma}(1) \\ \check{O}_3(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= \mathbf{p} \cdot \check{\sigma}(2) \\ \check{O}_4(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= \mathbf{p} \cdot \check{\sigma}(3) \\ \check{O}_5(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= \mathbf{q} \cdot \check{\sigma}(1) \\ \check{O}_6(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= \mathbf{q} \cdot \check{\sigma}(2) \\ \check{O}_7(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= \mathbf{q} \cdot \check{\sigma}(3) \\ \check{O}_8(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= \mathbf{q}_0 \cdot \check{\sigma}(1) \\ \check{O}_9(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= \mathbf{q}_0 \cdot \check{\sigma}(2) \\ \check{O}_{10}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= \mathbf{q}_0 \cdot \check{\sigma}(3) \\ \check{O}_{11}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= \check{\sigma}(1) \cdot \check{\sigma}(2) \\ \check{O}_{12}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= \check{\sigma}(1) \cdot \check{\sigma}(3) \\ \check{O}_{13}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= \check{\sigma}(2) \cdot \check{\sigma}(3) \\ \check{O}_{14}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= \mathbf{p} \times \check{\sigma}(1) \cdot \check{\sigma}(2) \\ \check{O}_{15}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= \mathbf{p} \times \check{\sigma}(1) \cdot \check{\sigma}(3) \\ \check{O}_{16}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= \mathbf{p} \times \check{\sigma}(2) \cdot \check{\sigma}(3) \\ \check{O}_{17}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= \mathbf{q} \times \check{\sigma}(1) \cdot \check{\sigma}(2) \\ \check{O}_{18}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= \mathbf{q} \times \check{\sigma}(1) \cdot \check{\sigma}(3) \\ \check{O}_{19}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= \mathbf{q} \times \check{\sigma}(2) \cdot \check{\sigma}(3) \\ \check{O}_{20}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= \mathbf{q}_0 \times \check{\sigma}(1) \cdot \check{\sigma}(2) \\ \check{O}_{21}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= \mathbf{q}_0 \times \check{\sigma}(1) \cdot \check{\sigma}(3) \\ \check{O}_{22}(\mathbf{p}, \mathbf{q}, \mathbf{q}_0) &= \mathbf{q}_0 \times \check{\sigma}(2) \cdot \check{\sigma}(3) \end{aligned}$$

$$\begin{aligned}
 A_{1414} &= A_{1515} = A_{1616} = A_{1634} = A_{2331} = 16\mathbf{p} \cdot \mathbf{p} \\
 A_{3030} &= A_{3838} = 24\mathbf{p} \cdot \mathbf{p} \\
 A_{3260} &= A_{4060} = -8\mathbf{p} \cdot \mathbf{p}(\mathbf{p} \times \mathbf{q}) \cdot \mathbf{q}_0 \\
 A_{3162} &= A_{3359} = A_{4159} = 8\mathbf{p} \cdot \mathbf{p}(\mathbf{p} \times \mathbf{q}) \cdot \mathbf{q}_0 \\
 A_{2424} &= A_{2525} = A_{3058} = A_{3535} = A_{3858} = 8(\mathbf{p} \cdot \mathbf{p})^2 \\
 A_{3131} &= A_{3939} = 16(\mathbf{p} \cdot \mathbf{p})^2 \\
 A_{5858} &= 8(\mathbf{p} \cdot \mathbf{p})^3 \\
 A_{2340} &= A_{2354} = A_{3450} = -16\mathbf{p} \cdot \mathbf{q} \\
 A_{3453} &= A_{3850} = -16i\mathbf{p} \cdot \mathbf{q} \\
 A_{25} &= A_{36} = A_{47} = A_{1126} = A_{1227} = A_{1336} = A_{3053} \\
 &= A_{3846} = 8\mathbf{p} \cdot \mathbf{q} \\
 A_{1417} &= A_{1518} = A_{1619} = A_{1650} = A_{1934} = A_{2332} \\
 &= A_{2347} = 16\mathbf{p} \cdot \mathbf{q} \\
 A_{3046} &= A_{3853} = 24\mathbf{p} \cdot \mathbf{q} \\
 A_{4062} &= A_{4860} = A_{5560} = -8\mathbf{p} \cdot \mathbf{q}(\mathbf{p} \times \mathbf{q}) \cdot \mathbf{q}_0 \\
 A_{3164} &= A_{3964} = A_{4161} = A_{4762} = A_{4959} = A_{5659} \\
 &= 8\mathbf{p} \cdot \mathbf{q}(\mathbf{p} \times \mathbf{q}) \cdot \mathbf{q}_0 \\
 A_{2426} &= A_{2527} = A_{3059} = A_{3536} = A_{3859} = A_{4658} \\
 &= A_{5358} = 8\mathbf{p} \cdot \mathbf{p}\mathbf{p} \cdot \mathbf{q} \\
 A_{3132} &= A_{3147} = A_{3940} = A_{3954} = 16\mathbf{p} \cdot \mathbf{p}\mathbf{p} \cdot \mathbf{q} \\
 A_{5859} &= 8(\mathbf{p} \cdot \mathbf{p})^2\mathbf{p} \cdot \mathbf{q} \\
 A_{2442} &= A_{2543} = A_{3551} = A_{3861} \\
 &= A_{4659} = A_{5359} = 8(\mathbf{p} \cdot \mathbf{q})^2 \\
 A_{3148} &= A_{3247} = A_{3955} = A_{4054} = 16(\mathbf{p} \cdot \mathbf{q})^2 \\
 A_{5861} &= 8\mathbf{p} \cdot \mathbf{p}(\mathbf{p} \cdot \mathbf{q})^2 \\
 A_{5863} &= 8(\mathbf{p} \cdot \mathbf{q})^3 \\
 A_{2341} &= -16\mathbf{p} \cdot \mathbf{q}_0 \\
 A_{28} &= A_{39} = A_{410} = A_{1128} = A_{1229} = A_{1337} \\
 &= A_{3857} = 8\mathbf{p} \cdot \mathbf{q}_0 \\
 A_{1420} &= A_{1521} = A_{1622} = A_{2234} = A_{2333} = 16\mathbf{p} \cdot \mathbf{q}_0 \\
 A_{3057} &= 24\mathbf{p} \cdot \mathbf{q}_0 \\
 A_{2428} &= A_{2529} = A_{3060} = A_{3537} = A_{3860} = A_{5758} \\
 &= 8\mathbf{p} \cdot \mathbf{p}\mathbf{p} \cdot \mathbf{q}_0 \\
 A_{3133} &= A_{3941} = 16\mathbf{p} \cdot \mathbf{p}\mathbf{p} \cdot \mathbf{q}_0 \\
 A_{5860} &= 8(\mathbf{p} \cdot \mathbf{p})^2\mathbf{p} \cdot \mathbf{q}_0 \\
 A_{2444} &= A_{2545} = A_{3552} = A_{3862} = A_{4660} \\
 &= A_{5360} = A_{5759} = 8\mathbf{p} \cdot \mathbf{q}\mathbf{p} \cdot \mathbf{q}_0 \\
 A_{3149} &= A_{3347} = A_{3956} = A_{4154} = 16\mathbf{p} \cdot \mathbf{q}\mathbf{p} \cdot \mathbf{q}_0 \\
 A_{5862} &= 8\mathbf{p} \cdot \mathbf{p}\mathbf{p} \cdot \mathbf{q}\mathbf{p} \cdot \mathbf{q}_0 \\
 A_{5864} &= 8(\mathbf{p} \cdot \mathbf{q})^2\mathbf{p} \cdot \mathbf{q}_0 \\
 A_{5760} &= 8(\mathbf{p} \cdot \mathbf{q}_0)^2 \\
 A_{2355} &= A_{5050} = -16\mathbf{q} \cdot \mathbf{q} \\
 A_{5053} &= -16i\mathbf{q} \cdot \mathbf{q} \\
 A_{55} &= A_{66} = A_{77} = A_{1142} = A_{1243} = A_{1351} \\
 &= A_{4653} = 8\mathbf{q} \cdot \mathbf{q} \\
 A_{1717} &= A_{1818} = A_{1919} = A_{1950} = A_{2348} = 16\mathbf{q} \cdot \mathbf{q} \\
 A_{4646} &= A_{5353} = 24\mathbf{q} \cdot \mathbf{q} \\
 A_{5562} &= -8\mathbf{q} \cdot \mathbf{q}(\mathbf{p} \times \mathbf{q}) \cdot \mathbf{q}_0 \\
 A_{4764} &= A_{5464} = A_{5661} = 8\mathbf{q} \cdot \mathbf{q}(\mathbf{p} \times \mathbf{q}) \cdot \mathbf{q}_0 \\
 A_{2626} &= A_{2727} = A_{3061} = A_{3636} = 8\mathbf{p} \cdot \mathbf{p}\mathbf{q} \cdot \mathbf{q} \\
 A_{3232} &= A_{4040} = A_{4747} = A_{5454} = 16\mathbf{p} \cdot \mathbf{p}\mathbf{q} \cdot \mathbf{q} \\
 A_{5959} &= 8(\mathbf{p} \cdot \mathbf{p})^2\mathbf{q} \cdot \mathbf{q} \\
 A_{2642} &= A_{2743} = A_{3063} = A_{3651} = A_{3863} = A_{4661} \\
 &= A_{5361} = 8\mathbf{p} \cdot \mathbf{q}\mathbf{q} \cdot \mathbf{q} \\
 A_{3248} &= A_{4055} = A_{4748} = A_{5455} = 16\mathbf{p} \cdot \mathbf{q}\mathbf{q} \cdot \mathbf{q} \\
 A_{5961} &= 8\mathbf{p} \cdot \mathbf{p}\mathbf{p} \cdot \mathbf{q}\mathbf{q} \cdot \mathbf{q} \\
 A_{5963} &= 8(\mathbf{p} \cdot \mathbf{q})^2\mathbf{q} \cdot \mathbf{q} \\
 A_{5362} &= A_{5761} = 8\mathbf{p} \cdot \mathbf{q}_0\mathbf{q} \cdot \mathbf{q} \\
 A_{4749} &= A_{5456} = 16\mathbf{p} \cdot \mathbf{q}_0\mathbf{q} \cdot \mathbf{q} \\
 A_{4242} &= A_{4343} = A_{4663} = A_{5151} = A_{5363} = 8(\mathbf{q} \cdot \mathbf{q})^2 \\
 A_{4848} &= A_{5555} = 16(\mathbf{q} \cdot \mathbf{q})^2 \\
 A_{6161} &= 8\mathbf{p} \cdot \mathbf{p}(\mathbf{q} \cdot \mathbf{q})^2 \\
 A_{6163} &= 8\mathbf{p} \cdot \mathbf{q}(\mathbf{q} \cdot \mathbf{q})^2 \\
 A_{6363} &= 8(\mathbf{q} \cdot \mathbf{q})^3 \\
 A_{2356} &= -16\mathbf{q} \cdot \mathbf{q}_0 \\
 A_{58} &= A_{69} = A_{710} = A_{1144} = A_{1245} \\
 &= A_{1352} = A_{5357} = 8\mathbf{q} \cdot \mathbf{q}_0 \\
 A_{1720} &= A_{1821} = A_{1922} = A_{2250} = A_{2349} = 16\mathbf{q} \cdot \mathbf{q}_0 \\
 A_{4657} &= 24\mathbf{q} \cdot \mathbf{q}_0 \\
 A_{2628} &= A_{2729} = A_{3062} = A_{3637} = 8\mathbf{p} \cdot \mathbf{p}\mathbf{q} \cdot \mathbf{q}_0 \\
 A_{3233} &= A_{4041} = 16\mathbf{p} \cdot \mathbf{p}\mathbf{q} \cdot \mathbf{q}_0 \\
 A_{5960} &= 8(\mathbf{p} \cdot \mathbf{p})^2\mathbf{q} \cdot \mathbf{q}_0 \\
 A_{2644} &= A_{2745} = A_{2842} = A_{2943} = A_{3064} = A_{3652} \\
 &= A_{3751} = A_{3864} = A_{4662} = 8\mathbf{p} \cdot \mathbf{q}\mathbf{q} \cdot \mathbf{q}_0 \\
 A_{3249} &= A_{3348} = A_{4056} = A_{4155} = 16\mathbf{p} \cdot \mathbf{q}\mathbf{q} \cdot \mathbf{q}_0 \\
 A_{5962} &= A_{6061} = 8\mathbf{p} \cdot \mathbf{p}\mathbf{p} \cdot \mathbf{q}\mathbf{q} \cdot \mathbf{q}_0 \\
 A_{5964} &= A_{6063} = 8(\mathbf{p} \cdot \mathbf{q})^2\mathbf{q} \cdot \mathbf{q}_0 \\
 A_{5762} &= 8\mathbf{p} \cdot \mathbf{q}_0\mathbf{q} \cdot \mathbf{q}_0 \\
 A_{4244} &= A_{4345} = A_{4664} = A_{5152} = A_{5364} \\
 &= A_{5763} = 8\mathbf{q} \cdot \mathbf{q}\mathbf{q} \cdot \mathbf{q}_0 \\
 A_{4849} &= A_{5556} = 16\mathbf{q} \cdot \mathbf{q}\mathbf{q} \cdot \mathbf{q}_0 \\
 A_{6162} &= 8\mathbf{p} \cdot \mathbf{p}\mathbf{q} \cdot \mathbf{q}\mathbf{q} \cdot \mathbf{q}_0
 \end{aligned}$$

$$A_{6164} = A_{6263} = 8\mathbf{p} \cdot \mathbf{q}\mathbf{q} \cdot \mathbf{q}\mathbf{q} \cdot \mathbf{q}_0$$

$$A_{6364} = 8(\mathbf{q} \cdot \mathbf{q})^2 \mathbf{q} \cdot \mathbf{q}_0$$

$$A_{5764} = 8(\mathbf{q} \cdot \mathbf{q}_0)^2$$

$$A_{88} = A_{99} = A_{1010} = 8\mathbf{q}_0 \cdot \mathbf{q}_0$$

$$A_{2020} = A_{2121} = A_{2222} = 16\mathbf{q}_0 \cdot \mathbf{q}_0$$

$$A_{5757} = 24\mathbf{q}_0 \cdot \mathbf{q}_0$$

$$A_{2828} = A_{2929} = A_{3737} = 8\mathbf{p} \cdot \mathbf{p}\mathbf{q}_0 \cdot \mathbf{q}_0$$

$$A_{3333} = A_{4141} = 16\mathbf{p} \cdot \mathbf{p}\mathbf{q}_0 \cdot \mathbf{q}_0$$

$$A_{6060} = 8(\mathbf{p} \cdot \mathbf{p})^2 \mathbf{q}_0 \cdot \mathbf{q}_0$$

$$A_{2844} = A_{2945} = A_{3752} = 8\mathbf{p} \cdot \mathbf{q}\mathbf{q}_0 \cdot \mathbf{q}_0$$

$$A_{3349} = A_{4156} = 16\mathbf{p} \cdot \mathbf{q}\mathbf{q}_0 \cdot \mathbf{q}_0$$

$$A_{6062} = 8\mathbf{p} \cdot \mathbf{p}\mathbf{p} \cdot \mathbf{q}\mathbf{q}_0 \cdot \mathbf{q}_0$$

$$A_{6064} = 8(\mathbf{p} \cdot \mathbf{q})^2 \mathbf{q}_0 \cdot \mathbf{q}_0$$

$$A_{4444} = A_{4545} = A_{5252} = 8\mathbf{q} \cdot \mathbf{q}\mathbf{q}_0 \cdot \mathbf{q}_0$$

$$A_{4949} = A_{5656} = 16\mathbf{q} \cdot \mathbf{q}\mathbf{q}_0 \cdot \mathbf{q}_0$$

$$A_{6262} = 8\mathbf{p} \cdot \mathbf{p}\mathbf{q} \cdot \mathbf{q}\mathbf{q}_0 \cdot \mathbf{q}_0$$

$$A_{6264} = 8\mathbf{p} \cdot \mathbf{q}\mathbf{q} \cdot \mathbf{q}\mathbf{q}_0 \cdot \mathbf{q}_0$$

$$A_{6464} = 8(\mathbf{q} \cdot \mathbf{q})^2 \mathbf{q}_0 \cdot \mathbf{q}_0$$

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