THREE NUCLEON SCATTERING USING A "THREE-DIMENSIONAL" APPROACH — CHALLENGES

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The so-called "three-dimensional" (3D) treatment of elastic nucleon–deuteron scattering and nucleon-induced deuteron breakup reactions has a potential to resolve certain issues related to the full understanding of these processes. 3D calculations, by working directly with the three-component momentum vectors of the nucleons, are in principle equivalent to using all partial waves simultaneously. It is expected that the advantages of the 3D formalism will be apparent for higher energies where traditional calculations require many partial waves to converge. The 3D description of neutron–deuteron scattering using first-order terms of the Faddeev equation seems to demonstrate these benefits. This paper outlines the 3D description of the elastic and the breakup channels of nucleon–deuteron scattering, points to difficulties related to the construction of a numerical realization, and suggests a workaround to some of these issues.

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1. Introduction

An accurate description of three-nucleon (3N) scattering is based on the Faddeev equation. Neglecting the 3N potential energy, this equation has the form [1] of

$$\check{T} \mid \boldsymbol{q}_0; \phi\rangle = \check{t}\check{P} \mid \boldsymbol{q}_0; \phi\rangle + \check{t}\check{P}\check{G}_0\check{T} \mid \boldsymbol{q}_0; \phi\rangle \,, \tag{1}$$

where $\mid \boldsymbol{q}_0; \phi\rangle$ is a 3N state composed from the deuteron in the space of particles $2, 3$ and a free particle with momentum $\boldsymbol{q}_0$ in the space of particle 1. The capital $\check{T}$ is the 3N transition operator (the inverted hat symbol is used to distinguish operators from unit vectors), $\check{t}$ is the two nucleon (2N) transition operator, satisfying the Lippmann–Schwinger equation and acting in the space of particles 2 and 3, $\check{G}_0$ is the free propagator and, finally, $\check{P}$ is

a permutation operator composed from operators $\check{P}_{ij}$ that exchange particles i and j

$$\check{P} = \check{P}_{12}\check{P}_{23} + \check{P}_{13}\check{P}_{23}\,. \tag{2}$$

The scattering amplitude $\check{T} \mid \boldsymbol{q}_0; \phi\rangle$ is the central object in equation (1), and together with the breakup operator $\check{U}_0$ and the elastic scattering operator $\check{U}$, it can be used to calculate observables in both the breakup and elastic channels of 3N scattering via the matrix elements [1]

$$\langle \phi_0 \mid \check{U}_0 \mid \boldsymbol{q}_0; \phi\rangle \;=\; \langle \phi_0 \mid \big(\check{1} + \check{P}\big)\,\check{T} \mid \boldsymbol{q}_0; \phi\rangle\,, \tag{3}$$

$$\langle \boldsymbol{q}_0'; \phi \mid \check{U} \mid \boldsymbol{q}_0; \phi\rangle \;=\; \langle \boldsymbol{q}_0'; \phi \mid \check{P}\check{G}_0^{-1} + \check{P}\check{T} \mid \boldsymbol{q}_0; \phi\rangle\,. \tag{4}$$

The state $\langle \phi_0 \mid$ in (3) describes the motion of three free particles and in (4) the free particle has a different momentum $\boldsymbol{q}_0'$ in the final state.

Solutions to equation (1) obtained using partial wave decomposition are available in the literature (see *e.g.* [1] and references therein). However, solving this equation using the so-called "three-dimensional" (3D) approach might provide new insights and more precise predictions that are necessary to verify new models of nuclear interactions against experimental data, especially in cases where traditional calculations require many partial waves to converge. An additional benefit of this approach is the possibility to skip the partial wave (PW) decomposition procedure for newly derived forces allowing researchers to perform calculations with new interactions in less time. These benefits are a result of the 3D formalism working directly with the three-component nucleon momentum vectors and by choosing two- or three-nucleon momentum eigenstates as the working basis in the calculations. This choice makes 3D calculations, in principle, equivalent to using all partial waves simultaneously. In practice, this is of course limited by the number of computing resources available. For an introduction to 3D calculations, please refer to [2] and references therein. More information on the 3D treatment of two nucleon systems, the ^{3}H bound state, the ^{3}He bound state with a screened Coulomb potential, and first-order neutron–deuteron scattering calculations can be found in [3–6].

An iterative approach to solving (1) with Padé summation or Krylov subspace methods will generally involve the repeated applications of operators from the right-hand side of this equation. This is the case for both traditional PW calculations and 3D calculations. Unfortunately, 3D calculations using only the first order of this equation and assuming

$$\check{T} \mid \boldsymbol{q}_0; \phi\rangle \approx \check{t}\check{P} \mid \boldsymbol{q}_0; \phi\rangle$$

are already quite complicated [6]. Going to the next order of the calculation

$$\check{T} \mid \boldsymbol{q}_0; \phi\rangle \approx \check{t}\check{P} \mid \boldsymbol{q}_0; \phi\rangle + \check{t}\check{G}_0\check{P}\check{t}\check{P} \mid \boldsymbol{q}_0; \phi\rangle$$

or higher orders introduces a substantial increase in the complexity of analytical expressions that make practical numerical implementations within the 3D formalism prohibitively difficult. Recently, following [7, 8], a template that can fit $\check{T} \mid \boldsymbol{q}_0, \phi\rangle$ at all orders of the calculation was proposed in [9]. This development can be used in solving problems related to the 3D description of neutron–deuteron scattering and was important for two reasons. Firstly, higher-order calculations or calculations that attempt to solve the entire Faddeev equation by reducing its dimensionality via Krylov subspace methods are necessary in order to obtain a precise description of 3N scattering. The operator form from [9] can be used to keep the complexity of analytical expressions constant across all orders and/or iterations of the calculation. Secondly, the operator template from [9] reduces the number of numerical resources required by the calculations by taking into account rotational symmetry.

This paper outlines problems related to the construction of a practical numerical implementation of a solution to the full Fadeev equation that is based on the operator template from [9]. The text is organized as follows. Section 2 contains a discussion of the postulated form of the 3N scattering amplitude. Next, Section 3 outlines problems with a practical numerical implementation of the calculation and suggests a partial solution. Finally, Section 4 contains the summary and outlook.

2. The operator form of the 3N scattering amplitude

Arguments presented in [9] lead to the following form of the 3N transition amplitude:

$$\langle \boldsymbol{pq} \mid \check{T}(E) \mid \boldsymbol{q}_0; \phi\rangle = \sum_{\gamma} \sum_{r=1}^{64} \tau_r^{\gamma}(E, \boldsymbol{p}, \boldsymbol{q}, \boldsymbol{q}_0) \mid \gamma\rangle \otimes \left(\check{O}_r(\boldsymbol{p}, \boldsymbol{q}, \boldsymbol{q}_0) \mid s\rangle\right) , \quad (5)$$

where E is the 3N energy and $\tau_r^{\gamma}(\boldsymbol{p}, \boldsymbol{q}, \boldsymbol{q}_0)$ are scalar functions of the final-state momenta $\boldsymbol{p}$, $\boldsymbol{q}$ and the momentum of the free particle in the initial state is $\boldsymbol{q}_0$. Furthermore, $\langle \boldsymbol{pq} \mid$ is a product state of Jacobi momenta, $\mid \gamma\rangle$ is one of the eight possible isospin states of the 3N system and, finally, $\check{O}_r(\boldsymbol{p}, \boldsymbol{q}, \boldsymbol{q}_0) \mid s\rangle$ is a spin state in which one of the 64 operators $\check{O}_r(\boldsymbol{p}, \boldsymbol{q}, \boldsymbol{q}_0)$ (listed in Appendix A in [9]) acts on a given 3N spin state $\mid s\rangle$.

The operator from (5) can be inserted into both parts of the right-hand side of (1)

$$\check{t}\check{P} \mid \boldsymbol{q}_0; \phi\rangle , \quad (6)$$

$$\check{t}\check{P}\check{G}_0\check{T} \mid \boldsymbol{q}_0; \phi\rangle \quad (7)$$

and numerical tests can be performed to verify whether the resulting states still match (5). In order to achieve this, it can be assumed that for a given 2N energy $E^{2\mathrm{N}}$, the 2N transition operator $\check{t}$ can be written in the following general, isospin conserving form in the space of two particles [10]:

$$\langle \boldsymbol{k}' \mid \check{t}^{\gamma_{2\mathrm{N}}}\left(E^{2\mathrm{N}}\right) \mid \boldsymbol{k}\rangle = \sum_{i=1}^{6} t_i^{\gamma_{2\mathrm{N}}}\left(E^{2\mathrm{N}}, k', k, \hat{\boldsymbol{k}}' \cdot \hat{\boldsymbol{k}}\right) \check{w}_i\left(\boldsymbol{k}', \boldsymbol{k}\right) . \tag{8}$$

In (8), $\gamma_{2\mathrm{N}}$ is a given 2N isospin state, $\boldsymbol{k}'$, $\boldsymbol{k}$ are relative particle momenta in the final and initial state, $t_i^{\gamma_{2\mathrm{N}}}(E^{2\mathrm{N}}, k', k, \hat{\boldsymbol{k}}' \cdot \hat{\boldsymbol{k}})$ are scalar functions of the initial and final momenta and, finally, $\check{w}_i(\boldsymbol{k}', \boldsymbol{k})$ are known 2N spin operators. More precisely, in the combined isospin–spin space of the 3N system, equation (8) turns into

$$\begin{aligned}\langle \boldsymbol{p}'\boldsymbol{q}' \mid \check{t}(E) \mid \boldsymbol{p}\boldsymbol{q}\rangle \;=\; & \sum_{i=1}^{6}\sum_{\gamma_{2\mathrm{N}}=1}^{4} t_i^{\gamma_{2\mathrm{N}}}\left(E - \frac{3}{4m}q^2; p', p, \hat{\boldsymbol{p}}' \cdot \hat{\boldsymbol{p}}\right) \delta^3\left(\boldsymbol{q}' - \boldsymbol{q}\right) \\ & \times \left(\check{1}^{\text{particle 1}} \otimes (\mid \gamma_{2\mathrm{N}}\rangle\langle\gamma_{2\mathrm{N}} \mid)^{\text{particle 2,3}}\right)^{\text{3N isospin}} \\ & \otimes \left(\check{1}^{\text{particle 1}} \otimes \check{w}_i\left(\boldsymbol{p}', \boldsymbol{p}\right)^{\text{particle 2,3}}\right)^{\text{3N spin}} , \end{aligned} \tag{9}$$

where m is the nucleon mass and the subspaces corresponding to different particles are marked explicitly together with the association to either the 3N spin or isospin spaces.

Since the isospin part, $\mid \gamma\rangle$, of (5) cannot depend on momenta, it is much simpler than the spin part $\check{O}_r(\boldsymbol{p}, \boldsymbol{q}, \boldsymbol{q}_0) \mid s\rangle$. If the isospin dependence is ignored, then checking whether (6) fits into the form of (5) reduces to verifying if operators of the type of

$$\left(\check{1} \otimes \check{w}\right) \check{P}_n \left(\check{1} \otimes \check{b}\right) \tag{10}$$

can be written as a linear combination of scalar functions τ and operators $\check{O}$ from the set used in equation (5). Similarly, checking whether (7) fits into (5) boils down to verifying if operators of the type of

$$\left(\check{1} \otimes \check{w}\right) \check{P}_n \check{O} \tag{11}$$

can be written in a similar way. In equations (10) and (11), $\check{w}$ are the 3N spin operators $\check{1} \otimes \check{w}_{i,j}(\boldsymbol{p}', \boldsymbol{p})$ from (8) with the momenta having values calculated by taking into account the permutations, $\check{P}_n$ is one of the two 3N spin permutation operators from $\check{P} = \check{P}_{12}\check{P}_{23} + \check{P}_{13}\check{P}_{23} \equiv \check{P}_1 + \check{P}_2$, and,

finally, $\check{b}$ is one of the two 2N operators appearing in the operator form of the deuteron bound state [3]

$$| \phi\rangle = \int \mathrm{d}^3\boldsymbol{p} \sum_{l=1}^{2} \phi_l(|\boldsymbol{p}|)\check{b}_l(\boldsymbol{p}) \mid \boldsymbol{p}\rangle \otimes \mid 1m_d\rangle \,, \tag{12}$$

where m_d is the deuteron spin projection. The Kronecker product of $\check{b}$ and an identity operator $\check{1}$ in equation (10) results in a 3N spin operator. Operators of both types (10) and (11) are a result of plugging the operator forms of the 3N scattering amplitude (5), the 2N transition operator (9) and the deuteron bound state (12) into the Faddeev equation (1).

In order to verify that (10) and (11) can be written using (5), the spin dependencies are removed by multiplying all equations from the left with one of the $\check{O}$ operators and taking a trace over spin states resulting in a set of coupled linear equations for the scalar functions τ. Numerical tests were conducted, where random values for selected vectors were assumed with the remaining vectors calculated by taking into account the permutation operators. In the tests, the scalar function values in (5) were calculated. Successfully running the tests a number of times, each time drawing different random values of the chosen vectors, suggested that the postulated operator form for the 3N scattering amplitude is correct and can be used in the construction of a numerical solution to the full Faddeev equation. However, for certain cases, the random values of momentum vector coordinates resulted in badly conditioned 64×64 matrices A whose elements are calculated by taking a trace over the spin states of the 3N system

$$A_{ij} \equiv \mathrm{Tr}\left(\check{O}_i \check{O}_j\right) \,, \tag{13}$$

where the trace operation over the spin states is used to remove spin dependence from the calculation. Since in practical calculations the inversion of the A matrix (13) would have to be performed many times, it is important to understand where the problem with these matrices originates.

3. Numerical considerations

Further investigations showed that the determinant A drops sharply to zero when the vectors $\boldsymbol{p}$, $\boldsymbol{q}$, $\boldsymbol{q}_0$ approach directions in which they are parallel to each other. This is not a new predicament, similar problems were encountered in some other 3D calculations but were alleviated when the relevant inverted matrix was multiplied by a separate array of scalar coefficients later in the calculation. This multiplication was typically performed analytically using symbolic programming inside Mathematica [11] and canceled out most

of the singularities. Unfortunately, the size of the A matrix does not allow direct analytical inversion. Additionally, each element of the inverted matrix would be a very complicated expression that could not be easily handled or simplified inside Mathematica [11].

A partial solution to this problem was found on the `math.stackexchange` mathematics forum [12]. The first step involves identifying all non-zero elements of A as shown in Fig. 1. Next, the algorithm separates the domain of A into seven vector subspaces such that if A is applied to a vector from a given subspace, then the resulting vector is also a member of the same subspace. As a result, the seven subspaces correspond to the seven blocks from the block-diagonal form of A in Fig. 2. The relation between the block diagonal form A_{d} and the original matrix A is:

$$A_{\mathrm{d}} = P_{\mathrm{d}}^{-1} A P_{\mathrm{d}}\,, \tag{14}$$

where P_{d} is the matrix form of the following permutation operator written using cycles:

$$\begin{aligned}\check{P}_{\mathrm{d}} \;=\; & (3\ \ 5)(4\ \ 8)(7\ \ 9)(12\ \ 14\ \ 20)(13\ \ 17\ \ 28\ \ 45)\\ & (15\ \ 24\ \ 27\ \ 43\ \ 22)(16\ \ 26\ \ 18\ \ 42)(19\ \ 44)(23\ \ 25\ \ 29)\,.\end{aligned}$$

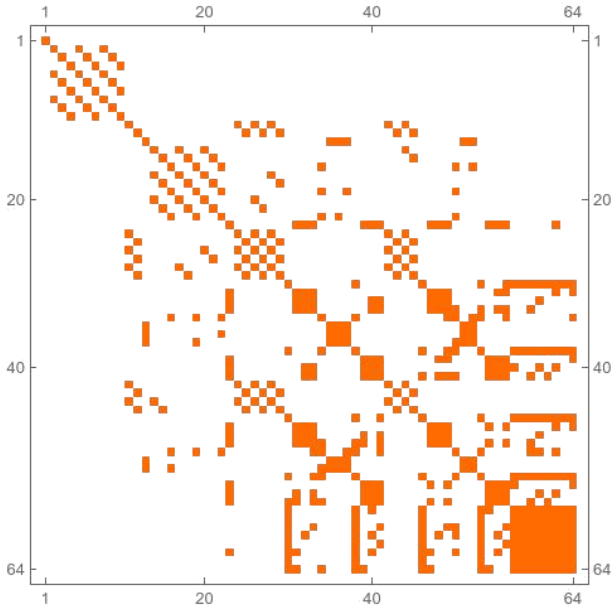

Fig. 1. (Color online) Non-zero elements of the A matrix are marked using gray/red squares.

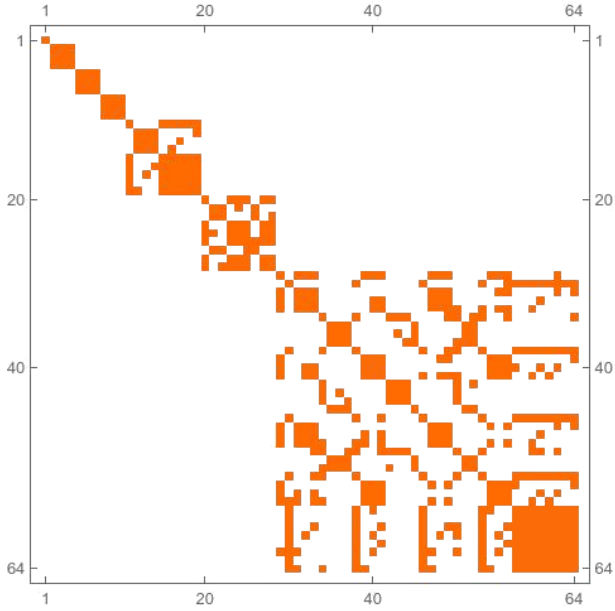

Fig. 2. (Color online) Block diagonal form of A : $A_{\rm d} = P_{\rm d}^{-1} A P_{\rm d}$. Non-zero elements are marked using gray/red squares.

The matrix form of this permutation is easy to obtain. Starting with a null 64×64 matrix, the number 1 is placed in appropriate rows and columns for each permutation of every cycle. For example, taking the fourth cycle (12 14 20), there will be a 1 in $P_{\rm d\ 12,20}$, $P_{\rm d\ 14,12}$ and $P_{\rm d\ 20,14}$ and when taking the second cycle (4 8), there will be a 1 in $P_{\rm d\ 8,4}$, $P_{\rm d\ 4,8}$. Additionally, since index values that do not appear in equation (15) are not permuted, a 1 should be placed in appropriate places on the diagonal. The inverse of this permutation is also easy to work out by simply reversing the cycles

$$\begin{aligned} \check{P}_{\rm d}^{-1} \;=\; & (3\ 5)(4\ 8)(7\ 9)(12\ 20\ 14)(13\ 45\ 28\ 17) \\ & (15\ 22\ 43\ 27\ 24)(16\ 42\ 18\ 26)(19\ 44)(23\ 29\ 25)\,. \end{aligned}$$

Inverting a block diagonal matrix $A_{\rm d}$ amounts to inverting each block separately. The inverse of the original matrix is then obtained via the relation

$$A^{-1} = P_{\rm d} A_{\rm d}^{-1} P_{\rm d}^{-1}\,. \tag{15}$$

Using this approach, it was possible to invert all but the largest block of $A_{\rm d}$. Here, new techniques need to be devised to handle the analytical inversion and simplification of this 36×36 matrix. Current efforts ran into problems related to the very large size of the resulting Wolfram Language

expressions. Working out and simplifying these expressions using standard algorithms was exhausting the time constraints of the calculation. Inverting the smaller blocks was greatly helped by identifying 16 distinct scalar expressions that make up the elements in A but unfortunately this was not enough to conclude the inversion of the largest fragment.

A separate obstacle in the implementation of a 3D numerical description of nucleon–deuteron scattering is the computational size of the problem. Solving the Faddeev equation (1) requires working out the τ functions from (5). Since these are scalar functions, instead of three vector arguments six real arguments are necessary, a typical choice [13] might be

$$|\boldsymbol{p}|\,, \qquad |\boldsymbol{q}|\,, \qquad |\boldsymbol{q}_0|\,, \qquad \hat{\boldsymbol{p}}\cdot\hat{\boldsymbol{q}}_0\,, \qquad \hat{\boldsymbol{q}}\cdot\hat{\boldsymbol{q}}_0\,, \qquad \widehat{\boldsymbol{p}\times\boldsymbol{q}_0}\cdot\widehat{\boldsymbol{q}\times\boldsymbol{q}_0}\,. \tag{16}$$

In the numerical realization, each of these arguments needs to be discretized and the τ functions represented as a multidimensional arrays. Consequently, (1) turns into a very heavy numerical problem even though the calculation can be performed separately for some arguments (for example, $|\boldsymbol{q}_0|$). In addition to this, handling the so-called "moving singularities" (as described *e.g.* in [13]) requires the implementation of multidimensional interpolations that work efficiently on a large computing cluster and can simultaneously utilize both the MPI and OPENMP protocols. These are, however, technical problems that can be solved by using appropriate libraries (an attempt at a Fortran/Wolfram Language library implementing these permutations is available upon request) and by allocating an appropriate amount of computing resources.

4. Summary and outlook

The "three-dimensional" description of the neutron–deuteron scattering process has potential to bring new insights into this process. Contrary to traditional calculations that utilize a finite set of partial waves, the "three-dimensional" calculations work directly with the three-dimensional degrees of freedom of the nucleon. This makes such calculations, in principle, equivalent to using all partial waves simultaneously. In practice, this property is of course limited by the available computing resources, nonetheless, the "three dimensional" might be able to more precisely describe certain kinematical situations. Additionally, the construction of a numerical solution to the Faddeev equation that uses the "three-dimensional" approach would be a valuable tool to test new models of nuclear forces since it does not require the potentials to undergo the partial wave decomposition procedure. Achieving these goals will require some fresh ideas in order to overcome problems related to the size and complexity of the resulting numerical problem and issues related to the inversion of the A matrix.

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