Editors' Suggestion

Solution of the n-^{4}He elastic scattering problem using the Faddeev-Yakubovsky equations

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The first numerical solution of the five-body Faddeev-Yakubovsky equations is presented. Modern realistic nucleon-nucleon Hamiltonians have been tested when describing low-energy elastic neutron scattering on the ^{4}He. Results obtained are compared with those available in the literature and based on the solution of the Schrödinger equation.

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I. INTRODUCTION

Solution of the nuclear bound state problem by *ab initio* methods has reached new heights during the last decade [1–5]. The accurate description of nuclei composed of several nucleons has become possible. However, bound-state properties, such as binding energies, nuclear densities, and radii, provide only a rather restricted set of data with which to test contemporary understanding of the nuclear force. It is the nuclear scattering experiment, where cross sections can be measured as a function of energy, reaction channel, angular distributions, and polarization phenomena, which provides the richest set of data involving nuclear interaction and dynamics.

However, the description of few-nucleon scattering in its full complexity turns out to be quite problematic. The main difficulty is related to the fact that unlike bound-state wave functions, which asymptotically approach zero for large values of any two-particle separation, scattering wave functions are non-compact. When solving a scattering problem in configuration space, the proper treatment of boundary conditions is required; in the Lippmann-Schwinger equation formulation of the scattering problem, such boundary conditions are ill-defined. In the early 1960s Faddeev formulated the t-matrix approach to the three-body problem [6], providing a proper way to formulate boundary conditions for continuum problems dominated by short-range interactions. Just a few years later Faddeev's revolutionary work was generalized to an arbitrary number of particles by Yakubovsky [7]. Regardless of these revolutionary mathematical developments, the progress toward solution of the Faddeev-Yakubovsky equations has been slow, and for many years was limited to $A = 3$ and $A = 4$ cases [8,9]. The main difficulty is related to the complexity of these equations. Indeed, the Faddeev-Yakubovsky (FY) approach transforms the few-particle Schrödinger equation into a set of differential equations for the so-called FY components, which are introduced for the purpose of uncoupling asymptotes of the binary scattering channels. The number of these components (channels) increases like a factorial of the particle number, resulting in very poor scaling of the FY formalism with particle number.

One should mention that the FY equations are not a unique way to solve scattering problems in configuration space. Diverse scattering problems may be solved accurately, also, based on the Schrödinger equation, if the Faddeev decomposition (or its equivalent) is used in order to enforce the proper boundary conditions [10]. Furthermore, due to poor scaling of the FY equations with particle number, approaches based on the Schrödinger equation, like [11], have much brighter prospects than the FY approach in describing systems containing more than five particles. However, when addressing the scattering problems using the Schrödinger equation, one should be cautious about the possibility of ending up with spurious solutions. Therefore, if computationally accessible, due to its mathematically rigorous nature, the FY equation formalism remains a reference for solving the few-particle scattering problems.

In this study the first solution of the FY equations in configuration space is presented for a five-body system. Modern realistic nucleon-nucleon interactions will be employed to describe neutron elastic scattering on the ^{4}He. Results will be compared with those available in the literature and obtained using methods based on solving the Schrödinger equation.

Calculations have been performed for three significantly different realistic Nucleon-Nucleon (NN) interaction models. The potentials considered describe very accurately NN scattering data and include the tail parts determined by pion exchange between the nucleons. Nevertheless these models differ significantly in the procedure adapted to parametrize their short-range components. The AV18 model is a local NN potential [12]; the INOY04 model contains a strongly nonlocal core within an $R = 2$ fm range for S and P waves [13]; the I-N3LO potential [14] is nonlocal in momentum space and is based on the χEFT approach, being derived up to next-to-next-to-next-to-leading order in chiral perturbation theory. All the results presented in that which follows have been obtained considering equal mass for neutrons and protons ($m_n = m_p = m$), defined as $\frac{\hbar^2}{m} = 41.471$ MeV fm^2.

II. FORMALISM FOR THE FIVE-BODY FY EQUATIONS

In the late 1960s Yakubovsky demonstrated a scheme to generalize the three-body Faddeev equations to an N-body

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system of particles governed by short-range interactions [7]. A detailed derivation of the five-body FY equations was performed in Ref. [15]. The derivation of the N-body FY equations starts by decomposing the total wave function into binary partitions, similar to the three-body Faddeev components:

$$\phi_{ij} = G_0 V_{ij} \Psi. \tag{1}$$

For a five-body system one may construct ten different binary components by permuting particle indexes (ij). In that which follows the letters $(ijklm)$ denote the possible combinations of particle indexes (12345). It is easy to verify that the total wave function is recovered by simply adding its binary components:

$$\Psi(x,y,z,w) = \sum_{i<j}^{5} \phi_{ij}(x,y,z,w). \tag{2}$$

The binary components $\phi_{ij}(x,y,z,w)$ are further split into four-body type components by following a pattern of breaking the five-body $(ijklm)$ partition into clusters and their subclusters. One has two types of four-body components, which are similar to those appearing in the four-body FY equations:

$$\begin{aligned} \psi_{ij}^{ijk} &= G_{ij} V_{ij} (\phi_{jk} + \phi_{ki}), \\ \psi_{ij}^{ij,kl} &= G_{ij} V_{ij} \phi_{kl}. \end{aligned} \tag{3}$$

Here the five-body Green's function G_{ij} includes a single interaction term V_{ij}: i.e., $G_{ij} = (E - H_0 - V_{ij})^{-1}$. For a five-body system there exist 30 different four-body components of the type ψ_{ij}^{ijk} as well as 30 components of the type $\psi_{ij}^{ij,kl}$. Using Yakubovsky's scheme one may easily decompose the binary components into the four-body terms:

$$\phi_{ij} = \psi_{ij}^{ijk} + \psi_{ij}^{ijl} + \psi_{ij}^{ijm} + \psi_{ij}^{ij,kl} + \psi_{ij}^{ij,km} + \psi_{ij}^{ij,lm}. \tag{4}$$

Finally, the four-body components can be decomposed into a sum of five-body FY components:

$$\begin{aligned} \psi_{ij}^{ijk} &= \mathcal{K}_{ij,k}^{l} + \mathcal{K}_{ij,k}^{m} + \mathcal{T}_{ij,k} \qquad \text{(30 amplitudes)}, \\ \psi_{ij}^{ij,kl} &= \mathcal{H}_{ij,kl} + \mathcal{S}_{ij,kl} + \mathcal{F}_{ij,kl} \qquad \text{(30 amplitudes)}. \end{aligned} \tag{5}$$

The Faddeev-Yakubovsky equations involve five different types of five-body FY components (see Fig. 1), denoted in this work by $\mathcal{K}_{ij,k}^{l}$, $\mathcal{H}_{ij,kl}$, $\mathcal{T}_{ij,k}$, $\mathcal{S}_{ij,kl}$, and $\mathcal{F}_{ij,kl}$. In total, there exist 60 components of the type $\mathcal{K}$ and 30 components for each of the types $\mathcal{H}$, $\mathcal{T}$, $\mathcal{S}$, and $\mathcal{F}$. The five-body FY equations constitute a set of 180 coupled equations, each of which may be associated with a particular FY component. One has five nontrivial equations, each highlighting one particular component of the various types. By separating terms associated with a highlighted component in the right-hand side of the relations, are obtains the equations summarized as follows:

$$\begin{aligned} (E - \widehat{H}_0 - V_{12})\mathcal{K}_{12,3}^{4} &= V_{12}\big(\mathcal{K}_{13,2}^{4} + \mathcal{K}_{23,1}^{4} + \mathcal{K}_{13,4}^{5} + \mathcal{K}_{23,4}^{5} \\ &\quad + \mathcal{K}_{13,4}^{2} + \mathcal{K}_{23,4}^{1} + \mathcal{T}_{13,4} + \mathcal{T}_{23,4} \\ &\quad + \mathcal{H}_{13,24} + \mathcal{H}_{23,14} + \mathcal{S}_{13,24} \\ &\quad + \mathcal{S}_{23,14} + \mathcal{F}_{13,24} + \mathcal{F}_{23,14}\big), \\ (E - \widehat{H}_0 - V_{12})\mathcal{H}_{12,34} &= V_{12}\big(\mathcal{H}_{34,12} + \mathcal{K}_{34,1}^{2} + \mathcal{K}_{34,2}^{1} \\ &\quad + \mathcal{K}_{34,1}^{5} + \mathcal{K}_{34,2}^{5} + \mathcal{T}_{34,1} + \mathcal{T}_{34,2}\big), \\ (E - \widehat{H}_0 - V_{12})\mathcal{T}_{12,3} &= V_{12}\big(\mathcal{T}_{13,2} + \mathcal{T}_{23,1} + \mathcal{H}_{13,45} + \mathcal{H}_{23,45} \\ &\quad + \mathcal{S}_{13,45} + \mathcal{S}_{23,45} + \mathcal{F}_{13,45} + \mathcal{F}_{23,45}\big), \\ (E - \widehat{H}_0 - V_{12})\mathcal{S}_{12,34} &= V_{12}(\mathcal{F}_{34,12} + \mathcal{S}_{34,15} + \mathcal{S}_{34,25} \\ &\quad + \mathcal{F}_{34,15} + \mathcal{F}_{34,25} + \mathcal{H}_{34,15} + \mathcal{H}_{34,25}), \\ (E - \widehat{H}_0 - V_{12})\mathcal{F}_{12,34} &= V_{12}\big(\mathcal{S}_{34,12} + \mathcal{K}_{34,5}^{1} + \mathcal{K}_{34,5}^{2} + \mathcal{T}_{34,5}\big). \end{aligned} \tag{6}$$

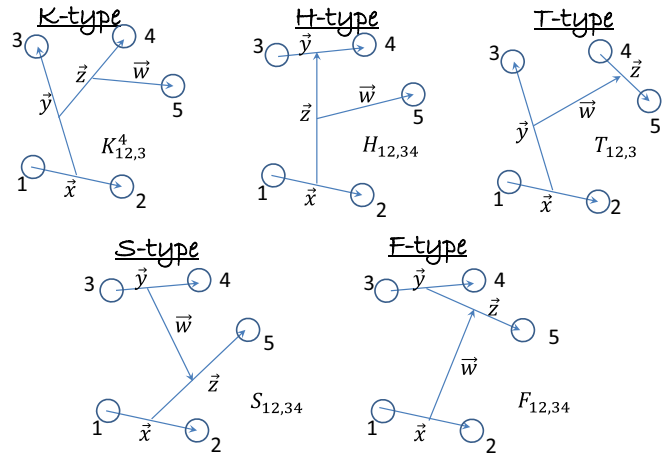

FIG. 1. Five-particle Jacobi coordinate sets used to describe FY components, denoted in this work as $\mathcal{K},\mathcal{T},\mathcal{H},\mathcal{S},\mathcal{F}$.

Other equations follow from this set by simply permuting particle indexes in an ordered way. For a system of five identical particles one can reduce the problem to solving only one set of the five equations, since there remain only five independent FY components ($\mathcal{K}_{ij,k}^{l}$, $\mathcal{H}_{ij,kl}$, $\mathcal{T}_{ij,k}$, $\mathcal{S}_{ij,kl}$, and $\mathcal{F}_{ij,kl}$). Other components may be obtained from the selected set of $(\mathcal{K},\mathcal{H},\mathcal{S},\mathcal{T},\mathcal{F})$ by using particle-permutation symmetry relations.

III. COORDINATES

Each FY component $F = (\mathcal{K},\mathcal{T},\mathcal{H},\mathcal{S},\mathcal{F})$ is a function of the twelve-dimensional configuration space determined by the four three-dimensional vectors $(\vec{x},\vec{y},\vec{z},\vec{w})$. It is convenient to express the FY components in their proper set of Jacobi coordinates; see Fig. 1. Jacobi coordinates connecting two clusters (s) and (t) are expressed using a general formula:

$$(\vec{x}, \vec{y}, \vec{z}, \vec{w}) = \sqrt{\frac{2m_s m_t}{m(m_s + m_t)}}(\vec{r}_s - \vec{r}_t), \tag{7}$$

where m_s and m_t are the masses of the clusters, while $\vec{r}_s$ and $\vec{r}_t$ are the respective positions of their centers of mass. An arbitrary mass factor m is introduced into the expression in order to retain the proper units of distance. When studying systems of identical particles it is convenient to identify this mass with the mass of a single particle (in this study, the mass of a nucleon). In terms of Jacobi coordinates, the center-of-mass

free Hamiltonian is expressed as

$$H_0 = -\frac{\hbar^2}{m}(\Delta_x + \Delta_y + \Delta_z + \Delta_w). \tag{8}$$

When studying low-energy processes, partial wave expansion turns out to be an efficient tool to express the angular dependence of the wave function. Without exception, in this work partial wave expansion is used to depict the angular dependence of the FY components as well as their dependence on spin and isospin quantum numbers:

$$F^{JM}(\vec{x},\vec{y},\vec{z},\vec{w}) = \sum \frac{f_\alpha(x,y,z,w)}{xyzw} |\{\{l_x l_y\}_{l_{xy}}\{l_z l_w\}_{l_{zw}}\}_L \times \{S\}\rangle_{JM}\{T\}_{TT_z}, \tag{9}$$

where $\alpha \equiv (l_x,l_y,l_z,l_w,l_{xy},l_{zw},L,\{S\},\{T\})$ is an index representing a set of intermediate state quantum numbers, coupled to the total angular momentum J and the total isospin T with its projection T_z (for the n-^{4}He scattering considered in this work, the total isospin and its projection are fixed to $T = 1/2$ and $T_z = 1/2^-$. $\{S\}$ and $\{T\}$ represent respectively partial-wave basis dependence on spin and isospin quantum numbers, which is provided by

$$\{S\} = |\{\{s_1 s_2\}_{s_x}\{s_3 s_4\}_{s_y}\}_{s_{xy}} s_5\rangle_{SS_Z}; \tag{10}$$

where s_1 to s_5 are spins of individual nucleons, and s_x,s_y,s_{xy},S represent quantum numbers of intermediate couplings. An equivalent expression is used to develop the isospin dependence $\{T\}$ of the FY components. The reduced components $f_\alpha(x,y,z,w)$ represent dependence on the radial parts of the coordinates. This dependence is expressed using Lagrange-Laguerre basis functions.

The last set of equations, (9) and (10), define the principal partial-wave basis set employed in this work. However, in parallel, two additional equivalent partial wave coupling schemes have been used: one utilizing coupling of angular momenta $\{l_y l_z\}_{l_{yz}}$, required in order to perform permutation operations acting in yz space, another explicitly using the two-particle angular momentum $\{l_x(s_1,s_2)_{s_x}\}_{j_x}$ needed to evaluate matrix elements of the NN interaction between particles 1 and 2.

IV. OPERATORS

In order to solve the FY equations, it is useful to define a set of operators which allow one to couple different FY components. First, a group of operators is introduced, which couple FY components of different types, but which share the same particle ordering:

$$\begin{aligned}
\mathcal{K}^4_{12,3} &= (P^{KH})^1_{yz}\mathcal{H}_{12,34}, \quad \mathcal{H}_{12,34} = (P^{HK})^1_{yz}\mathcal{K}^4_{12,3},\\
\mathcal{K}^4_{12,3} &= (P^{KT})^1_{zw}\mathcal{T}_{12,3}, \quad \mathcal{T}_{12,3} = (P^{TK})^1_{zw}\mathcal{K}^4_{12,3},\\
\mathcal{H}_{12,34} &= (P^{HS})^1_{zw}\mathcal{S}_{12,34}, \quad \mathcal{S}_{12,34} = (P^{SH})^1_{zw}\mathcal{H}_{12,34},\\
\mathcal{H}_{12,34} &= (P^{HF})^1_{zw}\mathcal{F}_{12,34}, \quad \mathcal{F}_{12,34} = (P^{FH})^1_{zw}\mathcal{H}_{12,34},\\
\mathcal{S}_{12,34} &= (P^{SF})^1_{zw}\mathcal{F}_{12,34}, \quad \mathcal{F}_{12,34} = (P^{FS})^1_{zw}\mathcal{S}_{12,34},\\
\mathcal{T}_{12,3} &= (\underline{P}^{TS})^0_{yz}\mathcal{S}_{12,45}, \quad \mathcal{S}_{12,34} = (\underline{P}^{ST})^0_{yz}\mathcal{T}_{12,5},\\
\mathcal{S}_{34,12} &= (\underline{P}^{SF})^0_{xy}\mathcal{F}_{12,34}, \quad \mathcal{F}_{34,12} = (\underline{P}^{FS})^0_{xy}\mathcal{S}_{12,34}.
\end{aligned} \tag{11}$$

The operators presented on each line are inverses of each other: i.e., as an example $((P^{HK})^1_{yz})^{-1} = (P^{HK})^1_{yz}$. The expressions for these operators split into tensor products of operators acting in coordinate, spin, and isospin spaces. When matrix elements of these operators are properly ordered, the inverse operator is directly obtained from the original operator by simply permuting its matrix elements and thus does not require separate evaluation or storage.

The second group of operators is used to change the particle ordering:

$$\begin{aligned}
\mathcal{K}^4_{12,3} &= (P^+)^1_{xy}\mathcal{K}^4_{23,1}, \quad \mathcal{K}^4_{12,3} = (P^-)^1_{xy}\mathcal{K}^4_{31,2},\\
\mathcal{T}_{12,3} &= (P^+)^1_{xy}\mathcal{T}_{23,1}, \quad \mathcal{T}_{12,3} = (P^-)^1_{xy}\mathcal{T}_{31,2},\\
\mathcal{K}^4_{12,3} &= (\varepsilon P^{34})^1_{yz}\mathcal{K}^3_{12,4},\\
\mathcal{K}^5_{12,3} &= (\varepsilon P^{45})^1_{zw}\mathcal{K}^4_{12,3},\\
\mathcal{H}_{12,34} &= (P^H)^0_{xy}\mathcal{H}_{34,12},\\
(\widetilde{P}^3)^1_{xy} &= (P^+)^1_{xy} + (P^-)^1_{xy},\\
(\widetilde{P}^4)^1_{yz} &= (\varepsilon P^{34})^1_{yz}, \quad (\widetilde{P}^5)^1_{zw} = (\varepsilon P^{45})^1_{zw}.
\end{aligned} \tag{12}$$

In these expressions the operators are defined using the general notation $(P^A)^n_{xy}$, where integer n indicates the number of angular integrations involved in coupling partial amplitudes; xy indicates that an operator transforms radial dependencies of the amplitude in coordinates x and y. The expressions for these operators are quite trivial, equivalent to ones used in solving the three-body or the four-body FY equations. Nevertheless their expressions become quite voluminous and will be published elsewhere. When applied successively, this set of operators is sufficient to couple any two FY components and thus solve the five-body FY equations as formulated in Eq. (7). Using these definitions the five-body FY equations read

$$\begin{aligned}
\mathcal{K}^4_{12,3} &= G_{12}V_{12}(\widetilde{P}^3)^1_{xy}\big(\mathcal{K}^4_{12,3} + (P^{KH})^1_{yz}\\
&\quad\times\big[\mathcal{H}_{12,34} + (P^{HS})^1_{zw}\mathcal{S}_{12,34} + (P^{HF})^1_{zw}\mathcal{F}_{12,34}\big],\\
&\quad+(\widetilde{P}^4)^1_{yz}\big[\mathcal{K}^4_{12,3} + (\widetilde{P}^5)^1_{zw}\mathcal{K}^4_{12,3} + (P^{KT})^1_{zw}\mathcal{T}_{12,3}\big]\big),\\
\mathcal{H}_{12,34} &= G_{12}V_{12}(\underline{P}^H)^0_{xy}\big(\mathcal{H}_{12,34} + 2(P^{HK})^1_{yz}\\
&\quad\times\big[\mathcal{K}^4_{12,3} + (\widetilde{P}^5)^1_{zw}\mathcal{K}^4_{12,3} + (P^{KT})^1_{zw}\mathcal{T}_{12,3}\big]\big),\\
\mathcal{T}_{12,3} &= G_{12}V_{12}(\widetilde{P}^3)^1_{xy}\big(\mathcal{T}_{12,3} + (\underline{P}^{TS})^0_{yz}\\
&\quad\times\big[\mathcal{S}_{12,34} + (P^{SF})^1_{zw}\mathcal{F}_{12,34} + (P^{SH})^1_{zw}\mathcal{H}_{12,34}\big]\big),\\
\mathcal{S}_{12,34} &= G_{12}V_{12}\big((\underline{P}^{ST})^0_{yz}(\widetilde{P}^3)^1_{xy}(\underline{P}^{TS})^0_{yz}(\underline{P}^{SF})^0_{xy}\\
&\quad\times\big[\mathcal{F}_{12,34} + (P^{FH})^1_{zw}\mathcal{H}_{12,34} + (P^{FS})^1_{zw}\mathcal{S}_{12,34}\big],\\
&\quad+(\underline{P}^{SF})^0_{xy}\mathcal{F}_{12,34}\big),\\
\mathcal{F}_{12,34} &= G_{12}V_{12}(\underline{P}^{FS})^0_{xy}\\
&\quad\times\big[\mathcal{S}_{12,34} + (\underline{P}^{ST})^0_{yz}\big(\mathcal{T}_{12,3} + 2(P^{TK})^1_{zw}\mathcal{K}^4_{12,3}\big)\big].
\end{aligned} \tag{13}$$

Since in this work a system of five formally identical particles is considered, this set of equations is written for components in which particles are ordered in a natural succession (12345).

The last set of equations is sufficient to solve the five-body problem and to obtain for this problem the related physical observables: binding energies or phase shifts. However, in order to estimate expectation values of the physical operators, one may find it necessary to generate the total wave function, which may be expressed in terms of the FY components as:

$$\begin{aligned}\Psi(x,y,z,w) &= \sum_{i<j}^{5}\phi_{ij}(x,y,z,w)\\ \phi_{12} &= \psi_{12}^{123}+\psi_{12}^{124}+\psi_{12}^{125}+\psi_{12}^{12,34}\\ &\quad+\psi_{12}^{12,35}+\psi_{12}^{12,45}\\ &= [1+P^{34}+P^{45}P^{34}]\big(\psi_{12}^{123}+\psi_{12}^{12,34}\big). \end{aligned} \quad (14)$$

where one denotes:

$$\begin{aligned}\widetilde{X} &= X + R_X,\\ X &\equiv (\mathcal{K},\mathcal{H},\mathcal{T},\mathcal{S},\mathcal{F}),\end{aligned} \quad (15)$$

where the term R_X represents a sum of components appearing on the right-hand side of the FY equation (7) relating to component X. For example,

$$X = \mathcal{K}_{12,3}^{4},$$

$$\begin{aligned}R_x &= \mathcal{K}_{13,2}^{4}+\mathcal{K}_{23,1}^{4}+\mathcal{K}_{13,4}^{5}+\mathcal{K}_{23,4}^{5}+\mathcal{K}_{13,4}^{2}+\mathcal{K}_{23,4}^{1}\\ &\quad+\mathcal{T}_{13,4}+\mathcal{T}_{23,4} \qquad (16)\\ &\quad+\mathcal{H}_{13,24}+\mathcal{H}_{23,14}+\mathcal{S}_{13,24}+\mathcal{S}_{23,14}+\mathcal{F}_{13,24}+\mathcal{F}_{23,14}, \qquad (17)\end{aligned}$$

such that

$$\begin{aligned}\widetilde{\psi}_{12}^{123} &= \widetilde{\mathcal{K}}_{12,3}^{4}+\widetilde{\mathcal{K}}_{12,3}^{5}+\widetilde{\mathcal{T}}_{12,3} = (1+P^{45})\widetilde{\mathcal{K}}_{12,3}^{5}+\widetilde{\mathcal{T}}_{12,3},\\ \widetilde{\psi}_{12}^{12,34} &= \widetilde{\mathcal{H}}_{12,34}+\widetilde{\mathcal{S}}_{12,34}+\widetilde{\mathcal{F}}_{12,34}.\end{aligned} \quad (18)$$

Finally

$$\Psi = [1+(1+P^{45})P^{34}]\big(\widetilde{\psi}_{12}^{123}+\widetilde{\psi}_{12}^{12,34}\big). \quad (19)$$

A. Boundary conditions

Solution of the differential equations is not complete unless the proper boundary conditions are formulated and imposed. The reduced components are both regular functions, when related to the solution of the bound state or scattering problems:

$$f_\alpha(0,y,z,w) = f_\alpha(x,0,z,w) = f_\alpha(x,y,0,w) = f_\alpha(x,y,z,0). \quad (20)$$

It is the boundary condition for the asymptotic region (at large radial distances) which turns out to be the more complicated when a scattering problem is considered. For the bound state problem the FY components are compact, and thus square-integrable basis functions might be readily used to describe the behavior of the reduced components. For the scattering problems, which do not involve system decomposed into more than two clusters (a case considered in this work), reduced components still remain compact in the x,y,z directions. On the other hand asymptotic parts of the elastic incoming (outgoing) wave of the scattered clusters are expressed in w-radial dependence of the reduced FY components. To fulfill this requirement but at the same time to be able to use square-integrable basis functions in solving scattering problems, the reduced components are split into two terms:

$$f_{\alpha,a}(x,y,z,w) = \widetilde{f}_{\alpha,a}^{sh}(x,y,z,w)+\widetilde{f}_{\alpha,a}^{ass}(x,y,z,w). \quad (21)$$

In this above expression, index a indicates an incoming channel number for which a solution is sought. The term $\widetilde{f}_{\alpha,a}^{sh}(x,y,z,w)$ is intended to describe only the interior part of the component $f_{\alpha,a}(x,y,z,w)$ based on an expansion employing compact basis functions. The term $\widetilde{f}_{\alpha,a}^{ass}(x,y,z,w)$ complements the expression by describing properly the asymptotic part of the reduced FY components. This term takes the form

$$\begin{aligned}\widetilde{f}_{\alpha,a}^{ass}(x,y,z,w) = \sum_b\sum_{\beta\subset b}\delta_{\beta,\alpha}\widetilde{\phi}_\beta(x,y,z)\Big(&\delta_{a,b}\hat{j}_{l_w^\alpha}(q_b w)\\ &+\sqrt{\frac{q_a}{q_b}}K_{b,a}\hat{n}_{l_w^\alpha}(q_b w)\eta_{l_w^\alpha}^{reg}(w)\Big). \end{aligned} \quad (22)$$

In the above expression the first sum runs over all open channels b, whereas the second sum runs over all the partial-wave amplitudes $\beta\subset b$, contributing in expanding asymptotes of this channel. The term $K_{b,a}$ represents K-matrix elements, describing the scattering processes, to be determined. $\hat{j}_{l_w^\alpha}(q_b w)$ and $\hat{n}_{l_w^\alpha}(q_b w)$ represent respectively Riccati-Bessel and Riccati-Neumann functions. Additionally a function $\eta_l^{reg}(w)$ is introduced in order to regularize the divergent behavior of the Riccati-Neumann function at the origin. This regularization function is chosen to be a form popularized by the numerical calculations of the Pisa group [10,16,17]:

$$\eta_l^{reg}(w) = [1-\exp(w/w_0)]^{2l+k}. \quad (23)$$

where in this parametrization, the power-k parameter must be chosen to be $k\geqslant 1$, and values of $k=1$ and $k=2$ turn out to be optimal. The range parameter w_0 determines the matching region between the dominance of the $\widetilde{f}_{\alpha,a}^{sh}$ and $\widetilde{f}_{\alpha,a}^{ass}$ terms and is chosen to lie in the interval $w_0=(1,2)$ fm. The selected regularization function satisfies natural conditions

$$\begin{aligned}\eta_l^{reg}(w)\hat{n}_l(q_b w)\big|_{w\to 0} &= 0,\\ \eta_l^{reg}(w)\hat{n}_l(q_b w)\big|_{w\to\infty} &= \hat{n}_l(q_b w).\end{aligned} \quad (24)$$

The calculated K-matrix elements turn out to be independent to high order of the two parameters encoded in $\eta_l^{reg}(w)$. This feature constitutes one of the tests for the reliability of the calculations.

Finally, the functions $\widetilde{\phi}_\beta(x,y,z)$ represent bound-state-like solutions of the five-body problem reduced for the four-body case. For the case considered in this work they represent the solution of the bound-state problem for the ^{4}He nucleus. These functions are obtained by reducing the five-body problem to the four-body one, which requires simply eliminating the w dependence in Eq. (14); that is, by equating the Laplacian operator (Δ_w), as well as all the permutation operators containing w dependence, to zero.

B. Lagrange-mesh method

The functions $f_{\alpha,a}(x,y,z,w)$, representing the radial dependence of the FY components, are expanded using basis

functions defined by the Lagrange-Laguerre mesh method [18]:

$$f_{\alpha,a}(x,y,z,w) = \sum_{i_x=1}^{N_{x,l_x)}} \sum_{i_y=1}^{N_{y,l_y}} \sum_{i_y=1}^{N_{z,l_z}} \sum_{i_y=1}^{N_{w,l_w}} C^{\alpha,a}_{i_x,i_y,i_z,i_w} u^{l_x}_{i_x}(x/h_{x,l_x}) \times u^{l_y}_{i_y}(y/h_{y,l_y}) u^{l_z}_{i_z}(z/h_{z,l_z}) u^{l_w}_{i_w}(w/h_{w,l_w}), \tag{25}$$

with $C^{\alpha,a}_{i_x,i_y,i_z,i_w}$ representing the expansion coefficients to be determined. For low-energy physics, the low-angular-momentum components are dominant, moreover their radial shapes often have more complicated structure than their high-momentum counterparts. Therefore in this work the number of basis functions is chosen as a function of the partial wave angular momentum they represent. This number is gradually reduced with increasing partial wave angular momentum number, in a manner similar to the cases of hyphersperical harmonics or harmonic oscillator bases for a fixed grand angular momentum number. The coefficients h_{x,l_x} are scaling parameters for the basis functions, defined as

$$u^{l_x}_i(x) = (-1)^i c_{i,l_x} \sqrt{\frac{x}{x_i(l_x)}} \frac{L^{2l_x+1}_{N_x(l_x)}(x)}{x - x_i(l_x)} e^{-x/2}, \tag{26}$$

In this expression $L^{\alpha}_N(x)$ denotes a Nth-degree generalized Laguerre polynomial, with $x_i(l_x)$ representing the zeroes of this polynomial. The coefficients c_{i,l_x} are fixed by imposing basis functions to be orthonormal, namely

$$\int_0^{\infty} u^{l_x}_i(x) u^{l_x}_{i'}(x) dx = \delta_{ii'}. \tag{27}$$

The set of differential equations (14) is transformed into a linear algebra problem by first projecting their angular dependence on the partial wave basis, defined by Eqs. (9) and (10), and then projecting radial parts on the Lagrange-Laguerre mesh basis, defined in Eq. (25). In this way a set of linear equations is obtained to determine the unknown expansion coefficients $C^{\alpha,a}_{i_x,i_y,i_z,i_w}$. This set of equations may be summarized as follows:

$$(\hat{H}^{FY} - E) C^{\alpha,a}_{i_x,i_y,i_z,i_w} = b^{(a)}. \tag{28}$$

Here $(H^{FY} - E)$ represents the kernel of the FY equations acting on the wave function's component defined by the term $\widetilde{f}^{sh}_{\alpha,a}(x,y,z,w)$ and represented by a set of linear coefficients $C^{\alpha,a}_{i_x,i_y,i_z,i_w}$. The inhomogeneous term $b^{(a)}$ is constructed by using the FY equation kernel on the part of the wave function's component defined by the $\widetilde{f}^{ass}_{\alpha,a}(x,y,z,w)$ term.

One may refer to [18,19] for a more detailed description of the numerical methods used in this work.

C. Kohn variational functional

The projection of the FY equations on Lagrange-mesh functions, given by Eq. (28), provides only as many linear equations as there exist unknown coefficients $C^{\alpha,a}_{i_x,i_y,i_z,i_w}$. However, there exist additional unknowns due to the presence of the K-matrix elements $(K_{a,b})$ encoded in the parametrization of the asymptotic parts of the FY amplitudes $\widetilde{f}^{ass}_{\alpha,a}(x,y,z,w)$; see Eq. (22). In order to balance the linear algebra problem, one has recourse via the Kohn variational functional.

Information on the scattering matrix is encoded in the asymptote of the system's wave function and at the same time in the separate FY components. Therefore there are two independent ways to apply Kohn's functional. The first one represents the conventional form of the Kohn variational principle, relying on the Wronskian relation combining the total wave function and the incoming wave:

$$K_{a,b} = \sqrt{\frac{1}{q_a q_b}} \big(\langle \psi_{in,b} | \big(\hat{H}^{\theta}_0 - E \big) | \Psi^a \rangle - \langle \Psi^a | \big(\hat{H}^{\theta}_0 - E \big) | \psi_{in,b} \rangle \big). \tag{29}$$

In this expression, wave function $\psi_{in,b}$ represents a free wave of channel b, defined by the FY partial amplitudes

$$f^{in}_{\alpha,a}(x,y,z,w) = \sum_b \sum_{\beta \subset b} \delta_{\beta,\alpha} \widetilde{\phi}_{\beta}(x,y,z) \delta_{a,b} \hat{j}_{l^{\alpha}_w}(q_b w). \tag{30}$$

An alternative approach is to replace the total wave function by a set of the Faddeev-Yakubovsky components containing the nonzero $\widetilde{f}^{ass}_{\alpha,a}(x,y,z,w)$ term and encompassing the required K-matrix element

$$K_{a,b} = \sqrt{\frac{1}{q_a q_b}} (\langle \psi_{in,b} | (\hat{H}_0 - E) | \Phi^a \rangle - \langle \Phi^a | (\hat{H}_0 - E) | \psi_{in,b} \rangle). \tag{31}$$

In principle, the relation (29) is more accurate mathematically, up to second-order terms in the system's wave function perturbation [16,17]. However, evaluation of this expression requires one to produce the total wave function, which involves calculation of the supplemental multidimensional integrals. In this work these integrals are evaluated based on the Lagrange-mesh approximation used to expand the FY components, which involves a relatively small number of the quadrature points. This approximation weighs heavily on the accuracy of the final result. In practice the second relation (that requires a much smaller numerical effort to evaluate) turns out to be of the similar accuracy at the first one. Comparison of the K-matrix elements extracted using the two different methods constitutes a critical test for the accuracy of the calculation and will be discussed in the next section.

V. RESULTS

Solution of the five-body FY equations turn out to be an extraordinary numerical task, which challenge current technical capacities. A careful choice of the parameter space should be made in order to optimize the solution. The key input is the choice of the Lagrange-mesh basis. One of the criteria used to judge the proper basis is the reproducibility of the ground-state binding energies of ^{4}He and ^{3}H, employing the same set of mesh points to be used in the n-^{4}He scattering calculations. Table I summarizes the binding energies of ^{4}He, obtained for the parameter space to be employed in the n-^{4}He scattering calculations. The partial wave expansion was constructed by limiting partial wave angular momenta to those satisfying

TABLE I. Binding energies of the ^{4}He ground state calculated using the basis limitations in this work, taking the same PW limitation but considerably larger size of the Lagrange-mesh basis ("Large basis"), which is converged for the radial basis. These results are compared with the literature values of the fully converged calculations.

	INOY04	I-N3LO	AV18
This work	−29.09	−25.24	−24.08
Large basis	−29.10	−25.39	−24.15
Refs. [20–23]	−29.11	−25.38(1)	−24.23(1)

$\max(l_x,l_y,l_z) \leqslant 4$ and $l_w \leqslant 3$ conditions. As can be seen in the table, for binding energy convergence, this is a reasonable choice.

When comparing the different interaction model results, the INOY04 values turn out to be the closest to the fully converged (large basis) result, whereas AV18 suffers from the largest deviation—but still only 150 keV. This is a natural consequence of the fact that among the three selected realistic Hamiltonians INOY04 is the softest interaction, and thus has the fastest convergence with respect to both PW expansion as well as to the number of the Lagrange-mesh functions used to describe the radial dependence of the FY amplitudes. In contrast, among the three interaction models, AV18 possesses the hardest core as well as the strongest tensor interaction term in the $^3SD_1$ wave, resulting in relatively slow convergence.

Although the FY equations are formulated for short-range potentials, in this work the repulsive Coulomb interaction, present between the protons within the ^{4}He core, is still included. Indeed, because the Coulomb interaction does not act in the asymptotic region of the open scattering channel, such a procedure does not violate the validity of the FY approach.

In Table II calculated phase shifts extracted using two different techniques, namely using Kohn's functional, Eq. (29), and the asymptote of Faddeev-Yakubovsky components, Eq. (31), are presented. These calculations were performed for the Hamiltonian based on the I-N3LO NN iteraction. One may observe quite a good agreement between the two methods: the differences do not exceed 2%. As explained in the previous section, due to approximations used in evaluating integrals involved in estimating the Kohn functional, the values extracted from the asymptote of the FY components turn out to be more reliable.

TABLE II. Calculated n-^{4}He scattering phase shifts at different energies for the $J^\pi = \frac{1}{2}^+$ and $\frac{3}{2}^-$ states and for the I-N3LO potential. Phase shifts have been calculated employing Kohn's variational functional (Kohn), Eq. (29), and from the asymptote of the Faddeev-Yakubovsky components (FY) via Eq. (31).

E_{cm} (MeV)	δ (deg.)			
	$J^\pi = \frac{1}{2}^+$		$J^\pi = \frac{3}{2}^-$	
	Kohn	FY	Kohn	FY
0.5	−22.0	−21.3	9.10	9.34
1.0	−30.8	−30.0	38.1	38.9
1.5	−37.5	−36.6	77.0	77.4
2.0	−43.5	−43.1	96.9	96.5
3.0	−49.2	−48.7	107.1	105.5
5.0	−61.6	−62.1	109.3	111.8
7.5	−71.2	−74.1	102.1	102.0

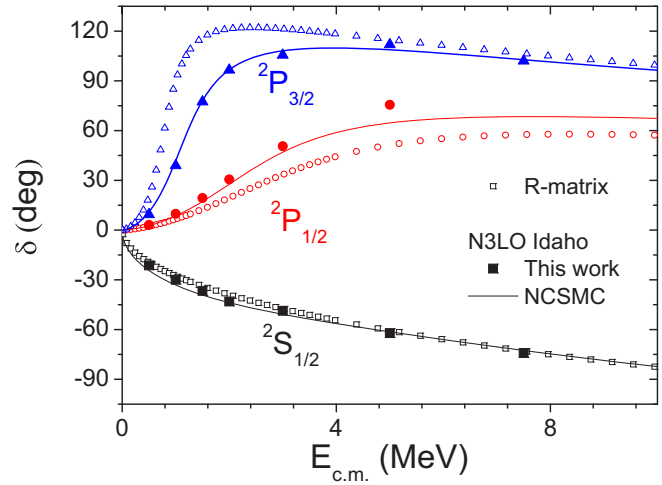

FIG. 2. Low energy n-^{4}He scattering phase shifts calculated for the Hamiltonian based on the I-N3LO nucleon-nucleon interaction. Results of this work (full symbols) are compared to the ones obtained by the NCSMC method [24] (full lines). Theoretical calculations are also compared with the phase shifts obtained from the R-matrix analysis of the experimental data [25] (open symbols).

In Fig. 2 $J^\pi = \frac{1}{2}^\pm$ and $J^\pi = \frac{3}{2}^-$ phase shifts calculated for the I-N3LO Hamiltonian are compared with the results obtained using the NCSMC technique [24] as well as with the phase shifts extracted from experimental data using an R-matrix analysis [25]. Keeping in mind that both theoretical calculations—those of this work and the ones obtained using the NCSMC technique [24]—have comparable numerical accuracy of 1°–2°, one may infer full agreement between the two completely different approaches to solving the elastic scattering problem. In comparison with the experimental data is good, one may also infer nice agreement for the S-wave scattering, dominated by strong Pauli repulsion between an incident neutron with the neutrons within the ^{4}He target. In contrast, the description of the resonant P waves is not satisfactory, revealing insufficient splitting between $J^\pi = \frac{1}{2}^-$ and $J^\pi = \frac{3}{2}^-$ partial waves.

In Fig. 3 the aforementioned I-N3LO Hamiltonian results are compared with those obtained for the INOY04 and the AV18 Hamiltonians. All the models describe well the S-wave phase shifts, indicating that the description of these waves are effectively model independent. In contrast, the different model predictions deviate in describing the resonant scattering in P waves. Both the INOY04 and the AV18 models lack attraction in the $J^\pi = \frac{3}{2}^-$ wave, predicting much flatter resonant structure than that provided by the R-matrix analysis of the experimental data [25] or even when compared to the I-N3LO results. As a consequence, the splitting between the two P waves for the AV18 model is smaller than for the I-N3LO model, which indicates a weaker effective

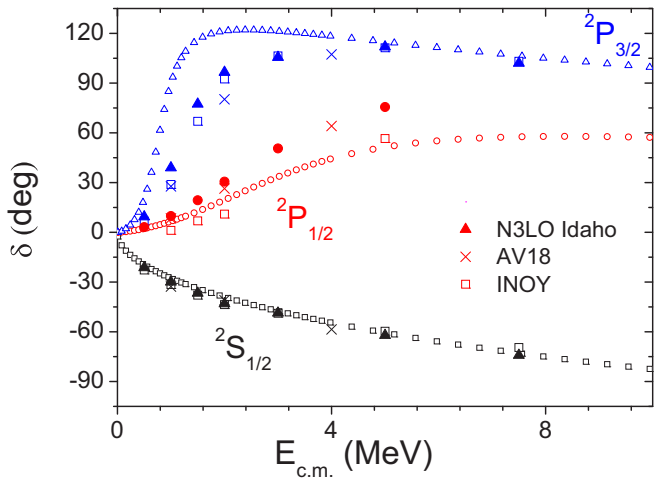

FIG. 3. Comparison of the low energy n-^{4}He scattering phase shifts calculated for three different realistic NN interaction Hamiltonians: the I-N3LO (full triangles), the AV18 (crosses), and the INOY04 (open squares). Theoretical calculations are also compared with the phase shifts obtained from the R-matrix analysis of the experimental data [25] (small open symbols).

spin-orbit interaction for the AV18 model than for the I-N3LO model. For the INOY04 interaction, the splitting of the P waves is not enough to explain the differences with the experimental data; for this model the P wave needs to be much more attractive overall. It is worth noting that very similar observations have been made when studying neutron scattering on the ^{3}H nucleus [20,26,27]: the INOY04 model lacks sufficiently strong attraction in the P waves and the AV18 model provides flatter-than-observed resonant structures in the ^{4}H nucleus, whereas the I-N3LO model provides the best description of the experimental data. This feature indicates a possible correlation between the P-wave states of ^{5}He and ^{4}H (or its isospin symmetry partner ^{4}Li) nuclei.

It is well accepted that a proper description of nuclear systems requires the presence of a three-nucleon force (3NF). Modern models of three-nucleon forces provide extra binding for the symmetric nuclei, like ground state of ^{4}He, but also are able to provide more attraction in the P-wave states. It is demonstrated in [26] for n-^{3}H scattering and in [24] for n-^{4}He, that inclusion of a local 3NF force, developed up to next-to-next-to-leading order terms in [21], in conjunction with the I-N3LO interaction improves significantly the description of the P-wave resonant states. Very similar effects are observed when including the phenomenological IL2 or IL7 three-nucleon forces [28,29] in conjunction with the AV18 NN interaction [26,30]. In this context, the INOY04 interaction turns out to be quite a typical. On the one hand this model provides proper binding energies for the trinucleon(s); however, it slightly overbinds the ^{4}He ground state by about 800 keV [20]. More importantly this model systematically underestimates the mean square radii of the light nuclei [31], resulting in large saturation densities for symmetric nuclear matter [32]. Finally, this model is unable to provide sufficient attraction for the P-wave structures. It would likely be highly nontrivial to correct all these defects by a simple model of the 3NF. The INOY04 NN interaction should be supplemented by a 3NF which is strongly repulsive at the origin in order to correct nuclear radii as well as saturation properties of nuclear matter. On the other hand this 3NF would need some attraction in the periphery with little effect on symmetric nuclei, while at the same time providing strong attraction for the P-wave structures.

VI. CONCLUSION

In the present paper the first solution of the five-body Faddeev-Yakubovsky equations is presented for neutron elastic scattering on ^{4}He. The numerical method involves only well controlled approximations, is numerically very efficient, and may include a large number of partial waves. These developments allow one to calculate five-nucleon system, scattering employing realistic nuclear Hamiltonians.

Three realistic nucleon-nucleon Hamiltonians have been tested, namely INOY04, I-N3LO, and AV18. All of the models provide an accurate description of low energy n-^{4}He scattering in the S wave, which is dominated by strong Pauli repulsion. In contrast, the model predictions deviate from the phase shifts derived from the experimental data for the resonant scattering in P waves. Similar effects have been observed when studying n-^{3}H and p-^{3}H scattering in [20,26,27], which indicates the possible existence of strong correlations between the four and five nucleon systems.

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