Modern nuclear force predictions for n-³H scattering above the three- and four-nucleon breakup thresholds

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Background: Description of the collision process, which includes breakup, is one of the most challenging problems of the quantum mechanics. Recently I have developed a formalism based on the complex-scaling method, which describes accurately nuclear collisions in three- and four-body systems.

Purpose: To provide accurate calculations for n^{-3} H scattering above the three- and four-nucleon breakup thresholds.

Method: A four-nucleon system is described in configuration space employing Faddeev-Yakubovsky equations. The complex-scaling method is applied to overcome the difficulties related with the complicated boundary conditions.

Results: Elastic observables as well as total breakup cross sections are calculated for neutron scattering on tritium at 14.1, 18, and 22.1 MeV using realistic *NN* interactions. Excellent agreement is found with the pioneering calculations of this process reported by A. Deltuva *et al.* [Phys. Rev. C **86**, 011001 (2012)]. Strong correlation of the calculated cross sections is established with model-predicted trinucleon binding energy. The forementioned observables reveal little sensitivity to the short-range details of *NN* interaction.

Conclusion: Reliable and accurate methods are now available to study four-nucleon scattering including the breakup.

DOI: 10.1103/PhysRevC.91.041001

PACS number(s): 21.45.-v, 21.60.-n, 21.30.-x, 25.10.+s

Establishing properties of the nuclear forces remains one of the most important challenges in nuclear physics. The success of this enterprize strongly depends on our ability to build accurate numerical tools, which could test modern nuclear interaction models in describing nuclear reactions. Proper formalisms for three-particle reactions have been introduced by Faddeev in 1961 [1] and a few years later generalized by Yakubovsky [2] for any number of particles. Regardless the fact that this formalism enables handling of binary collisions with relative ease, description of the breakup process into three or more fragments constitutes an important challenge. When formulated in momentum space, the kernels of the Faddeev-Yakubovsky (FY) equations contain singularities, whose complexity increases rapidly with a number of the available particle channels. When solving FY equations in configuration space, technical problems of the comparable complexity arise due to the necessity of handling the complicated boundary conditions, which are related with the behavior of the system wave function in the asymptotes. Therefore description of the breakup including collisions has been limited for a long time to the three-body case.

It is also quite obvious that a direct approach based on explicit treatment of the boundary conditions (or, equivalently, singularities of the integral equation kernels in momentum space equations) becomes overcomplex already for the systems containing more than three or four particles. In order to address such systems, it is necessary to find some tricks which enable us to bypass this problem. In the late sixties Nuttal proposed two different techniques, namely complex-energy [3] and complex-coordinate [4] methods, which makes possible the solution of a few-particle scattering problem by avoiding explicit use of the asymptotic form of the wave function. However, implementations of these two methods in treating nuclear collisions have lingered for more than three decades. The complex-energy method has been revived in a work of Uzu *et al.* [5] and after some technical improvements has been proved to be very efficient and accurate in describing the most complex four-nucleon reactions by Deltuva *et al.* [6]. Complex-coordinate (or complex-scaling) method has also been reintroduced in nuclear physics lately, mostly in studying nuclear reactions driven by the external probe [7-12]. In some of my previous studies, realized in collaboration with Carbonell, we have demonstrated validity of the last method in describing elastic rearrangement as well as breakup reactions for the three-body Hamiltonians which may combine short-range Coulomb as well as optical potentials [13,14]. Neutron-³H scattering has also been considered above the four-nucleon breakup threshold using the simplistic MT I-III variant of the Malfliet and Tjon potential [15]. At that time, the spline collocation method has been employed to solve the systems of integrodifferential equations. In this work I have replaced the method of spline collocation with a Lagrange-Laguerre mesh technique [16,17], which turned out to be more accurate and efficient. Recent numerical improvement permits addressing the $n^{-3}H$ reactions, employing fully realistic nuclear Hamiltonians.

Neutron scattering on ³H represents the simplest experimentally accessible four-nucleon system to handle theoretically. Regardless of its simplicity, this system presents several important features. First this system, made of three neutrons and only one proton, is one of the most neutron-rich systems produced in a laboratory and thus represents an ideal playground to study neutron-neutron interaction. On the other

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FIG. 1. (Color online) The FY components $K_{12,3}^4$ and H_{12}^{34} . As $z \to \infty$, the *K*-type components describe 3+1 particle channels, while the *H*-type components contain asymptotic states of 2+2 channels.

hand, this system in the region $E_{c.m.} \sim 2-6$ MeV exhibits four rather broad resonances. Description of this system in the region of resonances turns out to be quite challenging for the realistic interaction models [18,19]. At higher energies, when system breaks by releasing two or three neutrons, neutron correlations might provide some additional information about the *NN* and *NNN* interactions.

We use configuration space formulation based on the Faddeev-Yakubovsky (FY) equations to describe dynamics of a four-nucleon system [2,20]. In this formalism, the system wave function is decomposed into the so-called FY components (FYCs). There exist two distinct types of the FYCs for a four-body system, namely the components of type K ($K_{ij,k}^l$) and the components of type H (H_{ij}^{kl}) with *i*, *j*, *k*, *l* representing particle indexes. Furthermore, by permuting particle indexes one may construct the 12 independent components of type H. The components of type K are naturally associated with the 3 + 1 particle channels, whereas the components of type H are proper for the 2 + 2 ones; see Fig. 1.

Each FY component F = (K, H) is a function in ninedimensional configuration space, determined by the three three-dimensional (3D) vectors $(\vec{x}, \vec{y}, \vec{z})$. It is convenient to express the FYCs in their proper set of Jacobi coordinates; see Fig. 1. For a four-body system of identical mass particles, these coordinates are defined respectively by

$$\begin{aligned} \vec{x}_{K_{12,3}^4} &= \vec{r}_2 - \vec{r}_1 \quad \vec{x}_{H_{12}^{34}} = \vec{r}_2 - \vec{r}_1 \\ \vec{y}_{K_{12,3}^4} &= \sqrt{\frac{4}{3}} \left(\vec{r}_3 - \frac{\vec{r}_1 + \vec{r}_2}{2} \right) \quad \vec{y}_{H_{12}^{34}} = \vec{r}_4 - \vec{r}_3 \\ \vec{z}_{K_{12,3}^4} &= \sqrt{\frac{3}{2}} \left(\vec{r}_4 - \frac{\vec{r}_1 + \vec{r}_2 + \vec{r}_3}{3} \right) \\ \vec{z}_{H_{12}^{34}} &= \sqrt{2} \left(\frac{\vec{r}_3 + \vec{r}_4}{2} - \frac{\vec{r}_1 + \vec{r}_2}{2} \right). \end{aligned}$$
(1)

Partial-wave formalism is employed to express angular, spin, and isospin dependence of the FYCs. The angular dependence is described by using development in so-called tripolar

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harmonics $\mathcal{Y}_{\alpha}(\hat{x}, \hat{y}, \hat{z})$, i.e.,

$$\langle \vec{x} \, \vec{y} \vec{z} | F \rangle = \sum_{\alpha} \frac{F_{\alpha}(xyz)}{xyz} \, \mathcal{Y}_{\alpha}(\hat{x}, \hat{y}, \hat{z}). \tag{2}$$

The quantities $F_{\alpha}(xyz)$, which depend only on radial variables (xyz), are called regularized FY amplitudes. Here the label α holds for a set of 10 intermediate quantum numbers, expressing a given four-nucleon quantum state (J^{π}, T, T_z) . Using a LS-coupling scheme, they read

$$\begin{aligned} \mathcal{Y}_{\alpha_{K}} &\equiv \left\{ \left[(l_{x}l_{y})_{l_{xy}}l_{z} \right]_{L} \left[((s_{1}s_{2})_{s_{x}}s_{3})_{S3}s_{4} \right]_{S} \right\}_{J^{\pi}\mathcal{M}} \\ &\otimes \left[((t_{1}t_{2})_{t_{x}}t_{3})_{T3}t_{4} \right]_{T\mathcal{T}_{Z}}, \end{aligned} \tag{3} \\ \mathcal{Y}_{\alpha_{H}} &\equiv \left\{ \left[(l_{x}l_{y})_{l_{xy}}l_{z} \right]_{L} \left[(s_{1}s_{2})_{s_{x}}(s_{3}s_{4})_{s_{y}} \right]_{S} \right\}_{J^{\pi}\mathcal{M}} \\ &\otimes \left[(t_{1}t_{2})_{t_{x}}(t_{3}t_{4})_{t_{y}} \right]_{T\mathcal{T}_{Z}}, \end{aligned}$$

where the partial angular momenta are denoted with letters l, the spins of the particles by letters s, and the isospins by letters t.

Furthermore, isospin approximation is applied by considering neutrons and protons as two degenerate states of the same particle, nucleon with a mass set to $\hbar^2/m_N = 41.471$ MeV fm². Moreover, the total isospin of the four-nucleon system is considered to be conserved and set to T = 1.

Due to the particle permutation symmetry, the components K (or H), which differ in particle ordering, become formally identical. Therefore, in what follows particle indexing is dropped by retaining only one component of type K and one component of type H.

As has been demonstrated in a previous study [15], after applying the complex-scaling method it is convenient to separate an incoming wave solution. For the n-³H collisions, considered here, the incoming wave is fully absorbed by the components of type K, namely $K \equiv K^{\text{in}} + K^{\text{out}}$; $H \equiv H^{\text{out}}$. Here the incoming wave K^{in} is built from the ground-state wave function of ³H nucleus combined with the incoming wave of the neutron. Then for a system of four-identical fermions, the driven antisymmetrized FY equation reads [15,20]

$$(E-H_0 - V_{12})K^{\text{out}} - V_{12}(P^+ + P^-)[(1+Q)K^{\text{out}} + H^{\text{out}}]$$

= $V_{12}(P^+ + P^-)[QK^{\text{in}}],$
 $(E - H_0 - V_{12})H^{\text{out}} - V_{12}\tilde{P}[(1+Q)K^{\text{out}} + H^{\text{out}}]$
= $V_{12}\tilde{P}[(1+Q)K^{\text{in}}].$ (5)

where H_0 is a kinetic energy operator, whereas V_{ij} describes the interaction between *i*th and *j*th nucleons. FYCs are converted from one coordinate set to another by using the particle permutation/basis rotation operators, which are summarized as follows: $P^+ = (P^-)^{-1} \equiv P_{23}P_{12}$, $Q \equiv -P_{34}$, and $\tilde{P} \equiv P_{13}P_{24} = P_{24}P_{13}$, with P_{ij} standing for an operator with interchange particle indexes *i* and *j*. Using these definitions, total wave function of an A = 4 system may be expressed in terms of FYCs by

$$\Psi = [1 + (1 + P^{+} + P^{-})Q](1 + P^{+} + P^{-})K + (1 + P^{+} + P^{-})(1 + \tilde{P})H.$$
(6)

Asymptotes of the components K^{out} and H^{out} contain only various combinations of outgoing waves, thus bringing an

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TABLE I. Some calculated phase shifts δ and inelasticity parameters η for 22.1-MeV neutron scattering on triton using INOY04 potential. This work results are compared with the ones from Ref. [6].

PW	η		δ (deg)		
	This work	Ref. [6]	This work	Ref. [6]	
$1 S_0$	0.985	0.990	62.74	62.63	
${}^{3}P_{0}$	0.959	0.959	43.07	43.03	
${}^{3}P_{2}$	0.949	0.950	65.25	65.27	

interest to apply the complex-scaling (or coordinates) method, proposed by Nuttall and Cohen [4]. It is easy to see that by acting on outgoing wave with a complex-scaling operator (CSO),

$$\widehat{S} = e^{i\theta r \frac{\partial}{\partial r}} = e^{i\theta(x \frac{\partial}{\partial x} + y \frac{\partial}{\partial y} + z \frac{\partial}{\partial z})},\tag{7}$$

one gets exponentially bound functions, if the complex-scaling angle θ is chosen in the interval $(0,\pi)$.

Action of the complex-scaling operator on the set of Eqs. (5) gives

$$\widehat{S}(E - H_0 - V_{12})\widehat{S}^{-1}\widetilde{K}^{\text{out}} -\widehat{S}V_{12}\widehat{S}^{-1}(P^+ + P^-)[(1+Q)\widetilde{K}^{\text{out}} + \widetilde{H}^{\text{out}}] = \widehat{S}V_{12}\widehat{S}^{-1}(P^+ + P^-)[Q\widetilde{K}^{\text{in}}],$$
(8)

$$\widehat{S}(E - H_0 - V_{12})\widehat{S}^{-1}\widetilde{H}^{\text{out}}$$

$$\widehat{S}V_{12}\widehat{S}^{-1}\widetilde{D}[(1 + Q)\widetilde{K}^{\text{out}} + \widetilde{U}^{\text{out}}] \qquad (0)$$

$$-SV_{12}S^{-1}P[(1+Q)K^{out} + H^{out}]$$
(9)

$$= SV_{12}S^{-1}P[(1+Q)K^{\rm in}].$$
(10)

While action of the complex-scaling operator on outgoing waves gives exponentially bound functions, the same operation rends functions \tilde{K}^{in} (or \tilde{H}^{in}) exponentially divergent. Nevertheless these functions appear only in inhomogeneous term of the FY equations (8)–(10) readily premultiplied with a potential energy operator, and thus if interactions are exponentially bound the kernel of the complex-scaled equations may become compact. Still, as discussed in Refs. [13,21], to achieve this goal an additional kinematical condition should be satisfied for A > 2 systems.

The complex-scaled FY equations (10) are solved for the transformed FY components $\tilde{K}^{\text{out}} = \hat{S}K^{\text{out}}$ and $\tilde{H}^{\text{out}} = \hat{S}H^{\text{out}}$. The radial dependence of these complex-scaled FY components \tilde{K}^{out} and \tilde{H}^{out} is expanded on the Lagrange-Laguerre basis, whereas the system of integrodifferential equations is

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transformed into a linear algebra problem by using Lagrangemesh method [16,17]. Complex-scaled wave functions of ³H ground state, required to build the incoming wave functions, are obtained by solving Eq. (10) where dependence on the Jacobi coordinate z is removed. Scattering amplitudes including the breakup ones may be calculated from the transformed solutions \tilde{K}^{out} (or \tilde{H}^{out}) employing the integral relations; see Refs. [15,21] for the details.

In order to get numerically converged results one has to include in the expansion (3) partial waves with angular momenta $\max(l_x, l_y, l_z) \leq 4$. In addition, a 3D Lagrange-Laguerre mesh of ~30³ points is required to describe radial dependence of the regularized FY amplitudes $\tilde{F}_{\alpha}^{\text{out}}(xyz)$. This brings to solve a linear system with a typical size of ~10⁸ equations, which is realized using the BICGSTAB(L) algorithm [22].

A few years ago, the complex-scaling method was applied to study n^{-3} H scattering above the breakup threshold [15]. In that work, realized in collaboration with Carbonell, due to large numerical costs we were obliged to use the simplistic S-waves nucleon-nucleon interaction model. More recently, the spline collocation method, employed previously to discretize radial dependence of FY amplitudes, has been replaced by the Lagrange-mesh technique. This modification allowed significantly improved numerical accuracy and realistic description of the four-nucleon reactions above the three- and fourfragment breakup thresholds. As the first step of the longer program intended to cover fully the four-nucleon continuum, I have realized calculations of neutron scattering on the ³H nucleus. The calculations presented here have been performed using three formally and structurally different realistic nuclear Hamiltonians: INOY04 [23], xN3LO [24], and AV18 [25].

Three years ago pioneering realistic calculation on the n^{-3} H system above the breakup threshold was undertaken by Deltuva *et al.* [6]. Deltuva employs momentum-space formulation of the complex-energy method [3,21]. In Table I the phase shifts and inelasticity parameters obtained in this study are compared with the ones published by Deltuva for the INOY04 model. Excellent agreement is obtained between the two calculations, reaching three-digit accuracy. The largest discrepancy of 0.5% is observed for the inelasticity parameter in the ¹S₀ channel, which is due to the fact that this parameter is very close to unity.

Excellent agreement between the two calculations is also obtained for the integrated cross sections; see Table II. These calculations include all the scattering states with total angular momentum $J \leq 5$. Including more partial waves yields no change for the elastic cross section and only entirely

TABLE II. Integrated elastic (σ_{el}), breakup (σ_b), and total (σ_t) cross sections for neutron scattering on ³H. Calculations have been performed using INOY04 *NN* potential model. The results of this work are compared with the ones from Ref. [6] and experimental values from Refs. [26,27].

E_n (MeV)	This work			Ref. [6]			Exp.
	$\sigma_{\rm el} \ ({\rm mb})$	σ_b (mb)	$\sigma_{\rm tot}~({\rm mb})$	$\sigma_{\rm el} ({\rm mb})$	σ_b (mb)	$\sigma_{\rm tot}~({\rm mb})$	$\sigma_{\rm tot}~({\rm mb})$
14.1	927	19	947	928	19	947	978 ± 70
18.0	697	42	739	697	41	738	750 ± 40
22.1	535	61	596	536	61	597	620 ± 24

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FIG. 2. (Color online) Calculated n-³H elastic differential cross sections (left panel) and neutron analyzing power A_y (right panel) for incident neutrons at laboratory energy 22.1 MeV. Calculated values are compared with the experimental results of Seagrave *et al.* [28].

insignificant changes for the breakup one. The total cross sections are also in good agreement with the experimental data from Battat [26] and Phillips [27]; they fall within experimental error bars but favor slightly lower values than the experimental centroid.

In Fig. 2 the elastic differential cross section as well as the neutron analyzing power A_v are presented for 22.1-MeV neutron scattering on triton. In this figure, results obtained using three different realistic nuclear Hamiltonians, namely INOY04 [23], xN3LO [24], and AV18 [25], are presented. Before discussing agreement with the experimental data, one should notice that not all of the employed Hamiltonians are equally successful in describing bound-state properties of ³H (i.e., the target nucleus). It is commonly accepted that most of the nuclear interaction models require a three-nucleon force to provide extra binding for the trinucleon. The INOY04, χ N3LO, and AV18 models produce the tritons with binding energies of 8.48, 7.85, and 7.62 MeV respectively, and thus with the exception of the INOY04 model, they underbind triton (experimental binding energy of the triton is 8.482 MeV). However, correct positioning of the thresholds are crucial in describing low-energy scattering cross sections. In the vicinity of a threshold, due to the kinematical form factor, the breakup cross section increases with the available kinetic energy. This feature is clearly demonstrated in Fig. 3, where total cross sections provided by four different realistic nucleon-nucleon interaction models are plotted against the binding energy of ³H.¹ On the other hand, the total elastic cross section has the opposite behavior-it increases with the binding energy of the triton compensating effect from the breakup cross section. One may observe the linear correlation pattern for both cross sections. Existence of such a correlation indicates that at these energies the neutron cross sections are not very sensitive to the off-shell structure of a nuclear Hamiltonian, determined by the on-shell properties of the two-nucleon system and the binding energy of the triton. It is expected that once three-nucleon force is introduced to correct the binding energy of the trinucleons, different realistic nuclear Hamiltonian predictions should align with the result of the INOY04 model. While extensive model

dependence of the n^{-3} H cross sections has been performed only for 22.1-MeV neutrons, our other calculations suggest that this tendency should remain valid for the broader energy range above the three- and four-nucleon breakup thresholds. On the other hand, this tendency is clearly broken below the three-nucleon breakup threshold, where four pronounced neutron resonances are present [18,19].

The same correlation pattern is also observed for the differential elastic cross section; see Fig. 2. The elastic cross section increases with the trinucleon binding energy, which is the most pronounced at the cross-section minima. Cross sections provided by the INOY04 model, which must stand as a reference for any realistic Hamiltonian calculation with correct trinucleon threshold, provide the worst agreement with the experimental data of Ref. [28] at the cross-section minima. On the other hand, as demonstrated in Ref. [6], the calculated cross sections at $E_n = 18$ MeV lie in the middle between data sets of Refs. [28] and [29]. Thus one might expect a lack of reliability for the data from Ref. [28]. As disagreement is due to the cross-section minima, underestimation of the experimental error bars might be the reason of this discrepancy. New precise measurements are required to resolve this discrepancy.



FIG. 3. (Color online) Dependence of the calculated n^{-3} H total elastic and inelastic (breakup) cross sections on the triton binding energy. Calculations have been performed for neutrons with laboratory energy of 22.1 MeV.

¹CD-Bonn model result is taken from Ref. [6].

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Agreement between the theoretical and the experimental neutron analyzing powers is not perfect, but is much improved compared to one obtained for slower neutrons. In particular, it contrasts with the existence of the well-known Ay puzzle for p^{-3} He scattering below the p + p + d breakup threshold [30].

Conclusion. In this Rapid Communication new results for an n^{-3} H scattering above the four-nucleon breakup threshold are presented, which have been obtained using the three different realistic nuclear Hamiltonians. Correlation between the calculated elastic and breakup cross sections with a modelpredicted three-nucleon binding energy has been observed. On one hand, this proves an importance of the correct reproduction of the thresholds in such calculations; on the other hand, it reveals that 14- to 22-MeV neutron scattering on ³H is not a very sensitive tool in testing short-range details of the realistic nuclear Hamiltonians. This work is the first effort to apply the complex-scaling method in describing four-nucleon scattering above the

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breakup threshold using fully rigorous and realistic formalism. It is demonstrated that the level has been reached when four-nucleon scattering problem in its full complexity is solved accurately and reliably. The next step is to extend this study to other four-nucleon systems, related with the continuum of ⁴He and ⁴Li nuclei, which include repulsive Coulomb interaction. Pioneering works in this direction has already been undertaken based on momentum space formulation of the complex-energy method by Deltuva and Fonseca [31,32].

Acknowledgment. The author was granted access to the HPC resources of IDRIS under Allocation 2009-i2009056006 made by GENCI (Grand Equipement National de Calcul Intensif). I thank the staff members of the IDRIS for their constant help.

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