Few-nucleon systems with state-of-the-art chiral nucleon-nucleon forces

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We apply improved nucleon-nucleon potentials up to fifth order in chiral effective field theory, along with a new analysis of the theoretical truncation errors to study nucleon-deuteron (Nd) scattering and selected low-energy observables in ^{3}H ,^{4}He, and ^{6}Li. Calculations beyond second order differ from experiment well outside the range of quantified uncertainties, providing truly unambiguous evidence for missing three-nucleon forces within the employed framework. The sizes of the required three-nucleon-force contributions agree well with expectations based on Weinberg's power counting. We identify the energy range in elastic Nd scattering best suited to study three-nucleon-force effects and estimate the achievable accuracy of theoretical predictions for various observables.

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I. INTRODUCTION

Chiral effective field theory (EFT) provides a powerful framework for analyzing low-energy nuclear structure and reactions in harmony with the symmetries of quantum chromodynamics (QCD), the underlying theory of the strong interactions. It allows one to derive nuclear forces and currents in a systematically improvable way in terms of a perturbative expansion in powers of $Q \in (p/\Lambda_b, M_\pi/\Lambda_b)$, the so-called chiral expansion. Here, p refers to the magnitude of the nucleon three-momentum, M_π is the pion mass, and Λ_b is the breakdown scale of chiral EFT [1]. One finds, in particular, that the leading-order (LO) contribution to the Hamiltonian at order Q^0 and the first corrections at order Q^2 (NLO) are given solely by nucleon-nucleon (NN) operators while three-nucleon forces (3NFs) appear first at order Q^3 (N^{2}LO) (see Ref. [2] and references therein). Four-nucleon forces are even more suppressed and start contributing at order Q^4 (N^{3}LO). The chiral power counting thus provides a natural explanation of the observed hierarchy of nuclear forces.

With accurate N^{3}LO NN potentials being available for about a decade [3,4], the main focus of research has moved in recent years towards the 3NFs [5,6]. While providing small corrections to the nuclear Hamiltonian as compared to the dominant NN force, its inclusion seems to be necessary for quantitative understanding of nuclear structure and reactions. Historically, the importance of the 3NF has been conjectured already in the thirties [7] while the first phenomenological 3NF models date back to the fifties. However, in spite of extensive efforts, the spin structure of the 3NF is still poorly understood [5].

Chiral EFT is expected to provide a suitable theoretical resolution to the long-standing 3NF problem. Indeed, the leading chiral 3NF has already been extensively explored in *ab initio* calculations by various groups and found to yield promising results for nuclear structure and reactions [6,8]. The first corrections to the 3NF at order Q^4 (N^{3}LO) have also been derived [9–11] (and are parameter free) while the sub-sub-leading contributions at order Q^5 (N^{4}LO) are being derived [12–14].

On the other hand, understanding and validating the fine details of the 3NF clearly requires precise and systematic NN potentials and a reliable approach for estimating the accuracy of theoretical predictions at a given chiral order. References [15,16] initiated the direction that we follow here by developing a new generation of chiral EFT NN forces up to N^{4}LO, in which the amount of finite-cutoff artifacts has been substantially reduced by employing a novel ultraviolet regularization scheme, and by introducing a new procedure for estimating the theoretical uncertainty. In particular, the

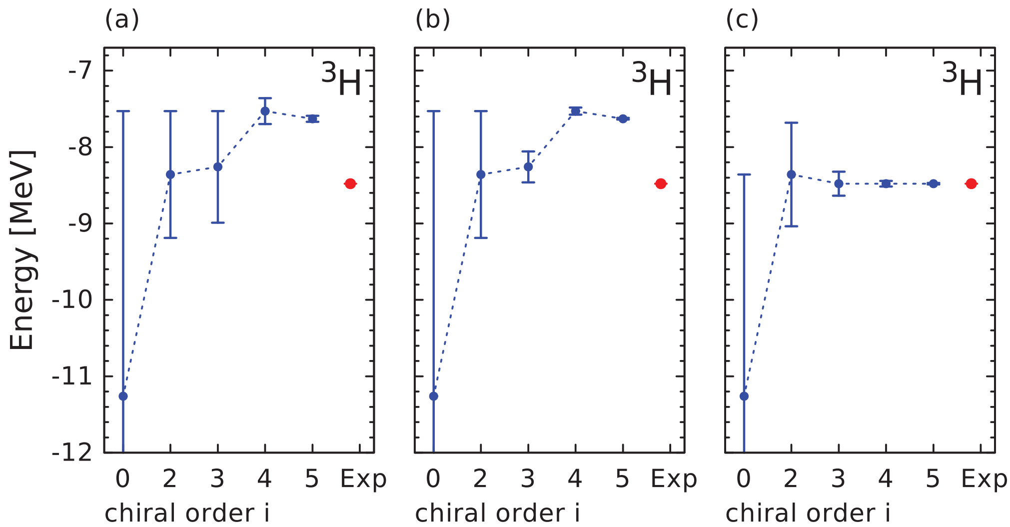

FIG. 1. Chiral expansion of the ^{3}H $E_{\rm g.s.}$ based on the NN potentials of Refs. [15,16] for the regulator $R = 1.0$ fm and using $Q = M_\pi/\Lambda_b$. Panel (a) shows incomplete results based on NN forces only, with uncertainties being estimated via Eqs. (5) and (6). Panel (b) shows incomplete results based on NN forces only, with uncertainties being estimated via Eqs. (5) and (6) for chiral order $i = 0,2$ and via Eqs. (7) and (8) for $i \geqslant 3$. Panel (c) shows the projected results assuming that the LECs in the N^{2}LO 3NF are tuned to reproduce the ^{3}H $E_{\rm g.s.}$ and using Eqs. (5) and (6) to specify the uncertainty.

long-range part of the NN potential is regularized in position space by multiplying with the function

$$f\left(\frac{r}{R}\right) = \left[1 - \exp\left(-\frac{r^2}{R^2}\right)\right]^6, \qquad (1)$$

with the cutoff R chosen in the range 0.8–1.2 fm.

In this paper we, for the first time, apply these novel chiral NN forces beyond the two-nucleon system and demonstrate their suitability for modern *ab initio* few- and many-body methods. By applying the new method for error analysis, we present unambiguous evidence for missing 3NF effects and demonstrate that the size of the required 3NF contributions agrees well with expectations based on Weinberg's power counting. We also estimate the theoretical accuracy for various observables achievable at N^{4}LO and identify the energy region in elastic N*d* scattering that is best suited for testing the chiral 3NF.

II. UNCERTAINTY QUANTIFICATION

We first describe our procedure for estimating the theoretical uncertainty. Let $X(p)$ be some observable with p referring to the corresponding momentum scale and $X^{(i)}(p)$, $i = 0,2,3,\ldots$, a prediction at order Q^i in the chiral expansion. We further define the order-Q^i corrections to $X(p)$ via

$$\Delta X^{(2)} \equiv X^{(2)} - X^{(0)}, \quad \Delta X^{(i)} \equiv X^{(i)} - X^{(i-1)}, \quad i \geqslant 3, \qquad (2)$$

so that the chiral expansion for X takes the form

$$X^{(i)} = X^{(0)} + \Delta X^{(2)} + \cdots + \Delta X^{(i)}. \qquad (3)$$

Generally, the size of the corrections is expected to be

$$\Delta X^{(i)} = \mathcal{O}(Q^i X^{(0)}). \qquad (4)$$

In Ref. [16], the validity of this estimate was confirmed for the total neutron-proton cross section. In Refs. [15,16], quantitative estimates of the theoretical uncertainty $\delta X^{(i)}$ of the chiral EFT prediction $X^{(i)}$ were made by using the expected and actual sizes of higher-order contributions. Specifically, the following procedure was employed:

$$\delta X^{(0)} = Q^2 |X^{(0)}|,$$
$$\delta X^{(i)} = \max_{2\leqslant j \leqslant i} \left(Q^{i+1}|X^{(0)}|,\ Q^{i+1-j}|\Delta X^{(j)}|\right), \qquad (5)$$

where $i \geqslant 2$ and $Q = \max(p/\Lambda_b,\ M_\pi/\Lambda_b)$ with $\Lambda_b =$ 600, 500, and 400 MeV for the regulator choices of $R =$ 0.8–1.0, 1.1, and 1.2 fm, respectively. The sizes of actual higher-order calculations provide additional information on

TABLE I. Ground-state energies $E_{\rm g.s.}$ of ^{3}H and ^{4}He (in MeV) and the point-proton radius r_p of ^{4}He (in fm) calculated by using the improved NN chiral potentials of Refs. [15,16] up to N^{4}LO for the cutoff $R = 1.0$ fm in comparison with empirical information. The quoted uncertainties for the theoretical predictions are estimated via Eqs. (5) and (6) for chiral order $i = 0,2$ and via Eqs. (7) and (8) for $i \geqslant 3$.

	LO	NLO	N^{2}LO	N^{3}LO	N^{4}LO	Empirical
$E_{\rm g.s.}$ (^{3}H)	−11.3(3.7)	−8.36(83)	−8.26(20)	−7.53(5)	−7.63(1)	−8.48
$E_{\rm g.s.}$ (^{4}He)	−45.5(21.7)	−28.6(4.8)	−28.1(1.2)	−23.75(28)	−24.27(6)	−28.30
r_p (^{4}He)	1.064(499)	1.389(174)	1.405(41)	1.563(9)	1.547(2)	1.462(6)

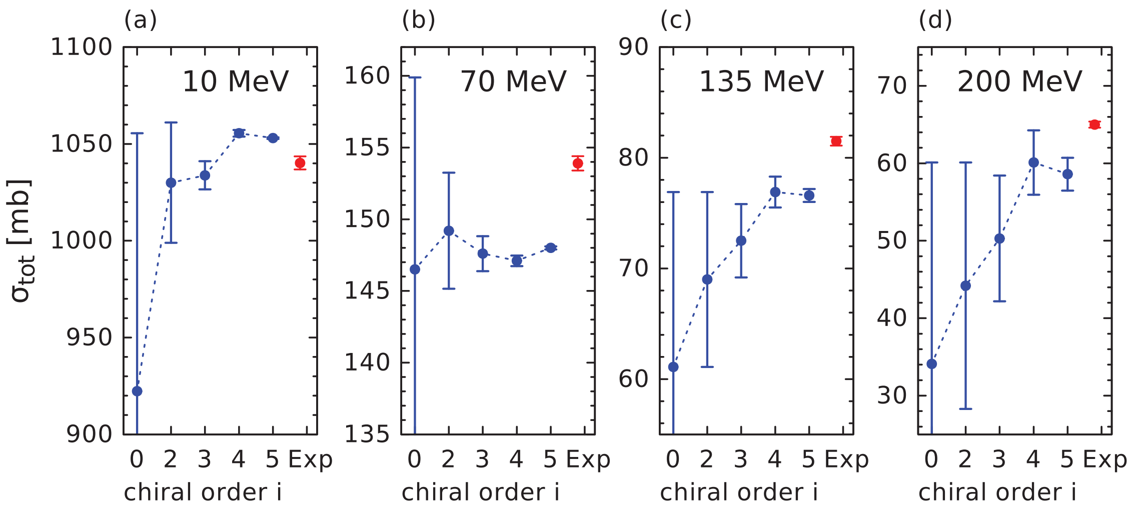

FIG. 2. Predictions for Nd total cross section based on the NN potentials of Refs. [15,16] for $R = 1.0$ fm without including the 3NF at (a) $E = 10$ MeV, (b) 70 MeV, (c) 135 MeV, and (d) 200 MeV. Theoretical uncertainties (blue) are estimated via Eqs. (5) and (6) for chiral order $i = 0,2$ and via Eqs. (7) and (8) for $i \geqslant 3$. Experimental data are taken from Ref. [19].

the theoretical uncertainties, which we use by imposing the constraint

$$\delta X^{(i)} \geqslant \max_{j,k}(|X^{(j\geqslant i)} - X^{(k\geqslant i)}|). \qquad (6)$$

The above procedure for estimating the uncertainty needs to be adjusted in order to account for the neglect of many-body forces in the present analysis. In particular, iterating the NN T matrix in the Faddeev equations generates contributions whose short-range behavior is order- and regulator-dependent. For low-energy Nd observables calculated in the EFT framework, approximate scheme independence is restored upon performing renormalization, i.e., upon expressing the bare low-energy constants (LECs) accompanying short-range 3NFs at orders Q^3, Q^5, ... in terms of observable quantities, such as the triton binding energy. In practice, this is achieved by fitting the corresponding LECs to experimental data. Therefore, when performing incomplete calculations based on NN interactions only, the estimate in Eq. (4) is not justified at or beyond N^{2}LO, the chiral order at which the contact 3NF starts contributing. Therefore, we adopt here a more appropriate procedure for estimating the uncertainty $\delta X^{(i)}$ for $i \geqslant 3$; namely,

$$\delta X^{(i)} = \max(Q^{i+1}|X^{(0)}|, Q^{i-1}|\Delta X^{(2)}|, Q^{i-2}|\Delta X^{(3)}|), \quad (7)$$

and do not employ Eq. (6). However, to be conservative in our estimates, we impose the additional constraints

$$\delta X^{(2)} \geqslant Q\,\delta X^{(0)}, \quad \delta X^{(i\geqslant 3)} \geqslant Q\,\delta X^{(i-1)}. \qquad (8)$$

In the future, more complete calculations will provide information on the actual size of contributions beyond N^{2}LO which should lead to a more reliable uncertainty quantification using Eqs. (5) and (6).

The dependence of the chiral NN forces on the local regulator R over the range 0.8–1.2 fm has been extensively investigated in Ref. [16] showing that cutoff artifacts become visible for $R > 1.0$ fm. On the other hand, we seek to obtain many-body results as close to convergence as possible, and this favors the largest feasible value of R. We therefore balance these competing conditions with the choice of $R = 1.0$ fm in this work.

III. PREDICTIONS FOR FEW-NUCLEON SYSTEMS

Our results for the chiral expansion of the ^{3}H ground-state energy ($E_{\text{g.s.}}$) using $Q = M_\pi/\Lambda_b$ are visualized in Fig. 1, see also Table I. In addition to the strong potentials, we have taken into account the electromagnetic interactions from the AV18 potential [17] for pp and nn interactions. Given that the ^{3}H $E_{\text{g.s.}}$ is commonly used to constrain the LECs entering the short-range part of the 3NF which implies that it is, as per construction, reproduced starting from N^{2}LO, we are able to show in the right panel of Fig. 1(a) the *complete* result for this quantity up to N^{4}LO already at this stage. As expected, we observe that Eqs. (7) and (8) provide a more reliable approach for error estimation in calculations based on NN interactions

TABLE II. Predicted values for Nd total cross section (in mb) based on the NN chiral potentials of Refs. [15,16] up to N^{4}LO for the cutoff $R = 1.0$ fm at laboratory energies of 10, 70, 135, and 200 MeV. The quoted uncertainties for the theoretical predictions are estimated via Eqs. (5) and (6) for chiral order $i = 0,2$ and via Eqs. (7) and (8) for $i \geqslant 3$. Experimental data are from Ref. [19].

E_N (MeV)	LO	NLO	N^{2}LO	N^{3}LO	N^{4}LO	Expt.
10	922(133)	1030(31)	1034(7.3)	1055(1.7)	1053(0.4)	1040.2(3.4)
70	146.5(13.4)	149.2(4.0)	147.6(1.2)	147.1(0.4)	148.0(0.1)	153.9(0.5)
135	61.1(15.8)	69.0(7.9)	72.5(3.3)	76.7(1.4)	76.6(0.6)	81.5(0.4)
200	34.1(26.0)	44.2(15.9)	50.3(8.1)	60.1(4.2)	58.6(2.1)	65.0(0.4)

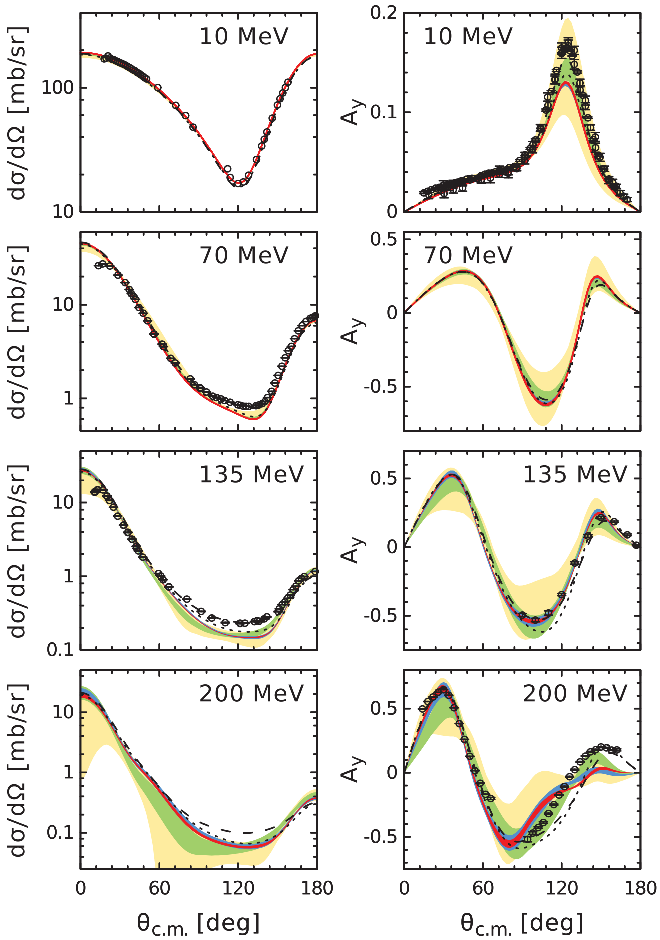

FIG. 3. Predictions for the differential cross section and nucleon A_y in elastic N*d* scattering based on the NN potentials of Refs. [15,16] for $R = 1.0$ fm without including the 3NF. Theoretical uncertainties are estimated via Eqs. (5) and (6) for chiral order $i = 2$ and via Eqs. (7) and (8) for $i \geqslant 3$. The bands of increasing width show the estimated theoretical uncertainty at N^{4}LO (red), N^{3}LO (blue), N^{2}LO (green), and NLO (yellow). The dotted (dashed) lines show the results based on the CD Bonn NN potential [20] (CD Bonn NN potential in combination with the Tucson–Melbourne 3NF [21]). For references to proton-deuteron data (symbols), see Ref. [5].

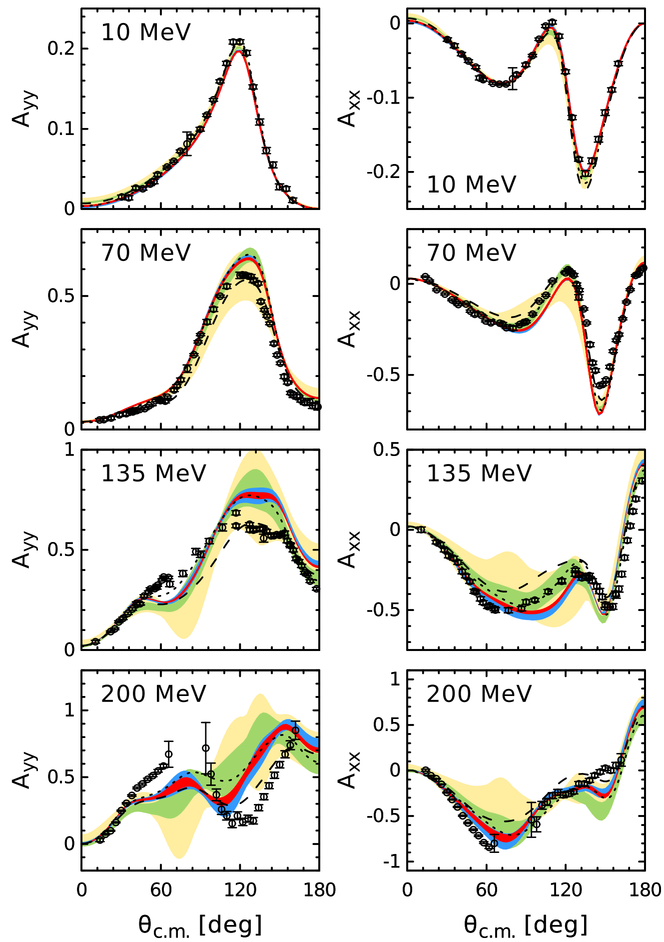

FIG. 4. Predictions for the tensor analyzing powers A_{yy} and A_{xx} in elastic N*d* scattering based on the NN potentials of Refs. [15,16] for $R = 1.0$ fm without including the 3NF. For notations see Fig. 3.

only, while using Eqs. (5) and (6) amounts to overestimating the actual error. The N^{3}LO (N^{4}LO) results for the ^{3}H $E_{\rm g.s.}$ are expected to be accurate at the level of ∼50 keV (∼10 keV) for the regulator choices of $R = 0.8$, 0.9, and 1.0 fm. Note that the size of the inferred 3NF contribution agrees well with the uncertainty at NLO, which reflects the estimated impact of the N^{2}LO contributions to the Hamiltonian. This is fully in line with expectations based on the Weinberg power counting [1,2]. We further emphasize that the sizable underbinding of the triton with the NN potentials at N^{3}LO and N^{4}LO is not limited to the employed regulator choice of $R = 1.0$ fm. We find $E_{\rm g.s.} = -7.47 \ldots -7.56$ MeV ($E_{\rm g.s.} = -7.48 \ldots -7.63$ MeV) for the variation of the regulator in the range $R = 0.8 \ldots 1.2$ fm at N^{3}LO (N^{4}LO).

We now turn to N*d* scattering observables, which are calculated by solving the Faddeev equation in the partial-wave basis. We take into account all partial waves up to the total angular momentum $j_{\rm max} = 5$ in two-nucleon subsystems. Isospin-breaking effects are taken into account in the standard way as described in Ref. [18]. Our predictions for the N*d* total cross section are visualized in Fig. 2, see also Table II. Similar to the ^{3}H $E_{\rm g.s.}$, one observes a significant discrepancy between the theoretical predictions based on the NN forces only and data, which provides clear evidence for missing 3NF contributions. The size of the discrepancy agrees within 1.5 times the estimated size of N^{2}LO corrections shown by the NLO error bars. Interestingly, the discrepancy at the lowest energy of 10 MeV is much smaller than the estimated size of N^{2}LO contributions. Given that the cross section at low energy is governed by the *S*-wave spin-doublet and spin-quartet N*d* scattering lengths, this observation can be naturally explained. Indeed, the spin-quartet scattering length is almost an order of magnitude larger than that of the spin-doublet and much less sensitive to the 3NF as a consequence of the Pauli principle.

Our predictions for N*d* differential cross section and analyzing powers A_y(N), A_{yy}, and A_{xx} are shown in Figs. 3 and 4. At the lowest energy of 10 MeV, there is little apparent need for 3NF effects except for A_y. Interestingly, the fine-tuning nature of this observable is clearly reflected in large theoretical

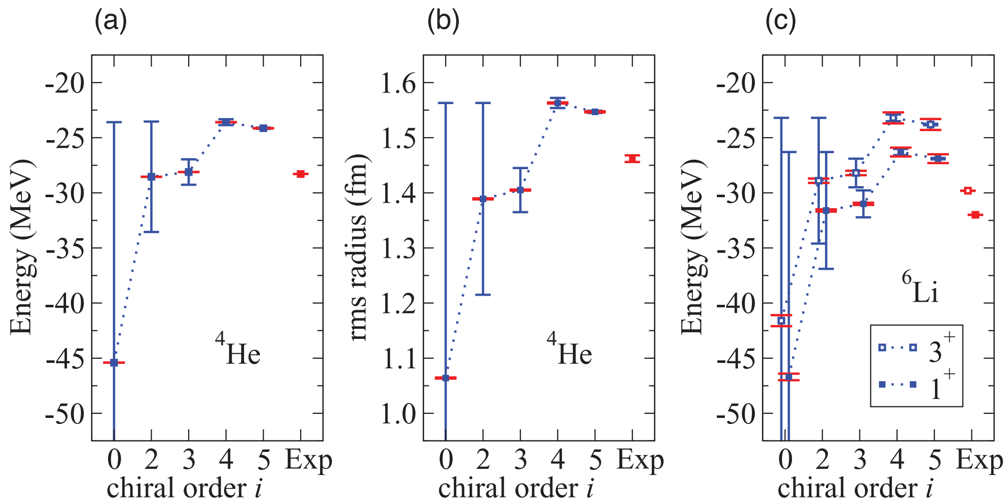

FIG. 5. Predictions for (a) $E_{\mathrm{g.s.}}$ and (b) r_p of ^{4}He and the energies of the lowest two states of (c) ^{6}Li based on the NN potentials of Refs. [15,16] for $R = 1.0$ fm without including the 3NF. Theoretical uncertainties (blue error bars with shorter horizontal lines) are estimated via Eqs. (5) and (6) for chiral order $i = 0,2$ and via Eqs. (7) and (8) for $i \geqslant 3$. Numerical uncertainties from the NCSM (red error bars with longer horizontal lines) are estimated following Ref. [23].

uncertainties at NLO and N^{2}LO. Starting from the laboratory energy of $E_N = 70$ MeV, one observes clear discrepancies between our predictions and data for the cross section and tensor analyzing powers which are expected to be explained by the 3NF. In all cases, the required 3NF contributions are of a natural size. Based on the width of the bands, one may expect Nd scattering observables at N^{4}LO to be accurately described up to energies of at least 200 MeV. It is also reassuring to see that the accuracy of chiral EFT predictions for Nd and NN [16] scattering observables at the same energy is comparable. We further emphasize that the improved NN potentials of Refs. [15,16] show clearly smaller finite-cutoff artifacts as compared to the N^{3}LO potentials of Ref. [4] and, in particular, do not lead to distortions in the cross-section minimum that were found in Ref. [22].

Next, we apply the improved NN potentials to $A > 3$ systems. We present in Fig. 5 order-by-order calculations of selected observables for ^{4}He and ^{6}Li. The results for ^{4}He are obtained both by solving the Faddeev–Yakubovsky (FY) equations and with the no-core shell model (NCSM) [8], which agree to within the estimated uncertainties of these methods. The numerical uncertainties in the FY solutions are a few keV for the energy and about 0.001 fm for the point-proton radius (r_p). The numerical uncertainties from incomplete convergence of the NCSM (see Ref. [23] for details) are shown as error bars (red) together with the estimated theoretical uncertainties from the truncated chiral expansion with $Q = M_\pi/\Lambda_b$ (blue).

The quoted empirical value for the point-proton radius of ^{4}He is extracted from the charge radius $r_c = 1.681(4)$ fm [24], measured in electron scattering experiments, by means of the relation [25]

$$r_p^2 = r_c^2 - \left(R_p^2 + \frac{3}{4m_p^2}\right) - \frac{N}{Z}R_n^2 - r_{\mathrm{so}}^2 - r_{\mathrm{mec}}^2, \qquad (9)$$

where R_p and R_n are the proton and neutron finite-size corrections, respectively, and m_p is the proton mass. Furthermore, r_{so}^2 is a relativistic correction due to spin-orbit coupling of the nucleons with nonzero orbital angular momentum while r_{mec}^2 denotes the contribution of meson-exchange currents. The quoted value of $r_p = 1.462(6)$ fm is taken from Ref. [26] which also gives the values for R_p, R_n and r_{so}. The contribution r_{mec}^2 is neglected. Notice that, within the theoretical uncertainties, our results for ^{3}H and ^{4}He are consistent with quantum Monte Carlo calculations using local chiral EFT NN potentials up to N^{2}LO [27].

For the ^{6}Li energies, we carried out similarity renormalization group (SRG) evolution [28] in order to enhance the convergence rate of the NCSM calculations that were performed in basis spaces up through $N_{\max} = 12$ and extrapolated to the infinite-matrix limit following Refs. [23,28]. We retained the induced 3NF arising from the SRG evolution (see Ref. [29] for details), and this produces results for the

TABLE III. Predicted values for the energies of the ground and the first excited state of ^{6}Li (in MeV) based on the NN chiral potentials of Refs. [15,16] up to N^{4}LO for the cutoff $R = 1.0$ fm. The first uncertainties for the theoretical predictions are estimated via Eqs. (5) and (6) for chiral order $i = 0,2$ and via Eqs. (7) and (8) for $i \geqslant 3$. The second uncertainties are the many-body uncertainties. See main text for additional details.

	LO	NLO	N^{2}LO	N^{3}LO	N^{4}LO	Expt.
$E_{\mathrm{g.s.}}$	−46.9(20.7)(0.3)	−31.7(5.5)(0.1)	−31.1(1.3)(0.1)	−26.2(0.3)(0.2)	−26.8(0.1)(0.2)	−31.99
E_{3^+}	−41.9(18.7)(0.6)	−29.0(5.8)(0.2)	−28.3(1.4)(0.2)	−23.2(0.3)(0.3)	−23.8(0.1)(0.3)	−29.81

^{6}Li energies in Fig. 5 that are independent of the SRG scale over the range $\alpha = 0.04$–0.08 fm^4 to within our quoted many-body uncertainties. For example, at N^{4}LO we obtain $E_{\text{g.s.}} = -26.9(4)$ [$-26.9(2)$] MeV at $\alpha = 0.04$ (0.08) fm^4 for ^{6}Li where the quantified numerical uncertainty in the last digit of the energy is quoted in parentheses. Our predictions for the energies of the ground and the first excited state of ^{6}Li are summarized in Table III for $\alpha = 0.08$ fm^4.

The patterns for the energies in Fig. 5 as well as for the r_p of ^{4}He are very similar to the pattern for the $E_{\text{g.s.}}$ of ^{3}H in Fig. 1 and the Nd total cross section at 10 MeV in Fig. 2. As in ^{3}H, we again observe underbinding, indicative of the need for 3NFs, especially at N^{3}LO and N^{4}LO. This underbinding is correlated with larger r_p in ^{4}He, which is expected to decrease toward the experimental result as $E_{\text{g.s.}}$ is lowered toward experiment with the inclusion of 3NFs. Note that the energy of the first excited state in ^{6}Li, with $J^\pi = 3^+$, follows the same pattern as the ground-state energy, leading to an excitation energy that depends much less on the chiral order than one might naively expect based on the theoretical uncertainties of the binding energies.

IV. SUMMARY AND CONCLUSIONS

To summarize, we study in this paper selected few-nucleon observables by using improved chiral NN potentials of Refs. [15,16] up to N^{4}LO. Our results suggest that these new chiral forces are well suited for modern *ab initio* few- and many-body methods. Using the novel approach for error analysis introduced in Ref. [15], we found truly unambiguous evidence for missing 3NF effects within the employed framework by observing discrepancies between our predictions and experimental data well outside the range of quantified uncertainties. The magnitude of these discrepancies is found to match well with the expected size of the chiral 3NF whose dominant contribution appears at N^{2}LO. Furthermore, we demonstrate that the predictions for Nd and NN scattering observables at the same energy have comparable accuracy, in agreement with the general principles of EFT. Most importantly, the expected theoretical uncertainty for Nd scattering observables at N^{3}LO and N^{4}LO in the energy range of $E_{\text{lab}} \simeq$ 70–200 MeV is shown to be substantially smaller than the observed discrepancies between state-of-the-art calculations and experimental data. This suggests that chiral EFT at these orders should be capable of resolving the long-standing 3NF problem in nuclear physics. Work on the explicit inclusion of the consistent 3NFs is in progress.

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