The importance of few-nucleon forces in chiral effective field theory

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We study the importance of few-nucleon forces in chiral effective field theory for describing many-nucleon systems. A combinatorial argument suggests that three-nucleon forces—which are conventionally regarded as next-to-next-to-leading order—should accompany the two-nucleon force already at leading order (LO) starting with mass number $A \simeq 10 - 20$. We find that this promotion enables the first realistic description of the ^{16}O ground state based on a renormalization-group-invariant LO interaction. We also performed coupled cluster calculations of the equation-of-state for symmetric nuclear matter and our results indicate that LO four-nucleon forces could play a crucial role for describing heavy-mass nuclei. The enhancement mechanism we found is very general and could be important also in other many-body problems.

Chiral effective field theory (χEFT) [1] promises a framework to incorporate pion physics—long believed to be important in nuclear physics—in an order-by-order improvable and renormalizable description of nuclear observables. The posited momentum scale where this EFT breaks down is in principle sufficiently high to control the interaction uncertainty for the entire nuclear chart and infinite nuclear matter. Few-nucleon forces emerge naturally in χEFT. The dramatic improvement in computational many-nucleon methods for the last couple of decades [2] now allows to quantitatively study the role and importance of such forces in nuclei well beyond the alpha particle [3].

When subjected to the organizing principle of Weinberg's power counting (WPC) [4, 5], Hamiltonians based on chiral two- (NN) and three-nucleon (NNN) forces typically describe few-nucleon systems well at sufficiently high orders [6, 7], but in most cases fail to predict essential bulk properties of finite nuclei as well as a realistic equation of state (EoS) of infinite matter [8–12]. Chiral interactions that accurately generate empirical saturation properties often provide a less accurate description of few-nucleon data [13]. The same problem is encountered when the $\Delta(1232)$ isobar—a relatively low-lying baryon excitation—is incorporated [14], albeit to a lesser degree [15, 16].

Though widely adopted, WPC is plagued by renormalizability problems [17] starting already at leading order (LO) [18–21], and persisting at higher orders [22–24]. Renormalization-group (RG) invariance can be achieved at LO with nonperturbative one-pion exchange restricted to low partial waves accompanied by contact interactions that are underestimated in WPC [18–21, 25]. Subleading corrections, to be treated in the distorted-wave Born approximation (DWBA) [26, 27], yield a reasonable description of NN data [28–33]. This renormalization approach, which we refer to as modified Weinberg's power counting (MWPC), provides realistic LO and next-to-LO (NLO) predictions of the ^{3}H and ^{3,4}He ground-state properties [34, 35]. However, these RG-invariant NN interactions predict unstable ground states in heavier nuclei such as ^{6}Li and ^{16}O [35]—an unrealistic feature also encountered [36–38] in lower-energy pionless EFT [1]. Although the slow convergence in the NN $^1S_0$ channel [39] can be mitigated with a dynamical dibaryon field [40] (which can also account for the amplitude zero [41]), the resulting energy-dependent potential makes it difficult to solve the many-nucleon Schrödinger equation in practice. A separable, and momentum-dependent, formulation (SEP) of the $^1S_0$ dibaryon potential [40] unfortunately yields results comparable to MWPC [35]. In summary, it appears that existing RG-invariant LO interactions in χEFT are deficient.

A common feature of existing power-counting schemes is that few-nucleon forces enter at subleading orders. The LO role of an NNN force [42] in pionless EFT led the authors of Refs. [43, 44] to promote a contact NNN interaction to LO also in χEFT. However, one would like to understand the promotion or demotion of interactions either on the basis of the RG coupled to naturalness [45] or another power-counting argument. In contrast to pionless EFT, the trinucleon system is RG invariant without NNN forces in χEFT up to NLO with either MWPC or SEP [34, 35].

Conspicuously absent from the application of EFT to heavier nuclei so far is any attempt to account for factors
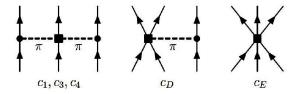
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Figure 1. Leading NNN interaction diagrams of pion-, pion-short, and short-range with LECs $c_{1,3,4}$, c_D, and c_E, respectively.

of the mass number $A \gg 1$ [46]. In this paper we put forward a combinatorial argument for promoting many-nucleon forces to LO as A increases. We also examine the quantitative consequences of this promotion for the description of ^{16}O, ^{40}Ca, and the EoS for symmetric nuclear matter (SNM).

Existing power-counting schemes rely on a perturbative expansion in the ratio $Q/M_{\mathrm{hi}} \ll 1$, where Q represents low-momentum scales and $M_{\mathrm{hi}} \lesssim 1$ GeV is the χEFT breakdown scale associated with nonperturbative QCD physics. The relevant low-momentum scales include the typical momentum p of a nuclear process, the pion mass $m_\pi \simeq 140$ MeV, and the pion decay constant $f_\pi \simeq 93$ MeV, which are normally assumed to be similar: $Q \sim f_\pi \sim m_\pi \sim p$. Here, for simplicity, we consider Deltaless χEFT, so formally considering the Delta-nucleon mass difference to be a high-energy scale like the nucleon mass $m_N \simeq 940$ MeV.

The size of multi-nucleon forces is usually estimated from "naive dimensional analysis" (NDA) [47–50], according to which a generic $2a$-nucleon, p-pion operator in the Lagrangian is

$$O_a = f_\pi^2 M_{\mathrm{hi}}^2 \left(\frac{m_\pi}{M_{\mathrm{hi}}}\right)^{2m} \left(\frac{\nabla}{M_{\mathrm{hi}}}\right)^d \left(\frac{\pi}{f_\pi}\right)^p \left(\frac{N^\dagger N}{f_\pi^2 M_{\mathrm{hi}}}\right)^a ,$$

(1)

where m and d are non-negative integers whose values are constrained by chiral symmetry and Lorentz invariance implemented in a Q/M_{hi} expansion. An n-nucleon force is constructed from combinations of O_a operators with $a \leq n$. The leading NNN forces consist of pion-, pion-short-, and short-range components [51, 52], as shown in Fig. 1. The $d = m = 0$ NNN and four-nucleon (NNNN) contact forces have low-energy constants (LECs) with additional factors of $(f_\pi^2 M_{\mathrm{hi}})^{2-a}$ relative to the LO NN forces. Five- and more-nucleon contact forces must, on spin-isospin considerations, have $d > 0$, which leads to additional suppression by factors of p/M_{hi}. At the same time, the importance of n-nucleon forces can be enhanced in an A-nucleon system by combinatorial factors as there are more ways to construct such interactions for $2 < n \lesssim A/2$. The simplest estimate of the contribution from the n-nucleon interaction relative to the NN

interaction for heavy nuclei is given by

$$R_n \equiv \frac{_A C_n}{_A C_2} \left(\frac{\langle N^\dagger N \rangle}{f_\pi^2 M_{\mathrm{hi}}}\right)^{n-2} ,$$

(2)

where $_A C_n = A!/[n!(A-n)!]$ is the binomial coefficient and $\langle N^\dagger N \rangle$ is the single-nucleon density. As A increases, both the combinatorial factor and the density of nucleons will increase. Approximating $\langle N^\dagger N \rangle$ by the saturation density $\rho_0 \simeq 0.16\,\mathrm{fm}^{-3}$, the relative contribution of NNN forces is $R_3 \sim A\rho_0/(3f_\pi^2 M_{\mathrm{hi}})$. Thus one might expect these forces to become as important as the NN force for $A \sim 3f_\pi^2 M_{\mathrm{hi}}/\rho_0$, which for a breakdown scale in the range $0.5 \lesssim M_{\mathrm{hi}}/\mathrm{GeV} \lesssim 1$ translates into a mass-number range $10 \lesssim A \lesssim 20$. Likewise, the NNNN force becomes comparable to the NNN force for $13 \lesssim A \lesssim 25$.

A similar estimate, but not limited to short-range operators, results from a diagrammatic analysis, where we count pion propagators as Q^{-2}, nucleon propagators as $m_N Q^{-2}$, and the loop measure involving nucleons as $Q^5 (4\pi m_N)^{-1}$. In this case, the penalty for the connection to an additional nucleon is Q/M_{hi} [1], in agreement with the power counting of Friar [53]. Combined with NDA, it leads to a suppression factor of $(Q/M_{\mathrm{hi}})^2$ instead of $\rho_0/(f_\pi^2 M_{\mathrm{hi}})$, for the leading short-range few-nucleon forces. The two estimates are numerically consistent if Q for nuclear matter is larger than f_π by a factor $\simeq 3$. If one uses instead Weinberg's estimate [5], where the penalty for the connection to an additional nucleon is $(Q/M_{\mathrm{hi}})^2$, the factor is instead $\simeq 4$. This argument suggests all leading three-nucleon forces are comparable.

These estimates suffer from a number of caveats. For one, they rely on NDA, which is based on purely perturbative arguments and is known to fail in the nuclear context where LO interactions must be treated nonperturbatively [45]. For example, renormalization of LO one-pion exchange in the NN $^1S_0$ channel requires an interaction with $a = 2$, $m = 1$, $d = 0$, and $p = 0$ [18, 19], which by Eq. (2) would appear only at next-to-NLO (N^{2}LO). This interaction is linked by chiral symmetry to a $p = 2$ interaction, and when the two pions are attached to two other nucleons it generates an enhanced NNNN force. Even with NDA, the leading NNNN forces [54] are not purely short ranged and are potentially more important than estimates on the basis of its short-range components. On the other hand, detailed spin-isospin structure might reduce the appearance of certain higher-body forces, particularly those involving pion exchange. Moreover, the critical values of A where few-nucleon forces enter tend to be shifted to higher values as saturation densities are not reached until $A \sim 60$ and the number of interacting nucleons is effectively limited by saturation.

A more reliable estimate of the importance of few-nucleon forces comes from numerical calculations. Throughout this work we start from the state-of-the-art LO and RG-invariant NN interactions MWPC40 and

SEP40 constructed in Ref. [35]. The relevant LECs are fitted to reproduce the deuteron energy $E(^2\text{H}) = -2.22$ MeV and the P-wave phase shifts of the Nijmegen analysis [55] up to laboratory energy $T_{\text{lab}} \approx 40$ MeV (center-of-mass momentum $p_{\text{cm}} = m_\pi$). The additional S-wave LEC in SEP40 is fitted to reproduce the $^1S_0$ effective range $r_0 = 2.7$ fm. For the NNN interactions we consider the diagrams from Deltaless χEFT in Fig. 1. We work in momentum space and employ a non-local super-Gaussian regulator in terms of relative nucleon momenta.

The few-nucleon calculations presented in this work were carried out using the Jacobi-coordinate formulation of the no-core shell-model [56, 57]. The ^{3}H (^{4}He) predictions were obtained in a harmonic-oscillator model space encompassing 41 (21) oscillator shells—that is $N_{\text{max}} = 40\,(20)$—and with an oscillator frequency $\hbar\omega = 36$ MeV. We find that the results are convergent with respect to N_{max} to within 1% for regulator-cutoff values in the range $\Lambda = 450 - 550$ MeV.

For predicting the properties of ^{16}O, ^{40}Ca and SNM we employed the coupled-cluster (CC) method [58–60]. For ^{16}O and ^{40}Ca our CC calculations started from a Hartree-Fock reference state expanded in a harmonic-oscillator basis consisting of up to 17 major shells ($N_{\text{max}} = 16$). The NNN force had an additional energy cut of $E_{3\text{max}} = 16\,\hbar\omega$, and to achieve convergent results we determined the optimal oscillator frequency for each model space. Furthermore, the NNN force was approximated at the normal-ordered two-body level (NO2B) which has been shown to be accurate for light- and medium-mass nuclei [61, 62]. The CC calculations were performed at the Λ-CCSD(T) approximation level which includes single-, double-, and perturbative triple-particle-hole excitations [63]. For the Λ-CCSD(T) calculations of ^{16}O we conservatively estimate that the energies are converged to within 1% (10%) for the regulator cutoffs $\Lambda = 450, 500$ (550) MeV, respectively. The calculations of SNM were done in the CCD(T) approximation with $A = 132$ nucleons placed in a momentum-space cubic lattice with $(2n_{\text{max}} + 1)^3$ mesh points for $n_{\text{max}} \leq 4$ and periodic boundary conditions [64]. Again, we approximated the NNN interaction at the NO2B level, and from calculations reported in Ref. [64] using interactions with similar cutoffs and regulators we estimate that the effects of residual NNN forces is at the order of $E/A \sim 1$ MeV for the densities considered in this work.

To gauge the effects of chiral NNN forces at LO in large-A nuclei, we first explored leading pion-range forces governed by the πN LECs $c_{1,3,4}$. With $c_{1,3,4} = -0.74, -3.61, 2.17$ GeV^{-1}, as inferred from πN scattering data in Ref. [65], the net NNN contribution is repulsive in ^{16}O, at least up to the highest cutoff (550 MeV) for which we can reliably perform CC calculations. A similar result was obtained with $c_{1,3,4}$ values from resonance saturation with the $\Delta(1232)$, which mimic the effects of the Fujita-Miyazawa force [66] expected to be dominant in

Deltaful χEFT [1]. However, a net attractive NNN force is required at LO, in MWPC, to generate a ^{16}O ground state that is also stable with respect to decay into four α particles. We are thus led to consider also the shorter-range components of the leading NNN interactions.

When we nonperturbatively include only the contact NNN interaction and fit the relevant LEC, c_E, to reproduce the triton ground-state energy $E(^3\text{H}) = -8.48$ MeV, we find that the ^{4}He binding energy increases without any sign of convergence with respect to increasing regulator cutoff, due to the singular and attractive c_E interaction at cutoffs $\gtrsim 550$ MeV. This is in stark contrast with pionless EFT, where a contact NNN force that ensures ^{3}H renormalization yields convergent results also for ^{4}He [67]. However, we are able to find convergent results when adding also the combined pion and short-range interaction with LEC c_D.

It is desirable to renormalize the combination of c_D and c_E to observables of nuclei where the NNN force can be considered LO but NNNN forces are not yet significant. Unfortunately, this will unavoidably involve non-trivial calculations of light-mass, open-shell nuclei. Since estimating $c_{D,E}$ using observables obeying few-nucleon universality, such as $A = 3, 4$ binding energies [68, 69], leads to highly degenerate solutions, we adopt instead the following procedure. First, we calculate the DWBA contributions to ^{3}H and ^{4}He from each of the NNN interaction terms. The perturbative treatment stems from our expectation of a small contribution from NNN interactions in few-nucleon systems. Indeed, it turns out that the net contribution from the $c_{1,3,4}$ diagrams to the binding energy is $\leq 10\%$. We then estimate a range for $c_{D,E}$ such that the sum of their DWBA contributions, $\langle V_{c_D} \rangle_A + \langle V_{c_E} \rangle_A$, does not exceed the expected magnitude of an N^{2}LO correction according to NDA, which we conservatively estimate as $\sim 1/6$ of the corresponding binding energy $|E_A|$ assuming $Q/M_{\text{hi}} \approx 1/3$ [70]. That is, we impose

$$|\langle V_{c_D} \rangle_A + \langle V_{c_E} \rangle_A| \leq \frac{|E_A|}{6}, \quad A = 3, 4. \qquad (3)$$

The allowed ranges are indicated as filled regions in Fig. 2 for the two NN interactions MWPC40 and SEP40. Expecting a non-negligible contribution from the NNN forces for larger A, we add the $c_{D,E}$ NNN interactions nonperturbatively in the ^{16}O CC calculations. We infer a (narrow) range of values of $c_{D,E}$ values (solid lines in Fig. 2) for which the predicted ground-state energy falls within 10% of the experimental value $E(^{16}\text{O}) \simeq -128$ MeV, only limited by a conservative CC method error and neglecting the EFT truncation error.

An overlap between the two constraints on $c_{D,E}$ exists in the cutoff range we were able to test and for values consistent with naturalness expectations. The solid lines shrink to the dots in Fig. 2 if $c_{D,E}$ interactions are treated nonperturbatively to reproduce the experimental values
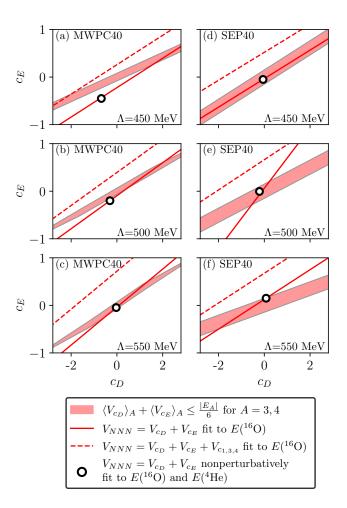
Figure 2. Inferred values of the NNN LECs $c_{D,E}$ at various cutoff Λ values for the NN potentials MWPC40 in panels (a)-(c) and SEP40 in panels (d)-(f).

Figure 3. Ground-state energy E of ^{16}O as a function of the cutoff Λ. CC results at three different cutoffs are marked with diamonds and connected with solid lines. Results from NN-only interactions are shown in panels (a) and (c) and from NN+NNN ($c_{D,E}$) in panels (b) and (d). The NN potential MWPC40 (SEP40) is used in the top (bottom) panels. The experimental energy (theoretical four-α threshold) is denoted by a dashed (dotted) line.

of $E(^3$H$)$, $E(^4$He$)$ and $E(^{16}$O$)$. Since most of the dots reside rather close to the filled regions, one could treat the $c_{D,E}$ NNN forces nonperturbatively also in $A = 3, 4$ nuclei without significant consequences. When additionally promoting the pion-range NNN force it is also possible to find $c_{D,E}$ values for which $E(^{16}$O$)$ falls within 10% of experiment. However, the repulsive character of this NNN force shifts the $c_{D,E}$ parametrization to the dashed lines in Fig. 2, which do not always overlap with the range of values (filled regions) that reproduce few-nucleon binding energies. Since Eq. (3) is merely an estimate, we cannot rule out the inclusion of pion-range NNN forces at LO completely. Nevertheless, in the following we analyze the role of NNN forces in many-nucleon systems using a minimal set of NNN interaction terms proportional the smallest values of $c_{D,E}$ in the overlap between the solid line and the filled area.

In Fig. 3(a),(c) we display the CC results for $E(^{16}$O$)$ without the $c_{D,E}$ NNN interactions. The NN-only results based on MWPC40 and SEP40 at LO [35] exhibit a strong cutoff dependence, and the former interaction
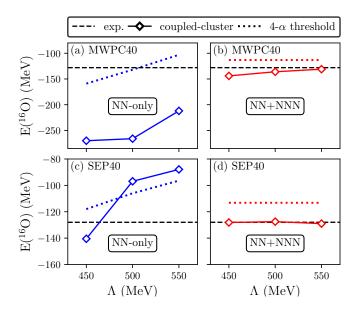
yields tremendous overbinding. For SEP40 and $\Lambda \gtrsim 500$ MeV, the ^{16}O ground state becomes energetically unstable with respect to decay into four α particles. In fact, the MWPC40 and SEP40 NN-only interactions also generate HF single-nucleon states that are starkly different from canonical shell-model expectations and allow, as we have verified numerically, for a deformed ^{16}O ground state [35]. Clearly, CC calculations including the minimal set of NNN interactions yield significantly improved results, see Fig. 3(b),(d). Both cutoff dependence and stability with respect to four-α breakup are rather satisfactory throughout the examined cutoff range, especially for an EFT at LO. In fact, this is the first time a realistic ^{16}O ground state is obtained with an EFT at LO. For the same set of NN+NNN interactions, we calculated the ^{40}Ca ground-state energy and we obtain predictions within 15% of the experimental value. For this nucleus we also estimated the CC method error $\lesssim 10\%$ up to $\Lambda = 500$ MeV. Although the ^{40}Ca ground state is below the 10-α threshold, the HF single-particle spectrum implies that this state is highly deformed, a feature similar to the NN-only prediction for the ^{16}O ground state [35]. This indicates the need for either a fine-tuning in LECs or NNNN forces, as suggested by Eq. (2). Note that N^{2}LO lattice calculations under WPC finds that an $SU(4)$-symmetric NNNN force is needed for accurate binding in α-particle nuclei [71].

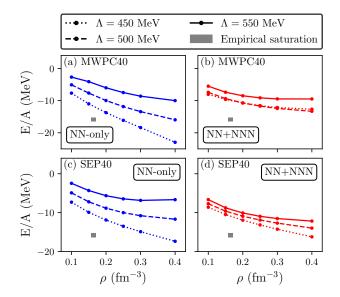To say something about LO predictions of larger-A nu-

Figure 4. Energy per nucleon (E/A) of SNM as a function of density (ρ) for various cutoff values Λ and the same interactions as in Fig. 3. The empirical saturation region [75] is marked by a grey square.

clear systems we calculated the EoS of SNM based on the NN+NNN interactions devised in this work. The predictions are shown in Fig. 4 for NN-only and NN+NNN forces. In most cases there is a rather strong cutoff dependence, qualitatively similar to the LO results in Ref. [72], and we detect no clear indication of saturation from our NN-only calculations, except with the SEP40 interaction at $\Lambda = 550$ MeV (albeit far from the empirical region). Including NNN ($c_{D,E}$) forces improves the convergence of the EoS results with Λ, however, it does not improve agreement with empirical EoS value, at least for $\Lambda \leq 550$ MeV. Moreover, even if one adds a generous $2-3$ MeV uncertainty, the NN+NNN results for the EoS will still be rather far from the empirical saturation point. We have verified that inclusion of (repulsive) pion-range NNN forces does not offer any improvement either. Calculations with very high-order NN-only [73] or NN+NNN [74] interactions in WPC also struggle to reproduce empirical saturation properties. Unless there are substantial changes at cutoff values currently accessible only in more approximate calculations [72], NNNN forces are likely to be needed at LO for describing large-A nuclei.

In conclusion, we found that NNN forces are crucial for a realistic LO description of the ^{16}O ground-state energy, and NNNN forces are likely to be needed in larger-A nuclei and to attain a realistic EoS for SNM. Our findings point to a missing ingredient in χEFT power counting—namely the dependence on mass number A through a combinatorial enhancement of few-body forces—that could be essential for making model-independent and reliable predictions of nuclear systems. Moreover, the en-

hancement mechanism of many-body forces found in this work is very general and could have foundational implications in fields other than low-energy nuclear physics.

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