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# Chiral Three-Nucleon Interactions in Light Nuclei, Neutron- $\alpha$ Scattering, and Neutron Matter

J. E. Lynn,<sup>1,\*</sup> I. Tews,<sup>2,3</sup> J. Carlson,<sup>1</sup> S. Gandolfi,<sup>1</sup> A. Gezerlis,<sup>4</sup> K. E. Schmidt,<sup>5</sup> and A. Schwenk<sup>2,3</sup>

<sup>1</sup>*Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*

<sup>2</sup>*Institut für Kernphysik, Technische Universität Darmstadt, 64289 Darmstadt, Germany*

<sup>3</sup>*ExtreMe Matter Institute EMMI, GSI Helmholtzzentrum für Schwerionenforschung GmbH, 64291 Darmstadt, Germany*

<sup>4</sup>*Department of Physics, University of Guelph, Guelph, Ontario, N1G 2W1, Canada*

<sup>5</sup>*Department of Physics, Arizona State University, Tempe, Arizona 85287, USA*

We present quantum Monte Carlo calculations of light nuclei, neutron- $\alpha$  scattering, and neutron matter using local two- and three-nucleon (3N) interactions derived from chiral effective field theory up to next-to-next-to-leading order (N<sup>2</sup>LO). The two undetermined 3N low-energy couplings are fit to the <sup>4</sup>He binding energy and, for the first time, to the spin-orbit splitting in the neutron- $\alpha$   $P$ -wave phase shifts. Furthermore, we investigate different choices of local 3N operator structures and find that chiral interactions at N<sup>2</sup>LO are able to simultaneously reproduce the properties of  $A = 4, 5$  systems and of neutron matter, in contrast to commonly used phenomenological 3N interactions.

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Three-nucleon (3N) interactions are essential for a reliable prediction of the properties of light nuclei and nucleonic matter [1–5]. In quantum Monte Carlo (QMC) calculations phenomenological 3N interactions such as the Urbana [6] and Illinois [7] models have been used with great success [3, 8]. However, such models suffer from certain disadvantages: They are not based on a systematic expansion and it was found that the Illinois forces tend to overbind neutron matter [9, 10]. It is therefore unlikely that these phenomenological models can be used to correctly predict the properties of heavy neutron-rich nuclei.

An approach which addresses these shortcomings is chiral effective field theory (EFT) [2, 11–14]. Chiral EFT is a low-energy effective theory consistent with the symmetries of quantum chromodynamics and provides a systematic expansion for nuclear forces. It includes contributions from long-range pion-exchange interactions explicitly and expands the short-distance interactions into a systematic set of contact operators accompanied by low-energy couplings fit to experimental data. Chiral EFT enables the determination of theoretical uncertainties and systematic order-by-order improvement; for recent work see Refs. [15–18].

Chiral EFT also predicts consistent many-body interactions. In Weinberg power-counting, 3N forces first enter at next-to-next-to-leading order (N<sup>2</sup>LO) [19, 20] and contain three contributions: a two-pion-exchange interaction  $V_C$ , a one-pion-exchange-contact interaction  $V_D$  and a 3N contact interaction  $V_E$ . While the first is accompanied by the couplings  $c_i$  from the pion-nucleon sector, the latter two are accompanied by the couplings  $c_D$  and  $c_E$  which have to be determined in  $A > 2$  systems.

In addition to systematic nuclear forces, reliable many-body methods are required to describe properties of light nuclei and to determine the properties of dense neutron matter. QMC methods, which solve the many-

body Schrödinger equation stochastically, are such a class of methods. Both the Green’s function Monte Carlo (GFMC) method and the auxiliary-field diffusion Monte Carlo (AFDMC) method rely on projection in imaginary time  $\tau$ ,

$$\lim_{\tau \rightarrow \infty} e^{-H\tau} |\Psi_T\rangle \rightarrow |\Psi_0\rangle, \quad (1)$$

with  $H$  the Hamiltonian of the system, and  $|\Psi_T\rangle$  a trial wave function not orthogonal to the many-body ground state  $|\Psi_0\rangle$ . For a recent review of developments and applications of QMC in nuclear physics, see Ref. [3]. Recently, we have developed chiral EFT interactions for QMC calculations [21–24], which provide nonperturbative results for testing the chiral expansion scheme [22] and benchmarks for neutron matter up to high density [21, 23]. However, these studies were limited to two-nucleon (NN) interactions only or to an exploratory study of neutron matter with only the long-range parts of the 3N interaction.

In this Letter, we include consistent 3N interactions at N<sup>2</sup>LO in coordinate space [24] in GFMC calculations of light nuclei and  $n$ - $\alpha$  scattering, and AFDMC calculations of neutron matter. We fit the two couplings  $c_D$  and  $c_E$  to the <sup>4</sup>He binding energy and low-energy  $n$ - $\alpha$  scattering  $P$ -wave phase shifts. The latter system has been studied using various approaches, see for example Refs. [25–27]. These observables are expected to be less correlated than fits to structure properties of  $A = 3, 4$  systems because the spin-orbit and  $T = \frac{3}{2}$  components of the 3N interaction enter directly.

In phenomenological 3N models, any short-range parts which arise from the Fourier transformation of pion exchanges are typically absorbed into other short-distance structures: we retain these explicitly. We choose the 3N cutoff  $R_{3N} = R_0$ , where  $R_0$  is the NN cutoff, and vary the cutoff in the range  $R_0 = 1.0 - 1.2$  fm [21–24]. Note that with a finite cutoff certain ambiguities appear including

the specific operator form associated with the shorter-

range interactions. In the Fourier transformation of  $V_D$  two possible operator structures arise:

$$V_{D1} = \frac{g_{ACD}m_\pi^2}{96\pi\Lambda_\chi F_\pi^4} \sum_{i<j<k} \sum_{\text{cyc}} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k \left[ X_{ik}(\mathbf{r}_{kj})\delta_{R_{3N}}(\mathbf{r}_{ij}) + X_{ik}(\mathbf{r}_{ij})\delta_{R_{3N}}(\mathbf{r}_{kj}) - \frac{8\pi}{m_\pi^2} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_k \delta_{R_{3N}}(\mathbf{r}_{ij})\delta_{R_{3N}}(\mathbf{r}_{kj}) \right], \quad (2a)$$

$$V_{D2} = \frac{g_{ACD}m_\pi^2}{96\pi\Lambda_\chi F_\pi^4} \sum_{i<j<k} \sum_{\text{cyc}} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k \left[ X_{ik}(\mathbf{r}_{ik}) - \frac{4\pi}{m_\pi^2} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_k \delta_{R_{3N}}(\mathbf{r}_{ik}) \right] \left[ \delta_{R_{3N}}(\mathbf{r}_{ij}) + \delta_{R_{3N}}(\mathbf{r}_{kj}) \right], \quad (2b)$$

where  $X_{ik}(\mathbf{r}) = [S_{ik}(\mathbf{r})T(r) + \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_k]Y(r)$  is the coordinate-space pion propagator,  $S_{ik}(\mathbf{r}) = 3\boldsymbol{\sigma}_i \cdot \hat{\mathbf{r}}\boldsymbol{\sigma}_k \cdot \hat{\mathbf{r}} - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_k$  is the tensor operator, and the tensor and Yukawa functions are defined as  $T(r) = 1 + 3/(m_\pi r) + 3/(m_\pi r)^2$  and  $Y(r) = e^{-m_\pi r}/r$ . The smeared-out delta function  $\delta_{R_{3N}}(\mathbf{r}) = \frac{1}{\pi\Gamma(3/4)R_{3N}^3} e^{-(r/R_{3N})^4}$  and the long-range regulator multiplying  $Y$ ,  $f_{\text{long}}(r) = 1 - e^{-(r/R_{3N})^4}$  are consistent with the choices made in the NN interaction [21–24]. The sum  $i < j < k$  runs over all particles 1 to  $A$ , and the cyclic sum runs over the cyclic permutations of a given triple.

The two possible  $V_D$  structures agree in the limit of  $R_{3N} \rightarrow 0$ , because the delta functions then enforce  $i = j$  ( $k = j$ ) in the first (second) term, in which case Eqs. (2a) and (2b) would coincide. The  $V_D$  interaction does not distinguish which of the two nucleons in the contact participates in the pion exchange. The second choice  $V_{D2}$  can be obtained with the exchange of a fictitious heavy scalar particle between the two nucleons in the contact. This ambiguity was also pointed out in [28]. The differences between Eqs. (2a) and (2b) are regulator effects and therefore higher order in the chiral expansion, but it is important to investigate how they affect different observables at this order.

Similar effects arise in the 3N contact interaction  $V_E$ . Here, the main ambiguity is the choice of the 3N contact operator. The same Fierz-rearrangement freedom that allows for a selection of (mostly) local contact operators in the NN sector up to N<sup>2</sup>LO exists in the 3N sector at this order. Symmetry considerations allow the choice of one of the following six operators [20]:

$$\{\mathbb{1}, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k, [(\boldsymbol{\sigma}_i \times \boldsymbol{\sigma}_j) \cdot \boldsymbol{\sigma}_k][(\boldsymbol{\tau}_i \times \boldsymbol{\tau}_j) \cdot \boldsymbol{\tau}_k]\}. \quad (3)$$

The usual choice is  $\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$ . Here, we investigate two other choices: first with the operator  $\mathbb{1}$ , and second with a projector operator  $\mathcal{P}$  on to triples with  $S = \frac{1}{2}$  and  $T = \frac{1}{2}$ :

$$\mathcal{P} = \frac{1}{36} \left( 3 - \sum_{i<j} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \right) \left( 3 - \sum_{k<\ell} \boldsymbol{\tau}_k \cdot \boldsymbol{\tau}_\ell \right), \quad (4)$$

where the sums are over pairs in a given triple. In the infinite-momentum cutoff limit only these  $S = \frac{1}{2}, T = \frac{1}{2}$

triples would contribute to  $V_E$  due to the Pauli principle. Thus, in the following we will explore three possible structures:

$$V_{E\tau} = \frac{c_E}{\Lambda_\chi F_\pi^4} \sum_{i<j<k} \sum_{\text{cyc}} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k \delta_{R_{3N}}(\mathbf{r}_{kj})\delta_{R_{3N}}(\mathbf{r}_{ij}), \quad (5a)$$

$$V_{E\mathbb{1}} = \frac{c_E}{\Lambda_\chi F_\pi^4} \sum_{i<j<k} \sum_{\text{cyc}} \delta_{R_{3N}}(\mathbf{r}_{kj})\delta_{R_{3N}}(\mathbf{r}_{ij}), \quad (5b)$$

$$V_{E\mathcal{P}} = \frac{c_E}{\Lambda_\chi F_\pi^4} \sum_{i<j<k} \sum_{\text{cyc}} \mathcal{P} \delta_{R_{3N}}(\mathbf{r}_{kj})\delta_{R_{3N}}(\mathbf{r}_{ij}). \quad (5c)$$

We stress that there are more possible operator structures for  $V_D$  and  $V_E$ , which will be investigated in future work.

Having specified all 3N structures, we vary the values of the couplings  $c_D$  and  $c_E$  to fit the <sup>4</sup>He binding energy as shown in Fig. 1a. We display curves for  $V_{D1}$  and  $V_{D2}$  using  $V_{E\tau}$  and both cutoffs  $R_0 = 1.0$  fm and  $R_0 = 1.2$  fm. In addition, we show curves for  $V_{D2}$  using the other two possible  $V_E$  structures and the cutoff  $R_0 = 1.0$  fm. For all of these possibilities, the stars give the values for the couplings which also fit  $P$ -wave  $n$ - $\alpha$  scattering phase shifts as shown in Fig. 1b. The resulting couplings  $c_D$  and  $c_E$  are given in Table I. In all cases  $\langle V_E \rangle$  is repulsive in <sup>4</sup>He except for the case with  $(D2, E\tau)$  with the softer cutoff ( $R_0 = 1.2$  fm), where it is mildly attractive.

For  $R_0 = 1.0$  fm and  $V_{E\tau}$ ,  $c_D \approx 0$  and both forms of  $V_D$  simultaneously fit the <sup>4</sup>He binding energy and  $P$ -wave  $n$ - $\alpha$  scattering phase shifts (see Fig. 1b). However, in the softer-cutoff case  $R_0 = 1.2$  fm,  $V_{D1}$  and  $V_{D2}$  lead to different couplings. For  $V_{D1}$ , the splitting between the two  $P$  waves appears to saturate in  $c_D$  for values of  $c_D > 2$ , e.g., the  $P \frac{3}{2}^-$  phase shift for  $c_D = 2.0, 3.0,$  and  $5.0$  at  $E_{\text{cm}} = 1.3$  MeV are each  $\sim 75$  deg., which is  $\sim 35$  deg. below the  $R$ -matrix value. Since we cannot fit the  $P$ -wave  $n$ - $\alpha$  scattering phase shifts in this case ( $V_{D1}$  and  $R_0 = 1.2$  fm) we do not consider it in the following. Instead for  $V_{D2}$  and  $R_0 = 1.2$  fm, the splitting can be fit, as is evident from Fig. 1b. For  $V_{D2}$  using  $V_{E\mathbb{1}}$  or  $V_{E\mathcal{P}}$  and  $R_0 = 1.0$  fm, both the <sup>4</sup>He binding energy and the  $P$ -wave  $n$ - $\alpha$  scattering phase shifts can be simultaneously fit: we show only the case with  $V_{E\mathcal{P}}$  in Fig. 1b. There we also show the NLO results which are a clear indication that 3N

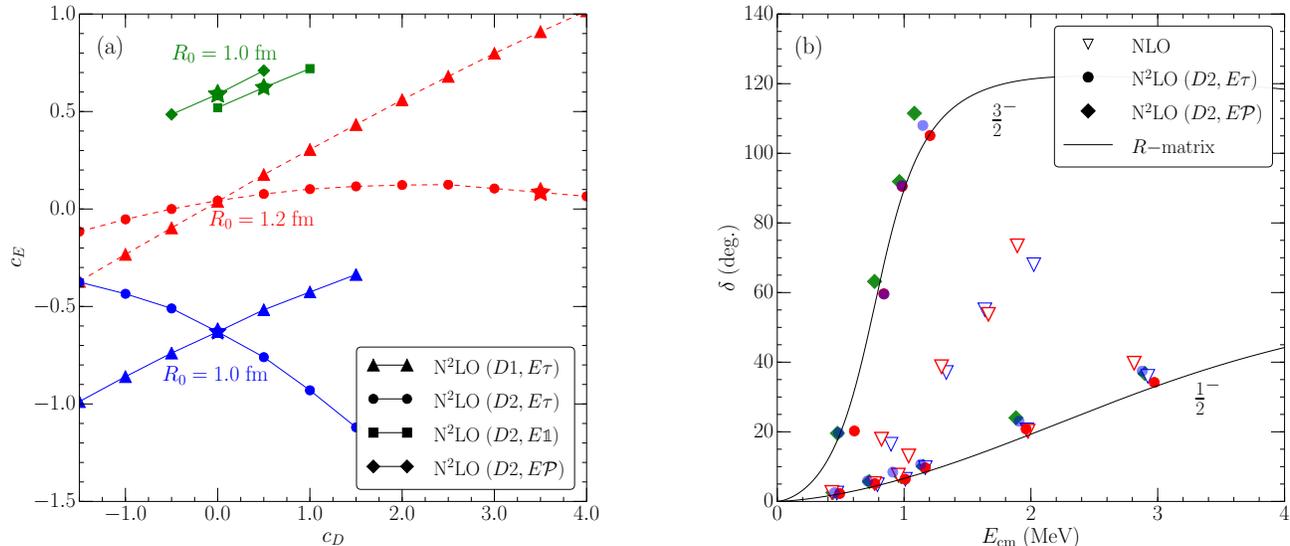


FIG. 1. (color online). (a) Couplings  $c_E$  vs.  $c_D$  obtained by fitting the  ${}^4\text{He}$  binding energy for different 3N-operator forms. Triangles are obtained by using  $V_{D1}$  and  $V_{E\tau}$  while the other symbols are obtained for  $V_{D2}$  and three different  $V_E$ -operator structures. Blue and green lines (lower and upper) correspond to  $R_0 = 1.0$  fm, while red lines (central) correspond to  $R_0 = 1.2$  fm. The GFMC statistical errors are smaller than the symbols. The stars correspond to the values of  $c_D$  and  $c_E$  which simultaneously fit the  $n$ - $\alpha$   $P$ -wave phase shifts (see Table I and right panel). No fit to both observables can be obtained for the case with  $R_0 = 1.2$  fm and  $V_{D1}$ . (b)  $P$ -wave  $n$ - $\alpha$  elastic scattering phase shifts compared with an  $R$ -matrix analysis of the data. Colors and symbols correspond to the left panel. We also include phase shifts calculated at NLO, which clearly indicate the necessity of 3N interactions to fit the  $P$ -wave splitting.

TABLE I. Fit values for the couplings  $c_D$  and  $c_E$  for different choices of 3N forces and cutoffs.

$V_{3N}$	$R_0$ (fm)	$c_E$	$c_D$
$N^2\text{LO}(D1, E\tau)$	1.0	-0.63	0.0
	1.2	-	-
$N^2\text{LO}(D2, E\tau)$	1.0	-0.63	0.0
	1.2	0.09	3.5
$N^2\text{LO}(D2, E\perp)$	1.0	0.62	0.5
$N^2\text{LO}(D2, EP)$	1.0	0.59	0.0

forces are necessary to properly describe  $n$ - $\alpha$  scattering. Similar results have been found in Ref. [29–31]. Because  $A = 3, 4$  systems are largely insensitive to odd-parity partial waves, we find no significant dependence on the choice of structures in  $V_D$ . However, our results in  $n$ - $\alpha$   $P$ -wave scattering show a substantial sensitivity:  $V_{D1}$  appears to have a smaller effect than  $V_{D2}$ .

In Fig. 2, we show ground-state energies and point-proton radii for  $A = 3, 4$  nuclei at NLO and  $N^2\text{LO}$  using  $V_{D2}$  and  $V_{E\tau}$  for  $R_0 = 1.0$  fm and  $R_0 = 1.2$  fm in comparison with experiment. The ground-state energies of the  $A = 3$  systems compare well with experimental values.

The ground-state energy of  ${}^4\text{He}$  is used in fitting  $c_D$  and  $c_E$ , and so is forced to match the experimental value to within  $\approx 0.03$  MeV. The point-proton radii also compare well with values extracted from experiment. The theoretical uncertainty at each order is estimated through the expected size of higher-order contributions, see Ref. [32] for details. We include results from LO, NLO, and  $N^2\text{LO}$  in the analysis using the Fermi momentum and the pion mass as the small scales for neutron matter and nuclei, respectively. The error bars presented here are comparable to those shown in Ref. [33], although it is worth emphasizing that our calculations represent a complete estimate of the uncertainty at  $N^2\text{LO}$  since we include 3N interactions. Other choices for 3N structures give similar results.

It is noteworthy that NN and 3N interactions derived from chiral EFT up to  $N^2\text{LO}$  have sufficient freedom such that  $n$ - $\alpha$  scattering phase shifts in Fig. 1b and properties of light nuclei in Fig. 2 can be simultaneously described. The failures of the Urbana IX model in underbinding nuclei and underpredicting the spin-orbit splitting in neutron-rich systems including the  $n$ - $\alpha$  system were among the factors motivating the addition of the three-pion exchange diagrams in the Illinois of 3N models [7]. Our results show that chiral 3N forces at  $N^2\text{LO}$ ,

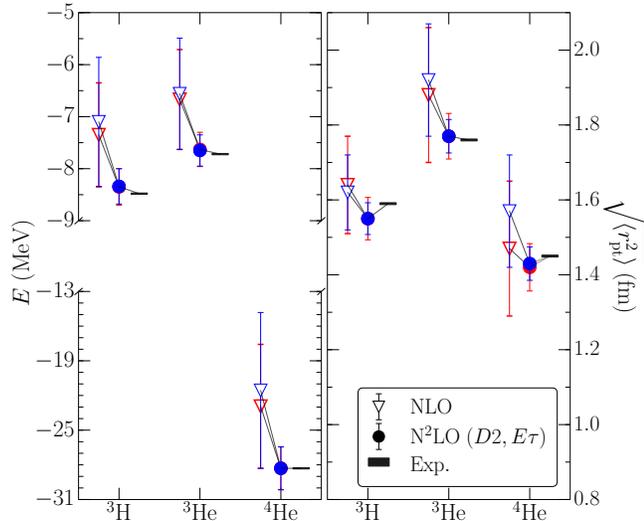


FIG. 2. (color online). Ground-state energies and point proton radii for  $A = 3, 4$  nuclei calculated at NLO and  $N^2$ LO (with  $V_{D2}$  and  $V_{E\tau}$ ) compared with experiment. Blue (red) symbols correspond to  $R_0 = 1.0$  fm ( $R_0 = 1.2$  fm). The errors are obtained as described in the text and also include the GFMC statistical uncertainties.

including the shorter-range parts in the pion exchanges, allow the simultaneous fit. These interactions should be tested further in light  $p$ -shell nuclei.

Finally, we study the full chiral  $N^2$ LO forces, including all 3N contributions, in neutron matter to extend the results from Ref. [24]. More specifically, we examine the effects of different  $V_D$  and  $V_E$  structures on the equation of state of neutron matter. Although these terms vanish in the limit of infinite cutoff, they contribute for finite cutoffs. In Fig. 3 we show results for the neutron matter energy per particle as a function of the density calculated with the AFDMC method as described in Refs. [3, 34, 35]. We show the energies for  $R_0 = 1.0$  fm for the NN and full 3N interactions. We use  $V_{D2}$  and the three different  $V_E$  structures:  $V_{E\tau}$  (blue band),  $V_{E1}$  (red band), and  $V_{EP}$  (green band). The error bands are determined as in the light nuclei case. The  $V_{EP}$  interaction fits  $A = 4, 5$  with a vanishing  $c_D$ , hence this choice of  $V_E$  leads to an equation of state identical to the equation of state with  $NN + V_C$  as in Ref. [24] (the projector  $\mathcal{P}$  is zero for pure neutron systems) and qualitatively similar to previous results using chiral interactions at  $N^2$ LO [36] and  $N^3$ LO [37].

As discussed, the contributions of  $V_D$  and  $V_E$  are only regulator effects for neutrons. However, they are sizable and result in a larger error band. At saturation density  $n_0 \sim 0.16$  fm $^{-3}$  the difference of the central value of

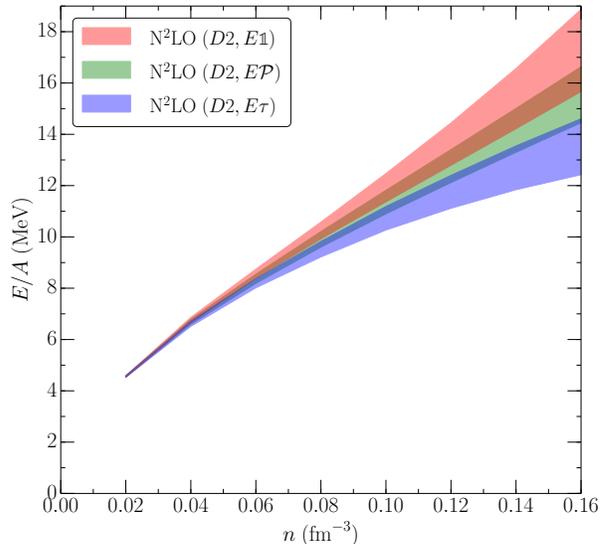


FIG. 3. (color online). The energy per particle in neutron matter as a function of density for the NN and full 3N interactions at  $N^2$ LO with  $R_0 = 1.0$  fm. We use  $V_{D2}$  and different 3N contact structures: the blue band corresponds to  $V_{E\tau}$ , the red band to  $V_{E1}$  and the green band to  $V_{EP}$ . The green band coincides with the  $NN + 2\pi$ -exchange-only result because both  $V_D$  and  $V_E$  vanish in this case. The bands are calculated as described in the text.

the energy per neutron after inclusion of the 3N contacts  $V_{E1}$  or  $V_{E\tau}$  is  $\sim 2$  MeV, leading to a total error band with a range of  $\sim 6.5$  MeV when considering different  $V_E$  structures. This relatively large uncertainty can be qualitatively explained when considering the following effects. Because the expectation value  $\langle \sum_{i<j} \tau_i \cdot \tau_j \rangle$  has a sign opposite to that of the expectation value  $\langle \mathbb{1} \rangle$  in  ${}^4\text{He}$ ,  $c_E$  will also have opposite signs in the two cases to fit the binding energy. However, in neutron matter both operators are the same, spreading the uncertainty band. A similar argument was made in Ref. [38].

With the regulators used here, the Fierz-rearrangement invariance valid at infinite cutoff is only approximate at finite cutoff, and hence the different choices of  $V_D$  and  $V_E$  can lead to different results. The different local structures can lead to finite relative  $P$ -wave contributions. These can be eliminated by choosing  $V_{EP}$ , which has a projection onto even-parity waves (predominantly  $S$  waves). The usual nonlocal regulator in momentum-space does not couple  $S$  and  $P$  waves.

In conclusion, we find for the first time that chiral interactions can simultaneously fit light nuclei and low-energy  $P$ -wave  $n$ - $\alpha$  scattering and provide reasonable estimates for the neutron matter equation of state. Other

commonly used phenomenological 3N models do not provide this capability. These chiral forces should be tested in light  $p$ -shell nuclei, medium-mass nuclei, and isospin-symmetric nuclear matter to gauge their ability to describe global properties of nuclear systems.

We also find that the ambiguities associated with contact-operator choices can be significant when moving from light nuclei to neutron matter and possibly to medium-mass nuclei where the  $T = \frac{3}{2}$  triples play a more significant role. The reason for the sizable impact may be the regulators used here, which break the Fierz-rearrangement invariance, making further investigations of regulator choices a priority. The impact of these ambiguities in the contact operators can contribute to the uncertainties and needs to be studied further.

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\* E-mail: [joel.lynn@gmail.com](mailto:joel.lynn@gmail.com)

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