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Phys. Rev. C **97**, 024332 — Published 26 February 2018

DOI: [10.1103/PhysRevC.97.024332](https://doi.org/10.1103/PhysRevC.97.024332)

# $\Delta$ isobars and nuclear saturation\*

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We construct a nuclear interaction in chiral effective field theory with explicit inclusion of the  $\Delta$ -isobar  $\Delta(1232)$  degree of freedom at all orders up to next-to-next-to-leading order (NNLO). We use pion-nucleon ( $\pi N$ ) low-energy constants (LECs) from a Roy-Steiner analysis of  $\pi N$  scattering data, optimize the LECs in the contact potentials up to NNLO to reproduce low-energy nucleon-nucleon scattering phase shifts, and constrain the three-nucleon interaction at NNLO to reproduce the binding energy and point-proton radius of  $^4\text{He}$ . For heavier nuclei we use the coupled-cluster method to compute binding energies, radii, and neutron skins. We find that radii and binding energies are much improved for interactions with explicit inclusion of  $\Delta(1232)$ , while  $\Delta$ -less interactions produce nuclei that are not bound with respect to breakup into  $\alpha$  particles. The saturation of nuclear matter is significantly improved, and its symmetry energy is consistent with empirical estimates.

PACS numbers: 21.30.-x, 21.10.-k, 21.45.-v, 21.60.De

## I. INTRODUCTION

In recent years, *ab initio* calculation of atomic nuclei with predictive power have advanced from light [1–4] to medium-mass nuclei [5–9]. Such calculations are only as good as their input, i.e. nucleon-nucleon ( $NN$ ) and three-nucleon ( $NNN$ ) interactions, therefore the quest for more accurate and more precise nuclear potentials is an ongoing endeavor at the forefront of research [10–20]. Here, potentials from chiral effective field theory ( $\chi\text{EFT}$ ) – based on long-ranged pion exchanges and short-ranged contact interactions – play a dominant role [21, 22], because they are expected to deliver accuracy (via fit to data) and precision (via increasingly higher orders in the power counting). As it turns out, however, state-of-the-art  $\chi\text{EFT}$  potentials that are accurate for the lightest nuclei with masses  $A = 2, 3$  vary considerably in their saturation point for nuclear matter [14] and in their binding energy for heavier nuclei [20, 23, 24].

This sensitivity of the saturation point to the details of the  $\chi\text{EFT}$  interaction is not well understood [25] and also puzzling from an EFT perspective. A practical approach to this dilemma consists of constraining  $\chi\text{EFT}$  potentials to reproduce experimentally determined binding energies and charge radii of nuclei as heavy as oxygen [18]. In this work, we will follow a different approach and explicitly include the  $\Delta$  isobar  $\Delta(1232)$ , abbreviated  $\Delta$  in the fol-

lowing, as a low-energy degree of freedom in addition to pions ( $\pi$ ) and nucleons ( $N$ ). We recall that the  $\Delta$ - $N$  mass-splitting  $\delta \equiv M_\Delta - M_N \approx 293$  MeV is roughly twice the pion mass ( $M_\pi \sim 140$  MeV) and well below the expected breakdown scale of  $\chi\text{EFT}$  potentials [21, 22]. Furthermore, the  $\Delta$  also couples strongly to the  $\pi N$  system. For these reasons, the early chiral  $NN$  interactions [26–28] included the  $\Delta$  degree of freedom. Indeed, van Kolck as well as Bernard *et al.* showed that the low-energy constants (LECs) of the  $\pi N$  interaction in a  $\Delta$ -less  $\chi\text{EFT}$  receive a substantial contribution via resonance saturation. As nuclear interactions from  $\chi\text{EFT}$  with and without  $\Delta$ 's have a similar structure otherwise, only little effort was invested in producing quantitative  $\Delta$ -full  $\chi\text{EFT}$  potentials. We refer the reader to the reviews [21, 22] for extensive discussions of this topic.

Recently, Piarulli *et al.* produced minimally non-local  $\chi\text{EFT}$   $NN$  potentials at next-to-next-to-next-to leading order ( $\text{N}^3\text{LO}$ ), with  $\Delta$ 's included up to next-to-next-to leading order (NNLO), using values for the subleading  $\pi N$  LECs  $c_1, c_2, c_3, c_4$  from Ref. [31]. Dropping the non-local terms led to the local potentials of Ref. [32]. Two different approaches augmented these local potentials with  $NNN$  forces up to NNLO. The corresponding diagrams of the  $NNN$  force, some  $NN$  diagrams, and the most relevant LECs are shown in Fig. 1. Logoteta *et al.* adjusted the LECs  $c_D$  and  $c_E$  of the short-ranged  $NNN$  terms to reproduce the saturation point of nuclear matter. However, they did not report results for few-nucleon systems. In contrast, Piarulli *et al.* adjusted  $c_D$  and  $c_E$  to reproduce properties of nuclear systems with mass number  $A = 3$ . Their quantum Monte Carlo calculations yielded accurate results for spectra of light nuclei up to  $^{12}\text{C}$ . We note that the potentials by Logoteta *et al.* and Piarulli *et al.* employ values for  $c_D$  and  $c_E$  that differ in signs and magnitudes.

In this paper we present a systematic construction and comparative analysis of non-local  $\Delta$ -full and  $\Delta$ -less  $\chi\text{EFT}$  potentials at LO, NLO, and NNLO, and report re-

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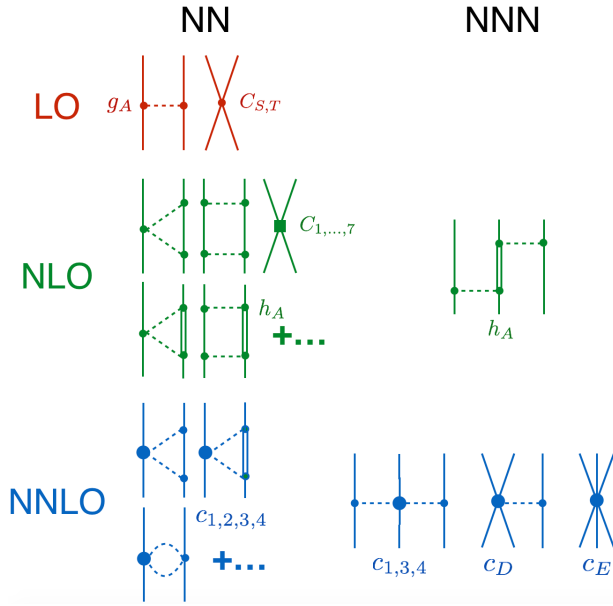


FIG. 1. (Color online) Schematic figure of relevant diagrams that enter in  $\Delta$ -full  $\chi$ EFT at leading order (LO), next-to-leading order (NLO), and next-to-next-to-leading order (NNLO). The leading  $\pi N$  and  $\pi N\Delta$  axial couplings are denoted by  $g_A$  and  $h_A$ , respectively. Note that there are no  $\Delta$  contributions at LO. At NLO, the  $NN$  contact interactions also remain unchanged. However, the leading-order  $NNN$  interaction, i.e. the well-known Fujita-Miyazawa term [35], appears at this order, see also Ref. [36]. The  $\Delta$  contributions to the  $NNN$  interaction at NNLO vanish due to the Pauli principle or are suppressed and demoted to a higher chiral order. Besides the subleading  $\pi N$  LECs  $c_1, c_2, c_3, c_4$ , the  $NNN$  diagrams contain two additional LECs;  $c_D$  and  $c_E$ .

sults for light- and medium-mass nuclei, and infinite nucleonic matter. We constrain the relevant short-ranged LECs using experimental data from nuclear systems with mass numbers  $A = 2, 4$  and use  $\pi N$  LECs determined in a recent high-precision analysis [37] based on the Roy-Steiner equations [38]. We do not include any additional contact operators beyond NNLO in Weinberg power counting. We find that the resulting  $\Delta$ -full potentials yield accurate charge radii and much improved binding energies for medium mass nuclei, and reproduce the saturation point of symmetric nuclear matter within estimated EFT-truncation errors. Furthermore, estimates of the EFT-truncation errors furnish a discussion of the improved convergence rate of the  $\Delta$ -full  $\chi$ EFT expansion compared to the  $\Delta$ -less theory.

## II. OPTIMIZATION OF INTERACTIONS

To isolate the effects of the  $\Delta$  isobar in the description of the saturation properties of nucleonic matter we compare our results with  $\Delta$ -less  $\chi$ EFT potentials at LO, NLO, and NNLO. Other than the inclusion of

the  $\Delta$ -isobar, the  $\Delta$ -full and the  $\Delta$ -less interactions are constructed following identical optimization protocols. For the description of the interaction we build on work [26, 31, 36, 39, 40] and treat the  $\Delta$ - $N$  mass difference  $\delta \equiv M_\Delta - M_N$  as an additional small scale. A power-counting for this approach is provided by the so-called small-scale expansion [39]. This is identical to the conventional heavy-baryon formulation of  $\chi$ EFT which is already used for including the nucleon mass-scale without any  $\Delta$  isobars. The  $\Delta$ -less pion-exchanges in the  $NN$  sector up to NNLO are given in Ref. [16]. The expressions for the  $NN$  contact potentials at LO and NLO are given in e.g. Ref. [22], and the  $\Delta$  contributions to the leading and sub-leading  $2\pi$ -exchanges in the  $NN$  potential are from Ref. [31]. Charge-independence breaking terms are included in the LO contact LECs as well as the one-pion exchange. Following Ref. [41] we remove all contributions that are proportional to the subleading  $\pi N\Delta$  coupling  $b_3 + b_8$  by renormalizing the  $\pi N\Delta$  axial coupling  $h_A$  and the subleading  $\pi N$  couplings  $c_{2,3,4}$ . We follow Siemens *et al.* and use  $h_A = 1.40$ ,  $g_A = 1.289$ , and the central Roy-Steiner values of the  $\pi N$  LECs for the  $\Delta$ -full and  $\Delta$ -less potentials up to third order. We recall that  $\Delta$ -less  $\chi$ EFT potentials often employ  $\pi N$  LECs with values that differ from what is found in  $\pi N$  scattering, because the absence of  $\Delta$ 's strongly renormalize the  $\pi N$  couplings  $c_{2,3,4}$  in the three-nucleon sector [42]. The  $\Delta$ -full theory is more consistent in this regard and the  $c_i$ 's appear to be more natural in size.

The expressions for the three-nucleon diagrams at NNLO are from Ref. [11]. The NLO  $NNN$ -force in the  $\Delta$ -full theory is given by the well-known Fujita-Miyazawa term [35]. This topology is identical in structure to the  $\Delta$ -less  $2\pi$ -exchange  $NNN$  interaction when using the resonance-saturation values for the relevant  $\pi N$  LECs

$$c_3^\Delta = -2c_4^\Delta = \frac{4h_A^2}{9\delta} = -2.972246 \text{ GeV}^{-1}.$$

To construct quantitative  $\Delta$ -full  $\chi$ EFT potentials we need to determine the numerical values of the LECs in the LO and NLO contact potentials and the  $c_D$  and  $c_E$  terms in the  $NNN$  interaction at NNLO. To optimize the contact LECs we use a Levenberg-Marquardt algorithm with machine-precise derivatives from automatic differentiation [20]. The objective function for the LO and NLO contact LECs consists of the sum of squared differences between the theoretical partial-wave  $NN$  scattering phase shifts and the corresponding values from the the Granada analysis [43] up to 200 MeV scattering energy in the laboratory system. At LO, we only use phase shifts up to 1 MeV. The neutron-neutron LEC  $\tilde{C}_{1S_0}^{(nn)}$  is constrained to reproduce the effective range expansion in the  $^1S_0$  channel. At NNLO we use the same optimization algorithm to find the  $c_D$  and  $c_E$  LECs that simultaneously reproduce the binding energy and point-proton radius of  $^4\text{He}$ . Although correlated, these  $A = 4$  observables provide enough information to identify a unique minimum in the  $c_D$ - $c_E$  plane that is sufficient for the purpose

of comparing the effects in nuclei and nucleonic matter due to the  $\Delta$  isobar. An extended regression analysis or Bayesian inference approach including additional data from many-nucleon systems or three-nucleon scattering would generate interactions for use in detailed analyses of atomic nuclei or model selection. In this work we focus on the effects of the  $\Delta$ -isobar in nucleonic matter.

To regulate the interactions we use the usual non-local regulators

$$f(p) = \exp \left[ - \left( \frac{p^2}{\Lambda^2} \right)^3 \right]$$

$$f(p, q) = \exp \left[ - \left( \frac{4p^2 + 3q^2}{4\Lambda^2} \right)^3 \right]$$

in the  $NN$  and  $NNN$  interactions, respectively. Here,  $p$  and  $q$  denote the Jacobi momenta in the two-body system and spectator nucleon, respectively, and  $\Lambda$  is the momentum cutoff. The non-local regulator acts multiplicatively, i.e.

$$V_{NN}(p', p) \rightarrow f(p') V_{NN}(p', p) f(p),$$

$$V_{NNN}(p', q'; p, q) \rightarrow f(p', q') V_{NNN}(p', q'; p, q) f(p, q).$$

To explore the sensitivity of the results with respect to changes in the cutoff  $\Lambda$  we employ two common choices, namely  $\Lambda = 450$  MeV and  $\Lambda = 500$  MeV. To regularize the  $2\pi$ -exchanges in conjunction with non-local regulation we use the standard spectral-function regularization (SFR) [44] with a cutoff  $\tilde{\Lambda} = 700$  MeV throughout. It should also be pointed out that recent work, e.g. Refs. [45–47], indicates that a carefully selected local regulation of the long-ranged  $2\pi$ -exchanges render SFR redundant and yields an improved analytical structure of the scattering amplitude. However, the overall existence of such scheme dependencies [48] will persist as long as the chiral interactions cannot be order-by-order renormalized, see e.g. Ref. [49] for a recent analysis. The numerical values of the employed  $\pi N$  LECs and the optimized short-ranged LECs for the  $\Delta$ -less as well as the  $\Delta$ -full potentials are given in Tables I and II. For the masses of the pions ( $\pi^{\pm,0}$ ), proton, neutron, nucleon ( $p, n, N$ ), and  $\Delta$  we use the following values (in MeV):  $M_{\pi^{\pm}} = 139.57018$ ,  $M_{\pi^0} = 134.9766$ ,  $M_p = 938.272046$ ,  $M_n = 939.565379$ ,  $M_N = 938.918267$ , and  $M_{\Delta} = 1232$ , respectively.

The statistical error from the Roy-Steiner analysis of the  $\pi N$  scattering data, documented in Ref. [37], as well as uncertainties due to the fit of the contact potentials, are not considered any further in this work. When contrasted with the much larger systematic uncertainties due to the truncation of the EFT, such statistical errors presently play a lesser role [20, 50, 51]. It is important to note that although the  $\pi N$  LECs are extracted from  $\pi N$  data using a high-precision Roy-Steiner analysis, the corresponding LECs in the  $\Delta$ -full sector are less precise due to the large uncertainty in the underlying determination of  $h_A$ .

To provide a crude estimate of the EFT-truncation uncertainty we follow Refs. [17, 52] and write the EFT expansion for an observable  $X$  as  $X = X_0 \sum_{n=0}^{\infty} a_n Q^n$ . Here  $X_0$  is the scale of the observable, given e.g. by the LO prediction,  $a_n$  are dimensionless expansion coefficients (with  $a_1 = 0$  in Weinberg power counting), and  $Q \equiv p/\Lambda_b$  is the ratio of the typical momentum  $p$  and the breakdown momentum  $\Lambda_b$ . The application of Bayes theorem with boundless and uniform prior distribution of the expansion coefficients  $a_n$  leads to an expression for the truncation error at order NjLO ( $j = 0$ : LO,  $j = 1$ : NLO,  $j = 2$ : NNLO) according to

$$\sigma_X(\text{NjLO}) = X_0 Q^{j+2} \max(|a_0|, |a_1|, \dots, |a_{j+1}|), \quad (1)$$

see Eq. (36) of Ref. [52]. This estimate is in semi-quantitative agreement with a Bayesian uncertainty quantification of the truncation error. The uncertainty at LO is further constrained to at least the size of the contribution of the higher chiral orders. For the breakdown scale  $\Lambda_b$ , we start from Ref. [17] but use a more conservative estimate of  $\Lambda_b = 500$  MeV. We also estimate the typical momentum-scale for bound state observables as  $p \sim m_{\pi}$ , and employ  $p \sim p_F$  (the Fermi momentum) for infinite nucleonic matter, whereas for  $NN$  scattering we extract the momentum scale  $\max(p_{\text{rel}}, m_{\pi})/\Lambda$ . We disregard detailed numerical factors in the various possible definitions of the relevant momentum scales for bound states since the estimate in Eq. (1) is only valid up to factors of order unity.

In Figs. 2, 3, and 4 we compare the quality of the  $NN$  scattering phase shifts of the  $\Delta$ -full and  $\Delta$ -less interactions with cutoff  $\Lambda = 450$  MeV. The results for the peripheral waves agree well with published interactions that were analyzed in the Born approximation [31]. The dashed lines show the  $\Delta$ -less results, order by order from red to green to blue. The full lines show the  $\Delta$ -full results, and we remind the reader that LO is not affected by the  $\Delta$  (see Fig. 1). Clearly, in several partial waves the  $\Delta$ -full  $\chi$ EFT interactions exhibit a faster order-by-order convergence than the corresponding  $\Delta$ -less formulations. Somewhat surprisingly, the  $\Delta$ NNLO results at higher scattering energies, in particular for  $^1S_0$  and selected peripheral waves, such as  $^1D_2$ , are slightly less accurate than the corresponding  $\Delta$ -less order. A more involved optimization strategy, such as Bayesian parameter estimation, could further illuminate this point. Nevertheless, the Granada phase shifts fall on the envelope of the estimated truncation errors and the results therefore seem reasonable. Although not shown, the computed phase shifts for the  $\Lambda = 500$  MeV interactions are very similar and exhibit the same features.

Tables III and IV summarize our results for selected bound-state observables in  $A \leq 4$  nuclei computed with a Jacobi-coordinate version [53] of the no-core shell model (NCSM) [3, 4]. All calculations are converged in 41 and 21 major oscillator shells with  $\hbar\Omega = 36$  MeV for  $A = 3$  and  $A = 4$ , respectively. The charge radius and binding energy of  $^4\text{He}$  were used to constrain the LECs  $c_D$  and

TABLE I. Numerical values of the LECs for  $\Delta$ -full  $\chi$ EFT potentials with a momentum cutoff  $\Lambda = 450$  MeV at LO, NLO, and NNLO. The  $\pi N$  LECs  $c_{1,2,3,4}$  are taken from the Roy-Steiner analysis in Ref. [37], and for consistency we use  $h_A = 1.40$ ,  $g_A = 1.289$ , and  $F_\pi = 92.2$  MeV.

LEC	LO(450)	$\Delta$ NLO(450)	$\Delta$ NNLO(450)	LO(500)	$\Delta$ NLO(500)	$\Delta$ NNLO(500)
$c_1$	—	—	-0.74	—	—	-0.74
$c_2$	—	—	-0.49	—	—	-0.49
$c_3$	—	—	-0.65	—	—	-0.65
$c_4$	—	—	+0.96	—	—	+0.96
$\tilde{C}_{1S_0}^{(nn)}$	-0.112927	-0.310511	-0.338023	-0.108522	-0.310256	-0.338223
$\tilde{C}_{1S_0}^{(np)}$	-0.112927	-0.310712	-0.338139	-0.108522	-0.310443	-0.338320
$\tilde{C}_{1S_0}^{(pp)}$	-0.112927	-0.309893	-0.337137	-0.108522	-0.309618	-0.337303
$\tilde{C}_{3S_1}$	-0.087340	-0.197951	-0.229310	-0.068444	-0.191013	-0.221721
$C_{1S_0}$	—	+2.391638	+2.476589	—	+2.395375	+2.488019
$C_{3S_1}$	—	+0.558973	+0.695953	—	+0.539378	+0.675353
$C_{1P_1}$	—	+0.004813	-0.028541	—	+0.015247	-0.012651
$C_{3P_0}$	—	+0.686902	+0.645550	—	+0.727049	+0.698454
$C_{3P_1}$	—	-1.000112	-1.022359	—	-0.951417	-0.937264
$C_{3P_2}$	—	-0.808073	-0.870203	—	-0.793621	-0.859526
$C_{3S_1-^3D_1}$	—	+0.362094	+0.358330	—	+0.358443	+0.354479
$c_D$	—	—	+0.790	—	—	-0.820
$c_E$	—	—	+0.017	—	—	-0.350

TABLE II. Numerical values of the LECs for  $\Delta$ -less  $\chi$ EFT potentials with a momentum cutoff  $\Lambda = 500$  MeV at LO, NLO, and NNLO. The  $\pi N$  LECs  $c_{1,3,4}$  are taken from the Roy-Steiner analysis in Ref. [37], and for consistency we use  $g_A = 1.289$ , and  $F_\pi = 92.2$  MeV

LEC	LO(450)	NLO(450)	NNLO(450)	LO(500)	NLO(500)	NNLO(500)
$c_1$	—	—	-0.74	—	—	-0.74
$c_3$	—	—	-3.61	—	—	-3.61
$c_4$	—	—	+2.44	—	—	+2.44
$\tilde{C}_{1S_0}^{(nn)}$	-0.112927	-0.149559	-0.152421	-0.108522	-0.148625	-0.152130
$\tilde{C}_{1S_0}^{(np)}$	-0.112927	-0.150034	-0.152630	-0.108522	-0.149167	-0.152327
$\tilde{C}_{1S_0}^{(pp)}$	-0.112927	-0.149336	-0.151775	-0.108522	-0.148236	-0.151463
$\tilde{C}_{3S_1}$	-0.087340	-0.152884	-0.166118	-0.068444	-0.147784	-0.158592
$C_{1S_0}$	—	+1.438619	+2.391093	—	+1.479889	+2.394670
$C_{3S_1}$	—	-0.684095	+0.446631	—	-0.692660	+0.426020
$C_{1P_1}$	—	+0.305070	+0.150981	—	+0.304204	+0.160280
$C_{3P_0}$	—	+1.207031	+0.909408	—	+1.225764	+0.949224
$C_{3P_1}$	—	-0.386920	-0.967768	—	-0.385154	-0.923166
$C_{3P_2}$	—	-0.167769	-0.696173	—	-0.137914	-0.681166
$C_{3S_1-^3D_1}$	—	+0.132948	+0.372585	—	+0.133834	+0.368968
$c_D$	—	—	+1.790	—	—	+0.400
$c_E$	—	—	+0.130	—	—	-0.270

$c_E$  of the short-ranged three-nucleon force whereas the NCSM results for  $A = 2, 3$  nuclei are predictions. At NNLO, all results except the binding energy of  $^2\text{H}$ , agree with the experimental values within the estimated EFT-truncation errors. The computed point-proton radii were transformed to charge radii using a standard expression, see e.g. Ref. [18].

### III. PREDICTIONS FOR MEDIUM MASS NUCLEI AND NUCLEONIC MATTER

In this Section we present results for selected finite nuclei and infinite nucleonic matter. For nucleonic matter we present results for both  $\Delta$ -less and  $\Delta$ -full interactions, while for finite nuclei we limit the discussion to the  $\Delta$ -full interactions since the  $\Delta$ -less interactions produce nuclei that are not bound with respect to breakup into  $\alpha$ -particles. The computed binding energies and radii of finite nuclei are consistent with our results for the saturation point in symmetric nuclear matter.

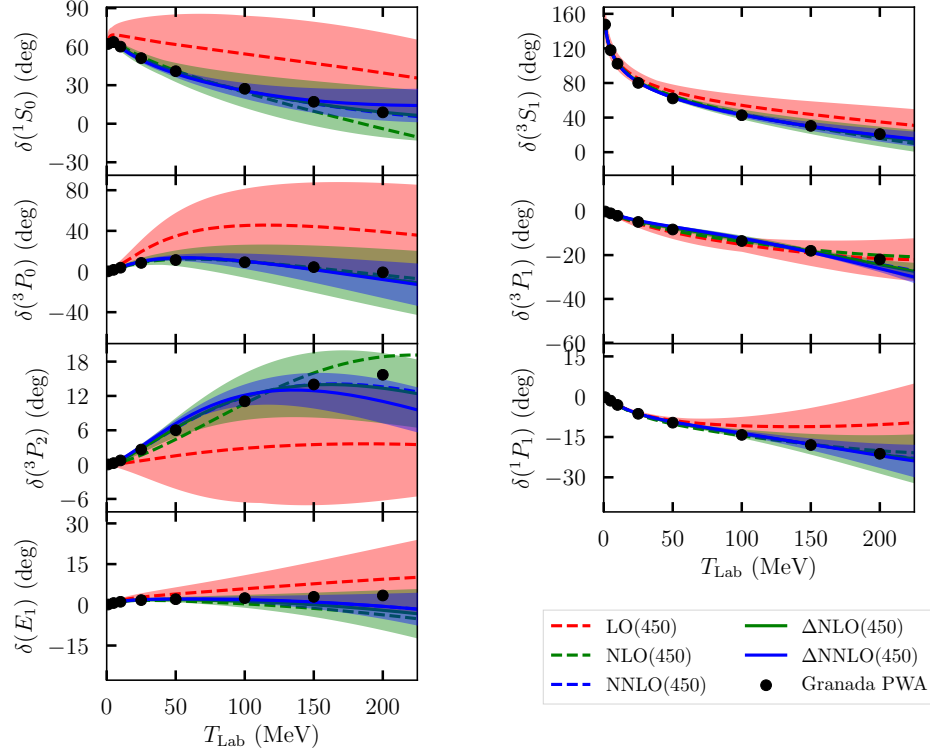


FIG. 2. (Color online) Neutron-proton scattering phase shifts for the contact partial waves using the  $\Delta$ -full and  $\Delta$ -less  $\chi$ EFT potentials with non-local cutoff  $\Lambda = 450$  MeV. All phases are compared to the results from the Granada phase shift analysis [43]. The bands correspond to the order-by-order EFT truncation error in the  $\Delta$ -full approach, as described in the main text.

TABLE III. Binding energies ( $E$ ) in MeV, charge radii ( $R_{\text{ch}}$ ) in fm, for  ${}^2, {}^3\text{H}$  and  ${}^3, {}^4\text{He}$  at LO, NLO, and NNLO with  $\Lambda = 450$  MeV, with and without the  $\Delta$ -isobar and compared to experiment. For the ground state of  ${}^2\text{H}$  we also present the quadrupole moment ( $Q$ ) in  $\text{e fm}^2$  and the  $D$ -state probability ( $P_D$ ) in %. Experimental charge radii are from Ref. [54]. Estimates of the EFT truncation-errors are given in parenthesis, and at LO we report the truncation error belonging to the  $\Delta$ -full expansion.

	LO(450)	NLO(450)	$\Delta$ NLO(450)	NNLO(450)	$\Delta$ NNLO(450)	Exp.
$E({}^2\text{H})$	2.01(15)	2.02(12)	2.10(5)	2.14(3)	2.16(2)	2.2245
$R_{\text{ch}}({}^2\text{H})$	2.16(16)	2.167(16)	2.156(7)	2.1511(44)	2.1486(19)	2.1421(88)
$P_D({}^2\text{H})$	7.15(3.51)	3.43(1.02)	3.63(97)	3.70(28)	3.74(27)	—
$Q({}^2\text{H})$	0.322(41)	0.276(13)	0.277(11)	0.277(3)	0.277(3)	0.27 <sup>a</sup>
$E({}^3\text{H})$	10.91(2.38)	8.54(65)	8.65(62)	8.56(18)	8.53(17)	8.48
$R_{\text{ch}}({}^3\text{H})$	1.52(23)	1.70(5)	1.72(6)	1.74(1)	1.74(2)	1.7591(363)
$E({}^3\text{He})$	9.95(2.21)	7.78(60)	7.85(58)	7.78(16)	7.73(16)	7.72
$R_{\text{ch}}({}^3\text{He})$	1.66(32)	1.91(7)	1.94(8)	1.96(2)	1.97(2)	1.9661(30)
$E({}^4\text{He})$	39.60(11.3)	30.10(2.62)	29.32(2.83)	28.30(72)	28.29(78)	28.30
$R_{\text{ch}}({}^4\text{He})$	1.37(30)	1.59(9)	1.63(7)	1.68(3)	1.67(2)	1.6755(28)

<sup>a</sup> CD-Bonn value [22]

### A. Finite nuclei

The many-body calculations for finite nuclei are performed with the coupled-cluster (CC) method [5, 55–57]. We employ the translationally invariant Hamiltonian

$$H = T - T_{\text{cm}} + V_{NN} + V_{NNN}. \quad (2)$$

Here,  $T$  denotes the total kinetic energy and  $T_{\text{cm}}$  the kinetic energy of the center of mass. As the Hamilto-

nian (2) does not reference the center-of-mass coordinate, the ground-state wave function is a product of an intrinsic and a Gaussian center-of-mass wave function [8, 58–61]. The CC method yields a similarity transformed Hamiltonian whose ground state is the product state corresponding to a closed-shell nucleus. In the coupled-cluster singles and doubles (CCSD) approximation, typically accounting for about 90% of the correlation energy, the ground-state is orthogonal to all 1-particle-1-

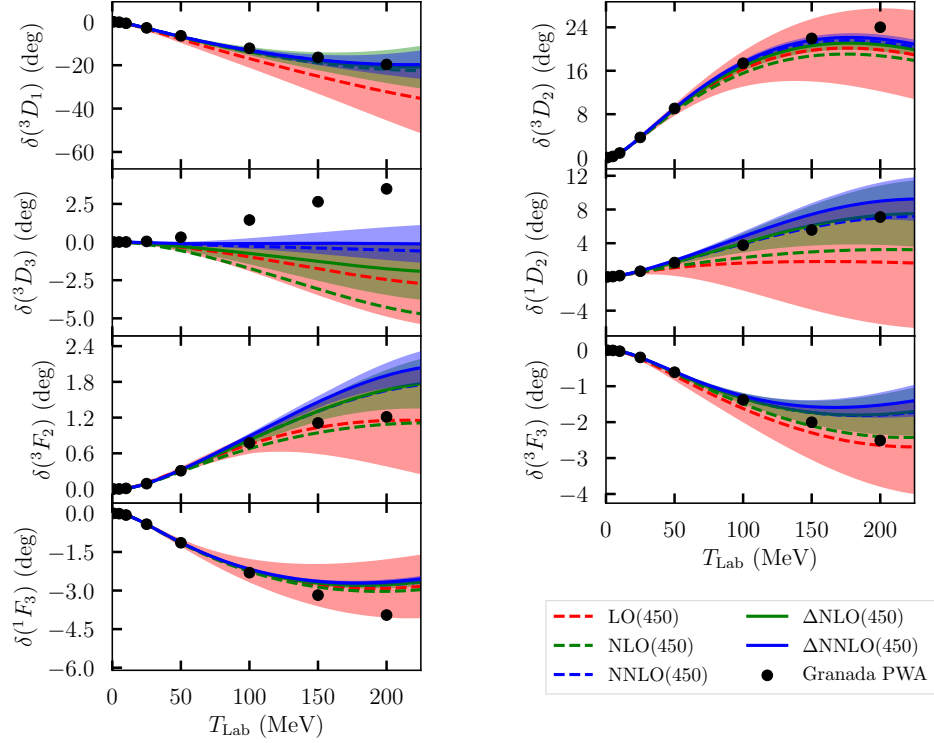


FIG. 3. (Color online) Neutron-proton scattering phase shifts for selected peripheral partial waves using the  $\Delta$ -full and  $\Delta$ -less  $\chi$ EFT potentials with non-local cutoff  $\Lambda = 450$  MeV. All phases are compared to the results from the Granada phase shift analysis [43]. The bands correspond to the order-by-order EFT truncation error in the  $\Delta$ -full approach, as described in the main text.

TABLE IV. Binding energies ( $E$ ) in MeV, charge radii ( $R_{\text{ch}}$ ) in fm, for  ${}^2,3\text{H}$  and  ${}^3,4\text{He}$  at LO, NLO, and NNLO with  $\Lambda = 500$  MeV, with and without the  $\Delta$ -isobar and compared to experiment. For the ground state of  ${}^2\text{H}$  we also present the quadrupole moment ( $Q$ ) in  $\text{e fm}^2$  and the  $D$ -state probability ( $P_D$ ) in %. Experimental charge radii are from Ref. [54]. Estimates of the EFT truncation-errors given in the parenthesis, and at LO we report the truncation error belonging to the  $\Delta$ -full expansion.

	LO(500)	NLO(500)	$\Delta$ NLO(500)	NNLO(500)	$\Delta$ NNLO(500)	Exp.
$E({}^2\text{H})$	2.04(16)	2.04(12)	2.12(5)	2.16(3)	2.18(2)	2.2245
$R_{\text{ch}}({}^2\text{H})$	2.15(16)	2.164(16)	2.153(7)	2.149(4)	2.1459(19)	2.1421(88)
$P_D({}^2\text{H})$	7.80(3.97)	3.55(1.17)	3.82(1.09)	3.93(32)	3.97(30)	—
$Q({}^2\text{H})$	0.317(42)	0.273(12)	0.276(11)	0.275(3)	0.276(3)	0.27 <sup>a</sup>
$E({}^3\text{H})$	10.47(1.97)	8.42(56)	8.91(43)	8.49(16)	8.50(12)	8.48
$R_{\text{ch}}({}^3\text{H})$	1.54(21)	1.71(5)	1.71(5)	1.75(1)	1.75(1)	1.7591(363)
$E({}^3\text{He})$	9.50(1.80)	7.66(51)	8.11(40)	7.72(14)	7.70(11)	7.72
$R_{\text{ch}}({}^3\text{He})$	1.68(30)	1.93(7)	1.92(7)	1.97(2)	1.98(2)	1.9661(30)
$E({}^4\text{He})$	37.00(8.69)	29.22(2.15)	30.70(2.38)	28.31(60)	28.31(65)	28.30
$R_{\text{ch}}({}^4\text{He})$	1.39(28)	1.60(7)	1.62(6)	1.68(2)	1.67(2)	1.6755(28)

<sup>a</sup> CD-Bonn value [22]

hole ( $1p$ - $1h$ ) and  $2p$ - $2h$  excitations. In addition to the CCSD approximation we include leading-order  $3p$ - $3h$  excitations perturbatively by employing the  $\Lambda$ -CCSD(T) method [59, 62, 63]. This approximation typically captures about 99% of the correlation energy. We employ a model space of 15 oscillator shells with  $\hbar\Omega = 16$  MeV, and a cutoff  $E_{3\text{max}} = 16\hbar\Omega$  for the maximum excita-

tion energy of three nucleons interacting via the three-nucleon potential  $V_{NNN}$ . This potential enters the CC calculations in the normal-ordered two-body approximation [64, 65] in the Hartree-Fock basis.

To assess the impact of the  $\Delta$ -isobar in finite nuclei we calculated the binding energies and charge radii for  ${}^4\text{He}$ ,  ${}^{16}\text{O}$ , and  ${}^{40}\text{Ca}$  order-by-order, i.e. at LO,

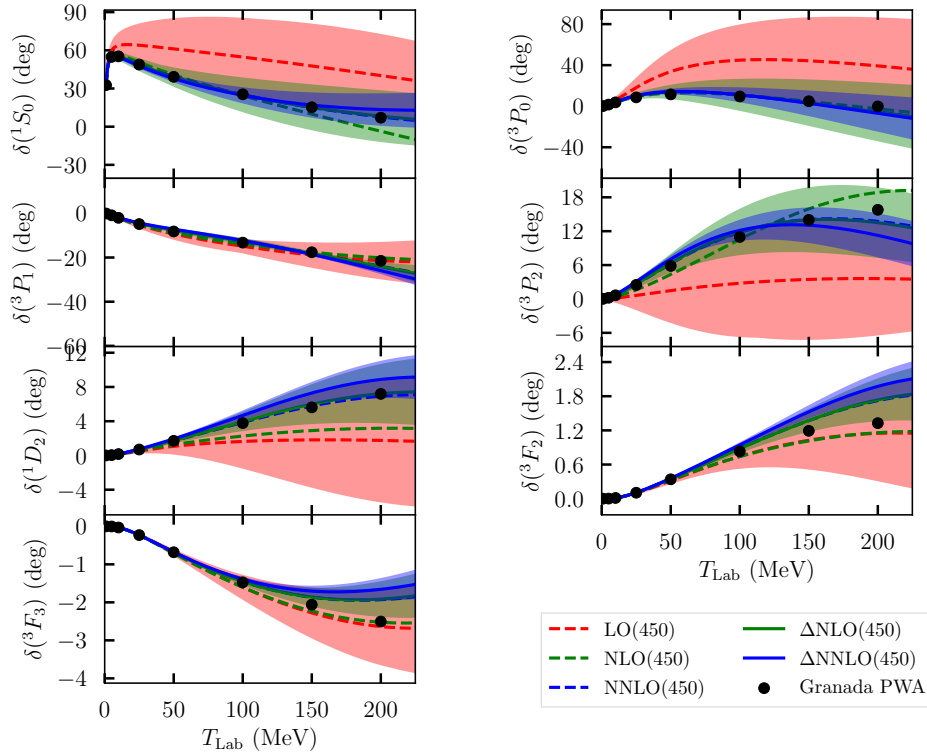


FIG. 4. (Color online) Proton-proton scattering phase shifts for the contact and selected peripheral partial waves using the  $\Delta$ -full and  $\Delta$ -less  $\chi$ EFT potentials with non-local cutoff  $\Lambda = 450$  MeV. All phases are compared to the results from the Granada phase shift analysis [43]. The bands correspond to the order-by-order EFT truncation error in the  $\Delta$ -full approach, as described in the main text.

NLO, and NNLO. Figure 5 shows the results using the  $\Delta$ -full interactions with a momentum cutoff  $\Lambda = 450$  MeV. The ground-state energies are  $E(^{16}\text{O}) = -108.8(11.4)$ ,  $-120.3(6.4)$ , and  $-117.0(1.8)$  MeV and  $E(^{40}\text{Ca}) = -216(97)$ ,  $-312(52)$ , and  $-309(14)$  MeV at LO, NLO, and NNLO, respectively. The charge radii are  $R_{\text{ch}}(^{16}\text{O}) = 1.96(0.76)$ ,  $2.63(0.36)$ , and  $2.73(0.10)$  fm and  $R_{\text{ch}}(^{40}\text{Ca}) = 2.29(1.25)$ ,  $3.41(0.61)$ , and  $3.55(0.17)$  fm at LO, NLO, and NNLO, respectively. Before we analyze the results, we estimate the systematic uncertainties due to the truncation of the EFT. Again we follow Refs. [17, 66], use Eq. (1) and set the momentum scale  $p = m_\pi$  for our low-energy observables. The predicted charge radii are accurate at each order within uncertainties. Already at NLO, which is independent of the sub-leading  $2\pi$ -exchange LECs  $c_i$ , we obtain an accurate description of both radii and binding energies of  $^4\text{He}$ ,  $^{16}\text{O}$  and  $^{40}\text{Ca}$ . At NNLO, the charge radii also exhibit a first sign of convergence in terms of the chiral expansion. Binding energies exhibit a nearly identical order-by-order increase in precision but somewhat underbind nuclei at NNLO. These results demonstrate that the  $\Delta$ -isobar can play an important role also in low-energy nuclear structure and nuclear saturation [14, 50].

The  $\Delta$  degree of freedom also impacts the stability of nuclei with respect to breakup into alpha particles. At

LO,  $^{16}\text{O}$  and  $^{40}\text{Ca}$  are not stable with respect to alpha emission. Similar results were observed in pionless EFT [67–69] and nuclear lattice EFT [25]. However, the  $\Delta$  modifies the  $2\pi$ -exchanges between nucleons, and we observe that the  $\Delta$ -full interactions at NLO and NNLO yield nuclei that are stable with respect to alpha emission. This is in stark contrast to results we obtained here using the  $\Delta$ -less NLO and NNLO interactions at cutoff  $\Lambda = 450$  MeV, and to those of Ref. [20].

Table V summarizes binding energies, radii, and also the neutron skins of nuclei with closed subshells up to  $^{48}\text{Ca}$ . Note that the lack of a spin-orbit (LS) force at LO results in energy-degeneracies that hamper CC calculations of non LS-closed nuclei. Therefore, we can obtain EFT truncation-errors only for  $^{16}\text{O}$  and  $^{40}\text{Ca}$  using Eq. (1). For  $^{48}\text{Ca}$  we predict a neutron skin of  $R_{\text{skin}} = 0.15$  fm at  $\Delta\text{NLO}$  and  $\Delta\text{NNLO}$ , consistent with the recent ranges 0.14–0.20 fm and 0.12–0.15 fm from Ref. [70] and Ref. [7], respectively.

Figure 6 shows the charge form-factor at  $\Delta\text{NLO}$  and  $\Delta\text{NNLO}$ , compared to  $\text{NNLO}_{\text{sat}}$  [18] and data. The charge form-factor is obtained by a Fourier transform of the intrinsic charge density [7, 72], and agrees with data for momentum transfers up to about  $q \approx 2.5 \text{ fm}^{-1}$ . Also for this quantity, the  $\Delta\text{NLO}$  results indicate an improved convergence of chiral expansion compared to the  $\Delta$ -less

TABLE V. Binding energies ( $E$ ) (in MeV), charge radii (in fm), proton point radii (in fm), neutron point radii (in fm), and neutron skin (in fm) for  $^8\text{He}$ ,  $^{16,22,24}\text{O}$ , and  $^{40,48}\text{Ca}$  at  $\Delta\text{NLO}$  and  $\Delta\text{NNLO}$ , and compared to experiment.

	$E$			$R_{\text{ch}}$			$R_p$		$R_n$		$R_{\text{skin}}$	
	$\Delta\text{NLO}$	$\Delta\text{NNLO}$	Exp. [71]	$\Delta\text{NLO}$	$\Delta\text{NNLO}$	Exp. [54]	$\Delta\text{NLO}$	$\Delta\text{NNLO}$	$\Delta\text{NLO}$	$\Delta\text{NNLO}$	$\Delta\text{NLO}$	$\Delta\text{NNLO}$
$^8\text{He}$	27.5	27.0	31.40	1.90	1.97	1.924(31)	1.77	1.85	2.63	2.70	0.85	0.85
$^{16}\text{O}$	120.3	117.0	127.62	2.63	2.73	2.699(5)	2.49	2.61	2.47	2.58	-0.02	-0.03
$^{22}\text{O}$	146.2	145.4	162.04	2.66	2.77		2.54	2.66	2.88	3.00	0.34	0.34
$^{24}\text{O}$	152.2	151.6	168.96	2.70	2.81		2.59	2.71	3.11	3.22	0.52	0.51
$^{40}\text{Ca}$	312.2	309.1	342.05	3.41	3.55	3.478(2)	3.31	3.45	3.26	3.40	-0.05	-0.05
$^{48}\text{Ca}$	373.4	373.8	416.00	3.45	3.56	3.477(2)	3.36	3.47	3.51	3.62	0.15	0.15

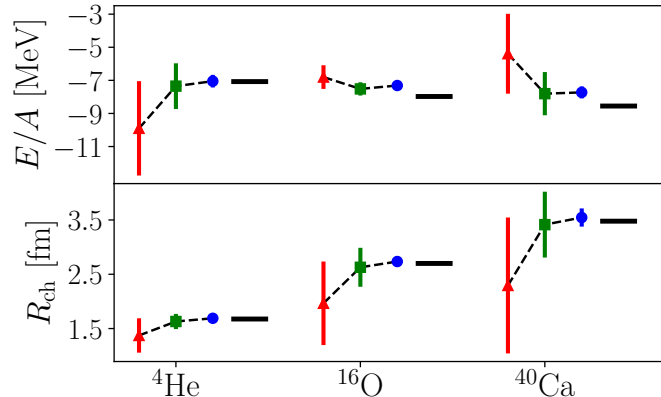


FIG. 5. (Color online) Ground-state energy (negative of binding energy) per nucleon and charge radii for selected nuclei computed with coupled cluster theory and the  $\Delta$ -full potential ( $\Lambda = 450$  MeV). For each nucleus, from left to right: LO (red triangle), NLO (green square), and NNLO (blue circle). The black bars are data. Vertical bars estimate uncertainties from the order-by-order EFT truncation errors  $\sigma(\text{LO})$ ,  $\sigma(\text{NLO})$ , and  $\sigma(\text{NNLO})$ . At NLO and NNLO we estimate a conservative 95% confidence interval, i.e.  $1.96 \times \sigma$ . See the text for details.

formulation.

We also computed spectra of various nuclei. These explorations exhibited mixed results: While the low-lying states in  $^{17}\text{O}$  were in good agreement with data,  $^{25}\text{O}$  is bound at  $\Delta\text{NNLO}$  with respect to  $^{24}\text{O}$  by about 0.5 MeV, and the  $J^\pi = 2^+$  state in  $^{24}\text{O}$  is too low. We believe that these shortcomings should not distract from the main results reported in this work: accurate saturation properties at NLO in the  $\Delta$ -full  $\chi\text{EFT}$ . We speculate that finer details such as spectra will require us to go to higher order in the  $NN$  interaction (as was done, e.g., in Ref. [34] by including  $N^3\text{LO}$  contacts), or to vary the  $\Delta$ -full  $\pi N$  couplings within their somewhat more generous uncertainty limits due to the rather poorly known  $\pi N \Delta$  coupling  $h_A$ , or to also use data of heavier nuclei in the optimization of the interaction. The interactions constructed in this work serve as excellent starting points for such endeavors.

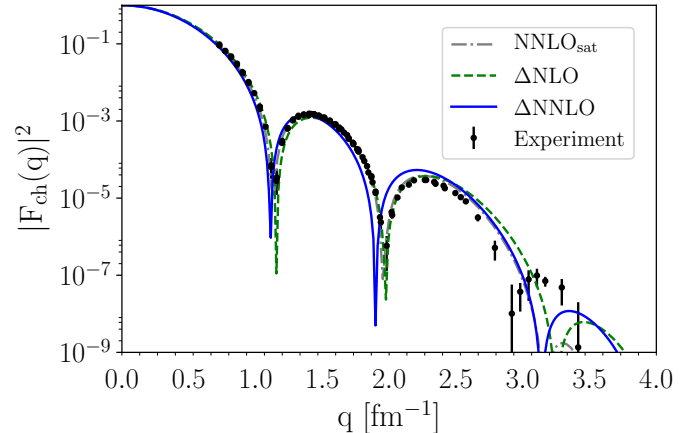


FIG. 6. (Color online) Elastic charge form factor of  $^{48}\text{Ca}$  from  $\text{NNLO}_{\text{sat}}$  (gray dash-dotted),  $\Delta\text{NLO}$  (green dashed), and  $\Delta\text{NNLO}$  (blue solid line) compared to experimental data (black).

## B. Nucleonic matter

We turn to the CC calculations of nuclear matter using  $\Delta$ -full and  $\Delta$ -less interactions up to NNLO. We follow Ref. [73] and employ a Hamiltonian  $H = T + V_{NN} + V_{NNN}$ . The basis is a discrete lattice in momentum space corresponding to periodic boundary conditions in a cubic box of length  $L$  in position space, and the discrete lattice momenta are given by  $2\pi\hbar n_i/L$ , with  $n_i = 0, \pm 1, \dots, \pm n_{\text{max}}$ , and  $i = x, y, z$ . We used  $n_{\text{max}} = 4$  as the maximum number of lattice points. The CC calculations were carried out at the doubles excitation level ( $2p\text{-}2h$ ) with perturbative triples ( $3p\text{-}3h$ ) corrections [CCD(T)]. Due to translational invariance, there are no  $1p\text{-}1h$  excitations. We use “closed-shell” lattice configurations with 66 neutrons for neutron matter, and 132 nucleons for symmetric nuclear matter. These nucleon numbers exhibit only small finite-size effects [73, 74]. The CCD(T) calculations were performed with the normal-ordered two-body approximation for the  $NNN$  interaction [64, 65], i.e. the three-nucleon force enters the normal-ordered Hamiltonian as 0-body, 1-body and 2-body interactions; summing over 3, 2, and 1 particles

in the reference state, respectively. All results are well converged for  $n_{\text{max}} = 4$  at all considered densities, i.e.  $\rho \leq 0.2 \text{ fm}^{-3}$ . To gauge the quality of the normal-ordered two-body approximation, we also included the “residual”  $NNN$  interaction (i.e. those that generate  $3p\text{-}3h$  excitations when acting on the reference) in perturbation theory. We found that the residual  $NNN$  contribution is negligible for neutron matter, and small (0.2-0.3 MeV per nucleon) in symmetric nuclear matter. This suggests that the normal-ordered two-body approximation for the three-nucleon force is sufficiently precise for the  $\Delta$ -full interactions considered in this work.

In Fig. 7 we compare the results for the energy per nucleon at different densities in symmetric nuclear matter and pure neutron matter using  $\Delta$ -full and  $\Delta$ -less interactions with a momentum cutoff  $\Lambda = 450 \text{ MeV}$  at LO, NLO, and NNLO. The saturation points in symmetric matter at NLO and NNLO shift towards considerably more realistic values upon inclusion of the  $\Delta$ . This observation is consistent with our results for finite nuclei. For the EFT truncation uncertainty we use Eq. 1, a relevant momentum scale  $p = p_F$ , and the breakdown momentum  $\Lambda_b = 500 \text{ MeV}$ . The uncertainties also make the accelerated convergence and consistency of the  $\Delta$ -full expansion more apparent. We note that our breakdown scale  $\Lambda_b$  is rather conservative. For  $\Lambda_b \gtrsim 650 \text{ MeV}$  the truncation-error bands of the  $\Delta$ -full and  $\Delta$ -less NNLO(450) interactions no longer overlap in the region of the empirical saturation density. We also note that nuclear matter does not saturate at LO in the range of densities we studied, and we remind the reader once more that the  $\Delta$  does not enter at this chiral order.

Figure 8 shows the difference between the equations of state for neutron matter and symmetric nuclear matter for the  $\Lambda = 450 \text{ MeV}$  cutoff. At the saturation density ( $\rho_0$ ), indicated as vertical lines for the different orders, this yields the symmetry energy ( $S_0$ ). Our results are  $\rho_0 = 0.18(1) \text{ fm}^{-3}$ ,  $22.8 \lesssim S_0 \lesssim 36.5 \text{ MeV}$ , and  $46 \lesssim L \lesssim 65 \text{ MeV}$  at  $\Delta\text{NLO}$ , and  $\rho_0 = 0.165(1) \text{ fm}^{-3}$ ,  $23.6 \lesssim S_0 \lesssim 33.3 \text{ MeV}$ , and  $32 \lesssim L \lesssim 67 \text{ MeV}$  at  $\Delta\text{NNLO}$ . The estimated EFT truncation error for  $\rho_0$  is very small at  $\Delta\text{NNLO}$  because its central value and lower and upper bounds have essentially the same saturation point. The estimated EFT truncation error for  $S_0$  is the maximum difference between the energies per particle in neutron matter and symmetric nuclear matter, at the saturation point. This uncertainty also decreases with increasing order. Finally, the estimated uncertainty in the slope ( $L$ ) of the symmetry energy is taken from the ranges of slopes of  $S_0$  at its upper and lower values. It is large even at  $\Delta\text{NNLO}$  and reflects that the slope in neutron matter exhibits a greater variance at  $\Delta\text{NNLO}$  than at  $\Delta\text{NLO}$ , see Fig. 7. We note that our predictions for the symmetry energy and its density derivative at  $\Delta\text{NLO}$  and  $\Delta\text{NNLO}$  are consistent with the recent estimates of Ref. [75, 76].

## IV. SUMMARY

We presented results for selected finite nuclei and infinite nucleonic matter using optimized interactions from  $\chi\text{EFT}$  with explicit  $\Delta$ -isobar degree-of-freedom. We optimized both  $\Delta$ -full and  $\Delta$ -less interactions order-by-order in the power counting up to NNLO, for two different cutoffs, and with  $\pi N$  LECs from a recent Roy-Steiner analysis of  $\pi N$  scattering. The  $NN$  contact potentials up to NNLO were adjusted to  $NN$  phase shifts, while the short-ranged parts of the  $NNN$  interactions were constrained by energy and radius data on  $^4\text{He}$ . We emphasize that the only differences between the  $\Delta$ -full and  $\Delta$ -less interactions are due to the explicit inclusion of the  $\Delta$  isobar. In a detailed comparison, we found that radii in nuclei up to  $^{48}\text{Ca}$  are accurate within EFT-truncation error estimates, and that binding energies – while improving order-by-order in precision – somewhat underbind heavier nuclei. The saturation point in nuclear matter is consistent with data within EFT error estimates. Our results also show that the inclusion of  $\Delta$ -isobars in the nuclear interaction can address the long-standing problem regarding nuclear saturation. This work therefore provides a valuable starting point for constructing more refined  $\Delta$ -full  $\chi\text{EFT}$  interactions, also at higher chiral orders, with improved uncertainty estimates.

## ACKNOWLEDGMENTS

We would like to thank Hermann Krebs for valuable discussions and input on the manuscript, Kai Hebeler for providing us with matrix elements in Jacobi coordinates for the three-nucleon interaction, and Gustav Jansen for providing us with the code that transforms three-nucleon matrix elements to the laboratory system. This material is based upon work supported by the Swedish Research Council under Grant No. 2015- 00225, and the Marie Skłodowska Curie Actions, Cofund, Project INCA 600398, the U.S. Department of Energy, Office of Science, Office of Nuclear Physics under Award Numbers DEFG02-96ER40963 (University of Tennessee), DE-SC0008499 and DE-SC0018223 (NUCLEI SciDAC collaboration), and the Field Work Proposal ERKBP57 at Oak Ridge National Laboratory. Computer time was provided by the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. This research used resources of the Oak Ridge Leadership Computing Facility located in the Oak Ridge National Laboratory, which is supported by the Office of Science of the Department of Energy under Contract No. DE-AC05-00OR22725, and used computational resources of the National Center for Computational Sciences, the National Institute for Computational Sciences, the Swedish National Infrastructure for Computing (SNIC).

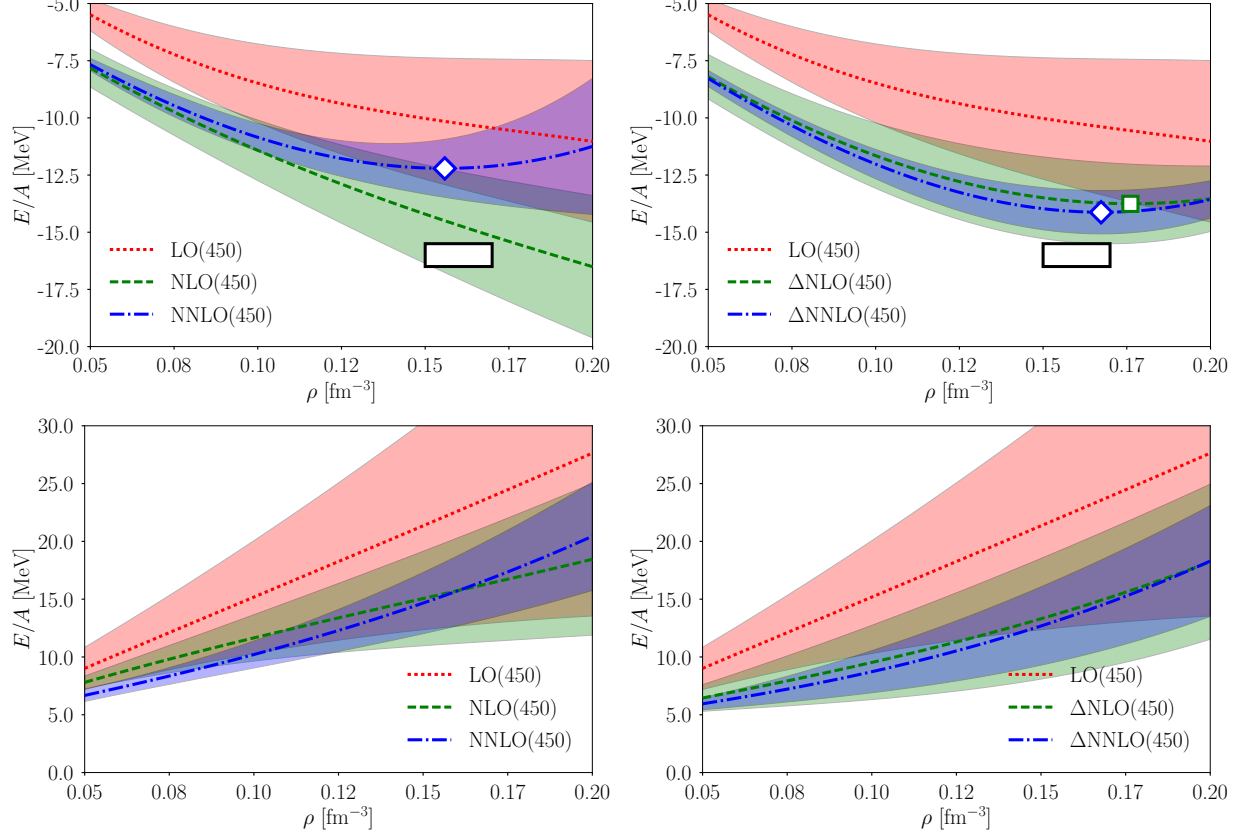


FIG. 7. (Color online) Energy per nucleon (in MeV) of symmetric nuclear matter (upper row) and pure neutron matter (lower row) up to third order in  $\chi$ EFT without (left column) and with (right column) explicit inclusion of the  $\Delta$ -isobar in  $\chi$ EFT. All interaction employ a momentum cutoff  $\Lambda = 450$  MeV. Shaded areas indicate the estimated EFT-truncation errors, and the (square) diamond marks the saturation point in symmetric nuclear matter for ( $\Delta$ NLO)  $\Delta$ NNLO. The black rectangle indicates the region  $E/A = -16 \pm 0.5$  MeV and  $\rho = 0.16 \pm 0.01 \text{ fm}^{-3}$ .

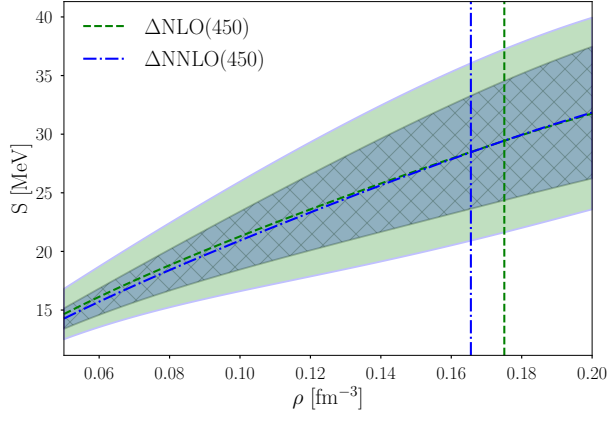


FIG. 8. (Color online) The symmetry energy as a function of the density for  $\Delta$ NLO (green), and  $\Delta$ NNLO (blue) with  $\Delta$ -full interaction at cutoff of 450 MeV, with uncertainties shown as shaded areas.

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