# **High-quality two-nucleon potentials up to fifth order of the chiral expansion**

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We present *NN* potentials through five orders of chiral effective field theory ranging from leading order (LO) to next-to-next-to-next-to-leading order  $(N<sup>4</sup>LO)$ . The construction may be perceived as consistent in the sense that the same power counting scheme as well as the same cutoff procedures are applied in all orders. Moreover, the long-range parts of these potentials are fixed by the very accurate  $\pi N$  low-energy constants (LECs) as determined in the Roy-Steiner equations analysis by Hoferichter, Ruiz de Elvira, and coworkers. In fact, the uncertainties of these LECs are so small that a variation within the errors leads to effects that are essentially negligible, reducing the error budget of predictions considerably. The *NN* potentials are fit to the world *NN* data below the pion-production threshold of the year 2016. The potential of the highest order  $(N<sup>4</sup>LO)$  reproduces the world *NN* data with the outstanding  $\chi^2$ /datum of 1.15, which is the highest precision ever accomplished for any chiral *NN* potential to date. The *NN* potentials presented may serve as a solid basis for systematic *ab initio* calculations of nuclear structure and reactions that allow for a comprehensive error analysis. In particular, the consistent order by order development of the potentials will make possible a reliable determination of the truncation error at each order. Our family of potentials is nonlocal and, generally, of soft character. This feature is reflected in the fact that the predictions for the triton binding energy (from two-body forces only) converges to about 8.1 MeV at the highest orders. This leaves room for three-nucleon-force contributions of moderate size.

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## **I. INTRODUCTION**

The quest for a practically feasible, and yet fundamental, theory of hadronic interactions at low energy (where QCD is nonperturbative) has spanned several decades. At the present time, there exists a general consensus that chiral effective field theory (chiral EFT) may provide the best answer to the quest. By its nature, chiral EFT is a model-independent approach with firm roots in QCD, due to the fact that interactions are subjected to the constraints of the broken chiral symmetry of low-energy QCD. Moreover, the approach is systematic in the sense that the various contributions to a particular dynamical process can be arranged as an expansion in terms of a suitable parameter. The latter is chosen to be the ratio of a typical external momentum (soft scale) to the chiral symmetry-breaking scale  $(\approx 1 \text{ GeV})$ , hard scale). Recent comprehensive reviews on the subject can be found in Refs. [\[1,2\]](#page-16-0).

In its early stages, chiral perturbation theory (ChPT) was applied mostly to  $\pi \pi$  [\[3\]](#page-16-0) and  $\pi N$  [\[4\]](#page-16-0) dynamics, because, due to the Goldstone-boson nature of the pion, these are the most natural scenarios for a perturbative expansion to exist. In the meantime, though, chiral EFT has been applied in nucleonic systems by numerous groups  $[1,2,5-30]$ . Derivations of the nucleon-nucleon (*NN*) interaction up to fourth order (next-to-next-to-next-to-leading order,  $N<sup>3</sup>LO$ ) can be found in Refs. [\[7,9,10,12,13,15\]](#page-16-0), with quantitative *NN* potentials making their appearance in the early 2000s [\[16,17\]](#page-16-0).

Since then, a wealth of applications of  $N<sup>3</sup>LO NN$  potentials together with chiral three-nucleon forces (3NFs) have been

reported. These investigations include few-nucleon reactions [\[31–34\]](#page-16-0), structure of light- and medium-mass nuclei [\[35–38\]](#page-16-0), and infinite matter [\[39–44\]](#page-16-0). Although satisfactory predictions have been obtained in many cases, persistent problems continue to pose serious challenges, such as the well-known  $A<sub>v</sub>$  puzzle of nucleon-deuteron scattering [\[45\]](#page-16-0). Naturally, one would invoke 3NFs as the most likely mechanism to solve this problem. Unfortunately, the chiral 3NF at NNLO does very little to improve the situation with nucleon-deuteron scattering [\[31,33\]](#page-16-0), while inclusion of the  $N<sup>3</sup>LO$  3NF produces an effect in the wrong direction [\[34\]](#page-16-0). The next step is then to proceed systematically in the expansion, namely to look at  $N<sup>4</sup>LO$  (or fifth order). This order is interesting for diverse reasons. From studies of some of the 3NF topologies at  $N<sup>4</sup>LO$  [\[46,47\]](#page-16-0), we know that a complete set of isospin-spin-momentum 3NF structures (a total of 20) are present at this order [\[48\]](#page-16-0) and that contributions can be of substantial size. Even more promising, at this order a new set of 3NF contact interactions appears, which has recently been derived by the Pisa group [\[49\]](#page-16-0). Contact terms are relatively easy to work with and, most importantly, come with free coefficients and thus provide larger flexibility and a great likelihood to solve persistent problems such as the  $A<sub>v</sub>$  puzzle as well as other issues (like the radius problem [\[50\]](#page-16-0) and the overbinding of intermediate-mass nuclei [\[51\]](#page-16-0)).

A principle of all EFTs is that, for meaningful predictions, it is necessary to include *all* contributions that appear at the order at which the calculation is conducted. Thus, when nuclear structure problems require for their solution the inclusion of  $3NFs$  at  $N<sup>4</sup>LO$ , then also the two-nucleon force involved in the calculation has to be of order  $N<sup>4</sup>LO$ . This is one reason why in Ref.  $[52]$  we derived the N<sup>4</sup>LO two-pion exchange (2PE) and three-pion exchange (3PE) contributions to the *NN* interaction and tested them in peripheral partial waves. In this

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<span id="page-1-0"></span>paper, we will present complete N4LO *NN* potentials that also include the lower partial waves which receive contributions from contact interactions.

In Ref. [\[52\]](#page-16-0), we also demonstrated that the next-tonext-to-leading order (NNLO), the  $N<sup>3</sup>LO$ , and the  $N<sup>4</sup>LO$ contributions to the *NN* interaction are all of about the same size, thus not showing much of a trend toward convergence. Therefore, in Ref. [\[53\]](#page-16-0) we calculated the  $N<sup>5</sup>LO$  (sixth-order) contribution which, indeed, turned out to be small. The latter result may be perceived as an indication of convergence showing up at  $N<sup>5</sup>LO$ . This adds to the significance of order N4LO.

Besides the above, we are faced with another set of convergence issues: The convergence of the predictions for the properties of nuclear few- and many-body systems, in which also chiral many-body forces are involved. To investigate these issues, one needs (besides those many-body forces) *NN* potentials at all orders of chiral EFT, ranging from leading order  $(LO)$  to  $N<sup>4</sup>LO$ , and constructed consistently, i.e., using the same power-counting scheme, consistent LECs, etc.

For that reason, we present in this paper *NN* potentials through five orders from LO to  $N<sup>4</sup>LO$ , constructed with the above-stated consistencies and with a reproduction of the *NN* data of the maximum quality possible at the respective orders. These potentials will allow for systematic investigations of nuclear few- and many-body systems with clear implications for convergence and uncertainty quantifications (truncation errors) [\[23,27,54,](#page-16-0)[55\]](#page-17-0).

This paper is organized as follows: In Sec. II, we present the expansion of the *NN* potential through all orders from LO to N4LO. The reproduction of the *NN* scattering data and the deuteron properties are given in Sec. [III.](#page-7-0) Some aspects regarding 3NFs are discussed in Sec. [IV,](#page-11-0) and uncertainty quantification is considered in Sec. [V.](#page-13-0) Section [VI](#page-14-0) concludes the paper.

#### **II. EXPANSION OF THE** *NN* **POTENTIAL**

### **A. Effective Langrangians**

In the  $\Delta$  less version of chiral EFT, which is the one we are pursuing here, the relevant degrees of freedom are pions (Goldstone bosons) and nucleons. Since the interactions of Goldstone bosons must vanish at zero momentum transfer and in the chiral limit ( $m_\pi \to 0$ ), the low-energy expansion of the effective Lagrangian is arranged in powers of derivatives and pion masses. This effective Lagrangian is subdivided into the following pieces,

$$
\mathcal{L}_{\text{eff}} = \mathcal{L}_{\pi\pi} + \mathcal{L}_{\pi N} + \mathcal{L}_{NN} + \cdots, \qquad (2.1)
$$

where  $\mathcal{L}_{\pi\pi}$  deals with the dynamics among pions,  $\mathcal{L}_{\pi N}$ describes the interaction between pions and a nucleon, and  $\mathcal{L}_{NN}$  contains two-nucleon contact interactions which consist of four nucleon-fields (four nucleon legs) and no meson fields. The ellipsis stands for terms that involve two nucleons plus pions and three or more nucleons with or without pions, relevant for nuclear many-body forces. The individual Lagrangians are organized in terms of increasing orders:

$$
\mathcal{L}_{\pi\pi} = \mathcal{L}_{\pi\pi}^{(2)} + \mathcal{L}_{\pi\pi}^{(4)} + \cdots, \qquad (2.2)
$$

$$
\mathcal{L}_{\pi N} = \mathcal{L}_{\pi N}^{(1)} + \mathcal{L}_{\pi N}^{(2)} + \mathcal{L}_{\pi N}^{(3)} + \mathcal{L}_{\pi N}^{(4)} + \cdots, \qquad (2.3)
$$

$$
\mathcal{L}_{NN} = \mathcal{L}_{NN}^{(0)} + \mathcal{L}_{NN}^{(2)} + \mathcal{L}_{NN}^{(4)} + \cdots, \qquad (2.4)
$$

where the superscript refers to the number of derivatives or pion mass insertions (chiral dimension) and the ellipses stand for terms of higher dimensions. We use the heavy-baryon formulation of the Lagrangians, the explicit expressions of which can be found in Refs. [\[1,46\]](#page-16-0).

#### **B. Power counting**

Based upon the above Langrangians, an infinite number of diagrams contributing to the interactions among nucleons can be drawn. Nuclear potentials are defined by the irreducible types of these graphs. By definition, an irreducible graph is a diagram that cannot be separated into two by cutting only nucleon lines. These graphs are then analyzed in terms of powers of small external momenta over the large scale:  $(Q/\Lambda_{\chi})^{\nu}$ , where Q is generic for a momentum (nucleon three-momentum or pion four-momentum) or a pion mass and  $\Lambda_{\chi} \sim 1$  GeV is the chiral symmetry-breaking scale (hardronic scale, hard scale). Determining the power  $\nu$  has become know as power counting.

Following the Feynman rules of covariant perturbation theory, a nucleon propagator is  $Q^{-1}$ , a pion propagator is  $Q^{-2}$ , each derivative in any interaction is Q, and each four-momentum integration is  $Q<sup>4</sup>$ . This is also known as naive dimensional analysis or Weinberg counting.

Since we use the heavy-baryon formalism, we encounter terms which include factors of  $Q/M_N$ , where  $M_N$  denotes the nucleon mass. We count the order of such terms by the rule  $Q/M_N \sim (Q/\Lambda_\chi)^2$ , for reasons explained in Ref. [\[5\]](#page-16-0).

Applying some topological identities, one obtains for the power of a connected irreducible diagram involving A nucleons [\[1,5\]](#page-16-0)

$$
\nu = -2 + 2A - 2C + 2L + \sum_{i} \Delta_{i}, \qquad (2.5)
$$

with

$$
\Delta_i \equiv d_i + \frac{n_i}{2} - 2, \qquad (2.6)
$$

where  $L$  denotes the number of loops in the diagram,  $d_i$  is the number of derivatives or pion-mass insertions, and  $n_i$  the number of nucleon fields (nucleon legs) involved in vertex  $i$ ; the sum runs over all vertexes  $i$ contained in the connected diagram under consideration. Note that  $\Delta_i \geq 0$  for all interactions allowed by chiral symmetry.

An important observation from power counting is that the powers are bounded from below and, specifically,  $v \ge 0$ . This fact is crucial for the convergence of the low-momentum expansion.

Furthermore, the power formula Eq.  $(2.5)$  allows us to predict the leading orders of connected multinucleon forces.

<span id="page-2-0"></span>

FIG. 1. Hierarchy of nuclear forces in ChPT. Solid lines represent nucleons and dashed lines represent pions. Small dots, large solid dots, solid squares, triangles, diamonds, and stars denote vertexes of index  $\Delta_i = 0, 1, 2, 3, 4$ , and 6, respectively. Further explanations are given in the text.

Consider a m-nucleon irreducibly connected diagram (mnucleon force) in an A-nucleon system ( $m \leq A$ ). The number of separately connected pieces is  $C = A - m + 1$ . Inserting this into Eq. [\(2.5\)](#page-1-0) together with  $L = 0$  and  $\sum_i \Delta_i = 0$  yields  $v = 2m - 4$ . Thus, two-nucleon forces  $(m = 2)$  appear at  $\nu = 0$ , three-nucleon forces (*m* = 3) appear at  $\nu = 2$  (but they happen to cancel at that order), and four-nucleon forces appear at  $v = 4$  (they do not cancel).

For an irreducible *NN* diagram ( $A = 2$ ,  $C = 1$ ), the power formula collapses to the very simple expression

$$
\nu = 2L + \sum_{i} \Delta_i \,. \tag{2.7}
$$

In summary, the chief point of the ChPT expansion of the potential is that, at a given order  $\nu$ , there exists only a finite number of graphs. This is what makes the theory calculable. The expression  $(Q/\Lambda_\chi)^{v+1}$  provides an estimate of the relative size of the contributions left out and thus of the relative uncertainty at order  $\nu$ . The ability to calculate observables (in principle) to any degree of accuracy gives the theory its predictive power.

Chiral perturbation theory and power counting imply that nuclear forces evolve as a hierarchy controlled by the power  $\nu$ ; see Fig. 1 for an overview. In what follows, we will focus on the two-nucleon force (2NF).

### **C. The long-range** *NN* **potential**

The long-range part of the*NN* potential is built up from pion exchanges, which are ruled by chiral symmetry. The various pion-exchange contributions may be analyzed according to the number of pions being exchanged between the two nucleons:

$$
V = V_{1\pi} + V_{2\pi} + V_{3\pi} + \cdots, \qquad (2.8)
$$

where the meaning of the subscripts is obvious and the ellipsis represents  $4\pi$  and higher pion exchanges. For each of the

<span id="page-3-0"></span>TABLE I. Basic constants used throughout this work [\[56\]](#page-17-0).

<b>Ouantity</b>	Value
Axial-vector coupling constant $g_A$	1.29
Pion-decay constant $f_{\pi}$	92.4 MeV
Charged-pion mass $m_{\pi^{\pm}}$	139.5702 MeV
Neutral-pion mass $m_{\pi^0}$	134.9766 MeV
Average pion-mass $\bar{m}_{\pi}$	138.0390 MeV
Proton mass $M_n$	938.2720 MeV
Neutron mass $M_n$	939.5654 MeV
Average nucleon-mass $M_N$	938.9183 MeV

above terms, we have a low-momentum expansion:

$$
V_{1\pi} = V_{1\pi}^{(0)} + V_{1\pi}^{(2)} + V_{1\pi}^{(3)} + V_{1\pi}^{(4)} + V_{1\pi}^{(5)} + \cdots, \qquad (2.9)
$$

$$
V_{2\pi} = V_{2\pi}^{(2)} + V_{2\pi}^{(3)} + V_{2\pi}^{(4)} + V_{2\pi}^{(5)} + \cdots, \qquad (2.10)
$$

$$
V_{3\pi} = V_{3\pi}^{(4)} + V_{3\pi}^{(5)} + \cdots, \qquad (2.11)
$$

where the superscript denotes the order  $\nu$  of the expansion.

Order by order, the long-range *NN* potential builds up as follows:

$$
V_{\text{LO}} \equiv V^{(0)} = V_{1\pi}^{(0)},\tag{2.12}
$$

$$
V_{\rm NLO} \equiv V^{(2)} = V_{\rm LO} + V_{1\pi}^{(2)} + V_{2\pi}^{(2)},\tag{2.13}
$$

$$
V_{\text{NNLO}} \equiv V^{(3)} = V_{\text{NLO}} + V_{1\pi}^{(3)} + V_{2\pi}^{(3)},\tag{2.14}
$$

$$
V_{\text{N}^3\text{LO}} \equiv V^{(4)} = V_{\text{NNLO}} + V_{1\pi}^{(4)} + V_{2\pi}^{(4)} + V_{3\pi}^{(4)},\qquad(2.15)
$$

$$
V_{\rm N^4LO} \equiv V^{(5)} = V_{\rm N^3LO} + V_{1\pi}^{(5)} + V_{2\pi}^{(5)} + V_{3\pi}^{(5)},\qquad(2.16)
$$

where LO stands for leading order, NLO stands for next-toleading order, etc.

#### *1. Leading order*

At leading order, only one-pion exchange (1PE) contributes to the long range; cf. Fig. [1.](#page-2-0) The charge-independent 1PE is given by

$$
V_{1\pi}^{(\text{CI})}(\vec{p}', \vec{p}) = -\frac{g_A^2}{4f_\pi^2} \,\tau_1 \cdot \tau_2 \, \frac{\vec{\sigma}_1 \cdot \vec{q} \,\vec{\sigma}_2 \cdot \vec{q}}{q^2 + m_\pi^2} \,, \tag{2.17}
$$

where  $\vec{p}$  and  $\vec{p}$  denote the final and initial nucleon momenta in the center-of-mass system, respectively. Moreover,  $\vec{q} = \vec{p}'$  –  $\vec{p}$  is the momentum transfer, and  $\vec{\sigma}_{1,2}$  and  $\tau_{1,2}$  are the spin and isospin operators of nucleons 1 and 2, respectively. Parameters  $g_A$ ,  $f_\pi$ , and  $m_\pi$  denote the axial-vector coupling constant, pion-decay constant, and the pion mass, respectively. See Table I for their values. Higher order corrections to the 1PE are taken care of by mass and coupling constant renormalizations. Note also that, on shell, there are no relativistic corrections. Thus, we apply 1PE in the form Eq.  $(2.17)$  through all orders.

For the *NN* potentials constructed in this paper, we take the charge dependence of the 1PE due to pion-mass splitting into account. Thus, in proton-proton  $(pp)$  and neutron-neutron  $(nn)$  scattering, we actually use

$$
V_{1\pi}^{(pp)}(\vec{p}',\vec{p}) = V_{1\pi}^{(nn)}(\vec{p}',\vec{p}) = V_{1\pi}(m_{\pi^0}), \qquad (2.18)
$$

and in neutron-proton  $(np)$  scattering, we apply

$$
V_{1\pi}^{(np)}(\vec{p}',\vec{p}) = -V_{1\pi}(m_{\pi^0}) + (-1)^{I+1} 2 V_{1\pi}(m_{\pi^{\pm}}), \quad (2.19)
$$

where  $I = 0,1$  denotes the total isospin of the two-nucleon system and

$$
V_{1\pi}(m_{\pi}) \equiv -\frac{g_A^2}{4f_{\pi}^2} \frac{\vec{\sigma}_1 \cdot \vec{q} \ \vec{\sigma}_2 \cdot \vec{q}}{q^2 + m_{\pi}^2} \,. \tag{2.20}
$$

Formally speaking, the charge dependence of the 1PE exchange is of order NLO [\[1\]](#page-16-0), but we include it also at leading order to make the comparison with the (charge-dependent) phase-shift analyses meaningful.

### *2. Subleading pion exchanges*

Two-pion exchange starts at NLO and continues through all higher orders. In Fig. [1,](#page-2-0) the corresponding diagrams show completely up to NNLO. Beyond that order, the number of diagrams increases so dramatically that we show only a few symbolic graphs. The situation is similar for the 3PE contributions, which start at  $N<sup>3</sup>LO$ . Also the mathematical formulas are getting increasingly involved. A complete collection of all formulas concerning the 2PE and 3PE contributions through all orders from NLO to  $N^4$ LO is given in Ref. [\[52\]](#page-16-0). Therefore, we will not reprint the complicated math here and refer the interested reader to the comprehensive compendium [\[52\]](#page-16-0). In all 2PE and 3PE contributions, we use the average pion mass,  $\bar{m}_{\pi} = 138.039$  MeV. The charge dependence caused by pion-mass splitting in 2PE has been found to be negligible in all partial waves with  $L > 0$  [\[57\]](#page-17-0). The small effect in  ${}^{1}S_{0}$ is absorbed into the charge dependence of the zeroth-order contact parameter  $C_{^{1}S_{0}}$ ; see below.

The contributions have the following general decomposition:

$$
V(\vec{p}', \vec{p}) = V_C + \tau_1 \cdot \tau_2 W_C
$$
  
+ 
$$
[V_S + \tau_1 \cdot \tau_2 W_S] \vec{\sigma}_1 \cdot \vec{\sigma}_2
$$
  
+ 
$$
[V_{LS} + \tau_1 \cdot \tau_2 W_{LS}] [-i\vec{S} \cdot (\vec{q} \times \vec{k})]
$$
  
+ 
$$
[V_T + \tau_1 \cdot \tau_2 W_T] \vec{\sigma}_1 \cdot \vec{q} \vec{\sigma}_2 \cdot \vec{q}, \qquad (2.21)
$$

where  $\vec{k} = (\vec{p}' + \vec{p})/2$  denotes the average momentum and  $\vec{S} = (\vec{\sigma}_1 + \vec{\sigma}_2)/2$  is the total spin. For on-shell scattering,  $V_\alpha$ and  $W_{\alpha}$  ( $\alpha = C, S, LS, T$ ) can be expressed as functions of  $q = |\vec{q}|.$ 

We consider loop contributions in terms of their spectral functions, from which the momentum-space amplitudes  $V_\alpha(q)$ and  $W_\alpha(q)$  are obtained via the subtracted dispersion integrals:

$$
V_{C,S}(q) = -\frac{2q^6}{\pi} \int_{nm_{\pi}}^{\tilde{\Lambda}} d\mu \, \frac{\text{Im} \, V_{C,S}(i\mu)}{\mu^5(\mu^2 + q^2)},
$$
  

$$
V_{T,LS}(q) = \frac{2q^4}{\pi} \int_{nm_{\pi}}^{\tilde{\Lambda}} d\mu \, \frac{\text{Im} \, V_{T,LS}(i\mu)}{\mu^3(\mu^2 + q^2)},
$$
(2.22)

and similarly for  $W_{C,S,T,LS}$ . The thresholds are given by  $n = 2$ for two-pion exchange and  $n = 3$  for three-pion exchange. For  $\tilde{\Lambda} \rightarrow \infty$  the above dispersion integrals yield the results of dimensional regularization, while for finite  $\tilde{\Lambda} \geq n m_{\pi}$  we employ the method known as spectral-function regularization (SFR) [\[58\]](#page-17-0). The purpose of the finite scale  $\tilde{\Lambda}$  is to constrain the imaginary parts to the low-momentum region where chiral effective field theory is applicable. Thus, a reasonable choice for  $\tilde{\Lambda}$  is to keep it below the masses of the vector mesons

<span id="page-4-0"></span>TABLE II. The  $\pi N$  low-energy constants (LECs) as determined in the Roy-Steiner equation analysis of  $\pi N$  scattering conducted in Ref. [\[60\]](#page-17-0). The given orders of the chiral expansion refer to the *NN* system. Note that the orders, at which the LECs are extracted from the  $\pi N$  system, are always lower by one order as compared of the  $NN$ system in which the LECs are applied. The  $c_i$ ,  $\bar{d}_i$ , and  $\bar{e}_i$  are the LECs of the second-, third-, and fourth-order  $\pi N$  Lagrangian [\[46\]](#page-16-0) and are in units of GeV<sup>-1</sup>, GeV<sup>-2</sup>, and GeV<sup>-3</sup>, respectively. The uncertainties in the last digits are given in parentheses after the values.

	NNLO	$N^3LO$	$N^4LO$
c <sub>1</sub>	$-0.74(2)$	$-1.07(2)$	$-1.10(3)$
c <sub>2</sub>		3.20(3)	3.57(4)
c <sub>3</sub>	$-3.61(5)$	$-5.32(5)$	$-5.54(6)$
$c_4$	2.44(3)	3.56(3)	4.17(4)
$\overline{d}_1 + \overline{d}_2$		1.04(6)	6.18(8)
$\bar{d}_3$		$-0.48(2)$	$-8.91(9)$
$\bar{d}_5$		0.14(5)	0.86(5)
$\bar{d}_{14} - \bar{d}_{15}$		$-1.90(6)$	$-12.18(12)$
$\bar{e}_{14}$			1.18(4)
$\bar{e}_{17}$			$-0.18(6)$

 $\rho(770)$  and  $\omega(782)$ , but above the  $f_0(500)$  [also know as  $\sigma$ (500)] [\[56\]](#page-17-0). This suggests that the region 600–700 MeV is appropriate for  $\tilde{\Lambda}$ . Consequently, we use  $\tilde{\Lambda} = 650$  MeV in all orders, except for  $N<sup>4</sup>LO$ , where we apply 700 MeV. We use this slightly larger value for  $N<sup>4</sup>LO$ , because it is suggestive that higher orders may permit an extension to higher momenta.

#### *3. The pion-nucleon low-energy constants*

Chiral symmetry establishes a link between the dynamics in the  $\pi N$  system and the NN system through common low-energy constants. Therefore, consistency requires that we use the LECs for subleading  $\pi N$  couplings as determined in analysis of low-energy  $\pi N$  scattering. Over the years, there have been many such determinations of questionable reliability. Fortunately, that has changed recently with the analysis by Hoferichter and Ruiz de Elvira [\[59\]](#page-17-0) and their coworkers [\[60\]](#page-17-0), in which the Roy-Steiner (RS) equations are applied. The RS equations are a set of coupled partial-wave dispersion relations constrained by analyticity, unitarity, and crossing symmetry. In the work of Ref. [\[60\]](#page-17-0), they are used to extract the LECs from the subthreshold point in  $\pi N$  scattering instead of the physical region. This is the preferred method for LECs to be applied in chiral potentials where, e.g., a one-loop  $\pi N$  amplitude leads to a two-loop contribution in *NN*. Such diagrams are best evaluated by means of Cutkosky rules [\[12,52,53\]](#page-16-0). The  $\pi N$  amplitude that enters the dispersion integrals is weighted much closer to subthreshold kinematics than to the threshold point. The LECs determined in Ref. [\[60\]](#page-17-0) carry very small uncertainties (cf. Table  $\Pi$ ) for, essentially, two reasons: first, because of the constraints built into the RS equations, and second, because of the use of the high-accuracy  $\pi N$  scattering lengths extracted from pionic atoms. In fact, the uncertainties are so small that they are negligible for our purposes. This makes the variation of the  $\pi N$  LECs in *NN* potential construction obsolete and reduces the error budget in applications of these potentials. For the potentials constructed in this paper, the central values of Table II are applied.

#### **D. The short-range** *NN* **potential**

The short-range *NN* potential is described by contributions of the contact type, which are constrained by parity, time reversal, and the usual invariances, but not by chiral symmetry. Terms that include a factor  $\tau_1 \cdot \tau_2$  (owing to isospin invariance) can be left out due to Fierz ambiguity. Because of parity and time reversal, only even powers of momentum are allowed. Thus, the expansion of the contact potential is formally written as

$$
V_{\rm ct} = V_{\rm ct}^{(0)} + V_{\rm ct}^{(2)} + V_{\rm ct}^{(4)} + V_{\rm ct}^{(6)} + \cdots, \qquad (2.23)
$$

where the superscript denotes the power or order.

The zeroth-order (leading order, LO) contact potential is given by

$$
V_{\rm ct}^{(0)}(\vec{p}', \vec{p}) = C_S + C_T \, \vec{\sigma}_1 \cdot \vec{\sigma}_2 \tag{2.24}
$$

and, in terms of partial waves,

$$
V_{\rm ct}^{(0)}(^1S_0) = \widetilde{C}_{\,S_0} = 4\pi \ (C_S - 3 \ C_T), \tag{2.25}
$$

$$
V_{\rm ct}^{(0)}(^{3}S_{1}) = \widetilde{C}_{^{3}S_{1}} = 4\pi (C_{S} + C_{T}). \tag{2.26}
$$

To deal with the isospin breaking in the <sup>1</sup>S<sub>0</sub> state, we treat  $\widetilde{C}_{^1S_0}$ in a charge-dependent way. Thus, we will distinguish among  $\widetilde{C}_{S_0}^{\text{pp}}, \widetilde{C}_{S_0}^{\text{np}}, \text{ and } \widetilde{C}_{S_0}^{\text{nn}}.$ 

At second order (NLO), we have

$$
V_{\text{ct}}^{(2)}(\vec{p}', \vec{p}) = C_1 q^2 + C_2 k^2 + (C_3 q^2 + C_4 k^2) \vec{\sigma}_1 \cdot \vec{\sigma}_2 + C_5[-i\vec{S} \cdot (\vec{q} \times \vec{k})] + C_6 (\vec{\sigma}_1 \cdot \vec{q}) (\vec{\sigma}_2 \cdot \vec{q}) + C_7 (\vec{\sigma}_1 \cdot \vec{k}) (\vec{\sigma}_2 \cdot \vec{k}),
$$
(2.27)

and partial-wave decomposition yields

 $\boldsymbol{V}$ 

 $\overline{V}$ 

$$
V_{\text{ct}}^{(2)}(^{1}S_{0}) = C_{1S_{0}}(p^{2} + p'^{2}),
$$
\n
$$
V_{\text{ct}}^{(2)}(^{3}P_{0}) = C_{3P_{0}} pp',
$$
\n
$$
V_{\text{ct}}^{(2)}(^{1}P_{1}) = C_{1P_{1}} pp',
$$
\n
$$
V_{\text{ct}}^{(2)}(^{3}P_{1}) = C_{3P_{1}} pp',
$$
\n
$$
V_{\text{ct}}^{(2)}(^{3}S_{1}) = C_{3S_{1}}(p^{2} + p'^{2}),
$$
\n
$$
V_{\text{ct}}^{(2)}(^{3}S_{1} - ^{3}D_{1}) = C_{3S_{1}-3D_{1}}p^{2},
$$
\n
$$
V_{\text{ct}}^{(2)}(^{3}D_{1} - ^{3}S_{1}) = C_{3S_{1}-3D_{1}}p'^{2},
$$
\n
$$
V_{\text{ct}}^{(2)}(^{3}P_{2}) = C_{3P_{2}} pp'.
$$
\n(2.28)

The relationship between  $C_{(2S+1)L_J}$  and  $C_i$  can be found in Ref. [\[1\]](#page-16-0).

<span id="page-5-0"></span>The fourth-order  $(N^3LO)$  contacts are

$$
V_{\text{ct}}^{(4)}(\vec{p}', \vec{p})
$$
  
=  $D_1 q^4 + D_2 k^4 + D_3 q^2 k^2 + D_4 (\vec{q} \times \vec{k})^2$   
+  $[D_5 q^4 + D_6 k^4 + D_7 q^2 k^2 + D_8 (\vec{q} \times \vec{k})^2] \vec{\sigma}_1 \cdot \vec{\sigma}_2$   
+  $(D_9 q^2 + D_{10} k^2) [-i \vec{S} \cdot (\vec{q} \times \vec{k})]$   
+  $(D_{11} q^2 + D_{12} k^2) (\vec{\sigma}_1 \cdot \vec{q}) (\vec{\sigma}_2 \cdot \vec{q})$   
+  $(D_{13} q^2 + D_{14} k^2) (\vec{\sigma}_1 \cdot \vec{k}) (\vec{\sigma}_2 \cdot \vec{k})$   
+  $D_{15} [\vec{\sigma}_1 \cdot (\vec{q} \times \vec{k}) \vec{\sigma}_2 \cdot (\vec{q} \times \vec{k})],$  (2.29)

with contributions by partial waves,

$$
V_{\text{ct}}^{(4)}(^{1}S_{0}) = \hat{D}_{1S_{0}}(p'^{4} + p^{4}) + D_{1S_{0}}p'^{2}p^{2},
$$
  
\n
$$
V_{\text{ct}}^{(4)}(^{3}P_{0}) = D_{3P_{0}}(p'^{3}p + p'p^{3}),
$$
  
\n
$$
V_{\text{ct}}^{(4)}(^{1}P_{1}) = D_{1P_{1}}(p'^{3}p + p'p^{3}),
$$
  
\n
$$
V_{\text{ct}}^{(4)}(^{3}P_{1}) = D_{3P_{1}}(p'^{3}p + p'p^{3}),
$$
  
\n
$$
V_{\text{ct}}^{(4)}(^{3}S_{1}) = \hat{D}_{3S_{1}}(p'^{4} + p^{4}) + D_{3S_{1}}p'^{2}p^{2},
$$
  
\n
$$
V_{\text{ct}}^{(4)}(^{3}D_{1}) = D_{3D_{1}}p'^{2}p^{2},
$$
  
\n
$$
V_{\text{ct}}^{(4)}(^{3}D_{1} - {}^{3}D_{1}) = \hat{D}_{3S_{1}}-{}^{3}D_{1}p^{4} + D_{3S_{1}}-{}^{3}D_{1}p'^{2}p^{2},
$$
  
\n
$$
V_{\text{ct}}^{(4)}(^{3}D_{1} - {}^{3}S_{1}) = \hat{D}_{3S_{1}}-{}^{3}D_{1}p'^{4} + D_{3S_{1}}-{}^{3}D_{1}p'^{2}p^{2},
$$
  
\n
$$
V_{\text{ct}}^{(4)}(^{1}D_{2}) = D_{1D_{2}}p'^{2}p^{2},
$$
  
\n
$$
V_{\text{ct}}^{(4)}(^{3}D_{2}) = D_{3D_{2}}p'^{2}p^{2},
$$
  
\n
$$
V_{\text{ct}}^{(4)}(^{3}P_{2}) = D_{3P_{2}}(p'^{3}p + p'p^{3}),
$$
  
\n
$$
V_{\text{ct}}^{(4)}(^{3}P_{2} - {}^{3}P_{2}) = D_{3P_{2}}-{}^{3}P_{2}p'^{3}p,
$$
  
\n
$$
V_{\text{ct}}^{(4)}(^{3}P_{2}
$$

Reference [\[1\]](#page-16-0) provides formulas that relate  $D_{(2S+1)L}$  to  $D_i$ .

The next higher order is sixth order  $(N<sup>5</sup>LO)$  at which, finally,  $F$  waves are also affected in the following way:

$$
V_{\text{ct}}^{(6)}({}^{3}F_{2}) = E_{^{3}F_{2}}p'^{3}p^{3},
$$
  
\n
$$
V_{\text{ct}}^{(6)}({}^{1}F_{3}) = E_{^{1}F_{3}}p'^{3}p^{3},
$$
  
\n
$$
V_{\text{ct}}^{(6)}({}^{3}F_{3}) = E_{^{3}F_{3}}p'^{3}p^{3},
$$
  
\n
$$
V_{\text{ct}}^{(6)}({}^{3}F_{4}) = E_{^{3}F_{4}}p'^{3}p^{3}.
$$
\n(2.31)

To obtain an optimal fit of the *NN* data at the highest order we consider in this paper, we include the above  $F$ -wave contacts in our  $N^4$ LO potentials.

#### **E. Charge dependence**

This is to summarize what charge dependence we include. Through all orders, we take the charge dependence of the 1PE due to pion-mass splitting into account, Eqs. [\(2.18\)](#page-3-0) and [\(2.19\)](#page-3-0). Charge dependence is seen most prominently in the  ${}^{1}S_{0}$  state at low energies, particularly in the  ${}^{1}S_{0}$  scattering lengths. The charge-dependent 1PE cannot explain it all. The remainder is accounted for by treating the  ${}^{1}S_{0}$  LO contact parameter,

 $C_{\text{1S}_0}$ , Eq. [\(2.25\)](#page-4-0), in a charge-dependent way. Thus, we will  $\mathsf{C}^1$ distinguish among  $\widetilde{C}_{1S_0}^{pp}$ ,  $\widetilde{C}_{1S_0}^{np}$ , and  $\widetilde{C}_{1S_0}^{nn}$ . For pp scattering at any order, we include the relativistic Coulomb potential [\[61,62\]](#page-17-0). Finally, at  $N<sup>3</sup>LO$  and  $N<sup>4</sup>LO$ , we take into account irreducible  $\pi$ - $\gamma$  exchange [\[63\]](#page-17-0), which affects only the *np* potential. We also take nucleon-mass splitting into account, or in other words, we always apply the correct values for the masses of the nucleons involved in the various charge-dependent *NN* potentials.

For a comprehensive discussion of all possible sources for the charge dependence of the *NN* interaction, see Ref. [\[1\]](#page-16-0).

### **F. The full potential**

The sum of long-range [Eqs.  $(2.12)$ – $(2.16)$ ] plus shortrange potentials [Eq. [\(2.23\)](#page-4-0)] results in

$$
V_{\rm LO} \equiv V^{(0)} = V_{1\pi} + V_{\rm ct}^{(0)},\tag{2.32}
$$

$$
V_{\rm NLO} \equiv V^{(2)} = V_{\rm LO} + V_{2\pi}^{(2)} + V_{\rm ct}^{(2)},\tag{2.33}
$$

$$
V_{\text{NNLO}} \equiv V^{(3)} = V_{\text{NLO}} + V_{2\pi}^{(3)},\tag{2.34}
$$

$$
V_{\text{N}^3\text{LO}} \equiv V^{(4)} = V_{\text{NNLO}} + V_{2\pi}^{(4)} + V_{3\pi}^{(4)} + V_{\text{ct}}^{(4)}, \quad (2.35)
$$

$$
V_{\rm N^4LO} \equiv V^{(5)} = V_{\rm N^3LO} + V_{2\pi}^{(5)} + V_{3\pi}^{(5)}, \tag{2.36}
$$

where we left out the higher order corrections to the 1PE because, as discussed, they are absorbed by mass and coupling constant renormalizations. It is also understood that the charge dependence discussed in the previous subsection is included.

In our systematic potential construction, we follow the above scheme, except for two physically motivated modifications. We add to  $V_{\text{N}^3\text{LO}}$  the  $1/M_N$  correction of the NNLO 2PE proportional to  $c_i$ . This correction is proportional to  $c_i/M_N$  and appears nominally at fifth order, because we count  $Q/M_N \sim$  $(Q/\Lambda_{\chi})^2$ . This contribution is given in Eqs. (2.19)–(2.23) of Ref. [\[52\]](#page-16-0) and we denote it by  $V_{2\pi, c_i/M_N}^{(5)}$ . In short, in Eq. (2.35), we replace

$$
V_{\mathrm{N}^3\mathrm{LO}} \longmapsto V_{\mathrm{N}^3\mathrm{LO}} + V_{2\pi, c_i/M_N}^{(5)}.
$$
 (2.37)

As demonstrated in Ref. [\[15\]](#page-16-0), the 2PE bubble diagram proportional to  $c_i^2$  that appears at N<sup>3</sup>LO is unrealistically attractive, while the  $c_i/M_N$  correction is large and repulsive. Therefore, it makes sense to group these diagrams together to arrive at a more realistic intermediate attraction at  $N<sup>3</sup>LO$ .

The second modification consists of adding to  $V_{N<sup>4</sup>LO}$  the four  $F$ -wave contacts listed in Eq. (2.31) to ensure an optimal fit of the *NN* data for the potential of the highest order constructed in this work.

The potential  $V$  is, in principal, an invariant amplitude (with relativity taken into account perturbatively) and thus satisfies a relativistic scattering equation, like, e.g., the Blankenbeclar-Sugar (BbS) equation [\[64\]](#page-17-0), which reads explicitly

$$
T(\vec{p}', \vec{p}) = V(\vec{p}', \vec{p}) + \int \frac{d^3 p''}{(2\pi)^3} V(\vec{p}', \vec{p}'') \frac{M_N^2}{E_{p''}} \times \frac{1}{p^2 - p''^2 + i\epsilon} T(\vec{p}'', \vec{p})
$$
 (2.38)

<span id="page-6-0"></span>with  $E_{p''} \equiv \sqrt{M_N^2 + p''^2}$  and  $M_N$  being the nucleon mass. The advantage of using a relativistic scattering equation is that it automatically includes relativistic kinematical corrections to all orders. Thus, in the scattering equation, no propagator modifications are necessary when moving up to higher orders.

Defining

$$
\widehat{V}(\vec{p}', \vec{p}) \equiv \frac{1}{(2\pi)^3} \sqrt{\frac{M_N}{E_{p'}}} V(\vec{p}', \vec{p}) \sqrt{\frac{M_N}{E_p}}
$$
(2.39)

and

$$
\widehat{T}(\vec{p}', \vec{p}) \equiv \frac{1}{(2\pi)^3} \sqrt{\frac{M_N}{E_{p'}}} T(\vec{p}', \vec{p}) \sqrt{\frac{M_N}{E_p}},
$$
\n(2.40)

where the factor  $1/(2\pi)^3$  is added for convenience, the BbS equation collapses into the usual, nonrelativistic Lippmann-Schwinger (LS) equation,

$$
\widehat{T}(\vec{p}', \vec{p}) = \widehat{V}(\vec{p}', \vec{p}) + \int d^3 p'' \widehat{V}(\vec{p}', \vec{p}'')
$$

$$
\times \frac{M_N}{p^2 - p''^2 + i\epsilon} \widehat{T}(\vec{p}'', \vec{p}). \tag{2.41}
$$

Since *V* satisfies Eq.  $(2.41)$ , it may be regarded as a nonrelativistic potential. By the same token,  $\overline{T}$  may be considered as the nonrelativistic  $T$  matrix. All technical aspects associated with the solution of the LS equation can be found in Appendix A of Ref. [\[65\]](#page-17-0), including specific formulas for the calculation of the  $np$  and  $pp$  phase shifts (with Coulomb). Additional details concerning the relevant operators and their decompositions are given in Sec. 4 of Ref. [\[66\]](#page-17-0). Finally, computational methods to solve the LS equation are found in Ref. [\[67\]](#page-17-0).

### **G. Regularization and nonperturbative renormalization**

Iteration of  $V$  in the LS equation, Eq.  $(2.41)$ , requires cutting  $\dot{V}$  off for high momenta to avoid infinities. This is consistent with the fact that ChPT is a low-momentum expansion which is valid only for momenta  $Q < \Lambda_{\chi} \approx 1$  GeV. Therefore, the potential V is multiplied with the regulator function  $f(p', p)$ ,

$$
\widehat{V}(\vec{p}', \vec{p}) \longmapsto \widehat{V}(\vec{p}', \vec{p}) f(p', p) \tag{2.42}
$$

with

$$
f(p', p) = \exp[-(p'/\Lambda)^{2n} - (p/\Lambda)^{2n}], \qquad (2.43)
$$

such that

$$
\widehat{V}(\vec{p}', \vec{p}) f(p', p)
$$
\n
$$
\approx \widehat{V}(\vec{p}', \vec{p}) \left\{ 1 - \left[ \left( \frac{p'}{\Lambda} \right)^{2n} + \left( \frac{p}{\Lambda} \right)^{2n} \right] + \cdots \right\}.
$$
\n(2.44)

For the cutoff parameter  $\Lambda$ , we apply three different values, namely, 450, 500, and 550 MeV.

Equation (2.44) provides an indication of the fact that the exponential cutoff does not necessarily affect the given order at which the calculation is conducted. For sufficiently large  $n$ , the regulator introduces contributions that are beyond the given order. Assuming a good rate of convergence of the chiral

expansion, such orders are small as compared to the given order and thus do not affect the accuracy at the given order. Thus, we use  $n = 2$  for 3PE and 2PE and  $n = 4$  for 1PE (except in LO and NLO, where we use  $n = 2$  for 1PE). For contacts of order  $\nu$ , *n* is chosen such that  $2n > \nu$ .

In our calculations, we apply, of course, the exponential form, Eq.  $(2.43)$ , and not the expansion, Eq.  $(2.44)$ . On a similar note, we also do not expand the square-root factors in Eqs.  $(2.39)$  and  $(2.40)$  because they are kinematical factors which guarantee relativistic elastic unitarity.

It is pretty obvious that results for the  $T$  matrix may depend sensitively on the regulator and its cutoff parameter. The removal of such regulator dependence is known as renormalization.

The renormalization of the *perturbatively* calculated *NN* potential is not a problem. The problem is nonperturbative renormalization. This problem typically occurs in *nuclear* EFT because nuclear physics is characterized by bound states and large scattering lengths, which are nonperturbative in nature. Or in other words, to obtain the nuclear amplitude, the potential has to be resummed (to infinite orders) in the LS equation, Eq. (2.41). EFT power counting may be different for nonperturbative processes as compared to perturbative ones. Such difference may be caused by the infrared enhancement of the reducible diagrams generated in the LS equation.

Weinberg's implicit assumption [\[5\]](#page-16-0) was that the counterterms introduced to renormalize the perturbatively calculated potential, based upon naive dimensional analysis ("Weinberg counting," cf. Sec.  $\overline{I}$  IB), are also sufficient to renormalize the nonperturbative resummation of the potential in the LS equation.

Weinberg's assumption may not be correct as first pointed out by Kaplan *et al.* [\[68\]](#page-17-0), and we refer the interested reader to Sec. 4.5 of Ref. [\[1\]](#page-16-0) for a comprehensive discussion of the issue. Even today, no generally accepted solution to this problem has emerged and some more recent proposals can be found in Refs. [\[69–76\]](#page-17-0). Concerning the construction of quantitative *NN* potential (by which we mean *NN* potentials suitable for use in contemporary many-body nuclear methods), only Weinberg counting has been used with success during the past 25 years  $[1,6,17,21,23,26]$ , which is why also in the present work we will apply Weinberg counting.

In spite of the criticism, Weinberg counting may be perceived as not unreasonable by the following argument. For a successful EFT (in its domain of validity), one must be able to claim independence of the predictions on the regulator within the theoretical error. Also, truncation errors must decrease as we go to higher and higher orders. These are precisely the goals of renormalization.

Lepage [\[77\]](#page-17-0) has stressed that the cutoff independence should be examined for cutoffs below the hard scale and not beyond. Ranges of cutoff independence within the theoretical error are to be identified using Lepage plots [\[77\]](#page-17-0). A systematic investigation of this kind has been conducted in Ref. [\[78\]](#page-17-0). In that work, the error of the predictions was quantified by calculating the  $\chi^2$ /datum for the reproduction of the *np* elastic scattering data as a function of the cutoff parameter  $\Lambda$  of the regulator function Eq.  $(2.43)$ . Predictions by chiral np potentials at order NLO and NNLO were investigated applying

Publication date	No. of <i>pp</i> data	No. of <i>np</i> data	References
Jan. 1955–Dec. 1992	1787	2514	[79.80]
Jan. 1993–Dec. 1999	1145	544	Tables XV and XVI of Ref. [65]
Jan. 2000–Dec. 2016	140	511	Ref. [81] and Table IV of present paper
Total	3072	3569	

<span id="page-7-0"></span>TABLE III. Publication history of the *NN* data below 350 MeV laboratory energy and references for their listings. Only data that pass the Nijmegen acceptance criteria [\[62\]](#page-17-0) are counted. "Total" defines the 2016 database.

Weinberg counting for the counter terms (*NN* contact terms). It is found that the reproduction of the  $np$  data at laboratory energies below 200 MeV is generally poor at NLO, while at NNLO the  $\chi^2$ /datum assumes acceptable values (a clear demonstration of order-by-order improvement). Moreover, at NNLO, a plateau of constant low  $\chi^2$  for cutoff parameters ranging from about 450 to 850 MeV can be identified. This may be perceived as cutoff independence (and, thus, successful renormalization) for the relevant range of cutoff parameters.

### **III.** *NN* **SCATTERING AND THE DEUTERON**

Based upon the formalism presented in the previous section, we have constructed *NN* potentials through five orders of the chiral expansion, ranging from LO  $(Q^0)$  to N<sup>4</sup>LO  $(Q^5)$ . In each order, we consider three cutoffs, namely,  $\Lambda = 450, 500$ , and 550 MeV. Since we take charge dependence into account, each *NN* potential comes in three versions: pp, np, and nn. The results from these potentials for *NN* scattering and the deuteron will be presented in this section.

### **A.** *NN* **database**

Since an important part of *NN* potential construction involves optimizing the reproduction of the *NN* data by the potential, we need to state, first, what *NN* database we are using.

Our database consists of all *NN* data below 350 MeV laboratory energy published in refereed physics journals between January 1955 and December 2016 that are not discarded when applying the Nijmegen rejection criteria [\[62\]](#page-17-0). We will refer to this as the "2016 database." This database was started by the Nijmegen group, who critically checked and assembled the data published up to December 1992. This 1992 database consists of 1787  $pp$  data (listed in Ref. [\[79\]](#page-17-0)) and 2514 *np* data (tabulated in Ref.  $[80]$ ); cf. Table III. In Ref. [\[65\]](#page-17-0), the database was then extended to include the data published up to December 1999 that survived the Nijmegen rejection criteria. This added 1145  $pp$  and 544  $np$  data (given in Tables XV and XVI of Ref. [\[65\]](#page-17-0), respectively). Thus, the 1999 database includes 2932  $pp$  and 3058  $np$  data.

To get to the 2016 database, we have added to the 1999 database the data published between January 2000 and December 2016 that are not rejected by the Nijmegen criteria. We are aware of the fact that modified rejection criteria have been proposed [\[82\]](#page-17-0) and applied in recent *NN* data analysis work [\[83\]](#page-17-0), but we continue to apply the classic Nijmegen criteria [\[62\]](#page-17-0) to be consistent with the pre-2000 part of the database.

Concerning after-1999 pp data, there exists only one set of 139 differential cross sections between 239.9 and 336.2 MeV measured by the EDDA group at COSY (Jűlich, Germany) with an overall uncertainty of 2.5% [\[81\]](#page-17-0). Thus, the total number of pp data contained in the 2016 database is 3072 (Table III).

In contrast to  $pp$ , there have been many new  $np$  measurements after 1999. We list the datasets that survived the Nijmegen rejection criteria in Table [IV.](#page-8-0) According to that list, the number of valid after-1999  $np$  data is 511, bringing the total number of np data contained in the 2016 database to 3569 (Table III).

For comparison, we mention that the 2013 Granada *NN* database [\[83\]](#page-17-0) consists of 2996 pp and 3717 np data. The larger number of pp data in our base is mainly due to the inclusion of 140  $pp$  data from Ref.  $[81]$  which are left out in the Granada base. On the other hand, the Granada base contains 148 more  $np$  data, which is a consequence of the modified rejection criteria applied by the Granada group, which allows for the survival of more *np* data.

Finally, we note that in the potential construction reported in this paper, we make use of the 2016 database only up to 290 MeV laboratory energy (pion-production threshold). Between 0 and 290 MeV, the 2016 database contains 2132 pp data and  $2721$  *np* data (cf. Table [V\)](#page-8-0).

#### **B. Data fitting procedure**

When we are talking about data fitting, we are referring to the adjustment of the *NN* contact parameters available at the respective order. Note that in our*NN* potential construction, the  $\pi N$  LECs are not fit parameters. The  $\pi N$  LECs are held fixed at their values determined in the  $\pi N$  analysis of Ref. [\[60\]](#page-17-0) displayed in Table  $II$  (we use the central values shown in that table). Thus, the *NN* contacts (Sec. [II D\)](#page-4-0) are the only fit parameters used to optimize the reproduction of the *NN* data below 290 MeV laboratory energy. As discussed, those contact terms describe the short-range part of the *NN* potentials and adjust the lower partial waves.

In the construction of any *NN* potential, we always start with the  $pp$  version since the  $pp$  data are the most accurate ones. The fitting is done in three steps. In the first step, the pp potential is adjusted to reproduce as closely as possible the *pp* phase shifts of the Nijmegen multienergy *pp* phase shift analysis [\[80\]](#page-17-0) up to 300 MeV laboratory energy. This is to ensure that phase shifts are in the right ballpark. In the second step, we make use of the Nijmegen pp error matrix [\[96\]](#page-17-0) to minimize the  $\chi^2$  that results from it. The advantage of this step is that it is computationally very fast and easy. Finally,

<span id="page-8-0"></span>TABLE IV. After-1999 np data below 350 MeV included in the 2016 np database. "Error" refers to the experimental overall normalization errors of the individual datasets. "None" signifies that the respective experimental data set does not carry a normalization error, i.e., the data are absolute. "Float" indicates that, in the analysis of the data set, the normalization was allowed to assume a value for which the  $\chi^2$  is a minimum disregarding a comparison with the experimental normalization error. This is done in cases where there is doubt about the alleged experimental normalization error. In the cases of "None" and "Float," the normalization is not counted as an observable. This table contains 473 observables plus 38 normalizations resulting in a total of 511 data. For the observables, we use in general the notation of Hoshizaki [\[84\]](#page-17-0), except for types which are undefined in the Hoshizaki formalism, where we use the Saclay notation [\[85\]](#page-17-0).

$T_{\text{lab}}$ (MeV)	No. type	Error $(\%)$	Institution	Ref.
$9.2 - 349.0$	92 $\sigma_{\text{tot}}$	None	Los Alamos	[86]
10.0	$6\sigma$	0.8	Ohio	[87]
95.0	$10\sigma$	5.0	Uppsala	[88]
95.0	$9\sigma$	4.0	Uppsala	[89]
96.0	$11\sigma$	5.0	Uppsala	[90]
96.0	$9\sigma$	3.0	Uppsala	[91]
96.0	$12\sigma$	None	Uppsala	[92]
260.0	8 P	1.8	<b>PSI</b>	[93]
260.0	16 P	1.8	<b>PSI</b>	$[93]$
260.0	$8A_{yy}$	3.9	<b>PSI</b>	[93]
260.0	$16 A_{yy}$	3.9	<b>PSI</b>	[93]
260.0	$9A_{zz}$	7.2	PSI	[93]
260.0	$5\ D$	2.4	<b>PSI</b>	[94]
260.0	8 D	Float	<b>PSI</b>	[94]
260.0	$8 D_{0s''0k}$	Float	<b>PSI</b>	[94]
260.0	$5 D_t$	2.4	PSI	[94]
260.0	$4A_t$	2.4	PSI	[94]
260.0	$8A_t$	2.4	<b>PSI</b>	[94]
260.0	$4 R_t$	2.4	<b>PSI</b>	[94]
260.0	$8 R_t$	2.4	<b>PSI</b>	$[94]$
260.0	$8 N_{0nkk}$	2.4	<b>PSI</b>	$[94]$
260.0	$4 N_{0s''kn}$	2.4	<b>PSI</b>	[94]
260.0	$8 N_{0s''kn}$	2.4	<b>PSI</b>	[94]
260.0	$4 N_{0s''sn}$	2.4	PSI	[94]
260.0	$8 N_{0s''sn}$	2.4	<b>PSI</b>	[94]
284.0	14 P	3.0	<b>PSI</b>	$[95]$
314.0	14P	3.0	<b>PSI</b>	[95]
315.0	16P	1.2	<b>PSI</b>	[93]
315.0	11 $A_{yy}$	3.7	<b>PSI</b>	[93]
315.0	16 $A_{yy}$	3.7	<b>PSI</b>	$[93]$
315.0	11 $A_{zz}$	7.1	PSI	$[93]$
315.0	6 D	Float	PSI	[94]
315.0	6 $D_{0s''0k}$	Float	<b>PSI</b>	[94]
315.0	$8\ D_{0s''0k}$	Float	<b>PSI</b>	[94]
315.0	$6 D_t$	1.9	<b>PSI</b>	[94]
315.0	$6A_t$	1.9	<b>PSI</b>	$[94]$
315.0	$8A_t$	1.9	<b>PSI</b>	[94]
315.0	$6 R_t$	1.9	<b>PSI</b>	[94]
315.0	$8 R_t$	1.9	PSI	[94]
315.0	$5 N_{0s''kn}$	1.9	PSI	[94]
315.0	$8 N_{0s''kn}$	1.9	<b>PSI</b>	$[94]$
315.0	6 $N_{0s''sn}$	1.9	<b>PSI</b>	[94]
315.0	$8 N_{0s''sn}$	1.9	<b>PSI</b>	[94]
315.0	$8 N_{0nkk}$	1.9	<b>PSI</b>	[94]
344.0	14 P	3.0	PSI	[95]

TABLE V.  $\chi^2$ /datum for the fit of the 2016 *NN* data base by *NN* potentials at various orders of chiral EFT ( $\Lambda = 500$  MeV in all cases).

$T_{\rm lab}$ bin (MeV) No. of data		LO <sub>1</sub>	NLO	NNLO $N^3LO$ $N^4LO$		
		Proton-proton				
$0 - 100$	795	520	18.9	2.28	1.18	1.09
$0 - 190$	1206	430	43.6	4.64	1.69	1.12
$0 - 290$	2132	360	70.8	7.60	2.09	1.21
			Neutron-proton			
$0 - 100$	1180	114	7.2	1.38	0.93	0.94
$0 - 190$	1697	96	23.1	2.29	1.10	1.06
$0 - 290$	2721	94	36.7	5.28	1.27	1.10
		<i>pp</i> plus <i>np</i>				
$0 - 100$	1975	283	11.9	1.74	1.03	1.00
$0 - 190$	2903	235	31.6	3.27	1.35	1.08
$0 - 290$	4853	206	51.5	6.30	1.63	1.15

in the third and final step, the  $pp$  potential contact parameters are fine-tuned by minimizing the  $\chi^2$  that results from a direct comparison with the experimental  $pp$  data contained in the 2016 database below 290 MeV. For this we use a copy of the SAID software package, which includes all electromagnetic contributions necessary for the calculation of *NN* observables at low energy. Since it turned out that the Nijmegen error matrix produces very accurate  $\chi^2$  for pp energies below 75 MeV, we use the values from this error matrix for the energies up to 75 MeV and the values from a direct confrontation with the data above that energy.

The  $I = 1$  np potential is constructed by starting from the *pp* version, applying the charge dependence discussed in Sec. [II E,](#page-5-0) and adjusting the nonderivative  ${}^{1}S_{0}$  contact such as to reproduce the  ${}^{1}S_{0}$  *np* scattering length. This then yields the preliminary fit of the  $I = 1 np$  potential. The preliminary fit of the  $I = 0$  *np* potential is obtained by a fit to the  $I = 0$  *np* phase shifts of the Nijmegen multienergy  $np$  phase shift analysis  $[80]$  below 300 MeV. Starting from this preliminary *np* fit, the contact parameters are fine-tuned in a confrontation with the *np* data below 290 MeV, for which the  $\chi^2$  is minimized. We note that during this last step we have also allowed for minor changes of the  $I = 1$  parameters (which also modifies the pp potential) to obtain an even lower  $\chi^2$  overall.

Finally the nn potential is obtained by starting from the pp version, replacing the proton masses by neutron masses, leaving out Coulomb, and adjusting the nonderivative  ${}^{1}S_{0}$ contact such as to reproduce the  ${}^{1}S_{0}$  nn scattering length for which we assume the empirical value of  $-18.95$  MeV [\[97,98\]](#page-17-0).

We note that our procedure for fitting *NN* potentials to data is essentially the same that was used to fit the high-precision *NN* potentials of the 1990s [\[65,99,100\]](#page-17-0) (fitted up to 350 MeV) and the first precision chiral *NN* potentials [\[1,16\]](#page-16-0) (fitted up to 290 MeV). This is quite in contrast to the procedure applied in the recent construction of the  $NNLO<sub>sat</sub>$  potential  $[26]$ , where the *NN* data up to 35 MeV and the ground-state energies and radii of nuclei up to  $40$ Ca are taken into acount to fix simulteneously the 2NF and 3NF. In Ref. [\[26\]](#page-16-0), the *NN* data up to 35 MeV are reproduced with a  $\chi^2$ /datum of 4.3. Similar procedures are applied in Ref. [\[27\]](#page-16-0).

<span id="page-9-0"></span>

FIG. 2. Chiral expansion of neutron-proton scattering as represented by the phase shifts in  $S$ ,  $P$ , and  $D$  waves and mixing parameters  $\epsilon_1$  and  $\epsilon_2$ . Five orders ranging from LO to N<sup>4</sup>LO are shown as denoted. A cutoff  $\Lambda = 500$  MeV is applied in all cases. The filled and open circles represent the results from the Nijmegen multienergy  $np$  phase-shift analysis [\[80\]](#page-17-0) and the GWU single-energy  $np$  analysis SP07 [\[102\]](#page-17-0), respectively.

Our fit procedures differ also substantially from the ones used in the recent chiral *NN* potential constructions of Refs. [\[23,24\]](#page-16-0), where the potentials are fitted to phase shifts. Already in the early 1990s, the Nijmegen group has pointed out repeatedly and demonstrated clearly [\[96\]](#page-17-0) that fitting to experimental data should be preferred over fitting to phase shifts, because a seemingly good fit to phase shifts can result in a bad reproduction of the data. Note that phase shifts are not experimental data.

## **C. Results for** *NN* **scattering**

The  $\chi^2$ /datum for the reproduction of the *NN* data at various orders of chiral EFT are shown in Table [V](#page-8-0) for different energy intervals below 290 MeV laboratory energy  $(T_{\text{lab}})$ . The bottom line of Table [V](#page-8-0) summarizes the essential results. For the close to 5000 pp plus np data below 290 MeV (pion-production threshold), the  $\chi^2$ /datum is 51.4 at NLO and 6.3 at NNLO. Note that the number of *NN* contact terms is the same for both orders. The improvement is entirely due to an improved description of the 2PE contribution, which is responsible for the crucial intermediate-range attraction of the nuclear force. At NLO, only the uncorrelated 2PE is taken into account, which is insufficient. From the classic meson-theory of nuclear forces [\[101\]](#page-17-0), it is well known that  $\pi$ - $\pi$  correlations and nucleon

resonances need to be taken into account for a realistic model of 2PE that provides a sufficient amount of intermediate attraction to properly bind nucleons in nuclei. In the chiral theory, these contributions are encoded in the subleading  $\pi N$ vertexes with LECs denoted by  $c_i$ . These enter at NNLO and are the reason for the substantial improvements we encounter at that order. This is the best proof that, starting at NNLO, the chiral approach to nuclear forces is getting the physics right.

To continue on the bottom line of Table [V,](#page-8-0) after NNLO, the  $\chi^2$ /datum then further improves to 1.63 at N<sup>3</sup>LO and, finally, reaches the almost perfect value of  $1.15$  at  $N<sup>4</sup>LO$ —a fantastic convergence.

Corresponding np phase shifts are displayed in Fig. 2, which reflect what the  $\chi^2$  have already proven, namely, an excellent convergence when going from NNLO to  $N<sup>3</sup>LO$  and, finally, to  $N<sup>4</sup>LO$ . However, at LO and NLO there are large discrepancies between the predictions and the empirical phase shifts as to be expected from the corresponding  $\chi^2$  values. This fact renders applications of the LO and NLO nuclear force useless for any realistic calculation (but they could be used to demonstrate truncation errors).

For order N<sup>4</sup>LO (with  $\Lambda = 500$  MeV), we also provide the numerical values for the phase shifts in the appendix. Our  $pp$  phase shifts are the phase shifts of the nuclear plus relativistic Coulomb interaction with respect to Coulomb

<span id="page-10-0"></span>TABLE VI. Scattering lengths (a) and effective ranges (r) in units of fm as predicted by *NN* potentials at various orders of chiral EFT  $(\Lambda = 500 \text{ MeV}$  in all cases).  $(a_{pp}^C$  and  $r_{pp}^C$  refer to the pp parameters in the presence of the Coulomb force.  $a^N$  and  $r^N$  denote parameters determined from the nuclear force only and with all electromagnetic effects omitted.)  $a_{nn}^N$  and  $a_{np}$  are fitted; all other quantities are predictions.

	LO	<b>NLO</b>	<b>NNLO</b>	$N^3LO$	$N^4LO$	Empirical
			${}^1S_0$			
$a_{\scriptscriptstyle{pp}}^{\scriptscriptstyle{C}}$	$-7.8153$	$-7.8128$	$-7.8140$	$-7.8155$	$-7.8160$	$-7.8196(26)$ [62]
						$-7.8149(29)$ [104]
$r_{pp}^C$	1.886	2.678	2.758	2.772	2.774	$2.790(14)$ [62]
						$2.769(14)$ [104]
		$-17.476$	$-17.762$	$-17.052$	$-17.123$	
$a_{\scriptstyle\scriptstyle\rm pp}^N \ r_{\scriptstyle\scriptstyle\rm pp}^N \ a_{\scriptstyle\scriptstyle\rm nn}^N \ r_{\scriptstyle\rm nn}^N$		2.752	2.821	2.851	2.853	
	$-18.950$	$-18.950$	$-18.950$	$-18.950$	$-18.950$	$-18.95(40)$ [97,98]
	1.857	2.726	2.800	2.812	2.816	$2.75(11)$ [105]
$a_{np}$	$-23.738$	$-23.738$	$-23.738$	$-23.738$	$-23.738$	$-23.740(20)$ [65]
$r_{np}$	1.764	2.620	2.687	2.700	2.704	$[2.77(5)]$ [65]
			${}^3S_1$			
$a_t$	5.255	5.415	5.418	5.420	5.420	$5.419(7)$ [65]
$r_t$	1.521	1.755	1.752	1.754	1.753	$1.753(8)$ [65]

wave functions. Note, however, that for the calculation of observables (e.g., to obtain the  $\chi^2$  in regard to experimental data), we use electromagnetic phase shifts, as *necessary*, which we obtain by adding to the Coulomb phase shifts the effects from two-photon exchange, vacuum polarization, and magnetic moment interactions as calculated by the Nijmegen group [\[62,103\]](#page-17-0). This is important for  ${}^{1}S_{0}$  below 30 MeV and negligible otherwise. For  $nn$  and  $np$  scattering, our phase shifts are the ones from the nuclear interaction with respect to Riccati-Bessel functions. The technical details of our phase shift calculations can be found in Appendix A3 of Ref. [\[65\]](#page-17-0).

The low-energy scattering parameters, order by order, are shown in Table VI. For  $nn$  and  $np$ , the effective range expansion without any electromagnetic interaction is used. In the case of pp scattering, the quantities  $a_{pp}^C$  and  $r_{pp}^C$  are obtained by using the effective range expansion appropriate in the presence of the Coulomb force (cf. Appendix A4 of Ref. [\[65\]](#page-17-0)). Note that the empirical values for  $a_{pp}^C$  and  $r_{pp}^C$  in Table VI were obtained by subtracting from the corresponding electromagnetic values the effects due to two-photon exchange and vacuum polarization. Thus, the comparison between theory and experiment for these two quantities is conducted correctly.  $a_{nn}^N$ , and  $a_{np}$  are fitted; all other quantities are predictions. Note that the  ${}^{3}S_{1}$  effective range parameters  $a_{i}$ and  $r_t$  are not fitted, but the deuteron binding energy is fitted (cf. next subsection) and that essentially fixes  $a_t$  and  $r_t$ .

## **D. Deuteron and triton**

The evolution of the deuteron properties from LO to N<sup>4</sup>LO of chiral EFT are shown in Table VII. In all cases, we fit the deuteron binding energy to its empirical value of 2.224575 MeV using the nonderivative  ${}^{3}S_{1}$  contact. All other deuteron properties are predictions. Already at NNLO, the deuteron has converged to its empirical properties and stays there through the higher orders.

At the bottom of Table VII, we also show the predictions for the triton binding as obtained in 34-channel chargedependent Faddeev calculations using only 2NFs. The results show smooth and steady convergence, order by order, toward

TABLE VII. Two- and three-nucleon bound-state properties as predicted by *NN* potentials at various orders of chiral EFT ( $\Lambda = 500$  MeV in all cases). (Deuteron: Binding energy  $B_d$ , asymptotic S state  $A_s$ , asymptotic  $D/S$  state  $\eta$ , structure radius  $r_{str}$ , quadrupole moment Q, D-state probability  $P_D$ ; the predicted  $r_{\text{str}}$  and Q are without meson-exchange current contributions and relativistic corrections. Triton: Binding energy  $B_t$ .)  $B_d$  is fitted; all other quantities are predictions.

	LO.	NLO	<b>NNLO</b>	$N^3LO$	$N^4LO$	Empirical <sup>a</sup>
Deuteron						
$B_d$ (MeV)	2.224575	2.224575	2.224575	2.224575	2.224575	2.224575(9)
$A_S$ (fm <sup>-1/2</sup> )	0.8526	0.8828	0.8844	0.8853	0.8852	0.8846(9)
$\eta$	0.0302	0.0262	0.0257	0.0257	0.0258	0.0256(4)
$r_{\rm str}$ (fm)	1.911	1.971	1.968	1.970	1.973	1.97507(78)
$Q~(\text{fm}^2)$	0.310	0.273	0.273	0.271	0.273	0.2859(3)
$P_D(\%)$	7.29	3.40	4.49	4.15	4.10	
Triton						
$B_t$ (MeV)	11.09	8.31	8.21	8.09	8.08	8.48

<sup>a</sup>See Table XVIII of Ref. [\[65\]](#page-17-0) for references; the empirical value for  $r_{\text{str}}$  is from Ref. [\[106\]](#page-17-0).

<span id="page-11-0"></span>a value around 8.1 MeV that is reached at the highest orders shown. This contribution from the 2NF will require only a moderate 3NF. The relatively low-deuteron D-state probabilities ( $\approx$ 4.1% at N<sup>3</sup>LO and N<sup>4</sup>LO) and the concomitant generous triton binding energy predictions are a reflection of the fact that our *NN* potentials are soft (which is, at least in part, due to their nonlocal character).

### **E. Cutoff variations**

As noted before, besides the case  $\Lambda = 500$  MeV, we have also constructed potentials with  $\Lambda = 450$  and 550 MeV at each order to allow for systematic studies of the cutoff dependence. In Fig. [3,](#page-12-0) we display the variations of the  $np$  phase shifts for different cutoffs at NNLO (left half of figure, green curves) and at  $N<sup>4</sup>LO$  (right half of figure, purple curves). We do not show the cutoff variations of phase shifts at  $N<sup>3</sup>LO$ , because they are about the same as at  $N<sup>4</sup>LO$ . Similarly, the variations at NLO are of about the same size as at NNLO. Figure [3](#page-12-0) demonstrates nicely how cutoff dependence diminishes with increasing order—a reasonable trend. Another point that is evident from this figure is that  $\Lambda = 450$  MeV should be considered as a lower limit for cutoffs, because obviously cutoff artifacts start showing up—above 200 MeV, particularly, in  ${}^{1}D_2$  and  ${}^{3}D_2$ . Concerning the upper limit for the cutoff: It has been discussed and demonstrated in length in the literature (see, e.g., Ref. [\[23\]](#page-16-0)) that for the *NN* interaction the breakdown scale occurs around  $\Lambda_b \approx 600$  MeV. The motivation for our upper value of 550 MeV is to stay below  $\Lambda_b$ .

In Table [VIII,](#page-13-0) we show the cutoff dependence for three selected aspects that are of great interest: the  $\chi^2$  for the fit of the *NN* data below 190 MeV, the deuteron properties, and the triton binding energy. The  $\chi^2$  does not change substantially as a function of cutoff, and crucial deuteron properties, like  $A<sub>S</sub>$  and  $\eta$ , stay within the empirical range, for both NNLO and  $N<sup>4</sup>LO$ . Thus, we can make the interesting observation that the reproduction of *NN* observables is not much affected by the cutoff variations. However, the D-state probability of the deuteron,  $P_D$ , which is not an observable, changes substantially as a function of cutoff at NNLO (namely, by  $\approx$ 1%) while it changes only by 0.25% at N<sup>4</sup>LO. Note that  $P_D$ is intimately related to the off-shell behavior of a potential and so are the binding energies of few-body systems. Therefore, in tune with the  $P_D$  variations, the binding energy of the triton varies by 0.25 MeV at NNLO, while it changes only by  $0.08$  MeV at  $N<sup>4</sup>LO$ . In this context, it is of interest to note that changes in the off-shell behavior of the 2NF can be compensated by corresponding changes in the 3NF, as demonstrated by Polyzou and Glőcke [[107\]](#page-17-0).

Even though cutoff variations are, in general, not the most reliable way to estimate truncation errors, in the above case they seem to reflect closely what we expect to be the truncation error.

### **IV. CHIRAL THREE-BODY FORCES**

As is well established, realistic *ab initio* nuclear structure calculations require the inclusion of 3NFs (and potentially also four-nucleon forces). The first 3NFs occur at NNLO (cf. Fig. [1\)](#page-2-0)

and were derived in Refs.  $[31,108]$  $[31,108]$ . The 3NFs at N<sup>3</sup>LO can be found in Refs.  $[109, 110]$ . Finally, at N<sup>4</sup>LO, the longestrange and intermediate-range 3NFs are given in Refs. [\[46,47\]](#page-16-0). Moreover, a new set of ten 3NF contact terms occurs at  $N^4LO$ , which has been derived by the Pisa group [\[49\]](#page-16-0). An efficient approach for calculating the matrix elements of chiral 3NF contributions up to  $N<sup>3</sup>LO$  has been published in Ref. [\[111\]](#page-17-0). This approach may eventually be extended to  $N^4LO$ .

In the derivation of all of the above-cited chiral 3NFs, the same power-counting scheme is applied as in the derivation of the 2NFs of this paper, namely, Weinberg counting and considering  $Q/M_N \sim (Q/\Lambda_\chi)^2$  (Sec. [II B\)](#page-1-0). Thus, those 3NF expressions are consistent with the present 2NFs, and they can be used together in *ab initio* calculations of nuclear structure and reactions.

In this context it is worth noting that, for convenience, the 3NFs are derived using dimensional regularization (DR), while we use SFR in the construction of the 2NFs [cf. Eq. [\(2.22\)](#page-3-0)]. This is, however, not a problem because, as shown in Ref. [\[58\]](#page-17-0), DR and SFR expressions differ only by higher order terms that are beyond the given order. Thus, the accuracy of the calculation conducted at a given order is not affected. An equivalent argument applies to the use of nonlocal regulators [Eq.  $(2.43)$ ] versus local ones (e.g., Eq.  $(11)$  of Ref.  $[18]$ ), since also these two types of regulators differ only by higher order terms beyond the given order.

Because of the complexity of the  $N<sup>4</sup>LO$  3NF, it may still take a few years until this force is available in a manageable form. Thus, for a while, we will have to live with incomplete calculations. However, there is one important component of the 3NF where, indeed, complete calculations up to  $N^4LO$  are possible: It is the 2PE 3NF. In Ref. [\[46\]](#page-16-0) it has been shown that the 2PE 3NF has essentially the same mathematical structure at NNLO,  $N<sup>3</sup>LO$ , and  $N<sup>4</sup>LO$ . Thus, one can add up the three orders of 3NF contributions and parametrize the result in terms of effective LECs. This was done in Ref. [\[46\]](#page-16-0), and we show the effective LECs they come up with in Table [IX,](#page-13-0) column  $N<sup>4</sup>LO$ , where we quote the numbers given in Eq.  $(5.2)$  of Ref. [\[46\]](#page-16-0), which are based upon the GW  $\pi N$  phase shifts [\[112\]](#page-18-0). Note that the LECs of Ref. [\[60\]](#page-17-0), which we are using for the 2NF, are also based upon GW input. Thus, there is consistency between the effective  $\bar{c}_i$  for the 3NF (column N<sup>4</sup>LO of Table [IX\)](#page-13-0) and our  $c_i$  for the 2NF (column N<sup>4</sup>LO of Table [II\)](#page-4-0).

Concerning, the 2PE 3NF at  $N<sup>3</sup>LO$ , Eq. (2.8) of Ref. [\[109\]](#page-17-0) provides the corrections to the  $c_i$  when the 2PE 3NF at  $N<sup>3</sup>LO$  is added in. Note, however, that there is a error in the numerical values given below Eq. (2.8) of Ref. [\[109\]](#page-17-0). While  $\delta c_1 = -0.13 \text{ GeV}^{-1}$  is correct, the correct values for  $\delta c_3$  and  $\delta c_4$  are  $\delta c_3 = -\delta c_4 = 0.89 \text{ GeV}^{-1}$ . When these corrections are applied to the  $N^3LO$  c<sub>i</sub> of our Table [II,](#page-4-0) then the values given in the  $N<sup>3</sup>LO$  column of Table [IX](#page-13-0) emerge. By using the  $\bar{c}_i$  of Table [IX](#page-13-0) in the mathematical expression of the NNLO 3NF, one can include at least the 2PE parts of the 3NF up to  $N<sup>3</sup>LO$  and even up to  $N<sup>4</sup>LO$  in a straightforward way.

The 2PE 3NF is the most obvious among all possible 3NF contributions. Historically, it is the first 3NF ever calculated [\[113\]](#page-18-0). The above-given prescriptions allow to take care of this very basic 3NF up to the highest orders considered in this paper.

<span id="page-12-0"></span>

FIG. 3. Cutoff variations of the *np* phase shifts at NNLO (left side, green lines) and N<sup>4</sup>LO (right side, purple lines). Dotted, dashed, and solid lines represent the results obtained with cutoff parameters  $\Lambda = 450, 500$ , and 550 MeV, respectively, as also indicated by the curve labels. Note that, at N<sup>4</sup>LO, the cases 500 and 550 MeV cannot be distinguished on the scale of the figures for most partial waves. Filled and open circles as in Fig. [2.](#page-9-0)

<span id="page-13-0"></span>TABLE VIII.  $\chi^2$ /datum for the fit of the *pp* plus np data up to 190 MeV and two- and three-nucleon bound-state properties as produced by *NN* potentials at NNLO and N<sup>4</sup>LO applying different values for the cutoff parameter  $\Lambda$  of the regulator function Eq. [\(2.43\)](#page-6-0). For some of the notation, see Table [VII,](#page-10-0) where also empirical information on the deuteron and triton can be found.

$\Lambda$ (MeV)		<b>NNLO</b>		$N^4LO$			
	450	500	550	450	500	550	
$\chi^2$ /datum pp and np							
0-190 MeV (2903 data)	4.12	3.27	3.32	1.17	1.08	1.25	
Deuteron							
$B_d$ (MeV)	2.224575	2.224575	2.224575	2.224575	2.224575	2.224575	
$A_S$ (fm <sup>-1/2</sup> )	0.8847	0.8844	0.8843	0.8852	0.8852	0.8851	
$\eta$	0.0255	0.0257	0.0258	0.0254	0.0258	0.0257	
$r_{\rm str}$ (fm)	1.967	1.968	1.968	1.966	1.973	1.971	
$Q~(\text{fm}^2)$	0.269	0.273	0.275	0.269	0.273	0.271	
$P_D(\%)$	3.95	4.49	4.87	4.38	4.10	4.13	
Triton							
$B_t$ (MeV)	8.35	8.21	8.10	8.04	8.08	8.12	

## **V. UNCERTAINTY QUANTIFICATIONS**

When applying chiral two- and many-body forces in *ab initio* calculations producing predictions for observables of nuclear structure and reactions, major sources of uncertainties are [\[54\]](#page-16-0) as follows:

- (1) Experimental errors of the input *NN* data that the 2NFs are based upon and the input few-nucleon data to which the 3NFs are adjusted.
- (2) Uncertainties in the Hamiltonian due to
	- (a) uncertainties in the determination of the *NN* and 3N contact LECs,
	- (b) uncertainties in the  $\pi N$  LECs,
	- (c) regulator dependence,
	- (d) EFT truncation error.
- (3) Uncertainties associated with the few- and many-body methods applied.

The experimental errors in the *NN* scattering and deuteron data propagate into the *NN* potentials that are adjusted to reproduce those data. To systematically investigate this error propagation, the Granada group has constructed smooth local potentials [\[114\]](#page-18-0), the parameters of which carry the uncertainties implied by the errors in the *NN* data. Applying 205 Monte Carlo samples of these potentials, they find an uncertainty of 15 keV for the triton binding energy [\[115\]](#page-18-0). In a more recent study [\[116\]](#page-18-0), in which only 33 Monte Carlo samples were used, the Granada group reproduced the uncertainty of 15 keV for the triton binding energy and, in addition, determined the uncertainty for the  $4$ He binding energy to be 55 keV. The

TABLE IX. Effective  $\pi N$  LECs (in units of GeV<sup>-1</sup>) recommended for the 2PE 3NF at the given orders. See text for explanations.

	<b>NNLO</b>	$N^3LO$	$N^4LO$
$\bar{c}_1$	$-0.74$	$-1.20$	$-0.73$
$\bar{c}_3$	$-3.61$	$-4.43$	$-3.38$
$\bar{c}_4$	2.44	2.67	1.69

conclusion is that the statistical error propagation from the *NN* input data to the binding energies of light nuclei is negligible as compared to uncertainties from other sources (discussed below). Thus, this source of error can be safely neglected at this time. Furthermore, we need to consider the propagation of experimental errors from the experimental few-nucleon data that the 3NF contact terms are fitted to. Also, this will be negligible as long as the 3NFs are adjusted to data with very small experimental errors; for example, the empirical binding energy of the triton is  $8.481795 \pm 0.000002$  MeV, which will definitely lead to negligible propagation.

Now turning to the Hamiltoninan, we have to first account for uncertainties in the *NN* and 3N LECs due to the way they are fixed. Based upon our experiences from Ref. [\[78\]](#page-17-0) and the fact that chiral EFT is a low-energy expansion, we have fitted the *NN* contact LECs to the *NN* data below 100 MeV at LO and NLO, below 190 MeV at NNLO, and below 290 MeV at  $N<sup>3</sup>LO$  and  $N<sup>4</sup>LO$ . One could think of choosing these fit intervals slightly different and a systematic investigation of the impact of such variation on the *NN* LECs is still outstanding. However, we do not anticipate that large uncertainties would emerge from this source of error.

The story is different for the 3NF contact LECs, since several very different procedures are in use for how to fix, e.g., the two contact parameters of the NNLO 3NF, known as the  $c_D$  and  $c_E$  parameters (and once the ten 3NF contacts at N<sup>4</sup>LO come into play, the situation will be even more diverse). Since at NNLO two parameters have to be fixed, two data are needed. In most procedures, one of them is the triton binding energy. For the second datum, the following choices have been made: the *nd* doublet scattering length  $^{2}a_{nd}$  [\[31\]](#page-16-0), the binding energy of  ${}^{4}$ He [\[117\]](#page-18-0), the point charge radius radius of  ${}^{4}$ He [\[40\]](#page-16-0), and the Gamow-Teller matrix element of tritium  $\beta$  decay [\[118–120\]](#page-18-0). Alternatively, the  $c_D$  and  $c_E$  parameters have also been pinned down by just an optimal overall fit of the properties of light nuclei [\[121\]](#page-18-0). The 3NF contact LECs determined by different procedures will lead to different predictions for the observables that were not involved in the fitting procedure. The differences in those results establish the uncertainty. Specifically, it would <span id="page-14-0"></span>be of interest to investigate the differences that occur for the properties of intermediate-mass nuclei and nuclear matter when 3NF LECs fixed by different protocols are applied.

The uncertainty in the  $\pi N$  LECs used to be a large source of uncertainty, in particular, for predictions for many-body systems [\[122–124\]](#page-18-0). With the new, high-precision determination of the  $\pi N$  LECs in the Roy-Steiner equations analysis [\[60\]](#page-17-0) (cf. Table [II\)](#page-4-0), this large uncertainty is essentially eliminated, which is great progress, since it substantially reduces the error budget. We have varied the  $\pi N$  LECs within the errors given in Table [II](#page-4-0) and find that the changes caused by these variations can easily be compensated by small readjustments of the*NN* LECs, resulting in essentially identical phase shifts and  $\chi^2$  for the fit of the data. Thus, this source of error is essentially negligible. The  $\pi N$  LECs also appear in the 3NFs, which also include contacts that can be used for readjustment. Future calculations of finite nuclei and nuclear matter should investigate what residual changes remain after such readjustment (that would represent the uncertainty). We expect this to be small.

The choice of the regulator function and its cutoff parameter create uncertainty. Originally, cutoff variations were perceived as a demonstration of the uncertainty at a given order (equivalent to the truncation error). However, in various investigations [\[23,44\]](#page-16-0) it has been demonstrated that this is not correct and that cutoff variations, in general, underestimate this uncertainty. Therefore, the truncation error is better determined by sticking literally to what "truncation error" means, namely, the error due to ignoring contributions from orders beyond the given order ν. The largest such contribution is the one of order  $(\nu + 1)$ , which one may therefore consider as representative for the magnitude of what is left out. This suggests that the truncation error at order  $\nu$  can reasonably be defined as

$$
\Delta X_{\nu} = |X_{\nu} - X_{\nu+1}|, \tag{5.1}
$$

where  $X_{\nu}$  denotes the prediction for observable X at order  $\nu$ . If  $X_{\nu+1}$  is not available, then one may use

$$
\Delta X_{\nu} = |X_{\nu-1} - X_{\nu}|Q/\Lambda , \qquad (5.2)
$$

choosing a typical value for the momentum Q, or  $Q = m_{\pi}$ . Alternatively, one may also apply more elaborate definitions, like the one given in Ref. [\[23\]](#page-16-0). Note that one should not add up (in quadrature) the uncertainties due to regulator dependence and the truncation error, because they are not independent. In fact, it is appropriate to leave out the uncertainty due to regulator dependence entirely and just focus on the truncation error [\[23\]](#page-16-0). The latter should be estimated using the same cutoff (e.g.,  $\Lambda = 500$  MeV) in all orders considered.

Finally, the last uncertainty to be taken into account is the uncertainty in the few- and many-body methods applied in the *ab inition* calculation. This source of error has nothing to do with EFT. Few-body problems are nowadays exactly solvable such that the error is negligible in those cases. For heavier nuclei and nuclear matter, there are definitely uncertainties no matter what method is used. These uncertainties need to be estimated by the practitioners of those methods. But with the improvements of algorithms and the increase of computing power, these errors are decreasing.

The bottom line is that the most substantial uncertainty is the truncation error. This is the dominant source of (systematic) error that should be carefully estimated for any calculation applying chiral 2NFs and 3NFs up to a given order.

## **VI. SUMMARY AND CONCLUSIONS**

We have constructed chiral *NN* potentials through five orders of chiral EFT ranging from LO to  $N<sup>4</sup>$ LO [\[125\]](#page-18-0). The construction may be perceived as consistent, because the same power counting scheme as well as the same cutoff procedures are applied in all orders. Moreover, the long-range part of these potentials are fixed by the very accurate  $\pi N$  LECs as determined in the Roy-Steiner equations analysis of Ref. [\[60\]](#page-17-0). In fact, the uncertainties of these LECs are so small that a variation within the errors leads to effects that are essentially negligible at the current level of precision. Another aspect that has to do with precision is that, at least at the highest order  $(N<sup>4</sup>LO)$ , the *NN* data below pion-production threshold are reproduced with the outstanding  $\chi^2$ /datum of 1.15. This is the highest precision ever accomplished with any chiral *NN* potential to date.

The *NN* potentials presented in this paper may serve as a solid basis for systematic *ab initio* calculations of nuclear structure and reactions that allow for a comprehensive error analysis. In particular, the order-by-order development of the potentials will make possible a reliable determination of the truncation error at each order.

Our family of potentials is nonlocal and, generally, of soft character. This feature is reflected in the fact that the predictions for the triton binding energy (from two-body forces only) converges to about 8.1 MeV at the highest orders. This leaves room for moderate three-nucleon forces.

These features of our potentials are in contrast to other families of chiral *NN* potentials of local or semilocal character that have recently entered the market  $[20-24]$ . Such potentials are less soft and consequently require stronger three-body force contributions.

The availability of families of chiral *NN* potentials of different character offers the opportunity for interesting systematic studies that may ultimately shed light on issues like the radius problem [\[50\]](#page-16-0), the overbinding of intermediate-mass nuclei [\[51\]](#page-16-0), and others.

Note that the differences between the above-mentioned families of potentials are in the off-shell character, which is not an observable. Thus, any off-shell behavior of a *NN* potential is legitimate. There is no wrong off-shell character. However, some off-shell behaviors may lead in a more efficient way to realistic results than others. That is of interest to the many-body practitioner. We are now in a position to systematically investigate this issue for chiral forces.

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<span id="page-15-0"></span>

$T_{\text{lab}}$ (MeV)	${}^1S_0$	$^{3}P_{0}$	${}^3P_1$	$D_2$	${}^3P_2$	${}^3F_2$	$\epsilon_2$	${}^3F_3$	${}^3F_4$
	32.79	0.14	$-0.08$	0.00	0.01	0.00	0.00	0.00	0.00
5	54.84	1.61	$-0.89$	0.04	0.23	0.00	$-0.05$	0.00	0.00
10	55.20	3.79	$-2.02$	0.17	0.69	0.01	$-0.20$	$-0.03$	0.00
25	48.62	8.66	$-4.84$	0.69	2.57	0.11	$-0.81$	$-0.23$	0.02
50	38.84	11.42	$-8.26$	1.67	5.87	0.35	$-1.69$	$-0.68$	0.12
100	24.97	9.15	$-13.48$	3.61	10.70	0.83	$-2.62$	$-1.46$	0.51
150	15.04	4.55	$-17.72$	5.45	13.57	1.16	$-2.83$	$-1.98$	1.07
200	7.10	$-0.47$	$-21.39$	7.22	15.54	1.20	$-2.71$	$-2.31$	1.67
250	0.11	$-5.89$	$-25.12$	8.85	17.01	0.92	$-2.42$	$-2.48$	2.20
300	$-6.43$	$-11.40$	$-29.35$	9.91	17.84	0.35	$-1.99$	$-2.46$	2.59

TABLE X. *pp* phase shifts (in degrees) up to F waves at  $N^4LO$  ( $\Lambda = 500$  MeV).

TABLE XI. *nn* phase shifts (in degrees) up to F waves at  $N^4LO$  ( $\Lambda = 500$  MeV).

$T_{\text{lab}}$ (MeV)	${}^{1}S_0$	$^{3}P_{0}$	${}^{3}P_1$	$D_2$	${}^3P_2$	${}^3F_2$	$\epsilon_2$	${}^3F_3$	${}^3F_4$
	57.62	0.21	$-0.12$	0.00	0.02	0.00	0.00	0.00	0.00
5	61.01	1.88	$-1.03$	0.05	0.28	0.00	$-0.06$	$-0.01$	0.00
10	57.82	4.16	$-2.21$	0.18	0.78	0.01	$-0.22$	$-0.04$	0.00
25	49.11	9.01	$-5.08$	0.73	2.77	0.11	$-0.84$	$-0.24$	0.02
50	38.71	11.55	$-8.52$	1.72	6.15	0.36	$-1.72$	$-0.70$	0.13
100	24.65	9.06	$-13.76$	3.68	11.02	0.84	$-2.62$	$-1.48$	0.53
150	14.70	4.40	$-17.98$	5.52	13.92	1.16	$-2.82$	$-2.00$	1.09
200	6.74	$-0.63$	$-21.62$	7.28	15.94	1.20	$-2.68$	$-2.32$	1.70
250	$-0.28$	$-6.02$	$-25.32$	8.88	17.42	0.91	$-2.36$	$-2.49$	2.23
300	$-6.87$	$-11.40$	$-29.48$	9.87	18.24	0.32	$-1.93$	$-2.46$	2.61

TABLE XII.  $I = 1 np$  phase shifts (in degrees) up to F waves at N<sup>4</sup>LO ( $\Lambda = 500$  MeV).

$T_{\text{lab}}$ (MeV)	${}^1S_0$	${}^3P_0$	${}^{3}P_1$	$D_2$	${}^3P_2$	${}^3F_2$	$\epsilon_2$	${}^3F_3$	${}^3F_4$
	62.00	0.18	$-0.11$	0.00	0.02	0.00	0.00	0.00	0.00
5	63.47	1.66	$-0.92$	0.04	0.27	0.00	$-0.05$	0.00	0.00
10	59.72	3.72	$-2.03$	0.16	0.75	0.01	$-0.19$	$-0.03$	0.00
25	50.48	8.25	$-4.79$	0.68	2.66	0.09	$-0.76$	$-0.20$	0.02
50	39.83	10.69	$-8.20$	1.68	5.96	0.31	$-1.62$	$-0.61$	0.11
100	25.68	8.25	$-13.44$	3.68	10.76	0.78	$-2.53$	$-1.35$	0.49
150	15.78	3.63	$-17.67$	5.56	13.63	1.08	$-2.76$	$-1.86$	1.04
200	7.90	$-1.37$	$-21.33$	7.34	15.63	1.12	$-2.64$	$-2.18$	1.64
250	0.96	$-6.75$	$-25.05$	8.96	17.12	0.83	$-2.35$	$-2.35$	2.17
300	$-5.57$	$-12.14$	$-29.23$	9.96	17.95	0.25	$-1.93$	$-2.34$	2.55

TABLE XIII.  $I = 0 np$  phase shifts (in degrees) at N<sup>4</sup>LO ( $\Lambda = 500$  MeV).



## **APPENDIX: PHASE-SHIFT TABLES**

<span id="page-16-0"></span>In this Appendix, we show the phase shifts as predicted by the N<sup>4</sup>LO potential with  $\Lambda = 500$  MeV in Tables [X–XIII.](#page-15-0) Note that our pp phase shifts are the phase shifts of the nuclear plus relativistic Coulomb interaction with respect to Coulomb

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wave functions. For  $nn$  and  $np$  scattering, our phase shifts are the ones from the nuclear interaction with respect to Riccati-Bessel functions. For more technical details of our phase-shift calculations, we refer the interested reader to Appendix A3 of Ref. [\[65\]](#page-17-0).

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