

Improved description of light nuclei through chiral effective field theory at leading order

M. Sánchez Sánchez^{1,*}, N. A. Smirnova^{1,†}, A. M. Shirokov^{2,3,4,‡}, P. Maris^{2,§} and J. P. Vary^{2,||}

¹*CENBG (CNRS/IN2P3–Université de Bordeaux), 33175 Gradignan cedex, France*

²*Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA*

³*Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Moscow 119991, Russia*

⁴*Pacific National University, 136 Tikhookeanskaya Street, Khabarovsk 680035, Russia*



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We propose an arrangement of the most commonly invoked version of the two-nucleon chiral potential such that the low-lying amplitude zero of the 1S_0 partial wave is captured at leading order of the effective expansion. Adopting other partial waves from the LENPIC interaction, we show how this modification yields an improved description of ground-state energies and point-proton radii of the ^3H , ^4He , and ^6He nuclei.

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I. INTRODUCTION

One of the fundamental challenges in nuclear physics is to provide a consistent—as well as phenomenologically successful—derivation of the nuclear potential grounded on first principles. The nuclear effective field theory (EFT) program offers a way to address this challenge. Here, the link with the underlying quantum chromodynamics (QCD) leans on the fact that the effective Lagrangian fulfills all QCD symmetries—most particularly the spontaneously and explicitly broken chiral symmetry, as in chiral EFT (χEFT) [1–4]. The latter aims at generalizing the scheme of chiral perturbation theory (χPT) [5] to nonperturbative physics, namely nuclear systems. The χEFT Lagrangian is written in terms of nucleons, pions, and other hadron fields instead of the underlying quarks and gluons of QCD. Since its symmetries are compatible with an infinite number of terms, it becomes mandatory to establish a hierarchical principle (“power counting”) that discriminates which terms should be used for consistency when computing observables. This enables one to express the EFT predictions as series in powers of a small parameter Q/M_{hi} . Here, Q (M_{hi}) stands for the magnitude of the typical external three-momentum of a process amenable to the EFT (the momentum scale at which the EFT breaks down and needs to be replaced by another theory that underlies the former); in χEFT , this is of the order of the pion mass, $Q \approx 100\text{ MeV}$ (the chiral-symmetry-breaking scale, $M_{\text{hi}} \approx 1\text{ GeV}$).

The initial applications of the nuclear EFT program were provided by pioneering studies in the early and middle 1990s [6–11]. They were grounded on the assumption that the

nuclear potential and currents obey a power counting corresponding with that of χPT , called naive dimensional analysis (NDA) [12,13] or simply “Weinberg power counting.” However, in nonperturbative physics this program has been criticized for leading to inconsistencies with the renormalization-group-invariance (RGI) (or cutoff-convergence) principle, i.e., for displaying model dependence (see, e.g., Refs. [14–16]); for a different interpretation in terms of a framework valid at a defined scale, see, e.g., Refs. [17–20].

From a purely phenomenological point of view, it is worth noting that, at leading order (LO) in the expansion, the Weinberg counting fails to produce a qualitatively correct description of two-nucleon (NN) scattering in the 1S_0 channel at momenta $Q \sim m_\pi$ due to a lack of repulsion among the nucleons. This may be remedied through an enhancement of beyond-LO terms in the effective potential. As proposed in Ref. [21], this enhancement is sufficient to reproduce the amplitude zero that shows up in this wave at a relatively soft scattering momentum. Consequently, the convergence of the effective expansion is improved.

In modern calculations, χEFT plays a leading role, chiral potentials being a basic ingredient for understanding nuclear structure and reactions with *ab initio* methods (see Ref. [22] for an overview). Among such methods, one of the most versatile is the no-core shell model (NCSM) [23]. In this approach, the A -body nonrelativistic Schrödinger equation is solved in a basis representation which is most often chosen to be the spherical harmonic-oscillator (HO) basis. All the (structureless) nucleons are treated as active degrees of freedom, and the Slater-determinant expansion is built up from HO single-particle wave functions depending on the HO frequency. This allows one to reformulate the many-body problem as a symmetric sparse eigenvalue problem, whose solution has the finite size of the model space as its only source of uncertainty. One version of the chiral potential that is employed in current NCSM calculations is essentially given by Weinberg power counting. However, the abovementioned lack of repulsion in the 1S_0 channel results in an overbinding

* sanchez@cenbg.in2p3.fr

† smirnova@cenbg.in2p3.fr

‡ shirokov@nucl-th.sinp.msu.ru

§ pmaris@iastate.edu

|| jvary@iastate.edu

pattern of light nuclei at LO; see the work by the LENPIC Collaboration in Refs. [24–26].¹ The convergence of the expansion may be thus accelerated by means of a modification of the original prescription along the lines explored in Ref. [21]. In particular, we replace the bare, partial-wave projected NN potential of the 1S_0 wave (where the centrifugal suppression that appears for channels with $\ell \geq 1$ [28] is absent) and we retain the isospin-conserving LO interactions present in all the remaining channels, namely one-pion exchange (OPE) plus a single, nonderivative contact term affecting the 3S_1 wave. This produces a very significant improvement in the predictions for ground-state energies and point-proton RMS radii of three light nuclei, namely ^3H , ^4He , and ^6He , as we show in the present work. Our efforts are framed in the context of other studies such as Refs. [15,27,29], where alternative LO descriptions of few-nucleon systems are explored in order to achieve an improved and theoretically consistent convergence of the χEFT expansion. In addition, an improvement at the LO level such as the one we propose here may potentially give rise to future works based on perturbation theory beyond LO.

This article is structured as follows. In Sec. II, the issues with Weinberg power counting in the 1S_0 two-nucleon channel are examined, the strategy used here to improve on such problems is described, and the details of our calculation at the two-body level are provided. In Sec. III, we show the LO results for the ground-state energies and radii of ^3H , ^4He , and ^6He both for the LO original LENPIC interaction (see Ref. [30]) and for the LO modified one, examine the convergence of the energies in the infinite-basis limit, and argue that the overestimation of binding energies and the underestimation of radii coming from the LO original LENPIC potential are significantly alleviated after the modification we propose. Finally, in Sec. IV we present our conclusions and outline our ideas for future research work.

II. THE TWO-NUCLEON 1S_0 CHANNEL IN CHIRAL EFT

The emergence of a pole in the NN 1S_0 amplitude at imaginary momentum $k \approx i/a$ (note that the $\hbar = c = 1$ units are used all through this work), where $a = -23.7 \text{ fm} = -(8.3 \text{ MeV})^{-1}$ is the scattering length in the neutron-proton channel,² has long been identified as a very shallow virtual

¹Related to the RGI issues of the Weinberg counting that were previously mentioned, we remark that such overbinding holds true only when relatively soft momentum cutoffs are considered, as is the case in the present work. Note also that Refs. [15,27], where a modified, RGI-consistent power counting is invoked, predict an underbound ^3H nucleus already at moderate cutoff values.

²Unlike the Coulomb repulsion in the two-proton channel, the effects of charge-independence and charge-symmetry breakings that are inherent to the strong force have been neglected in our first-order approach. We recall [31] that those two phenomena may be respectively quantified in terms of the 1S_0 neutron-neutron (nn), proton-proton (pp), and neutron-proton (np) scattering lengths [32,33] as

$$\frac{a_{np} - (a_{nn} + a_{pp}^{\text{(strong)}})/2}{a_{np}} \approx 0.24; \quad \frac{a_{nn} - a_{pp}^{\text{(strong)}}}{a_{np}} \approx 0.05.$$

state. This, together with the loosely bound deuteron, anticipates the nonperturbative nature of nuclear physics already in its simplest manifestation—the two-nucleon system. As a consequence, the LO part of the NN interaction has to be fully iterated when inserted in a dynamical equation (e.g., Schrödinger) that governs the system. In particular, the attraction provided by the OPE contribution—the main long-range effect—to the 1S_0 potential is relatively mild. This introduces an attractive short-range contribution also at LO, sufficient to render the aforementioned almost-bound state. The momentum-space representation of this short-range part reads as a pure constant C_0 . Its inclusion as a first-order effect is grounded on two complementary arguments. On the one hand, this contact force comes from a four-nucleon vertex *without* derivative or pion-mass insertions; hence, according to NDA, it will be parametrically enhanced by $O(M_{\text{hi}}^n/Q^n)$ with respect to a diagram with n of such insertions.³ On the other hand, from an RGI perspective, the cutoff-independent contact piece of the 1S_0 -projected OPE as it emerges from the effective Lagrangian would pose an ill-defined solution unless such a piece is reabsorbed into the running coupling C_0 .

There is, however, another relevant feature of the 1S_0 partial wave that was recognized early on. This is the fact that the NN scattering amplitude changes from positive to negative at momentum $k \equiv k_0 \approx 350 \text{ MeV}$. It is worth recalling that this fact motivated the inclusion of a short-range repulsive core in some of the earliest phenomenological models of the NN interaction (see, e.g., Refs. [34,35]). From a more modern perspective, provided that the hard scale in χEFT , usually identified as the typical mass of the lightest non-Goldstone hadrons, respects $M_{\text{hi}} \approx 1 \text{ GeV}$, then one should identify⁴ $k_0 \sim Q$. Hence, χEFT should be well convergent in the $k \sim k_0$ momentum region—in other words, beyond-LO corrections should not offset a significant deficiency in the LO result. In addition, it seems appealing to have a LO interaction that provides a satisfactory description of the phenomenological scattering matrix on a qualitative level, i.e., in its gross features—for instance, not only its poles but also its eventual zeros and changes of sign. This concept appears particularly reasonable if one adheres to the idea that only the LO part of the potential should be treated nonperturbatively, while N^{th} LO terms should start contributing at ν^{th} order in distorted-wave perturbation theory, as argued in Refs. [15,27,37–42].

To accomplish the vision just described, one confronts the fact that the attraction provided by the short-range term C_0

³Actually, for the particular case of the 1S_0 wave, the four-nucleon diagram with no derivative and two pion-mass insertions, which gives rise to a pointlike $D_2 m_\pi^2$ interaction, happens to break this rule and is nominally as relevant as the C_0 vertex [14]. This observation, however, remains inconsequential in the pure-nucleon sector, provided that the pion mass is treated as a constant.

⁴Such an assumption is in good agreement with the LO nature of OPE in the 1S_0 wave since, in terms of power counting, this relies on $M_{NN} \sim Q$, where M_{NN} sets the inverse strength of OPE in this wave; recall that k_0 happens to be only $\approx 15\%$ numerically larger than M_{NN} (see Ref. [36] for a different approach to this).

in the Weinberg scheme is too strong to capture the amplitude zero at any reasonable momentum. Actually, the LO Weinberg prediction for this channel is a phase shift that becomes approximately constant ($\approx 60^\circ$) in the middle-range region ($k \gtrsim 100$ MeV all the way up to the pion-production threshold) provided that a reasonably hard momentum cutoff is employed ($\Lambda \gtrsim 500$ MeV, where a more precise estimate depends on the chosen regularization prescription). In Ref. [21], another formulation of the short-range part of the LO potential was proposed in order to subsume the amplitude zero.

To see how this fact can be exploited here, start by considering the part of the χ EFT Lagrangian relevant for the two-nucleon 1S_0 channel in the standard arrangement,

$$\begin{aligned} \mathcal{L}_\chi^{(W)} = & \frac{1}{2} (\partial_\mu \boldsymbol{\pi} \cdot \partial^\mu \boldsymbol{\pi} - m_\pi^2 \boldsymbol{\pi}^2) \\ & + N^\dagger \left[i\partial_0 + \frac{\vec{\nabla}^2}{2m_N} - \frac{g_A}{2f_\pi} \boldsymbol{\tau} \cdot (\vec{\sigma} \cdot \vec{\nabla}) \boldsymbol{\pi} \right] N \\ & - C_0 (N^T \mathbf{P}_{1S_0} N)^\dagger \cdot (N^T \mathbf{P}_{1S_0} N) + \dots, \end{aligned} \quad (1)$$

where $\boldsymbol{\pi}$ and N denote the pion isotriplet and nucleon isodoublet fields with isospin-averaged masses $m_\pi = 138.04$ MeV and $m_N = 938.92$ MeV, $g_A = 1.26$ and $f_\pi = 92.4$ MeV are the axial-coupling and pion-decay constants, $\mathbf{P}_{1S_0} = \sigma_2 \boldsymbol{\tau} \tau_2 / \sqrt{8}$ is the two-nucleon projector in terms of the Pauli matrices $\vec{\sigma}$ ($\boldsymbol{\tau}$) acting on spin (isospin) space, and the ellipsis stands for more complicated terms suppressed by negative powers of the breakdown scale. Applying the usual Feynman rules in momentum space, the 1S_0 partial-wave projected two-nucleon potential is obtained to be

$$V_\chi^{(W)}(p', p) = C_0 + V_\pi(p', p), \quad (2)$$

where p (p') is the magnitude of the relative momentum of the incoming (outgoing) nucleons, while the long-range component of the interaction is

$$V_\pi(p', p) = \frac{1}{m_N} \int_0^\infty dr r^2 j_0(p'r) U_\pi(r) j_0(pr), \quad (3)$$

$j_0(x) = x^{-1} \sin x$ being the zeroth-order spherical Bessel function of the first kind, and

$$U_\pi(r) = -\frac{m_\pi^3}{M_{NN}} Y(m_\pi r), \quad M_{NN} = \frac{16\pi f_\pi^2}{g_A^2 m_N}, \quad Y(x) = \frac{e^{-x}}{x}. \quad (4)$$

Besides, C_0 has been redefined with respect to Eq. (1) through $C_0 + 4\pi/(m_N M_{NN}) \rightarrow C_0$. The off-shell scattering matrix is then nonperturbatively found by solving the S -wave projected Lippmann-Schwinger equation

$$T(p', p; k) = V(p', p) + \frac{2}{\pi} \int_0^\infty dq \frac{V(p', q) q^2 T(q, p; k)}{(k^2 - q^2)/m_N + i0^+} \quad (5)$$

for $V(p', p) \equiv V_\chi^{(W)}(p', p)$. However, this happens to be singular, as one can see by the fact that the integral in Eq. (5) is linearly divergent; thus, a regularization prescription must be used. To be consistent with our adoption of potentials in the remaining partial waves from Ref. [30], we will apply

a nonlocal regulator for the short-range component of the interaction and a local regulator for the long-range one,

$$C_0 \rightarrow f_S(p'/\Lambda) C_0 f_S(p/\Lambda), \quad f_S(x) = e^{-x^2}; \quad (6)$$

$$U_\pi(r) \rightarrow U_\pi(r) f_L(r/R), \quad f_L(x) = (1 - e^{-x^2})^6, \quad (7)$$

where the coordinate and momentum cutoffs R and Λ verify $R\Lambda = 2$, so that

$$\int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}\cdot\vec{r}} f_S(k/\Lambda) \propto f_S(r/R) \quad (8)$$

is fulfilled. The nonperturbative phase shift is obtained from the on-shell scattering matrix,

$$\delta(k) = \frac{1}{2i} \log [1 - 2ikm_N T(k, k; k)]. \quad (9)$$

The value of C_0 is found by imposing the renormalization condition

$$\lim_{k \rightarrow 0} k \cot \delta(k) = -\frac{1}{a}. \quad (10)$$

If one chooses $R = 0.9$ fm ($\Lambda = 439$ MeV), then $C_0 = -(440 \text{ MeV})^{-2}$.

The proposal of Ref. [21] is to remedy the excess of attraction of the interaction (2) through resumming into LO subleading terms that are repulsive enough to render the amplitude zero. This is done by means of a reparametrization of Eq. (1) grounded on the introduction of two auxiliary ‘‘dibaryon’’ [43] fields $\boldsymbol{\phi}_1$ and $\boldsymbol{\phi}_2$ such that the effective Lagrangian becomes

$$\begin{aligned} \mathcal{L}_\chi^{(2\phi)} = & \frac{1}{2} (\partial_\mu \boldsymbol{\pi} \cdot \partial^\mu \boldsymbol{\pi} - m_\pi^2 \boldsymbol{\pi}^2) \\ & + N^\dagger \left[i\partial_0 + \frac{\vec{\nabla}^2}{2m_N} - \frac{g_A}{2f_\pi} \boldsymbol{\tau} \cdot (\vec{\sigma} \cdot \vec{\nabla}) \boldsymbol{\pi} \right] N \\ & + \sum_{j=1,2} \left\{ \boldsymbol{\phi}_j^\dagger \cdot \left[\Delta_j + c_j \left(i\partial_0 + \frac{\vec{\nabla}^2}{4m_N} \right) \right] \boldsymbol{\phi}_j \right. \\ & \left. - \sqrt{\frac{4\pi}{m_N}} (\boldsymbol{\phi}_j^\dagger \cdot N^T \mathbf{P}_{1S_0} N + \text{H.c.}) \right\} + \dots, \end{aligned} \quad (11)$$

where the two-dibaryon low-energy couplings (LECs)—the residual masses Δ_j and the kinetic factors c_j —admit expansions in powers of Q/M_{hi} ; for notational simplicity, here we will abbreviate $\Delta_j \equiv \Delta_j^{[0]}$ and $c_j \equiv c_j^{[0]}$, with the superscript [0] referring to the LO contribution. Then, the number of free parameters at LO is reduced from four to three by adopting the prescription $c_1 \equiv 0$, thus yielding a potential given by an energy-dependent term (associated with two LECs) plus a constant, namely

$$V_\chi^{(2\phi)}(p', p, k) = \frac{1}{m_N} \left(\frac{1}{\Delta_1} + \frac{1}{\Delta_2 + c_2 k^2/m_N} \right) + V_\pi(p', p) \quad (12)$$

$(1/\Delta_1 + 1/M_{NN} \rightarrow 1/\Delta_1)$. Then one can fit to [21]

$$\begin{aligned} \lim_{k \rightarrow 0} k \cot \delta(k) &= -\frac{1}{a}, \\ \lim_{k \rightarrow 0} \frac{\partial}{\partial k^2} k \cot \delta(k) &= \frac{r_0}{2}, \\ \delta(k_0) &= 0, \end{aligned} \quad (13)$$

with $r_0 = 2.7$ fm being the 1S_0 np effective range. In Ref. [21], it is shown that Eq. (12) yields a surprisingly good description of the phenomenological 1S_0 phase shift [33] in the whole elastic regime. However, note that this interaction is energy dependent, which is often a drawback in calculations beyond the two-body sector—in general, it is unclear how to define the pair energy on which the pair potential would depend.

In this work, we adopt a heuristic approach by exploring a momentum-dependent interaction such that its on-shell version coincides with Eq. (12). This can be done [44] in terms of the introduction of an auxiliary isovector field

$$\begin{aligned} \Phi &= N^T \left[\gamma^2 - \frac{1}{4} (\vec{\nabla} - \overleftarrow{\nabla})^2 \right]^{-\frac{1}{2}} \mathbf{P}_{1S_0} N \\ &= N^T \left[\frac{1}{\gamma} + \frac{1}{8\gamma^3} (\vec{\nabla} - \overleftarrow{\nabla})^2 + \dots \right] \mathbf{P}_{1S_0} N, \end{aligned} \quad (14)$$

so that the effective Lagrangian becomes

$$\begin{aligned} \mathcal{L}_\chi^{(\Phi)} &= \frac{1}{2} (\partial_\mu \boldsymbol{\pi} \cdot \partial^\mu \boldsymbol{\pi} - m_\pi^2 \boldsymbol{\pi}^2) \\ &+ N^\dagger \left[i\partial_0 + \frac{\vec{\nabla}^2}{2m_N} - \frac{g_A}{2f_\pi} \boldsymbol{\tau} \cdot (\vec{\sigma} \cdot \vec{\nabla}) \boldsymbol{\pi} \right] N \\ &- \frac{4\pi}{m_N} \left[\frac{\gamma^2}{\Delta_1} \Phi^\dagger \cdot \Phi + \frac{1}{\Delta_2} (N^T \mathbf{P}_{1S_0} N)^\dagger \cdot (N^T \mathbf{P}_{1S_0} N) \right] \\ &+ \dots, \end{aligned} \quad (15)$$

giving rise to a separable-plus-constant short-range potential

$$\begin{aligned} V_\chi^{(\Phi)}(p', p) &= \frac{1}{m_N} \left[\frac{1}{\Delta_1} \mathcal{F}(p'/\gamma) \mathcal{F}(p/\gamma) + \frac{1}{\Delta_2} \right] + V_\pi(p', p), \\ \mathcal{F}(x) &= (1 + x^2)^{-\frac{1}{2}} \end{aligned} \quad (16)$$

$(1/\Delta_2 + 1/M_{NN} \rightarrow 1/\Delta_2)$, which is again supplemented by Eq. (13).⁵ The constant term $1/\Delta_2$ in the potential (16)

⁵In the $M_{NN} \rightarrow \infty$ limit of the interaction (16), Eq. (5) admits an analytic solution and one can see explicitly that the resulting on-shell amplitude coincides with the one arising from the $M_{NN} \rightarrow \infty$ version of the interaction (12). Also, it is interesting to note that this “pionless” limit of Eq. (16) is compatible with a positive effective range, thus circumventing the Wigner-bound issues [45,46] of momentum-dependent contact potentials such as the ones explored in Ref. [47]. This observation is consistent with the conclusions of Ref. [48], provided that the structure in Eq. (16) is seen as the infinite resummation of interaction terms that appear in standard pionless EFT, where the coefficients in front of those terms are fixed beforehand.

emerges from the four-nucleon term in the Lagrangian (15), similar to the case of C_0 in the potential (2) and the Lagrangian (1). Furthermore, the equivalence between Eqs. (15) and (16) can be checked by expanding both expressions at low momenta and comparing term by term using the standard formalism employed in the literature; see, e.g., Ref. [49]. We solve Eq. (5) with $V(p', p) \equiv V_\chi^{(\Phi)}(p', p)$, by means of a regularization strategy analogous to the one of Eqs. (6) and (7), for $R = 0.9$ fm. Through the best fit to Eq. (13), we find $\Delta_1 = -58$ MeV, $\Delta_2 = 96$ MeV, and $\gamma = 476$ MeV.

In Fig. 1, we plot the 1S_0 phase shifts arising from the potentials $V_\chi^{(W)}(p', p)$ and $V_\chi^{(\Phi)}(p', p)$ incorporating the regularization prescription and the renormalization conditions detailed above, together with the partial-wave analysis (PWA) of Ref. [32]. Note that the best fit corresponding to the $V_\chi^{(\Phi)}(p', p)$ interaction yields a good reproduction of the phenomenological curve for momenta up to ≈ 300 MeV, but fails to reproduce the amplitude zero at the correct location, shifting it $\approx 10\%$ to the right. However, this is a regulator artifact—increasing slightly the momentum cutoff Λ would remedy this flaw [21]. Besides, for larger cutoffs ($\Lambda \gtrsim M_{\text{hi}}$), the difference between the curves emerging from both potentials becomes greater (see Fig. 7 of Ref. [21], where a sharp-cutoff regularization prescription is adopted).

While it might seem reasonable to investigate the regulator dependence of our proposed interaction, this would take us beyond the scope of our present goal. That is, we aim here only to demonstrate the order or magnitude of the effects that are obtained with an existing regulator scheme.

Once the LECs of Eq. (16) are determined, the two-body matrix elements (TBMEs) of this interaction in the HO basis are found through sandwiching between corresponding HO states $|n, \ell\rangle$:

$$\begin{aligned} \mathcal{V}_{n'n}^{(1S_0)} &\equiv \langle n', 0 | V_\chi^{(\Phi)} | n, 0 \rangle \\ &= \frac{2}{\pi} \int_0^\infty dp' \int_0^\infty dp p'^2 p^2 \psi_{n'0}^*(p') V_\chi^{(\Phi)}(p', p) \psi_{n0}(p) \\ &= \frac{1}{m_N} \left\{ \frac{2}{\pi} \int_0^\infty dp' \int_0^\infty dp p'^2 p^2 \psi_{n'0}^*(p') f_S(p'/\Lambda) \right. \\ &\quad \times \left[\frac{1}{\Delta_1} \mathcal{F}(p'/\gamma) \mathcal{F}(p/\gamma) + \frac{1}{\Delta_2} \right] f_S(p/\Lambda) \psi_{n0}(p) \\ &\quad \left. + \int_0^\infty dr r^2 \Psi_{n'0}^*(r) U_\pi(r) f_L(r/R) \Psi_{n0}(r) \right\}, \end{aligned} \quad (17)$$

with $\psi_{n\ell}(p)$ and $\Psi_{n\ell}(r)$ the momentum- and coordinate-space representations of the radial basis functions at radial quantum number n and orbital angular momentum ℓ , given by [50]

$$\begin{aligned} \psi_{n\ell}(p) &= (-1)^n \sqrt{\frac{2\Gamma(n+1)b^3}{\Gamma(n+\ell+\frac{3}{2})}} (pb)^\ell e^{-\frac{p^2 b^2}{2}} L_n^{(\ell+\frac{1}{2})}(p^2 b^2); \\ \Psi_{n\ell}(r) &= \sqrt{\frac{2\Gamma(n+1)}{\Gamma(n+\ell+\frac{3}{2})b^3}} (r/b)^\ell e^{-\frac{r^2}{2b^2}} L_n^{(\ell+\frac{1}{2})}(r^2/b^2), \end{aligned} \quad (18)$$

where $b = \sqrt{2/(m_N \Omega)}$ is the HO length, Ω being the HO frequency, and $L_n^{(\ell+\frac{1}{2})}$ is a generalized Laguerre polynomial. These TBMEs are then transformed to the single-particle

basis, supplementing contributions in other partial waves from the LENPIC^[0] two-nucleon interaction [24–26] for implementing in our many-body calculations.

III. STUDY OF LIGHT NUCLEI

For our initial application to light nuclei, we selectively investigate the ground-state properties of ³H, ⁴He, and ⁶He using the NCSM approach. Our NCSM calculations have been carried out on the supercomputer Cori, a Cray XC40 system at the National Energy Research Scientific Computing Center (NERSC), by means of the highly parallelized nuclear-structure eigensolver known as many-fermion dynamics for nuclei (MFDn) [51–53]. The nuclear observables have been calculated as functions of the HO energy $\hbar\Omega = 15$ MeV, 17.5 MeV, \dots , $\hbar\Omega_{\max}$, where $\hbar\Omega_{\max}$ has been chosen for each nucleus to provide a visual impression of the convergence (ranging from $\hbar\Omega_{\max} = 50$ MeV for the loosely bound ⁶He to $\hbar\Omega_{\max} = 70$ MeV for the tightly bound ⁴He). Our results have been obtained for different values of the parameter $N_{\max} = 6, 8, \dots, 20$ (for ³H); 6, 8, \dots , 16 (for ⁴He); and 4, 6, \dots , 14 (for ⁶He). These values of N_{\max} are both convenient and sufficient for our purposes. We recall that this parameter represents the maximum number of HO excitation quanta that can be shared among the A nucleons above the minimum-energy configuration. Both $\hbar\Omega$ and N_{\max} give a measure of the infrared and ultraviolet cutoffs and fully determine the model space [54–56]. The accurate infrared scale for the model-space truncation of the NCSM basis was derived and demonstrated in Ref. [57]. However, instead of an infrared-extrapolation prescription, here we use the simplest extrapolation methods for energies and radii suggested in Refs. [58,59], respectively. These are sufficiently accurate for our purposes and clearly show, for those nuclei studied here, the improvements induced by the suggested modification to the NN interaction.

A. Ground-state energies

The results on ground-state energies of ³H, ⁴He, and ⁶He are shown in Fig. 2: Left panels present the results obtained with the original LENPIC^[0] interaction [24–26,30], while right panels show the results obtained with the same interaction modified in the ¹S₀ channel as described above. We observe that the proposed modification removes much of the overbinding inherent to the conventional LO potential. At the same time, the convergence of the calculations as a function of N_{\max} remains of a similar quality. This can be inferred from the fact that, for increasing N_{\max} parameter, the results become gradually independent of the HO energy quanta.

In order to extract the extrapolated ground-state energy E_{∞} , we adopt the simple Extrapolation B of Ref. [58], based on the phenomenological relation

$$E(N_{\max}, \hbar\Omega) = A(\hbar\Omega) \exp[-c(\hbar\Omega)N_{\max}] + E_{\infty}(\hbar\Omega). \quad (19)$$

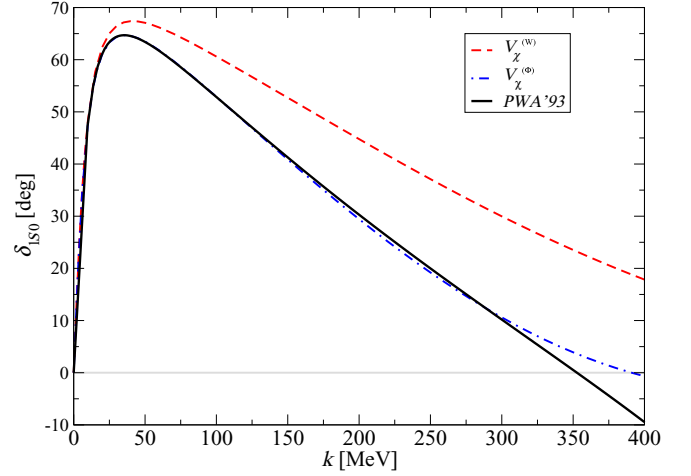


FIG. 1. ¹S₀ phase shift (in degrees) as a function of the center-of-mass momentum (in MeV) for the potentials (2) and (16), with the regularization prescriptions (6) and (7) ($R = 0.9$ fm) and the renormalization conditions (10) and (13) respectively, depicted as dashed (red) and dot-dashed (blue) curves. The solid (black) line is the phase shift extracted from the partial-wave analysis of Ref. [32].

Knowing $E(N_{\max}, \hbar\Omega)$ for $N_{\max} = \{N_{\max}^* - 2, N_{\max}^*, N_{\max}^* + 2\}$, one can easily solve

$$E_{\infty}(\hbar\Omega) = \frac{E^2(N_{\max}^*, \hbar\Omega) - E(N_{\max}^* - 2, \hbar\Omega)E(N_{\max}^* + 2, \hbar\Omega)}{2E(N_{\max}^*, \hbar\Omega) - E(N_{\max}^* - 2, \hbar\Omega) - E(N_{\max}^* + 2, \hbar\Omega)}. \quad (20)$$

In our extrapolations, we have taken $N_{\max}^* = 18, 14, 12$ for ³H, ⁴He, ⁶He respectively. We have observed that the extrapolated ground-state energies display a reasonable $\hbar\Omega$ independence in the intermediate region $\hbar\Omega = (30-50)$ MeV. To be specific, we choose $E_{\infty}(\hbar\Omega)$ such that the difference $E(N_{\max}^* + 2, \hbar\Omega) - E_{\infty}(\hbar\Omega)$ is minimized [58].

The uncertainties in $E_{\infty}(\hbar\Omega)$, depicted as horizontal bands in Fig. 2, have been determined through applying Eq. (20) with $N_{\max}^* = 16, 12, 10$ for ³H, ⁴He, ⁶He respectively. Still, there is the caveat that the upper uncertainty of an extrapolated result should not extend higher than the result for the largest N_{\max} in consideration; note that the variational principle guarantees that, for any finite truncation of the model space, each eigenvalue provides an upper bound for the ground-state energy in the full model space. We apply such principle in its strong (or global) version, meaning that our extrapolated energy can never lie above the minimum of the largest N_{\max} curve. This said, one also needs to be careful to not simply choose the error associated to the optimal $\hbar\Omega$ from which the corresponding central value was extracted. This is due to the fact that the extrapolated results from two consecutive sets of N_{\max} tend to cross in the close neighborhood of such optimal $\hbar\Omega$, thus leading to underestimated uncertainties when a small $\hbar\Omega$ step is used. Instead, we examined the uncertainties around the optimal $\hbar\Omega$ value (mostly above it) in order to obtain such uncertainties.

We summarize our results in Table I, showing that the overbinding is reduced by about 70% for the three nuclei. Besides, notice that in our calculations the ⁴He ground state

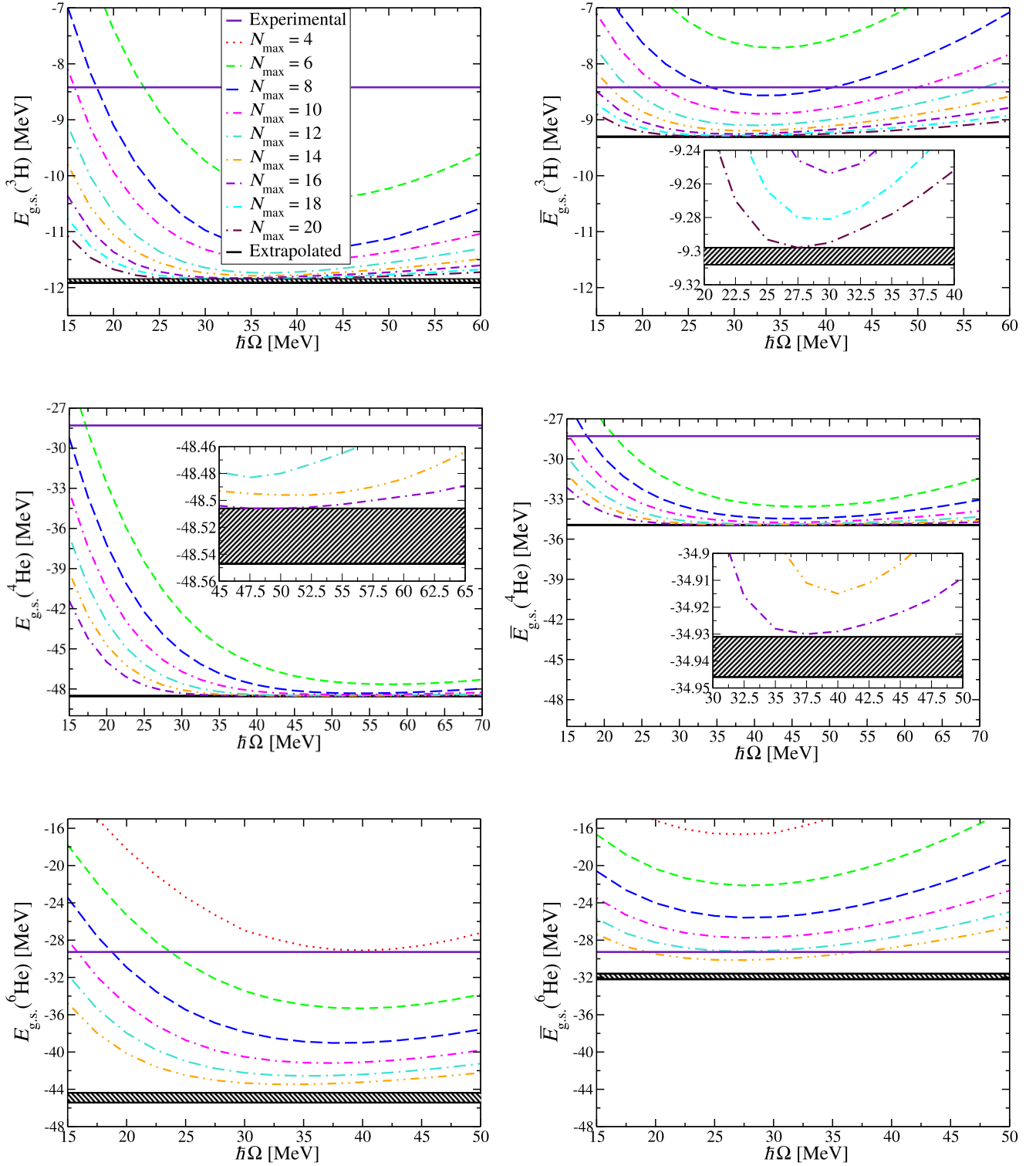


FIG. 2. Ground-state energies $E_{\text{g.s.}}$ and $\bar{E}_{\text{g.s.}}$ of ${}^3\text{H}$, ${}^4\text{He}$, and ${}^6\text{He}$ with LENPIC^[0] (2) [24–26,30] and modified LENPIC^[0] (16) interactions respectively, with the regularization prescription of Eqs. (6) and (7) and a coordinate cutoff $R = 0.9$ fm, together with the corresponding experimental values. For both potentials, the infinite- N_{max} extrapolated results and the associated uncertainties shown by black bands have been obtained through Eq. (20) (see the main text for further explanations).

exhibits a faster N_{max} convergence than the ${}^3\text{H}$ ground state, similar to what is observed with other NN interactions (see, e.g., Refs. [58,60]). However, note that for both potentials

studied here, we find that ${}^6\text{He}$ is above the ${}^4\text{He} + n + n$ threshold. This is an inconvenience that appears with other interactions though; see, e.g., Ref. [61] and the beyond-LO

TABLE I. Extrapolated ground-state energies $E_{g.s.}$ and $\bar{E}_{g.s.}$ of ${}^3\text{H}$, ${}^4\text{He}$, ${}^6\text{He}$ with LENPIC^[0] [24–26,30] and *modified*LENPIC^[0] interactions respectively. Note that the asymmetric character of the ${}^4\text{He}$ intervals of confidence is due to the suppression of the positive error by the variational principle. Our results for $E_{g.s.}({}^3\text{H})$ and $E_{g.s.}({}^4\text{He})$ are to be compared with the ones reported in Ref. [25] (-11.747 and -48.39 MeV, respectively), where the charge dependence of the NN interaction is explicitly taken into account, allowing us to conclude that its effect is small for these nuclei.

Ground-state energies			
Nucleus	$E_{g.s.}$ [MeV]	$\bar{E}_{g.s.}$ [MeV]	$E_{g.s.}^{(\text{exp})}$ [MeV]
${}^3\text{H}$	-11.88 ± 0.03	-9.303 ± 0.005	-8.42
${}^4\text{He}$	$-48.507^{+0.001}_{-0.040}$	$-34.936^{+0.005}_{-0.010}$	-28.30
${}^6\text{He}$	-44.9 ± 0.5	-31.9 ± 0.3	-29.27

results of Ref. [25]. Yet, the Daejeon16 and JISP16 NN interactions do succeed in amending such an issue; see, e.g., Ref. [60] and references therein.

B. Point-proton RMS radii

Our results for the point-proton RMS radii of ${}^3\text{H}$ and ${}^4\text{He}$ are plotted in Fig. 3. Note that, since ${}^6\text{He}$ appears unbound with respect to the ${}^4\text{He} + n + n$ threshold (see Table I), the ${}^6\text{He}$ point-proton radius is not meaningful for the two interactions studied here.

Unlike the energy, which is sensitive to intermediate- and short-range correlations, the RMS-radius operator is a long-range operator. In general, long-range operators display a poorer convergence with N_{max} . This is due to the fact that the HO basis produces density distributions with Gaussian fall-off at large distances, while exponential fall-off is the physically expected behavior. Hence, increasing the size of the model space increases the radial extent of the NCSM density distribution, but it does not circumvent its unphysical damping with respect to the true density distribution. Extracting a robust extrapolation of the point-proton RMS radii would thus require new developments and/or larger basis spaces. We note that in the literature there are phenomenological prescriptions accounting for the dependence of the radii on the size of the model space analogous to Eq. (20) for the energies [62].

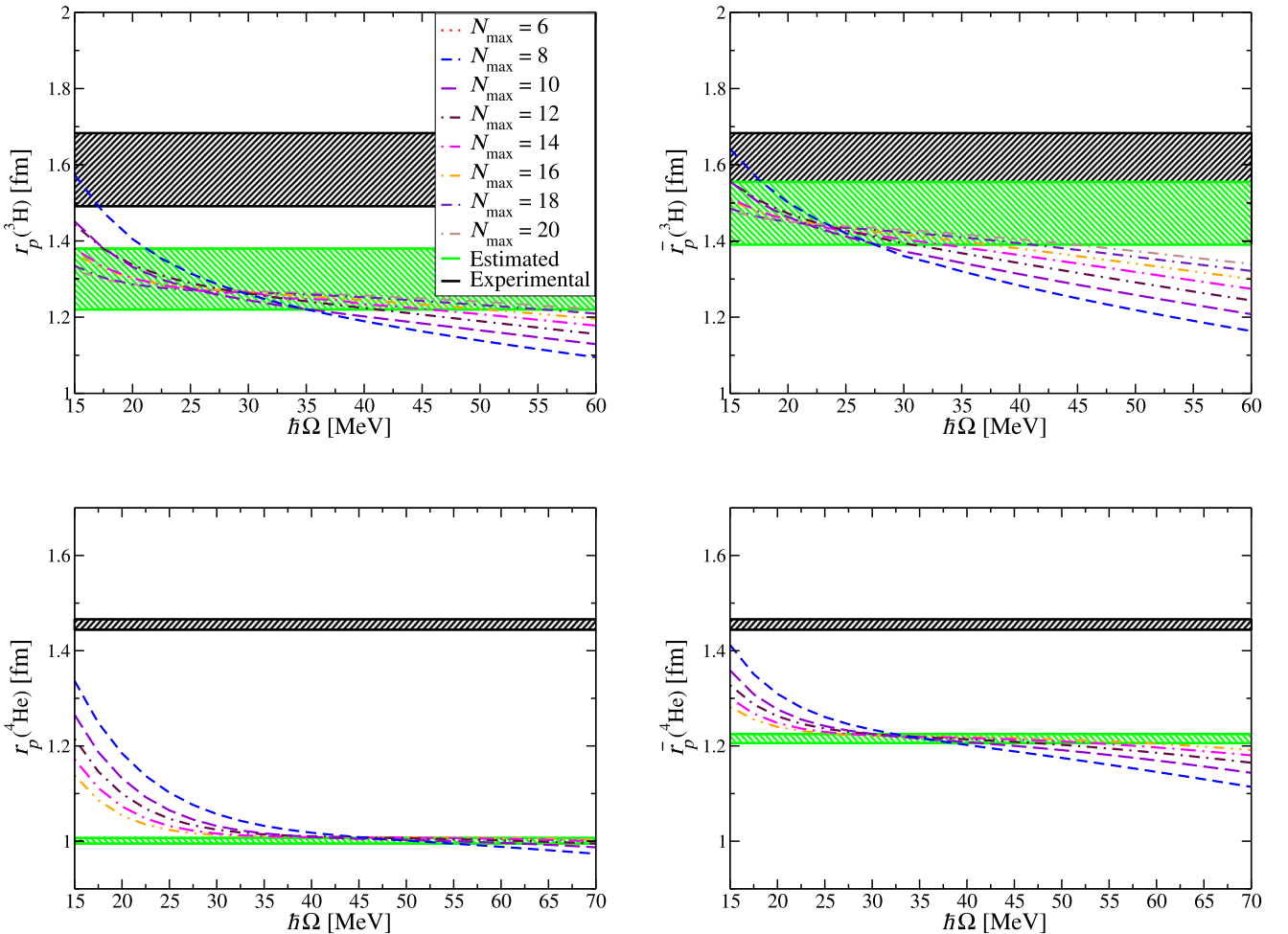


FIG. 3. Point-proton RMS radii r_p and \bar{r}_p of ${}^3\text{H}$ and ${}^4\text{He}$ with LENPIC^[0] (2) [24–26] and *modified*LENPIC^[0] (16) interactions respectively, with the regularization prescription of Eqs. (6) and (7) and a coordinate cutoff $R = 0.9$ fm. The dashed black (green) band represents the experimental error (the uncertainty of our estimated result). Note that the upper (lower) limit of the latter was obtained from the highest (lowest) point where two curves with different N_{max} cross each other.

TABLE II. Point-proton RMS radii r_p and \bar{r}_p of ${}^3\text{H}$ and ${}^4\text{He}$ with LENPIC^[0] [24–26,30] and *modified* LENPIC^[0] interactions respectively. Note that the “experimental” point-proton radii are extracted from the experimental charge radii given in Refs. [64,65].

Nucleus	Point-proton RMS radii		
	r_p [fm]	\bar{r}_p [fm]	$r_p^{(\text{exp})}$ [fm]
${}^3\text{H}$	1.3 ± 0.1	1.5 ± 0.1	1.587 ± 0.096
${}^4\text{He}$	0.99 ± 0.01	1.22 ± 0.01	1.455 ± 0.011

Theoretical approaches, able to obtain extrapolations of long-range observables through analyses of infrared properties of the HO basis, are also available [55,63]. However, in this work we will adopt the prescription of taking as our guess for the estimated radius the crossing point of the $\hbar\Omega$ dependence of the radii obtained with different N_{max} [59]; see Table II. For both nuclei, we note that the extra repulsion induced by the modified LENPIC^[0] interaction results in the crossing point being shifted to the left (i.e., it appears for smaller values of $\hbar\Omega$) with respect to the original LENPIC^[0] interaction. The overall effect of the modified interaction is to produce a point-proton RMS radius that is larger than the one produced by the original interaction, in closer agreement with experiment.

We see that the modification of the LO chiral potential described in Sec. II allowed us to produce new LO results for two nuclear magnitudes, namely the ground-state energy and the point-proton RMS radius, of three positive-parity light nuclei. These predictions are closer to experiment than the LO results of Ref. [25] obtained under the assumption of NDA. In particular, we notice that the excess of NN attraction anticipated by Weinberg power counting at LO generates, for these nuclei, an overestimation of the binding energies and an underestimation of the radii that can be both easily and significantly improved with our proposal.

IV. CONCLUSIONS AND PERSPECTIVES

In this work, we have explored the consequences in the description of light nuclei produced by a rearrangement of the short-range part of a two-nucleon chiral potential that is most commonly employed in current *ab initio* calculations of light nuclei, i.e., the one grounded on the Weinberg power counting. We have followed Ref. [21] in promoting subleading (repulsive) interaction terms that capture, already at leading order in the effective expansion, the zero of the 1S_0 partial-wave amplitude—a zero that appears at a relatively soft scattering momentum according to experiment. We remark that the proposal here relies merely on the treatment of such momentum as a low-energy scale. Furthermore, the 1S_0 channel amplitude is unique in displaying such a low-lying zero along with a very shallow pole. We distinguish the situation in the 1S_0 channel from the 3S_1 channel (where the amplitude zero lies beyond the pion-production threshold) and from the 3P_0 amplitude (which turns around at a lower energy but contains no low-energy pole). The scattering in these latter two channels is qualitatively well captured at

leading order—either by the Weinberg scheme for cutoffs below the breakdown scale of the theory [66,67] or for a wider cutoff range through certain renormalization-consistent modifications of the Weinberg prescription [15,38–41].

We have shown that the minimal change in the power counting invoked in this work significantly helps to improve the leading-order results, at the level of the ground-state energies and point-proton radii, of the ${}^3\text{H}$, ${}^4\text{He}$, and ${}^6\text{He}$ nuclei. In particular, the excess of attraction of the 1S_0 two-nucleon interaction brought by the Weinberg scheme at leading order yields a pattern of overbinding in the ground-state energies and underprediction of the radii for those nuclei [25]. We show that this deficiency can be addressed by the inclusion of repulsive terms as leading-order effects. This may also help to alleviate the pressure on higher orders of the effective expansion, thus opening a new avenue for potentially improved convergence with respect to increasing chiral order.

Of course, before a claim of convergence of this rearrangement can be made, one needs to produce results beyond leading order in the expansion for observables. We intend to pursue this task in future work. Then, getting ${}^6\text{He}$ bound with respect to ${}^4\text{He}$, unlike what we found at leading order (see Sec. III), will be a relevant test of consistency for our approach. We also need to study how charge-dependent and charge-asymmetric terms should be encoded in our proposed potential expansion, in the spirit of what was done in Ref. [68] for Weinberg’s power counting; see also the recent work of Ref. [69], which demonstrates that a charge-independence-breaking short-range term needs to be promoted to leading order for consistency with the nonperturbative inclusion of electromagnetic effects in the two-nucleon potential.

The path forward has significant uncertainties. Note that—in spite of some exceptions, such as the recent work of Ref. [70]—the general way to proceed in current *ab initio* calculations is, following Weinberg’s original idea [6,7], to treat subleading terms of the potential on the same footing as its leading part (i.e., nonperturbatively). However, some authors [15,27,37–42] argue that, in order not to undermine cutoff independence of observables, such subleading contributions need to be added as perturbations on top of the infinitely iterated leading-order potential. Still, other authors [17–20] disagree with this conception, as they claim that cutoff dependence of observables is guaranteed to be reasonably mild provided that one sticks to cutoff values that are softer than the breakdown scale of the EFT—typically, below (500–600) MeV in *ab initio* calculations.

It is worth recalling that cutoff-convergence issues of the Weinberg counting already emerge in the two-nucleon sector at leading order itself, as first noticed in Ref. [15]. Such issues arise in those channels where one-pion exchange—which is prescribed to be leading order under the assumption of naive dimensional analysis—is both singular and attractive. That is, in light of the $1/r^3$ divergence of the potential at small r , the leading-order amplitude does not converge for large enough cutoffs if no repulsive contact term is employed. However, in Weinberg power counting a contact term

affecting a partial wave with orbital angular momentum ℓ is prescribed to contribute no less than 2ℓ orders down with respect to leading order. Yet, one can easily check that the 3P_0 amplitude becomes ill defined when cutoffs in the range 500 MeV–1 GeV are used unless an unexpected contact term with two derivatives is promoted from next-to-next-to-leading order to leading order. But, since there is an infinite number of partial waves where one-pion exchange is both singular and attractive, Refs. [15,38–41] advocate to treat one-pion exchange as a subleading (perturbative) correction in those channels where the centrifugal barrier becomes effective. In particular, the 3P_0 channel might be the only partial wave with $\ell \geq 1$ where one-pion exchange needs to be retained at leading order, as first pointed out in Ref. [71]; such a hypothesis is backed by the more recent work of Refs. [72,73]. Hence, in the future we plan to promote the 3P_0 contact term to leading order and see how this may improve the description of heavier nuclei. We remark, however, that such a modification in the Weinberg counting is mainly motivated by renormalization requirements, unlike the one proposed here, which was aimed at improving the agreement with phenomenological evidence. Finally, we comment that cutoff dependence of observables

was not studied here, but it will be addressed in future work.

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