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Effective Field Theory for Lattice Nuclei

N. Barnea,[1] L. Contessi,[2] D. Gazit,[1] F. Pederiva,[2,3] and U. van Kolck[4,5]

[1]*Racah Institute of Physics, The Hebrew University, Jerusalem 91904, Israel*
[2]*Physics Department, University of Trento, via Sommarive 14, I-38123 Trento, Italy*
[3]*INFN-TIFPA Trento Institute for Fundamental Physics and Applications, Trento, Italy*
[4]*Institut de Physique Nucléaire, CNRS/IN2P3, Université Paris-Sud, F-91406 Orsay, France*
[5]*Department of Physics, University of Arizona, Tucson, AZ 85721, USA*

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We show how nuclear effective field theory (EFT) and *ab initio* nuclear-structure methods can turn input from lattice quantum chromodynamics (LQCD) into predictions for the properties of nuclei. We argue that pionless EFT is the appropriate theory to describe the light nuclei obtained in LQCD simulations carried out at pion masses heavier than the physical pion mass. We solve the EFT using the effective-interaction hyperspherical harmonics and auxiliary-field diffusion Monte Carlo methods. Fitting the three leading-order EFT parameters to the deuteron, dineutron and triton LQCD energies at $m_\pi \approx 800$ MeV, we reproduce the corresponding alpha-particle binding and predict the binding energies of mass-5 and 6 ground states.

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Introduction – Understanding the low-energy dynamics of quantum chromodynamics (QCD), which underlies the structure of nuclei, is a longstanding challenge posed by its non-perturbative nature. After many years of development, lattice QCD (LQCD) simulations are fulfilling their promise of calculating static and dynamical quantities with controlled approximations. Progress has reached the point where meson and single-baryon properties can be predicted quite accurately, see for example Ref. [1]. Following the pioneering studies in quenched [2] and fully-dynamical [3] LQCD, a substantial effort is now in progress to study light nuclei [4–7]. Multinucleon systems are significantly more difficult to calculate than single-baryon states, as they are more complex, demand larger lattice volumes, and better accuracy to account for the fine-tuning of the nuclear force. At heavier light-quark masses, the formation of quark-antiquark pairs is suppressed, the computational resources required to generate LQCD configurations are reduced, and the signal-to-noise ratio in multinucleon correlation function improves [7]. Therefore, present multinucleon LQCD simulations are performed at heavy up and down quark masses, which result in unphysical values for hadronic quantities. Once lattice artifacts are accounted for using large enough volumes and extrapolating to the continuum, LQCD results depend on a single parameter, the pion mass m_π. However, sufficiently large volumes are harder to achieve as the number of nucleons increases due to the the saturation of nuclear forces.

A hadronic effective field theory (EFT) that incorporates chiral symmetry (chiral EFT) provides a tool to extrapolate LQCD results to a smaller, more realistic pion mass [3, 8]. Here we show how EFTs, combined with *ab initio* methods for the solution of the Schrödinger equation, provide a way to extend LQCD results also to the larger distances involved in nuclei with several nucleons. Of course, solving the nuclear many-body problem is not a small challenge, yet it is considerably simpler than solving QCD on the lattice.

We devise an EFT for existing lattice nuclei, that is, nuclei composed of neutrons and protons living in a world where m_π is much larger than the physical pion mass. Pion effects can be considered short-ranged, and the appropriate theory is pionless EFT ($\not\pi$EFT), an EFT based on the most general dynamics among nucleons which is consistent with the symmetries of QCD. (For a review, see *e.g.* Ref. [9]). We solve this EFT in leading order (LO) using the effective-interaction hyperspherical harmonics (EIHH) method [10] for systems with $A \leq 6$ nucleons, and the auxiliary-field diffusion Monte Carlo (AFDMC) method [11, 12] for $A \geq 4$. Binding energies of nuclei with $A \leq 3$ are used as input. The energy of the $A = 4$ ground state provides a consistency check between both *ab initio* methods, and between them and LQCD. Binding energies for $A \geq 5$ are predictions that extend LQCD into new territory. In order to evaluate the feasibility of our approach, we present here the first analysis of the problem using recent multinucleon LQCD results at $m_\pi = 805$ MeV from the NPLQCD collaboration [6]. Table I summarizes nucleon and light nuclear data in nature and in the LQCD world, including our results.

The modern approach to nuclear physics deploys *ab initio* methods such as EIHH and ADFMC in the solution of chiral EFT with coupling constants tuned to experimental few-body data. Since the latter are replaced here by LQCD data, our approach illustrates how eventually one will be able to derive the structure of real nuclei directly from QCD. Our method can be extended straightforwardly to hypernuclei.

Effective Field Theory – Identification of the relevant energy scales and the selection of the appropriate degrees of freedom is essential for a successful application of EFT

TABLE I. Available experimental and LQCD data at various values of the pion mass [MeV], and our results: the neutron and proton masses and binding energies of the lightest nuclei [MeV]. Fitted values are marked with *. Error estimates are discussed in the text.

m_π	140	510	805	805
Nucleus	[Nature]	[5]	[6]	[This work]
n	939.6	1320.0	1634.0	1634.0
p	938.3	1320.0	1634.0	1634.0
nn	-	7.4 ± 1.4	15.9 ± 3.8	15.9 ± 3.8 *
D	2.224	11.5 ± 1.3	19.5 ± 4.8	19.5 ± 4.8 *
^{3}n	-			-
^{3}H	8.482	20.3 ± 4.5	53.9 ± 10.7	53.9 ± 10.7 *
^{3}He	7.718	20.3 ± 4.5	53.9 ± 10.7	53.9 ± 10.7
^{4}He	28.30	43.0 ± 14.4	107.0 ± 24.2	89 ± 36
^{5}He	27.50			98 ± 39
^{5}Li	26.61			98 ± 39
^{6}Li	32.00			122 ± 50

TABLE II. Variation of the nuclear energy scales with the pion mass.

Scale	$m_\pi \sim 140$ MeV	$m_\pi \sim 500$ MeV	$m_\pi \sim 800$ MeV
M_{QCD}	1000 MeV	1300 MeV	1600 MeV
M_Δ	300 MeV	300 MeV	180 MeV
M_π	140 MeV	500 MeV	800 MeV
M_{ope}	20 MeV	200 MeV	400 MeV
M_{nuc}	10 MeV	15 MeV	25 MeV

to a physical problem. In Table II we present the relevant energy scales for natural nuclear physics and for lattice nuclei, as inferred from Table I.

In nature, nuclear physics comprises several scales. The higher is the QCD scale $M_{QCD} \sim m_N \sim 1$ GeV that characterizes the nucleon mass m_N, most other hadron masses, and the chiral-symmetry-breaking scale. The second and third scales are given by the energies of the lightest nucleon excitation and meson, respectively, $M_\Delta \sim m_\Delta - m_N \sim 300$ MeV associated with the Delta-nucleon mass difference and $M_\pi \sim m_\pi \sim 140$ MeV. Both these scales are numerically not very different from the pion decay constant and the Fermi momentum in heavy nuclei. Another energy scale, which we call the one-pion-exchange scale, emerges when the inverse pion Compton wavelength is combined with the QCD mass scale, $M_{ope} \sim m_\pi^2/m_N \sim 20$ MeV. This is also the characteristic magnitude of the nuclear binding energy per nucleon, $M_{nuc} \sim B/A$.

For lattice nuclei these scales can be different. We observe that the approximate degeneracy between M_{ope} and M_{nuc}, so important in nature, is removed and a clear separation develops between M_{nuc} and the other scales. Barring a dramatic, unforeseen relative decrease in the mass of another nucleon excitation or meson, nucleons are expected to be the only relevant degrees of freedom for low-energy lattice nuclei. An EFT involving the most general dynamics of only the non-relativistic four-component nucleon field (two spin and two isospin states), without any mesons, is the appropriate theory for these systems. For a process with external momenta $Q \sim \sqrt{m_N M_{nuc}}$ it produces the same S matrix as QCD, but in an expansion in Q/M, where M is the typical scale of higher-energy effects. The resulting theory coincides with $\not\pi$EFT for natural nucleons [9], except for different values of parameters and scales. While in nature $\sqrt{m_N M_{nuc}} \sim 100$ MeV and $M \sim M_\pi$, for $m_\pi \sim 800$ MeV the numbers in Table II suggest instead $\sqrt{m_N M_{nuc}} \sim 200$ MeV and $M \sim \sqrt{M_{QCD} M_\Delta} \simeq 500$ MeV (*cf.* Ref. [13]).

The Hamiltonian – The EFT Lagrangian contains all possible terms compatible with QCD symmetries and ordered by the number of derivatives and nucleon fields. The corresponding Hamiltonian is naturally formulated in momentum space, where the potential takes the form of a momentum expansion that must be regulated in high momentum. Dependence only on transferred momenta leads to local interactions, while more general momentum dependence yields non-local interactions as well.

Due to the Pauli principle we need consider only antisymmetric multinucleon states. Restricting the Lagrangian to this subspace we are free to choose a subset of the terms in the EFT Lagrangian without loss of generality. As in Ref. [14], here we aim at formulating a local EFT nuclear potential that will allow us to study the many-body problem utilizing techniques, such as AFDMC [11, 12], that are restricted to local interactions. In order not to introduce non-local terms in the regularization, we assume a regulator function of Gaussian form, $f_\Lambda(q) = \exp(-\boldsymbol{q}^2/\Lambda^2)$ in terms of the momentum transfer $\boldsymbol{q}$ and a regulator parameter (or cutoff) Λ.

For this regulator the coordinate-space Hamiltonian takes the form

$$H = -\sum_i \frac{\nabla_i^2}{2m_N} + \sum_{i<j} \left(C_1 + C_2\, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j\right) e^{-\Lambda^2 r_{ij}^2/4} + \sum_{i<j<k} \sum_{cyc} D_1 \left(\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j\right) e^{-\Lambda^2 (r_{ik}^2 + r_{jk}^2)/4} + \dots, \quad (1)$$

where $\sum_{cyc}$ stands for the cyclic permutation of a particle triplet (ijk), and "…" for terms containing more derivatives and/or more-body forces. The expansion coefficients $C_{1,2}(m_\pi, \Lambda), D_1(m_\pi, \Lambda), \dots$, commonly called low-energy constants (LECs), are unknown parameters that encompass physics at the scale M and above, and thus change with m_π. They depend on the arbitrary cutoff Λ in such a way that low-energy observables are (nearly) cutoff-independent, and they should be fitted through comparison between the EFT and the available data.

Naïve scaling arguments suggest that the LECs should scale as $1/M^{1+d+\frac{3}{2}(n-4)}$, where d is the number of derivatives and n is the number of nucleon fields [15]. However, the existence of shallow S-wave two-body bound states at $\sqrt{m_N M_{nuc}} \ll M$ requires enhancements in operators that connect S waves. The LO two-body operators are those without derivatives [16]. While a surprising enhancement in the non-derivative three-body interaction promotes it to LO [17], the same is thought not to happen for four-body forces [18]. More-body forces require derivatives and are expected to be further suppressed. To match current lattice calculations we can neglect isospin violation. For the first attempts at a description of real light nuclei with the leading interactions, see Ref. [19]. The m_π dependence of two- and three-nucleon observables in $\not\pi$EFT has been studied with input from chiral EFT in Ref. [20]. The quark mass dependence of the triple-α process was estimated in Ref. [21].

Some comments are in order about the EFT truncation. Expanding the regulator around $q = 0$, we see that it introduces terms of $\mathcal{O}(Q/\Lambda)^2$. Moreover, the regulator does not commute with the permutation operator, which gives rise to more general momentum dependence of the same order. These terms can be lumped with higher-order interactions in the "…" of Eq. (1) without increasing the expected truncation error, $\mathcal{O}(Q/M)$, because we consider here $\Lambda \gtrsim M$. A conservative estimate of the $\not\pi$EFT truncation error at LO is about 40%. However, we note that in application of $\not\pi$EFT to the physical ^{4}He nucleus an accuracy of 10-20% is achieved [18, 19], even though a naive estimate suggests a 50% uncertainty.

Input data – The online publication of the NPLQCD data for the spectrum of the $A \leq 4$ nuclei last year [6] provided the motivation for the current work. The measured lattice binding energies of the deuteron, dineutron and triton, together with that of the alpha particle, provided us with the three data points to which we fit our LO LECs, plus one data point to validate it. In the meanwhile new lattice results have appeared. Unquenched calculations of light nuclear binding energies at $m_\pi = 510$ MeV were reported [5], and also the two-nucleon (NN) scattering lengths and effective ranges at $m_\pi = 805$ MeV [7]. We assume here that the interaction has range $\sim 1/m_\pi$ and comparable effective ranges, but much larger scattering lengths. Since the reported effective ranges are smaller than the scattering lengths, our expansion should converge, albeit at a slow rate. Note, however, that the data from Ref. [7] indicates an almost degenerate double bound state pole in the NN T matrix, which is thought to be incompatible with a short-range non-relativistic potential [22]. Worse still, Ref. [4] finds no NN bound states in a large range of pion masses that includes the values in Table I. Until the dust settles, we concentrate on the LQCD data in Table I for $m_\pi = 805$ MeV, as a first check of our proposed approach.

TABLE III. The LO LECs [GeV] for lattice nuclei at $m_\pi = 805$ MeV, as a function of the momentum cutoff Λ [fm^{-1}].

Λ	$C_{1,0}$	$C_{0,1}$	D_1
2	−0.1480	−0.1382	−0.07515
4	−0.4046	−0.3885	−0.3902
6	−0.7892	−0.7668	−1.147
8	−1.302	−1.273	−2.648

Calibration and predictions – For the calibration of the NN LECs we turn to the spin-isospin (S, T) basis and define the channel constants $C_{S,T} \equiv C_1 + [2S(S+1) - 3]C_2$. We solve the two-body Schrödinger equation using the Numerov method, and fit $C_{S,T}$ to the deuteron ($S = 1,\ T = 0$) and dineutron ($S = 0,\ T = 1$) binding energies. To calibrate the LEC D_1 using the ^{3}H binding energy B_3, we solve the three-body Schrödinger equation with the EIHH method, where we expand the wavefunction into a set of antisymmetrized hyperspherical-harmonics spin-isospin states. Convergence is controlled by the hyper-angular quantum number K_{max}, results being obtained by extrapolation to the limit $K_{max} \to \infty$ [10]. The corresponding error in our results is estimated to be smaller (for the lighter systems, much smaller) than the EFT truncation error.

The LECs fitted to the central values of the lattice results are presented in Table III. The cutoff dependence of the NN LECs $C_{S,T}$ is qualitatively similar to other regulators [16]. We see no limit-cycle behavior [17] in D_1, possibly because our cutoff values are not large enough to probe the second branch of the periodic function.

A simple check of $\not\pi$EFT at LO, which is equivalent to the large-scattering-length approximation to the two-body problem, is that for large cutoffs the $S = 1,\ T = 0$ scattering length is related to deuteron binding energy B_{31} by $a_{31} \approx 1/\sqrt{m_N B_{31}}$ [16]. This relation suggests that a_{31} should approach 1.12 fm for the lattice deuteron. For our Gaussian cutoff we find $a_{31} = (1.2 \pm 0.5)$ fm, where we use the wide range of cutoff variation $2 - 14\,\mathrm{fm}^{-1}$ to estimate the EFT error. With a sharper cutoff function $f_\Lambda(q) \to \exp(-\boldsymbol{q}^4/\Lambda^4)$ there is quicker convergence to the expected number, $a_{31} = (1.1 \pm 0.1)$ fm in the same cutoff range.

With LECs fixed, we now have a complete LO potential that can be used to predict other properties of lattice nuclei. As a first step in this direction we shall estimate the binding energies B_A for $A = 4, 5, 6$. To solve the Schrödinger equation for these systems we use, in addition to EIHH, also the AFDMC method. In the latter technique [11, 12], the ground-state energies are projected from an arbitrary initial state by means of a stochastic imaginary-time propagation. The numerical complexity related to the presence of operatorial

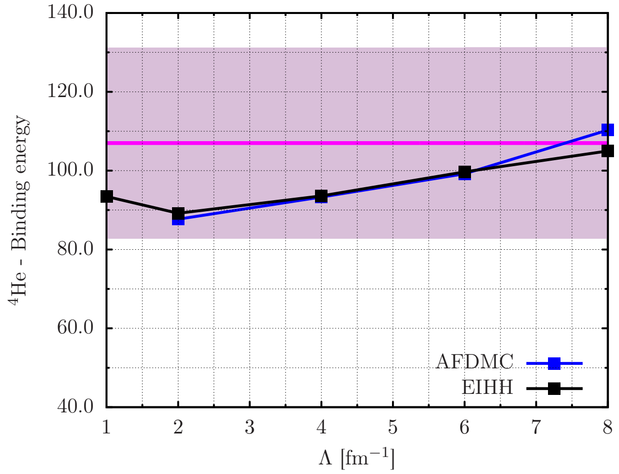

FIG. 1. (Color online) ^{4}He binding energy B_4 [MeV] as function of the momentum cutoff Λ [fm^{-1}]. The (magenta) horizontal line and the (pink) band give the LQCD central value and error. The (black and blue) solid lines are (respectively the EIHH and AFMDC) LO EFT results.

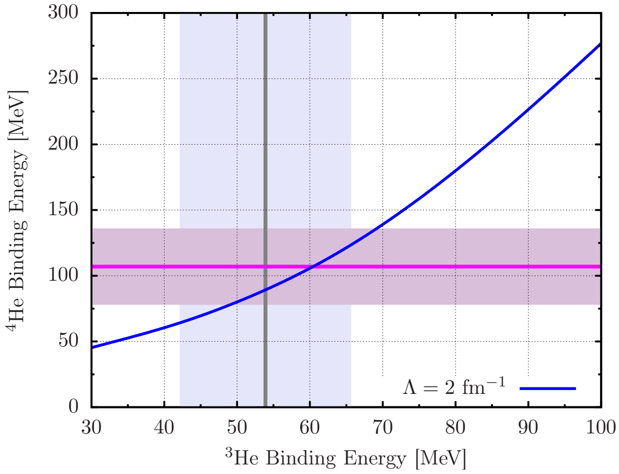

FIG. 2. (Color online) Correlation between the ^{4}He and ^{3}He binding energies, B_4 [MeV] and B_3 [MeV]. Horizontal and vertical lines and bands represent LQCD results. The (blue) solid line is the Tjon line in LO EFT from EIHH at $\Lambda = 2$ fm^{-1}.

terms in the interaction is reduced by using the Hubbard-Stratonovich transformation, at the price of introducing auxiliary fields as additional degrees of freedom.

In properly renormalized EFT, observables should be asymptotically invariant to the value of Λ. In practice, this goal is hard to achieve because in heavier systems our cutoff range is limited and variation of calculated properties tends to be smaller than the expected EFT truncation error. Therefore we aim for a more modest goal, that observables depend only weakly on the cutoff. In Fig. 1 we present the calculated binding energy of ^{4}He, B_4, as a function of Λ. Over a wide cutoff range the EFT prediction reproduces the LQCD result within the measurement error, evidence that the EFT in LO captures the essence of the strong-interaction dynamics, and that 40% is an overestimate of the EFT truncation error. Our results are not cutoff invariant, however the cutoff dependence is rather moderate: B_4 changes by 20% when Λ grows by a factor of 4.

In Fig. 2 we present the correlation between ^{3}He and ^{4}He binding energies. When we allow D_1 to vary at fixed $C_{S,T}$, LO EFT gives a line [18], which corresponds to the phenomenological Tjon line [23]. One can see how the measurement error in B_3 is propagated into an error in the predicted B_4 value. Using this figure alone one would conclude that the EFT error estimate for B_4 is about ±27 MeV, very close to the measurement error. Our estimate of a 40% error in the LO EFT is likely *very* conservative. Our reproduction of the LQCD central value and error estimate for B_4 indicates consistency of the LQCD values [6] for the $A = 2, 3, 4$ systems.

The power of the EFT formulated above is the relative ease with which it can be extended to different few- and many-body systems. Using $\Lambda = 2$ fm^{-1} we have looked for excited states in $A = 2, 3, 4$ systems, but much to our surprise found none. Similarly, we have found no evidence for ^{3}n droplets, for which our ground-state binding energy coincides with the two-body threshold. Results for the $A = 5, 6$ ground states at $\Lambda = 2$ fm^{-1} are shown in Table I, with errors estimated from the EFT truncation.

For ^{5}He we found a bound state with binding energy $B_5 = 98.2$ MeV, which reflects a 9 MeV binding relative to ^{4}He at the same cutoff. However, examining the evolution of B_5 with the cutoff we found that for $\Lambda = 4$ fm^{-1} the five-body ground-state energy coincides with the four-body threshold. This suggests that the $A = 5$ nuclear gap found in nature persists for larger quark masses.

We have also calculated the ^{6}Li ground state for $\Lambda = 2$ fm^{-1}, obtaining $B_6 \approx 122$ MeV. In this case the error in K_{max} extrapolation is about 3 MeV, which is somewhat larger than for lighter systems but still small compared with input and truncation errors. Thus $B_6/A \approx 20$ MeV, similar to lattice ^{4}He. We conjecture that nuclear saturation survives the increase in pion mass, but this conclusion remains to be confirmed by larger calculations.

Conclusion – One of the main challenges of current research in nuclear physics is to provide a unified look at the nuclear regime, from QCD to heavy nuclei. Using results from recent lattice QCD simulations of few-nucleon systems, we took important steps in this direction by demonstrating the consistency of $\not{\pi}$EFT and LQCD for $m_\pi \approx 800$ MeV. Our results suggest that some of the defining properties of nuclei might be relatively insensitive to the value of the pion mass. More LQCD data are needed in order to go beyond LO EFT and assess the systematic uncertainty of the EFT approach, while more extensive calculations with the EFT should settle the issue of the importance of quark masses to nuclear properties, with implications for the analysis of fundamental constant variability [24].

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