Extrapolating Lattice QCD Results using Effective Field Theory

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Lattice simulations are the only viable way to obtain ab-initio Quantum Chromodynamics (QCD) predictions for low energy nuclear physics. These calculations, however, are done in a finite box and therefore extrapolation is needed to get the free space results. Here we use nuclear Effective Fields Theory (EFT), designed to provide a low energy description of QCD using baryonic degrees of freedom, to extrapolate the lattice results from finite to infinite volume. To this end, we fit the EFT to the results calculated with nonphysical high quark masses and solve it with the stochastic variational method in a finite and infinite volume. Moreover, we perform similar EFT calculations for physical quark mass and predict the finite-volume effects to be found in future Lattice QCD calculations.

I. INTRODUCTION

At low energies, characterizing the nuclear structure, Quantum Chromodynamics (QCD), the fundamental theory of the strong interactions, is non-perturbative. The only feasible way to obtain *ab-initio* QCD predictions for nuclear physics is through Lattice simulations of QCD, dubbed LQCD [1].

These calculations are done via numerical evaluation of path integrals on a discrete space- and time-like lattice and summing over all possible paths. When the volume of the lattice is taken to be infinitely large and its sites infinitesimally close to each other, the continuum is recovered.

After years of development, LQCD simulations are fulfilling their promise of calculating static and dynamical quantities with controlled approximations. Progress has been made to a point where meson and single-baryon properties can be predicted quite accurately; see, e.g., [2–4]. However, the complexity and peculiar fine-tuning aspects in nuclear systems make this fundamental approach significantly more difficult relative to the extraction of single-baryon observables. For a recent reviews, see, e.g. [5, 6].

Currently, a few LQCD collaborations are studying multi-baryon systems, including HAL QCD [7, 8], PACS [9, 10], NPLQCD [11–13], CalLat [14], and the Mainz group [15]. Most teams try to extract the nuclear binding energies directly from the lattice simulations. HAL QCD collaboration takes a different approach, trying to extract the nuclear potential from the lattice simulation, and then calculate observables using standard nuclear physics techniques with the resulting potential. At this point, HAL QCD results are different from the results of the other groups.

A more common approach to study nuclear physics is based on Effective Field Theories (EFTs). In nuclear EFTs, baryons and mesons replace the quarks and gluons as the fundamental degrees of freedom. This framework provides a practical theory to analyze nuclear physics while incorporating the essential features of QCD. For low energy aspects of nuclear physics, like the descrip-

tion of light nuclei, even the mesons are not needed, and one is left with baryonic EFT, commonly referred to as pionless EFT, which will be employed here. This EFT is especially appropriate in a heavy pion mass world, where the pion dynamic is suppressed.

The first application of EFT for LQCD faced the challenge of using LQCD results to predict the binding energies of larger nuclei. A pionless EFT was fitted to the LQCD results and then used to predict the ground-state energies of ⁵He and ⁶Li [16], as well as ¹⁶O [17].

As mentioned above, LQCD calculations necessarily take place in finite volumes, thus affecting their infrared properties. For two-body systems, it is fair to claim that the implications of the finite volume on the spectrum are well understood through the Lüscher formalism in the asymptotic regime [18, 19]. The formalism pertinent for systems beyond the 2-body system has not yet reached this level of maturity, while significant progress is achieved in recent years, see e.g., [20–25].

The complexity of the problem suggests that an alternative road map towards the determination of infinite-volume quantities is called for.

Such an approach could be to build a nuclear EFT with the same boundary conditions as LQCD. This way the EFT is built directly matching the LQCD results in a finite lattice, and the extrapolation to the infinite lattice can be easily carried out through the nuclear EFT. Doing so, LQCD calculations may be performed with smaller lattice volumes, giving more accurate results, leaving the extrapolation to be done with the EFT.

Here we use the NPLQCD results for pion mass of $m_\pi=806$ MeV [11] to calibrate a leading order pionless EFT at finite box size and extrapolate the results toward the free space limit. Moreover, we perform the inverse procedure for the case of physical pion mass, i.e. we fit our EFT to the experimental results in the continuum and then predict the finite-box effect to be calculated in future LQCD calculations.

II. THEORY

LQCD calculations are done in a finite volume, making the challenge of correcting the lattice size effects to get the physical relevant results.

The common approach to do so is based on Lüscher's work [18, 19], which solves the two-body problem in a large box. Doing so, one can get the first order correction for the free-space binding energy,

$$E_B - E_L = -24\pi |A|^2 \frac{e^{-\kappa L}}{mL} + O\left(e^{-\sqrt{2}\kappa L}\right) \tag{1}$$

where E_B is the free space binding energy, E_L is the binding energy in a lattice with size L, $|A|^2 \sim 1$ is a normalization constant, and $\kappa = \sqrt{mE_B}$ is the binding momentum. To utilize Lüscher formula one has to calculate the binding energies for a few lattice sizes and fit the results with Eq. (1) to extract the free space parameters. Similar method enables the extraction of free space scattering parameters from finite box bound state calculations, avoiding the complication of dealing with continuum states.

A few years ago a different variant was proposed [26, 27], which is to calculate in a single lattice several boosted states differ by their total angular momentum. Using the asymptotic solution of boosted states in a box, the free space parameters can be extracted.

However, the generalization of such methods to larger systems is a challenge. The three-body case can be solved in some simple cases, and based on that several methods to correct the finite lattice effects were developed [20–24].

Here we would like to take a different path, relevant to arbitrary particle number, based on the construction of a relevant EFT which can be solved in any lattice size.

Effective field theories are a powerful tool to study the low energy properties of a system whenever a separation of scales exists between the energy scale of the studied process and the typical scale of the underlying theory.

Weinberg [28] has formulated the idea that in order to calculate low-energy observables of a given theory, it is sufficient to write down the most general Lagrangian, whose form is only limited by general properties like analyticity, unitarity, and the symmetries of the theory under investigation. In the case of QCD, it is Lorentz symmetry, parity, time reversal, and charge conjugation. Chiral symmetry, which is an approximated symmetry for the physical u and d quarks, does not apply in our case of heavy quarks. The fields used as degrees of freedom in this effective Lagrangian should be those which are seen as asymptotic states in the regime one is interested in. For low-energy nuclear physics, the relevant degrees of freedom are the nucleons.

A general Lagrangian constructed this way contains an infinite number of terms. The key ingredient to resolve this obstacle is the scale separation mentioned above: Being only interested in low-energy observables, one can assume that the terms in the Lagrangian are ordered by a

small parameter, which is the ratio of the energy scales involved.

The resulting theory for baryonbaryon interactions, which does not contain explicit pions but only contact interactions, is known as pionless EFT. The process of establishing the order of terms in the EFT is called power counting. For pionless EFT it is well known that the naive power counting, based on counting powers of momentum, fails due to the emergence of Efimov physics [29], and the three-body contact term is to be promoted to leading order [30]; see, however, [31].

The relevant Lagrangian at leading order is therefore,

$$\mathcal{L} = N^{\dagger} \left(i \partial_0 + \frac{\nabla^2}{2m} \right) N - \frac{C_0}{2} (N^{\dagger} N)^2 - \frac{C_1}{2} (N^{\dagger} \sigma N)^2 - \frac{D}{6} (N^{\dagger} N)^3$$
(2)

where N is the nuclaon field operator, and C_0 , C_1 and D are the low-energy constants (LECs). This lagrangian can be supplemented with terms containing more fields and/or more derivatives, which are subdominant. Since in this work we focus on the leading order, such terms will be neglected in the following.

Contact interactions are singular and therefore regularization is needed; here we use a Gaussian regulator $\tilde{g}(p) = \exp[-(p/\Lambda)^2]$ that suppresses momenta above an ultraviolet cutoff Λ . Since the cutoff is not a physical quantity, the theory observables must not be depend on it. This is achieved via renormalization, i.e. by fitting the values of the LECs $C_0 = C_0(\Lambda)$, $C_1 = C_1(\Lambda)$ and $D = D(\Lambda)$ such that chosen physical quantities are fixed at their observed values.

The leading order interaction in pionless EFT is to be iterated, which is equivalent to solving the nonrelativistic Schrödinger equation with the Hamiltonian

$$H = -\frac{1}{2m} \sum_{i} \nabla_{i}^{2} + \sum_{i < j} V_{2}(r_{ij}) + \sum_{i < j < k} V_{3}(r_{ij}, r_{jk}), (3)$$

where the two-body interaction is

$$V_2(r_{ij}) = (C_0 + C_1 \sigma_i \cdot \sigma_j) g_{\Lambda}(r_{ij}), \tag{4}$$

the three-body interaction is

$$V_3(r_{ij}, r_{jk}) = D \sum_{cyc} g_{\Lambda}(r_{ij}) g_{\Lambda}(r_{jk})$$
 (5)

where $g_{\Lambda}(r) = \frac{\Lambda^3}{8\pi^{3/2}} \exp(-\Lambda^2 r^2/4)$ and \sum_{cyc} stands for cyclic permutation of $\{i, j, k\}$.

Putting our system in a box with periodic boundary conditions, one has to solve

$$H\Psi_L = E_L \Psi_L \tag{6}$$

where the subscript L denotes that the wavefunction Ψ_L is to obey periodic boundary condition,

$$\Psi_L(\mathbf{r}_1, \mathbf{r}_2, \dots) = \Psi_L(\mathbf{r}_1 + \mathbf{n}_1 L, \mathbf{r}_2 + \mathbf{n}_2 L, \dots).$$
 (7)

for arbitrary integers trios $\{n_1, n_2, ...\}$. For finite volume the potential V transforms into a periodic potential

$$V_L(\mathbf{r}_1, \mathbf{r}_2, \ldots) = \sum_{\mathbf{n}_1, \mathbf{n}_2, \ldots} V(\mathbf{r}_1 + \mathbf{n}_1 L, \mathbf{r}_2 + \mathbf{n}_2 L, \ldots) .$$
 (8)

For example, the x-axis component of the two-body potential becomes

$$\exp[-\Lambda^2 x_{ij}^2/4] \longrightarrow \sum_{q} \exp[-\Lambda^2 (x_{ij} - qL)^2/4],$$

where in principle the sum over q runs over all integers from minus infinity to infinity. In practice, due to the short-range nature of the interaction, far boxes are negligible and the sum is limited to $-N_{\rm box} \leq q \leq N_{\rm box}$. We have verified that our results are fully converged for $N_{\rm box} = 5$

III. METHODS

To solve the N-body Schrödinger equation we first note that with the leading order interactions (4),(5) spin and isospin are good quantum number. Thus we can write the wave-function as a product of a spatial function time a spin state $\chi_{SS_z}(s_1, s_2, \dots)$ and an isospin state $\xi_{TT_z}(t_1, t_2, \dots)$ antisymmetrized to ensure Fermi statistics. To satisfy the periodic boundary conditions we follow Ref. [32] and expand the spatial part of the wavefunction using a correlated Gaussians basis. Using the abbreviations $\mathbf{r} = (\mathbf{r}_1, \mathbf{r}_2, \dots \mathbf{r}_A)$ for the A-body coordinates, and $\mathbf{x} = (x_1, \dots x_A)$ for the x component (same for y, z) these basis function are written as a product of periodic functions in the x, y, z directions

$$G_L(\mathbf{r}) = G_{Lx}(\mathbf{x})G_{Ly}(\mathbf{y})G_{Lz}(\mathbf{z}). \tag{9}$$

The x-component basis functions G_{Lx} (same for G_{Ly}, G_{Lz}) are defined by a symmetric positive definite $A \times A$ matrices A_x , a positive definite diagonal matrix B_x , and a shift vector $\mathbf{d} = (d_1, \dots d_N)$,

$$G_{Lx} = \sum_{\boldsymbol{n}_x} G(A_x, B_x, \boldsymbol{d}_x; \boldsymbol{x} - L\boldsymbol{n}_x)$$
 (10)

with

$$G = \exp\left[-\frac{1}{2}\boldsymbol{x}^T A_x \boldsymbol{x} - \frac{1}{2}(\boldsymbol{x} - \boldsymbol{d})^T B_x (\boldsymbol{x} - \boldsymbol{d})\right], \quad (11)$$

and $\mathbf{n}_x = (n_1, n_2, \dots n_N), n_i \in \mathbb{Z}.$

The desired solution for the Schrodinger equation

$$\Psi = \sum_{k} c_k \Phi(A_k, B_k, \boldsymbol{d}_k; \boldsymbol{r}, \mathbf{s}, \mathbf{t}), \tag{12}$$

is then expanded on the basis,

$$\Phi_k = \hat{\mathcal{A}} \left[G_L(A_k, B_k, \boldsymbol{d}_k; \boldsymbol{r}) \chi_{SS_z}(\boldsymbol{s}) \xi_{TT_z}(\boldsymbol{t}) \right], \quad (13)$$

where \hat{A} is the antisymmetrization operator, $s = (s_1, s_2, \dots s_A)$, and same for t. The linear parameters c_k are obtained solving the generalized eigenvalue problem $H\mathbf{c} = EN\mathbf{c}$, where $H_{ij} = \langle \Phi_i | H | \Phi_j \rangle$ are the Hamiltonian matrix elements, and $N_{ij} = \langle \Phi_i | H | \Phi_j \rangle$ the normalization matrix elements. One of the advantages of the Gaussian basis is that the matrix elements can be calculated analytically [32].

To optimize our basis we use the Stochastic Variational Method (SVM) [33]. To add a function to our basis, the elements of A_k , B_k , and d_k are chosen randomly one by one, and the values which give the lowest energy are taken.

IV. RESULTS

A. $m_{\pi} = 806 \text{ MeV}$

First, we would like to deal with the results of the NPLQCD collaboration [11]. These calculations assume SU(3) symmetry, where the mass of the u and d quarks were enlarged to the value of the s quark mass. The resulting pion mass was calculated to be $m_{\pi}=806$ MeV and the nucleon mass was m=1.634 GeV.

Calculations were done for three lattice sizes, $L\approx 3.4$ fm, 4.5 fm and 6.7 fm. The masses of light nuclei and hypernuclei with atomic number $A\leq 4$, and strangeness $|s|\leq 2$, were calculated. Here we focus on nuclei with $A\leq 3$.

Given a cutoff value, three data points are needed to calibrate the EFT. Here we choose to use the binding energies of the deuteron, di-neutron (which is found to be bound for such heavy pion) and triton.

To verify that our results are cutoff independent we perform calculations with different cutoff values (from $2 \, \mathrm{fm^{-1}}$ to $10 \, \mathrm{fm^{-1}}$). The results of the largest cutoff values, which are fully converged, are shown hereafter.

Tab. I summarizes the results from NPLQCD collaboration [11] for the finite-volume binding energies of two and three-nucleon systems calculated at pion mass of $m_{\pi}=806$ MeV. For each state three energies were calculated, corresponding to zero total momentum (n=0) as well as two lowest boosted states (n=1,2). For the largest lattice, we use all three states, while for the two smaller lattices the boosted states deviate from the ground state, and therefore we did not use them. We checked, however, that our results do not change substantially when all states are taken into account.

Solving the Schrödinger equation for each box size, we find the LECs that best fit the LQCD results of Tab. I employing least-squares fit. One can then predict the values for the continuum by solving the Schrödinger equation in the limit of $L\longrightarrow\infty$.

Two systems are bound in the two-body s=0 sector, namely the deuteron and the di-neutron. The di-neutron binding energy calculated from the EFT is shown in Fig. 1 as function of lattice size. NPLQCD results, which were

TABLE I. Light nuclei binding energies (in MeV) calculated in [11] using LQCD with $m_{\pi}=806$ MeV for different lattice size L (in fm).

system	L = 3.4	L = 4.5	L = 6.7
nn	17.8 ± 3.3	15.1 ± 2.8	15.9 ± 3.8
$^{2}\mathrm{H}$	25.4 ± 5.4	22.5 ± 3.5	19.5 ± 4.8
³ H	65.6 ± 6.8	63.2 ± 8.0	53.9 ± 10.7

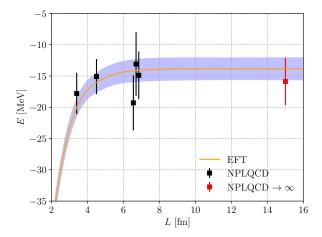


FIG. 1. The dineutron ground state energy as a function of the lattice size. EFT results (for $\Lambda=10~{\rm fm}^{-1}$) are shown in blue curve, and the NPLQCD results used for fitting are shown in black squares. The red square shows Ref. [11] estimate for infinte lattice.

used to fit our EFT, are also shown. The band stands for the error estimation of the EFT, where the main source of the error is the uncertainty and scatter of the LQCD results.

In Fig. 2 we show the deuteron binding energy calculated from the EFT, as well as the data points from LQCD used for fitting. Here also the main source of error (shown as a band) comes from the LQCD results.

Two bound states exist for nuclei in the three-body sector, namely ³H and ³He. Following the LQCD calculations, we eliminate charge-symmetry breaking terms as well as Coulomb forces and therefore their energies are degenerate. The triton ground state energy is shown in Fig. ³ as a function of the lattice size.

Due to the deeper binding of the triton, its wavefunction is more compact and therefore finite lattice corrections are less important here, as one can see comparing Fig. 3 to Figs. 1 and 2.

The extrapolated results are summarized in Tab. II and compared to the values of the largest lattice which were taken as the infinite lattice limit in Ref. [11]. From this comparison as well as from the Figs. it can be seen that our infinite volume results are consistent with

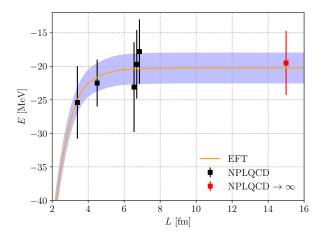


FIG. 2. The deuteron ground state energy as a function of the lattice size. EFT results (for $\Lambda=10~{\rm fm}^{-1}$) are shown in blue curve, and the NPLQCD results used for fitting are shown in black squares. The red square shows Ref. [11] estimate for infinte lattice.

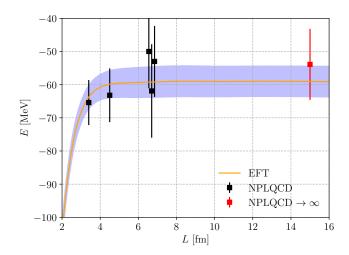


FIG. 3. The triton ground state energy as a function of the lattice size. EFT results (for $\Lambda=10~{\rm fm}^{-1}$) are shown in blue curve, and the NPLQCD results used for fitting are shown in black squares. The red square shows Ref. [11] estimate for infinte lattice.

NPLQCD [11], to within one standard deviation. The errors associated with our $L \to \infty$ extrapolations are smaller due to the use of more data points, associated with smaller error bars.

B. Physical pion mass

In the near future, one would hope to see LQCD calculation for the physical pion mass. Here we try to predict the lattice size corrections to the binding energies of light

TABLE II. Light nuclei binding energies (in MeV) from the largest lattice of Ref. [11] and extrapolated to to infinite lattice with out EFT.

system	Ref. [11]	This work
	. ,	
nn	15.9 ± 3.8	13.8 ± 1.8
$^{2}\mathrm{H}$	19.5 ± 4.8	20.2 ± 2.3
$^{3}\mathrm{H}$	53.9 ± 10.7	58.2 ± 4.7

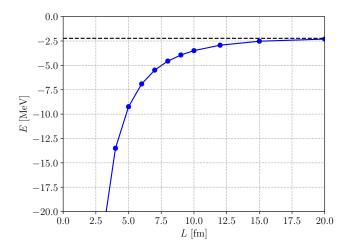


FIG. 4. The deuteron energy as a function of box-size for physical pion mass.

nuclei, which may be utilized to choose the appropriate lattice size for such calculations.

Three bound nuclei are known with $A \leq 3$, namely the deuteron, triton and ³He. Charge symmetry breaking is typically ignored in LQCD calculation, and we adopt this assumption here.

In Fig. 4 the results for the deuteron are shown. The deuteron binding is very shallow, resulting in a large spatial extent state. As a consequence, the deuteron binding energy is converged to its asymptotic value only for very large lattices, $L \gtrsim 20$ fm. This emphasizes the importance of an extrapolation technique to such calculations.

In Fig. 5 the triton binding energy is shown as a function of the lattice size. Here the results converge faster to the infinite volume limit, and asymptotic results are shown for $L \gtrsim 12$ fm.

V. CONCLUSION

The effect of the finite lattice size on the light nuclei binding energies is explored by the construction of pionless effective field theory. This theory, fitted to the LQCD results for small lattices, is then used to extrapolate to the infinite volume limit by solving the Schrödinger equation in a finite and infinite boxes.

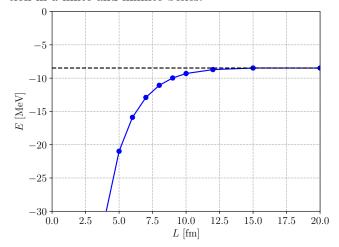


FIG. 5. The triton energy as a function of box-size for physical pion mass.

We study the results of NPLQCD collaboration for pion mass of 806 MeV and present values for the infinite lattice limit. Our extrapolated binding energies are similar to those extracted by the NPLQCD collaboration, albeit with smaller error bars reflecting the use of more data points with better accuracy.

With an eye on future calculations with physical pion mass, we predict the lattice size correction for light nuclei, showing that results are converging to the infinite lattice size limit only for $L\gtrsim 20$ fm for the deuteron and for $L\gtrsim 12$ fm for the triton. This emphasizes the importance of proper technique to extrapolate the results from small lattices.

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