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Two Nucleons on a Lattice

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Abstract

The two-nucleon sector is near an infrared fixed point of QCD and as a result the S-wave scattering lengths are unnaturally large compared to the effective ranges and shape parameters. It is usually assumed that a lattice QCD simulation of the two-nucleon sector will require a lattice that is much larger than the scattering lengths in order to extract quantitative information. In this paper we point out that this does not have to be the case: lattice QCD simulations on much smaller lattices will produce rigorous results for nuclear physics.

I. INTRODUCTION

One of the central goals of nuclear physics is to make rigorous predictions for both elastic and inelastic processes in multi-nucleon systems directly from QCD. The only presently-available technique to achieve this goal is lattice QCD, where space-time is discretized and QCD Green functions are evaluated in Euclidean space. Unfortunately, at present, the variety of processes that can be addressed with lattice QCD is quite limited. The currently-available computational power restricts not only the sizes of lattices that can be utilized, but also the lattice spacings and quark masses that can be simulated. Moreover, the Maiani-Testa theorem [1] precludes determination of scattering amplitudes away from kinematic thresholds from Euclidean-space Green functions at infinite volume. However, by generalizing a result from non-relativistic quantum mechanics [2] to quantum field theory, Lüscher [3, 4] realized that one can access $2 \rightarrow 2$ scattering amplitudes from lattice simulations performed at finite volume. Significant progress has been made using this finite-volume technique to determine the low-energy $\pi\pi$ phase shifts directly from QCD, e.g. Ref. [5]. However, only one lattice QCD calculation of the nucleon-nucleon (NN) scattering lengths [6] has been attempted, and it was a quenched simulation with heavy pions¹.

When contemplating computing nuclear observables with lattice QCD one naively assumes that the lattice must be much larger than the systems being simulated, so that the systems on the lattice resemble those at infinite-volume. This would mean, for instance, that when computing the rate for the simplest inelastic nuclear process, $np \rightarrow d\gamma$, which near threshold involves radiative capture from the 1S_0 channel, a lattice of size $L \gg |a^{(^1S_0)}|, |a^{(^3S_1)}|$ is required, where $a^{(^1S_0)}$ and $a^{(^3S_1)}$ are the 1S_0 and 3S_1 NN scattering lengths, respectively. Given that $a^{(^1S_0)} = -23.714$ fm, such a calculation would have to await a future in which computational power is sufficient to handle volumes of this size. Fortunately, as we will see, this argument is not correct.

There is a sizable separation of length scales in nuclear physics, due to the fact that nature has chosen to be very near an infrared fixed point of QCD [8, 9, 10]. As a result, the scattering lengths in both S -wave channels are unnaturally-large compared to all typical strong-interaction length scales, including the range of the nuclear potential which is determined by the pion Compton wavelength. Perhaps counter-intuitively, in simulating two-nucleon processes, the relevant lengths scales are those of the nuclear potential and *not* the scattering lengths, and thus as long as the lattice is large compared to the inverse of the pion mass one can in principle “simply” determine matrix elements and scattering parameters. Furthermore, quantitative information about the two-nucleon sector can be extracted from simulations on even smaller lattices. However, the theoretical analysis that would be required for such an extraction is significantly more complex, and in this work we restrict ourselves to lattices that are much larger than the pion Compton wavelength².

¹ For a recent review of hadron-hadron interactions on the lattice, see Ref. [7].

² There is a second technique that can be used to extract information about nuclear processes from small lattices. If simulations are performed on lattices with quark masses that are somewhat different from their physical values, the scattering lengths will, most likely, no longer be unnaturally large [11, 12, 13]. By using the pionful effective field theory to calculate the quark mass dependence of the scattering parameters, the results of such simulations can be related to those at the physical values of the quark masses. The expansion parameters in the pionful theory are not exceptionally small, and so higher order calculations will need to be performed in order to have reliable extrapolations. We do not explore this option in this

Perhaps the motivation for a lattice calculation of the radiative-capture process $np \rightarrow d\gamma$ is less than compelling as the cross-section and contributing multipoles at low-energies are well-measured. High-precision data recently collected [14] with HI γ S agrees well with calculations [15, 16] in the pionless effective field theory [17, 18], EFT($\not{\pi}$), and also with the best modern potential models (see Ref. [14]). However, weak processes such as $\nu d \rightarrow \nu np$, which play a central role in the determination of solar-neutrino fluxes from the sun, depend upon two-body weak currents [19, 20] that presently are determined with significant uncertainties from reactor experiments [21] and are also determined from the β -decay of tritium [22] with unknown systematic uncertainties. Recently they have been determined by the Sudbury Neutrino Observatory (SNO) from a fit to the neutrino fluxes [23], but again with large uncertainty. As we move into an era of high-precision neutrino astronomy, and considering the potential impact this will have on our understanding of particle physics, it is imperative that we have a precision determination of these weak currents. Lattice QCD may be the only rigorous method with which to determine these capture rates with high precision unless a precise experimental determination is made [24].

In this work we explore the scattering states and bound states of the two-nucleon sector at finite lattice volumes. We first develop the finite-volume effective field theory relevant to the very-low energy interactions of two-nucleons, and we recover the exact eigenvalue equation as well as several approximate formulas due to Lüscher [3, 4]. We find several new approximate formulas; we derive the leading finite-volume corrections to the bound-state energy and we find perturbative formulas for the lowest-lying energy levels for the case of a scattering length which is large compared to the lattice size. Armed with this technology, we consider simple unphysical limits of the scattering parameters to gain some intuition, and then explore the two-nucleon sector itself.

II. THE PIONLESS THEORY OF NN INTERACTIONS IN A BOX

An effective field theory (EFT) without pions, EFT($\not{\pi}$), has been developed [8, 9, 17, 18] to describe the very low-momentum interactions of two nucleons, with and without electroweak probes. EFT($\not{\pi}$) exploits the sizable hierarchy between the S -wave NN scattering lengths on the one hand, and the effective ranges, shape parameters and pion Compton wavelength on the other, and has been used successfully to perform relatively high-precision calculations, some at the $\sim 1\%$ level. Therefore, an EFT exists that can be used to rigorously determine the behavior of low-momentum nuclear observables in a finite volume, i.e. a lattice, and conversely can be used to extract infinite-volume limits of lattice simulations of two-nucleon observables. Furthermore, EFT($\not{\pi}$) has been used to successfully compute the properties of three-nucleon systems [25], and therefore calculations of three-nucleon systems at finite volume should be possible as well ³.

For NN scattering, the interaction between nucleons is described by a series of local operators with an increasing number of derivatives acting on the nucleon fields. The scattering amplitude can be computed in an elegant form using dimensional-regularization with power-divergence subtraction (PDS) [8, 9]. In this scheme, the coefficients of the operators

work.

³ As a point of interest, it has been conjectured recently in Ref. [26] that QCD is very near the critical trajectory for a renormalization-group limit cycle in the three-nucleon sector.

in the Lagrange density have natural size, even for unnaturally-large scattering lengths. The scattering amplitude is identical to that of effective-range theory, and that found by solving the Schrödinger equation with a pseudo-potential [18]. An important feature that distinguishes EFT($\not{\pi}$) from other constructions is that electroweak interactions can be included systematically, in the same way they are included in chiral perturbation theory (χ PT).

In EFT($\not{\pi}$) (describing non-relativistic baryons ⁴ each of mass M) the exact two-body elastic scattering amplitude in the continuum arises from the diagrams shown in Fig. 1, which can be resummed [8, 9] to give

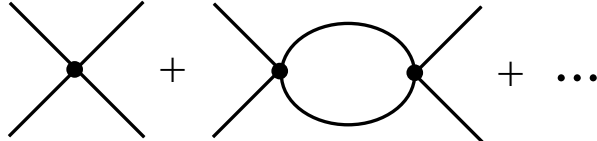


FIG. 1: *The diagrams in EFT($\not{\pi}$) which can be summed to give the scattering amplitude. The small solid circle denotes an insertion of the infinite tower of contact operators, $\sum C_{2n}(\mu) p^{2n}$.*

$$\mathcal{A} = \frac{\sum C_{2n}(\mu) p^{2n}}{1 - I_0 \sum C_{2n}(\mu) p^{2n}} \quad , \quad I_0 = \left(\frac{\mu}{2}\right)^{4-D} \int \frac{d^{D-1}\mathbf{q}}{(2\pi)^{D-1}} \frac{1}{E - \frac{|\mathbf{q}|^2}{M} + i\epsilon} \quad , \quad (1)$$

where the $C_{2n}(\mu)$ are the renormalization-scale dependent coefficients of operators with $2n$ derivatives acting on the nucleon fields (or equivalently with n time derivatives), μ is the dimensional-regularization scale, and D is the number of space-time dimensions. The loop integral I_0 is linearly divergent, and when defined with the PDS subtraction scheme [8, 9] becomes

$$I_0^{(PDS)} = -\frac{M}{4\pi} (\mu + ip) + \mathcal{O}(D - 4) \quad , \quad (2)$$

where $p = \sqrt{ME}$ is the momentum of each nucleon in the center-of-mass, and hence the scattering amplitude takes the usual form

$$\mathcal{A} = \frac{4\pi}{M} \frac{1}{p \cot \delta - ip} \quad . \quad (3)$$

This unitary expression describes NN scattering below the onset of the first inelastic threshold; that is, it is valid for $|\mathbf{p}| < \sqrt{m_\pi M}$, where m_π is the pion mass. The subtraction-scale dependence of the one-loop diagrams is exactly compensated by the corresponding dependence of the coefficients $C_{2n}(\mu)$. δ is the energy-dependent S -wave phase shift (we will only consider S -wave scattering but this construction generalizes to all partial waves). It is clear from eq. (1) that $p \cot \delta$ is an analytic function of p^2 for momenta less than the cut-off of EFT($\not{\pi}$), which is $\sim m_\pi/2$. We may therefore adopt the effective-range expansion,

$$p \cot \delta = -\frac{1}{a} + \frac{1}{2} r_0 p^2 \sum_{i=0}^{\infty} (r_i^2 p^2)^i \quad , \quad (4)$$

⁴ Relativistic corrections can be included in perturbation theory [17]

where a is the scattering length, r_0 is the effective range, and the other r_i correspond to higher-order shape parameters⁵.

We are interested in the energy-eigenvalues of the NN system placed in a box with sides of length L with periodic boundary conditions. The scattering-state and bound-state energy-eigenvalues can be found by requiring the real part of the inverse scattering amplitude computed in the box to vanish,

$$\frac{1}{\sum C_{2n}(\mu) p^{2n}} - \text{Re}(I_0^{(PDS)}(L)) = 0 \quad , \quad (5)$$

where the infinite-volume integral in eq. (1) is replaced by a discrete sum over the momentum states allowed on the lattice,

$$I_0(L) = \frac{1}{L^3} \sum_{\mathbf{k}} \frac{1}{E - \frac{|\mathbf{k}|^2}{M}} \quad . \quad (6)$$

This discrete sum is also linearly divergent as the ultra-violet behavior of the theory is unchanged, and its value in the PDS scheme is found by adding and subtracting the corresponding infinite-volume integrals evaluated at $E = 0$. One of the infinite-volume integrals is evaluated with a momentum cut-off, $|\mathbf{k}| \leq \Lambda$, that is equal to the mode cut-off introduced to regulate the discrete sum, while the other is evaluated with dimensional-regularization and PDS, to give

$$I_0^{(PDS)}(L) = -\frac{M}{4\pi}\mu + \frac{1}{L^3} \sum_{\mathbf{k}}^{\Lambda} \frac{1}{E - \frac{|\mathbf{k}|^2}{M}} + M \int^{\Lambda} \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{1}{|\mathbf{k}|^2} \quad , \quad (7)$$

and the limit $\Lambda \rightarrow \infty$ is taken, assuming that the lattice spacing vanishes. For any realistic simulation there will be an upper bound on Λ , given by the edge of the first Brillouin zone [27].

A. The Eigenvalue Equation

The energies of the low-lying energy levels of two-nucleons in a box with sides of length L with periodic boundary conditions [3, 4, 28, 29] and with their center-of-mass at rest can now be determined in terms of $p \cot \delta$, from eq. (5) and eq. (7). Values of p^2 that solve⁶

$$p \cot \delta(p) = \frac{1}{\pi L} \mathbf{S} \left(\left(\frac{Lp}{2\pi} \right)^2 \right) \quad , \quad (8)$$

⁵ We use the sign convention for the scattering length that is traditionally used in nuclear physics. This is opposite to the sign convention used by Lüscher [3, 4]

⁶ Lüscher writes this expression as [3, 4]

$$e^{2i\delta_0(k)} = \frac{\mathcal{Z}_{00}(1; q^2) + i\pi^{3/2}q}{\mathcal{Z}_{00}(1; q^2) - i\pi^{3/2}q}$$

where $q = pL/(2\pi)$. The three-dimensional zeta-functions are

$$\mathcal{Z}_{00}(s; q^2) = \frac{1}{\sqrt{4\pi}} \sum_{\mathbf{n}} (\mathbf{n}^2 - q^2)^{-s}$$

where the formally divergent functions are defined via analytic continuation.

with

$$\mathbf{S}(\eta) \equiv \sum_{\mathbf{j}}^{\Lambda_j} \frac{1}{|\mathbf{j}|^2 - \eta} - 4\pi\Lambda_j \quad , \quad (9)$$

give the location of all of the energy-eigenstates in the box, including the bound states (with $p^2 < 0$). The sum is over all three-vectors of integers \mathbf{j} such that $|\mathbf{j}| < \Lambda_j$ and where the limit $\Lambda_j \rightarrow \infty$ is implicit (corresponding to the $\Lambda \rightarrow \infty$ limit in eq. (7)). In Fig. 2 we plot $\mathbf{S}(\eta)$ vs. η from eq. (9). While our derivation of eq. (8) is valid within the radius of convergence of EFT($\not{\pi}$), that is for $|\mathbf{p}| < m_\pi/2$, we expect that eq. (8) remains valid as long as the energy of the two-nucleon states are below the pion-production threshold, $|\mathbf{p}| < \sqrt{m_\pi M}$ [4].

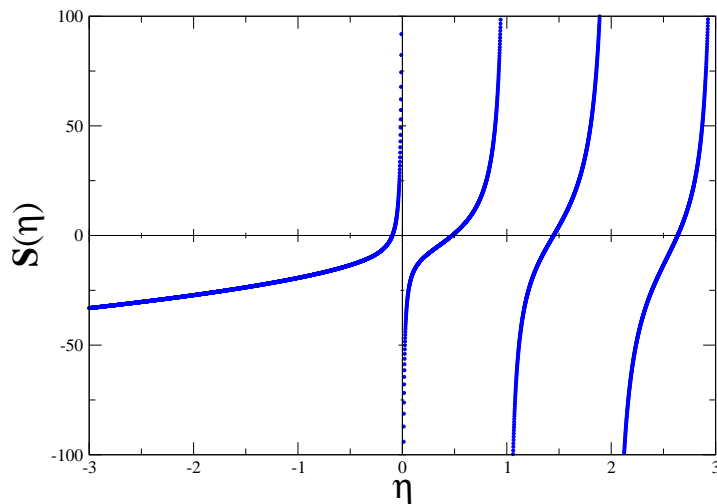


FIG. 2: A plot of $\mathbf{S}(\eta)$ vs. η from eq. (9). The function has poles for $\eta \geq 0$ and does not have poles for $\eta < 0$.

B. Approximate Formulas

There are two extreme limits that can be considered for the solution of eq. (8). First, there is the limit that Lüscher considers in his work in which $L \gg |a|$. In this limit the solution of eq. (8) smoothly approaches the infinite-volume limit. The energy of the two lowest-lying continuum states in the A_1 representation of the cubic group [30] are

$$E_0 = +\frac{4\pi a}{ML^3} \left[1 - c_1 \frac{a}{L} + c_2 \left(\frac{a}{L} \right)^2 + \dots \right] + \mathcal{O}(L^{-6}) \quad , \quad (10)$$

where the coefficients are $c_1 = -2.837297$, $c_2 = +6.375183$, and

$$E_1 = \frac{4\pi^2}{ML^2} - \frac{12 \tan \delta_0}{ML^2} \left[1 + c'_1 \tan \delta_0 + c'_2 \tan^2 \delta_0 + \dots \right] + \mathcal{O}(L^{-6}) \quad , \quad (11)$$

where $c'_1 = -0.061367$, $c'_2 = -0.354156$. In addition, in the limit $L \gg a$, we have solved eq. (8) for the location of the bound state that exists for $a > 0$ with an attractive interaction ⁷

$$E_{-1} = -\frac{\gamma^2}{M} \left[1 + \frac{12}{\gamma L} \frac{1}{1 - 2\gamma(p \cot \delta)'} e^{-\gamma L} + \dots \right] , \quad (13)$$

where $(p \cot \delta)' = \frac{d}{dp^2} p \cot \delta$ evaluated at $p^2 = -\gamma^2$. The quantity γ is the solution of

$$\gamma + p \cot \delta|_{p^2=-\gamma^2} = 0 , \quad (14)$$

which yields the bound-state binding energy in the infinite-volume limit.

In the limit where $L \ll |(p \cot \delta)^{-1}|$ (which is a useful limit to consider when systems have unnaturally-large scattering lengths), the solution of eq. (8) gives the energy of the lowest-lying state to be

$$\tilde{E}_0 = \frac{4\pi^2}{ML^2} [d_1 + d_2 L p \cot \delta_0 + \dots] , \quad (15)$$

where the coefficients are $d_1 = -0.095901$, $d_2 = +0.0253716$ and where $p \cot \delta_0$ is evaluated at an energy $E = \frac{4\pi^2}{ML^2} d_1$. The energy of the next level is

$$\tilde{E}_1 = \frac{4\pi^2}{ML^2} [d'_1 + d'_2 L p \cot \delta_0 + \dots] , \quad (16)$$

where $d'_1 = +0.472895$, $d'_2 = +0.0790234$ and where $p \cot \delta_0$ is evaluated at an energy $E = \frac{4\pi^2}{ML^2} d'_1$. The values of the $d_i^{(\prime)}$ are determined by zeroes of the three-dimensional zeta-functions, and the expressions for E_i and \tilde{E}_i , excluding E_{-1} , are valid for both-sign scattering lengths.

C. A Toy Model : $a = \pm 1$ and $r_i = 0$

Let us consider an unphysical limit of NN scattering in which the NN potential has zero-range but a scattering length of $|a| = \pm 1$ in the infinite-volume limit. Therefore, the scattering amplitude is $p \cot \delta = -1/a$, as the effective range and all shape parameters vanish, $r_i = 0$.

The system with $a = -1$ must result from an attractive interaction, but one not attractive enough to yield a bound state. One might imagine that the potential is extremely attractive and that the state with $a = -1$ is the one near threshold with many other deep states present. However, the deep states will be at the cut-off of the theory, set by the range of the potential, and in the limit we are considering these are infinitely deep. The system with $a = +1$ could result from a repulsive interaction in which case there will be no bound state in this channel. However, $a = +1$ could also result from an attractive interaction that is attractive enough to give rise to a bound state near threshold. In the infinite-volume limit of

⁷ The extension of the Chowla-Selberg formula to higher dimensions [31] gives

$$\mathbf{S}(-x^2) \rightarrow -2\pi^2 x + 6\pi e^{-2\pi x} + \dots , \quad (12)$$

for large x , where the ellipses denote terms exponentially suppressed by factors of $e^{-4\pi x}$, or more.

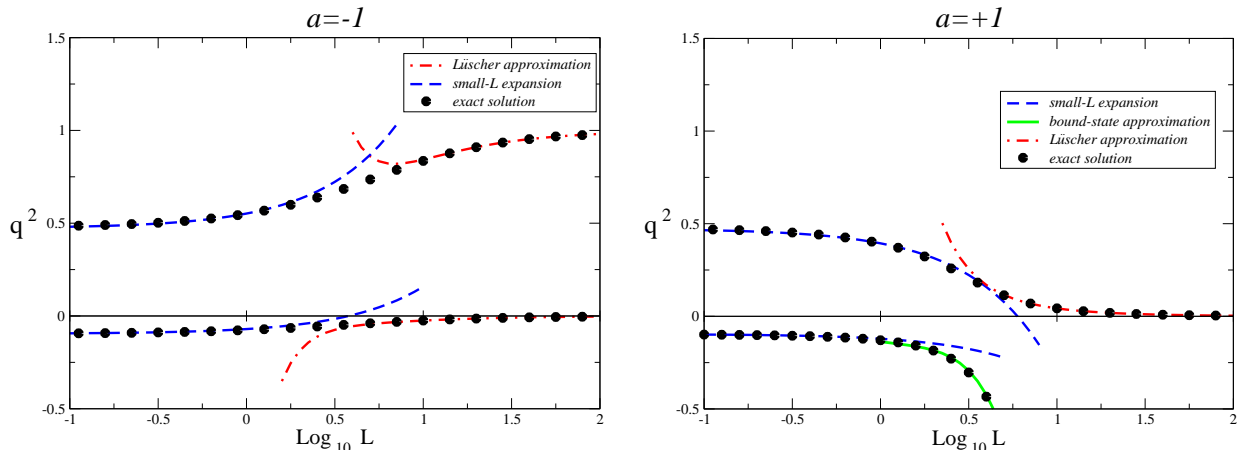


FIG. 3: The two lowest-lying solutions to eq. (8) for $a = \pm 1$ fm and $r_i = 0$. The vertical axis is q^2 , which is related to the energy by $E = q^2 \frac{4\pi^2}{ML^2}$, while the horizontal axis is $\log_{10} L$. The left panel corresponds to $a = -1$ which can only arise from an attractive potential. The right panel corresponds to $a = +1$ which can arise from both an attractive and a repulsive potential. For a repulsive potential the lower solution is absent. The solid circles correspond to exact numerical solutions of eq. (8). The curves that match the exact solution at small L result from eq. (15) and eq. (16), while the curves that match the exact solution at large L result from eq. (10), eq. (11), and eq. (13).

this second scenario, one must recover the continuum of scattering states at positive energy and also the bound state.

As $L \rightarrow 0$ the scattering lengths of opposite signs can be identified with each other (as this is equivalent to taking the $|a| \rightarrow \infty$ limit of the model) and so the levels become degenerate. One is tempted to think that the levels that are degenerate in the $L \rightarrow 0$ limit are the same as those that are degenerate in the $L \rightarrow \infty$ limit. However, this cannot be the case as the lowest state at $L = 0$ in the system with $a = +1$ smoothly becomes the bound state at $L = \infty$ (as a function of L) and a bound state does not exist in the $a = -1$ system. This can be seen clearly in Fig. 3.

It is apparent in both the $L \gg |a|$ and $L \ll |a|$ limits that the parameter arising in the asymptotic expansion of the energies of the levels is $\sim 3|a|/L$. This can be seen clearly in Fig. 3 where Lüscher's expressions in a/L break down at $L \sim 3$ fm while the expressions in eq. (15) and eq. (16), which are an expansion in L/a , remain close to the exact solution out to $L \sim 3$ fm.

D. Low-energy NN Scattering in the S-wave

It is well known that the scattering lengths and effective ranges alone are sufficient to describe low-energy NN scattering data to quite high precision. This results in part from the fact that the shape-parameters are much smaller than one would naively guess. We therefore truncate the effective-range expansion in our numerical analysis, and the power-counting of EFT(π) dictates how the shape-parameters can be included in perturbation theory. At this

order, the energy-levels of two-nucleons in the 1S_0 channel whose center-of-mass is at rest in a periodic box of size L are found by solving

$$\frac{1}{a^{(1S_0)}} - \frac{1}{2}r^{(1S_0)} p^2 + \frac{1}{\pi L} \mathbf{S} \left(\left(\frac{Lp}{2\pi} \right)^2 \right) = 0 \quad , \quad (17)$$

for p^2 , which is related to the energy of the NN system via $E = p^2/M$. In the 1S_0 channel the scattering length and effective range are

$$a^{(1S_0)} = -23.714 \text{ fm} \quad , \quad r^{(1S_0)} = 2.734 \text{ fm} \quad . \quad (18)$$

Despite the fact that the NN interaction is attractive in this channel at long- and interme-

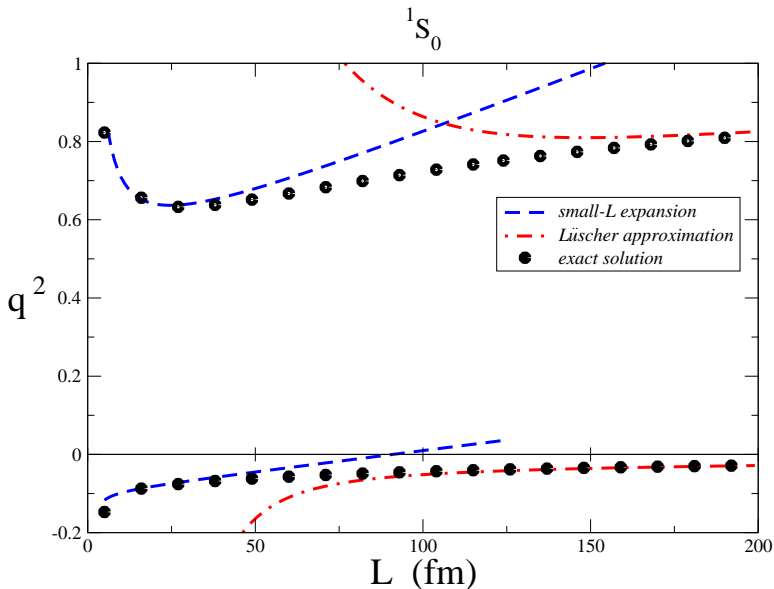


FIG. 4: *The two lowest-lying energy-eigenstates of two nucleons in the 1S_0 channel on a lattice of size L . The vertical axis is q^2 , where $E = q^2 \frac{4\pi^2}{ML^2}$, while the horizontal axis is the lattice size L . The solid circles correspond to the exact solution of eq. (17). The curves that are asymptotic to the exact solution at large L correspond to Lüscher's relations in eq. (10), eq. (11), while the curves that are asymptotic to the exact solution at smaller values of L correspond to the expressions in eq. (15) and eq. (16).*

diate distances, there are no bound states of pp , np nor nn in the 1S_0 channel at the physical values of the quark masses or Λ_{QCD} ⁸.

One can see from Fig. 4 that Lüscher's power-series expansion of the energy-levels converges slowly in the 1S_0 channel. For the ground state one needs a box of size

⁸ One finds that in all likelihood there is no bound state in this channel for quark masses smaller than their physical values but it is possible that bound states exists for quark masses somewhat larger than their physical values [11, 12, 13]. This is an exciting possibility that can be explored with lattice QCD.

$L \gtrsim 80 \text{ fm} \sim 3a^{(1S_0)}$ while for the first excited state one needs a box of size $L \gtrsim 150 \text{ fm}$ before these perturbative expansions converge to the exact result. Therefore, these asymptotic expressions will not be of great utility to nuclear physicists in the near future. By contrast, the expressions we have derived in the $L \rightarrow 0$ limit, eq. (15) and eq. (16), are applicable for boxes smaller than $L \lesssim 50 \text{ fm}$. However, the crucial assumption, $L \gg r_i$, begins to break down for volumes with $L \lesssim 5 \text{ fm}$. In table I we show the momenta of the first two states in the $1S_0$ channel. The lowest-level can be described by EFT($\not{\pi}$) on a lattice with $L \sim 10 \text{ fm}$ but a lattice with $L \gtrsim 15 \text{ fm}$ is required in order for EFT($\not{\pi}$) to describe the second state. This is not to say that we cannot use the location of all the states on a lattice with $L \sim 10 \text{ fm}$; for momenta outside the range of validity of EFT($\not{\pi}$) and below pion-production threshold, i.e. for $m_\pi/2 < |\mathbf{p}| < \sqrt{m_\pi M}$, lattice results will have to be matched directly to $p \cot \delta$ in the $1S_0$ channel as there is no effective-range expansion.

TABLE I: Momenta of the lowest-lying levels of two-nucleons on the lattice. An asterisk denotes momenta outside the range of validity of the effective-range expansion, $|\mathbf{p}|^{\text{max.}} = m_\pi/2 \sim 70 \text{ MeV}$. The energy of the state is $E = |\mathbf{p}|^2/M$, and the appearance of an “i” indicates a $-ve$ energy.

	$1S_0$ $ \mathbf{p} $ (MeV)		$3S_1$ $ \mathbf{p} $ (MeV)	
Lattice Size L (fm)	1st	2nd	Deuteron	1st
1000	0.1 i	1.21	45.5 i	0.052
100	2.6 i	10.52	45.5 i	1.76
25	13.8 i	39.3	45.8 i	18.25
15	24.6 i	67.0	49.9 i	44.61
10	39.0 i	104.3 (*)	61.3 i	83.1 (*)
5	94.4 i (*)	224.7 (*)	116.5 i (*)	206.5 (*)

The $3S_1 - 3D_1$ channel is somewhat complicated by the fact that the tensor interaction gives rise to mixing between the $3S_1$ and the $3D_1$ channels. On the lattice this means that different representations of the cubic group will mix due to the tensor component of the NN interaction. In particular, the A_1 representation will mix with the E and T_2 representations [30]. However, the power-counting of EFT($\not{\pi}$) dictates that we can ignore contributions from this mixing and the $3D_1$ channel at the order to which we are working [17]. Therefore, at this order, the energy levels of two nucleons in the $3S_1$ channel can be found by solving

$$\frac{1}{a^{(3S_1)}} - \frac{1}{2}r^{(3S_1)} p^2 + \frac{1}{\pi L} \mathbf{S} \left(\left(\frac{Lp}{2\pi} \right)^2 \right) = 0 \quad . \quad (19)$$

In the $3S_1$ channel the effective-range parameters are

$$a^{(3S_1)} = +5.425 \text{ fm} \quad , \quad r^{(3S_1)} = 1.75 \text{ fm} \quad . \quad (20)$$

One can see from Fig. 5 that Lüscher’s power-series expansion of the energy-levels converges to the exact solution for the lowest-lying continuum state when $L \gtrsim 15 \text{ fm} \sim 3a^{(3S_1)}$. However, our expression for the deuteron binding energy at finite-volume appears to work even at significantly smaller volumes. Unfortunately, the expressions that we have derived for small volumes do not converge well to the exact solution in this channel. This is because the scattering length is only a factor of ~ 3 larger than the effective range and thus

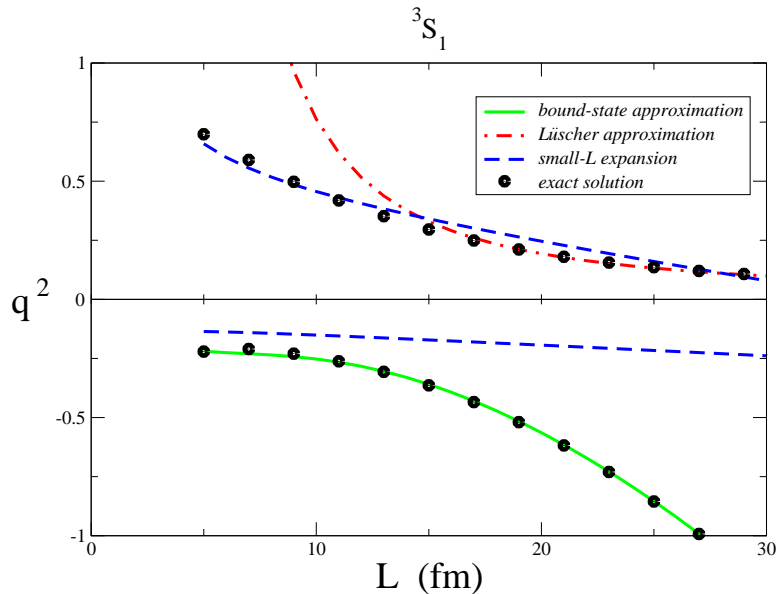


FIG. 5: The two lowest-lying energy-eigenstates of two nucleons in the 3S_1 channel on a lattice of size L . The vertical axis is q^2 , where $E = q^2 \frac{4\pi^2}{ML^2}$, while the horizontal axis is L . The solid circles correspond to exact solutions of eq. (19). The curves that are asymptotic to the exact solution at large L correspond to Lüscher's relation in eq. (10) and the relation for the bound-state energy, eq. (13), while the curves that are asymptotic to the exact solution at small L correspond to the expressions in eq. (15) and eq. (16).

the expansion parameter $Lp \cot \delta$ is not small enough over the entire range of L . Perhaps higher-order contributions will improve the agreement. The deuteron state can be described with EFT($\not{\pi}$) for lattices with $L \gtrsim 10$ fm, but the lowest-lying continuum state can be described by EFT($\not{\pi}$) only for $L \gtrsim 15$ fm. In table I we show the momenta of the deuteron bound state and the lowest-lying scattering state in the 3S_1 channel.

Beyond the range of validity of EFT($\not{\pi}$), the 3S_1 channel is significantly different than the 1S_0 channel. As mentioned above, in EFT($\not{\pi}$) ${}^3S_1 - {}^3D_1$ mixing is subleading in the expansion. However in the pionful theory, i.e. for $m_\pi/2 < |\mathbf{p}| < \sqrt{m_\pi M}$, ${}^3S_1 - {}^3D_1$ mixing appears at leading order in the EFT expansion [32]. Therefore, in this range of energies eq. (19) is *not* valid and one must solve a coupled system of integral equations.

III. CONCLUSIONS

Lattice QCD calculations of the scattering lengths and effective ranges in the two-nucleon sector would be a significant milestone toward rigorous calculations of nuclear properties and decays. Aside from providing essential information about the quark-mass dependence of nuclear physics, such calculations by themselves will not significantly improve our ability to compute nuclear properties, as the scattering amplitudes are already well-known experimentally. However, we would be in a position to compute electroweak matrix elements between two-nucleon states, and thereby provide information that will be vital to future

calculations of electroweak processes involving nuclei. Knowledge of these processes will directly affect analysis of data from present and future neutrino observatories.

Exact solutions to Lüscher's general formula for the energy-levels of the two-nucleon system on a lattice with periodic boundary conditions will allow for the extraction of scattering parameters from simulations with lattice volumes that are much smaller than naively estimated. It would appear that simulations on lattices with $L \gtrsim 15$ fm will make it possible to extract both the scattering lengths and effective ranges in the two-nucleon sector in a straightforward way. This is contrary to the expectation that lattices with $L \gg |a|$ are required to determine the scattering parameters. The extraction of useful information from simulations with lattices $L \lesssim 10$ fm will require direct matching to $p \cot \delta$ in the spin singlet channel, as the pionless theory and thus the effective-range expansion, will no longer be appropriate. In the spin-triplet channel there remains the additional challenge of formulating the finite-volume eigenvalue equations which account for mixing between S - and D -waves. These finite-volume calculations are a vital component of the technology required to make rigorous statements about nuclear processes directly from QCD.

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