Multi-Pion Systems in Lattice QCD and the Three-Pion Interaction

Silas R. Beane,1 William Detmold,2 Thomas C. Liu,3 Kostas Orginos,4,5 Assumpta Parreño,6 Martin J. Savage,2 and Aaron Torok1
(NPLQCD Collaboration)

1 Department of Physics, University of New Hampshire, Durham, NH 03824-3568, USA
2 Department of Physics, University of Washington, Box 351560, Seattle, WA 98195, USA
3 N Division, Lawrence Livermore National Laboratory, Livermore, CA 94551, USA.
4 Department of Physics, College of William and Mary, Williamsburg, VA 23187-8795, USA
5 Jefferson Laboratory, 12000 Jefferson Avenue, Newport News, VA 23606, USA.
6 Departament d’Estructura i Constituents de la Matè ria and Institut de Ciències del Cosmos, Universitat de Barcelona, E–08028 Barcelona, Spain.

(Dated: October 3, 2007)

The ground-state energies of 2, 3, 4 and 5 \( \pi^+ \)’s in a spatial-volume \( V \sim (2.5 \text{ fm})^3 \) are computed with lattice QCD. By eliminating the leading contribution from three-\( \pi^+ \) interactions, particular combinations of these \( n-\pi^+ \) ground-state energies provide precise extractions of the \( \pi^+ \pi^+ \) scattering length that are in agreement with that obtained from calculations involving only two \( \pi^+ \)'s. The three-\( \pi^+ \) interaction can be isolated by forming other combinations of the \( n-\pi^+ \) ground-state energies, and we find a result that is consistent with a repulsive three-\( \pi^+ \) interaction for \( m_\pi \lesssim 350 \text{ MeV} \).

A major goal of strong-interaction physics is to determine the spectrum and interactions of hadrons and nuclei from Quantum Chromodynamics (QCD). Lattice QCD is the only known way to rigorously compute strong-interaction quantities, and an increasing effort is being put into understanding the lattice QCD calculations that will be required to extract even the most basic properties of light nuclei. It is clear that at some level, the interactions among three or more hadrons play a significant role in nuclei, and an important goal for lattice practitioners is to determine the parameters of such interactions. We report on the first lattice QCD calculation of systems comprised of more than two hadrons.

The simplest multi-hadron systems (both conceptually, and from a numerical perspective) consist of \( n \) pseudoscalar mesons of maximal isospin. Interactions between multiple pions are important to explore for phenomenological reasons. Three pion interferometry is currently a topic of interest in heavy-ion collisions [1]) and, further, such interactions impact the formation of a pion condensate which is energetically favored in systems with large isospin chemical potential, and will impact the properties of (hot) pion gases. In this work we perform lattice QCD calculations of the ground-state energies of \( \pi^+\pi^+, \pi^+\pi^+\pi^+, \pi^+\pi^+\pi^+\pi^+, \pi^+\pi^+\pi^+\pi^+\pi^+\pi^+\pi^+\pi^+ \) in a spatial volume of \( V \sim (2.5 \text{ fm})^3 \) with periodic boundary conditions and a lattice spacing of \( b \sim 0.125 \text{ fm} \). These systems serve as an ideal laboratory for investigating multi-particle interactions as chiral symmetry guarantees relatively weak interactions among pions, and multiple pion correlation functions computed with lattice QCD do not suffer from signal to noise issues that are expected to plague analogous calculations in multi-baryon systems.

A result that is consistent with a repulsive three-pion interaction of magnitude expected from naive dimensional analysis (NDA) is found for \( m_\pi \lesssim 350 \text{ MeV} \). The \( \pi^+\pi^+ \) scattering length is extracted from the \( n > 2 \) pion systems with precision that is comparable to (and in some cases better than) the \( n = 2 \) determination [10].

Recently, the volume dependence of the energy of the \( n \)-boson (of mass \( M \)) ground state in a periodic cubic spatial volume of periodicity \( L \) has been computed [2] (see also [3–8]). The finite-volume shift to the ground-state energy is

\[
\Delta E_n = \frac{4\pi a}{ML^3} \left( \frac{n}{2} \right) \left[ 1 - \frac{aI}{\pi L} + \left( \frac{a}{\pi L} \right)^2 \left[ I^2 + (2n-5)J \right] - \left( \frac{a}{\pi L} \right)^3 \left[ I^3 + (2n-7)IJ + (5n^2 - 41n + 63)K \right] \right] + \left( \frac{n}{2} \right) \frac{8\pi^2a^3r}{ML^6} + \left( \frac{n}{3} \right) \frac{\eta_3^L}{L^6} + O(1/L^7),
\]

where \( a \) and \( r \) are the two-boson scattering length and effective range parameters, respectively and \( \eta_3^L \) is the renormalization-group invariant (RGI) three-boson interaction (\( \eta_3^R \) is renormalization scheme and scale independent, but depends logarithmically on \( L \); in terms of the three particle interaction defined in Ref [2], \( \eta_3^R = \eta_3(\mu) + \frac{64\pi^2a^5}{M}(3\sqrt{3} - 4\pi) log(\mu L) - \frac{96\pi^4}{\pi^2M} \langle 2Q + R \rangle \)). The geometric constants appearing in Eq. (1) are \( I = -8.9136329, J = 16.532316 \) and \( K = 8.4019240 \). At this order the energy is only sensitive to a combination of the effective range and scattering length, \( a = a + \frac{24\pi^2}{\pi^2}r \) and in what follows we replace \( a \rightarrow \bar{a} \), eliminating \( r \). The above expansion is valid provided \( a, r \ll L \) with an additional
constraint on $n$.

Two combinations of energies are particularly useful in what follows. The first combination

$$L^3 M (\Delta E_n, m^2 - 3m + 2) - \Delta E_n n (n^2 - 3n + 2) \over 2 (m - 1)m (m - n)(n - 1) \pi n$$

$$= \pi \left\{ 1 - {\pi \over \pi L} + \left[ {\pi \over \pi L} \right]^2 \left[ I^2 - J \right] \right\}$$

$$\times \left[ -I^3 + 3IJ + (19 + 5m n - 10(n + m)) K \right] \right\}, \quad (2)$$

(for $n, m > 2$) is independent of $\pi^L$ and allows a determination of $\pi$ up to $O(1/L^3)$ corrections (combinations achieving the same result using all of the $n = 3, 4, 5$ energies can also be constructed). Second, the three body parameter can be determined from

$$\pi^L = L^6 \left( \frac{n}{3} \right)^{-1} \left\{ \Delta E_n - \frac{n}{2} \Delta E_2 - 6 \left( \frac{n}{3} \right) M^2 \Delta E_2^3 \right\}$$

$$\times \left( \frac{L}{2\pi} \right)^4 \left[ J + \frac{L^2 M \Delta E_2}{2\pi^2} \left( I J - \frac{1}{5n} - \frac{31}{5n} \right) K \right] \right\}, \quad (3)$$

($n > 2$) with corrections arising at $O(1/L)$. Additionally, the dimensionless combination

$$1 - {2 \Delta E_3 \over 3 \Delta E_2 + 1 \Delta E_4 \over 6 \Delta E_2 + 5M^3 L^6 K \over 32\pi^6} \Delta E_2^3 \sim O(1/L^7), \quad (4)$$

provides a useful check of the convergence of the expansion. Combinations involving $\Delta E_{2,3,5}$ and $\Delta E_{2,4,5}$ can also be constructed that also vanish at this order.

The requisite ground-state energies are extracted from the $n-\pi^+$ correlation functions defined by

$$C_n(t) = \left\langle 0 \left| \sum \chi_{n+}(x, t) \chi_{n+}^\dagger (0, 0) \right|^n \right\rangle,$$  \quad (5)

where $\chi_{n+}(x) = u^a(x) \gamma_0 \bar{a}_n(x)$ is an interpolating operator for the $\pi^+$ ($a$ is a color index). The sums in Eq. (5) project the correlation functions onto the $A_1$ representation of the cubic symmetry group (in the continuum this corresponds to angular momentum $\ell = 0, 4, \ldots$). As $n$ increases, the number of Wick contractions involved in computing $C_n(t)$ increases as $n^2$. In the limit of isospin symmetry, the correlation functions in Eq. (5) with $n < 13$ require the computation of only a single quark propagator, $S(x; t)$ (for $n > 12$ additional propagators are required to circumvent the Pauli exclusion). As an example, the $n = 3$ correlator can be expressed as

$$C_3(t) = \text{tr} \left[ \Pi \right]^3 - 3 \text{tr} \left[ \Pi \right] \text{tr} \left[ \Pi^2 \right] + 2 \text{tr} \left[ \Pi^3 \right], \quad (6)$$

where $\Pi = \sum_y \gamma_5 S(x; t) 0 \gamma_0 S^\dagger (x, t; 0)$ and the trace is over Dirac and color indices.

In this work we have computed the $C_{1,2,3,4,5}(t)$ in mixed-action lattice QCD, using domain-wall valence quark propagators from a Gaussian smeared-source on the rooted-staggered coarse MILC gauge-configurations ($20^3 \times 64$) after HYP-smearing and chopping (see Refs. [9, 10] for details). These are computed at pion masses of $m_\pi \sim 290, 350, 490, 590$ MeV. Details of the propagators used in the correlation functions are given in Table I and can be found in Ref. [10].

| $m_\pi$ (MeV) | $N_{cfg}$ | $N_{src}$ | $m_\pi/f_n$ |
|-----------------|-----------|-----------|------------|
| 291.3(1.0)(1.0) | 468       | 16        | 1.990(11)(14) |
| 351.9(0.5)(0.2) | 769       | 20        | 2.323(57)(30)  |
| 491.4(0.4)(0.3) | 486       | 24        | 3.0585(49)(95) |
| 590.5(0.8)(0.2) | 564       | 8         | 3.4758(98)(60)  |

TABLE I: Parameters of the domain-wall propagators used herein. A lattice spacing of $b = 0.125$ fm has been used to convert from lattice to physical units. The number of gauge configurations is $N_{cfg}$, and the number of sources per configuration is $N_{src}$. For further details see Ref. [10].

The energies of $n$ pion states are dominated by the $n$ single pion energies, with the interactions contributing a small fraction of the total energy. To extract the resulting energy shifts, $\Delta E_n$, the ratios of correlators

$$G_n(t) = \left( C_n(t) \right)^{\pi^+ \to \infty} \left( C_1(t) \right)^{\pi^+ \to \infty} \left( A e^{\Delta E_n t} \right), \quad (7)$$

are formed, where the second relation holds in the limit of infinite temporal extent and infinite number of gauge-configurations. Inclusion of effects of temporal boundaries is complicated for multi-hadron systems, and our analysis is restricted to regions where an effective mass plot clearly shows the ground state is dominant.

For the quantities discussed below, fits are performed using both jackknife and bootstrap analyses of the effective masses ($e.g.$, $\log \left( G_n(t) / G_n(t - 1) \right)$) for each energy or combination thereof. A systematic uncertainty is determined by a comparison of the various fit procedures and fitting ranges. To avoid uncertainties arising from scale setting, we focus on the dimensionless quantities $m_{\pi} \pi_{\pi^+} + \pi_{\pi^+}$ and $m_{\pi} f_{\pi}^4 \pi_{\pi^+}$ ($\pi_{\pi^+}$ is expected to scale as $m_{\pi}^{-1} f_{\pi}^{-3}$ by NDA).

The $\pi^+ \pi^+$ scattering length (more precisely, the combination $\pi_{\pi^+ \pi^+}$) has been studied repeatedly in lattice QCD using the finite volume formalism of L"uscher [6] (for $a/L \ll 1$ a perturbative expansion gives the $n = 2$ case of Eq. (1)). In particular, a precise extraction of this scattering length has been performed using the same propagators as used in this work [10]. Therefore, the utility of multi-pion energies in extracting the scattering length can be ascertained, as summarized in Figs. 1, 2 and 3.

In Fig. 1, the energy shifts for $n = 2, 3, 4,$ and 5 are displayed for the highest precision calculation, $m_\pi \sim 350$ MeV. Clear plateaus are visible for each $n$; indeed,
the relative uncertainty decreases significantly with increasing $n$ in the range explored; this is particularly clear for the calculation with $m_\pi \sim 290$ MeV. Since multiple combinations of pions interact in an $n$-pion state over a larger volume of the lattice, a statistically improved signal results.

Figure 2 presents extractions of the scattering length at all four orders in the $1/L$ expansion in Eq. (1) for the same pion mass as in Fig. 1. For $n > 2$, the N$^3$LO ($1/L^6$) extraction is performed using Eq. (2) with the point at $n = 3$ arising from the energy shifts $\Delta E_1$ and $\Delta E_5$, and so on. Significant dependence on $n$ in the lower order extractions (LO, NLO and NNLO) is observed, indicating the presence of residual effects. However the most accurate extractions using Eq. (2), which eliminates the three-$\pi^+$ interaction, (Eq. (1) for $n=2$) are in close agreement for all $n$. Since the construction of the combinations in Eq. (2) have specific forms for the $n$-dependence, we interpret this as being consistent with the form of this equation and the presence of a term that scales as $1/n$ which can be identified as the three-pion interaction.

The effective $m_\pi \pi^+\pi^+$ plots for $\{n,m\} = \{3,5\}$ are shown in Fig. 3. Agreement is found at the level of correlation functions with those of $n=2$, $\{n,m\} = \{3,4\}$ and $\{n,m\} = \{4,5\}$, although the $n=2$ correlation function at $m_\pi \sim 291$ MeV suffers from somewhat larger statistical fluctuations than at the other pion masses. Combining these results, we can conclude that higher order effects in $1/L$ (such as higher-derivative interactions and four-particle interactions, which occur at $O(1/L^8)$ and $O(1/L^9)$, respectively) are small. For the calculations with $m_\pi \sim 290$ MeV, the $n > 3$ effective $m_\pi \pi^+\pi^+$ plots are significantly “cleaner” than for $n = 2$.

![Figure 2: Extracted values of $m_\pi \pi^+\pi^+$ at $m_\pi \sim 350$ MeV. LO, NLO and N$^3$LO correspond to extractions of $\pi$ at $O(1/L^3,1/L^4,1/L^5)$ from Eq. (1), respectively. The N$^3$LO results for $\{n,m\} = \{3,4\}, \{3,5\}$, and $\{4,5\}$ are determined from Eq. (2). For $n = 2$, the exact solution of the eigenvalue equation [6] is denoted by “Lüscher”.

![Figure 3: Effective $m_\pi \pi^+\pi^+$ plot for $\{n,m\} = \{3,5\}$ using Eq. (2). The statistical and systematic uncertainties of the fits have been combined in quadrature.

To isolate the three-body interaction, we turn now to the combinations defined in Eq. (3), and the effective $m_\pi f_{\pi^+\pi^+\pi}$ plots are shown in Fig. 4. As expected from the previous discussion, a nonzero value of $m_\pi f_{\pi^+\pi^+\pi}^L$ is found for $m_\pi \sim 290$ and 350 MeV. Figure 5 and Table II summarize the results for the RGI three-$\pi^+$-interaction, $m_\pi f_{\pi^+\pi^+\pi}^L$, at $L = 2.5$ fm. The magnitude of the result is consistent with NDA. In Table II, we also present $m_\pi f_{\pi^+\pi^+\pi}^L(\mu = 1/b)$, a quantity that has a well-defined infinite-volume limit (unlike $\eta_N^L$) but is scale and scheme
dependent. Its scale dependence is given below Eq. (1), and we use the MS subtraction scheme; see Ref. [2] for details.

\[ m_{\pi} f_{\pi} \eta_{3} \]

The statistical and systematic uncertainties have been combined in quadrature. The vertical dashed line denotes the physical value of \( m_{\pi} / f_{\pi} \).

| \( m_{\pi} \) (MeV) | 291 | 352 | 491 | 591 |
|----------------------|------|------|------|------|
| \( m_{\pi} f_{\pi} \eta_{3} \) (2.5 fm) | 1.3(2)(7) | 0.8(1)(2) | 0.4(2)(4) | -0.4(3)(4) |
| \( m_{\pi} f_{\pi} \eta_{3} (\mu = 1/b) \) | 1.2(2)(7) | 0.7(1)(2) | -0.1(2)(4) | -1.3(3)(4) |

TABLE II: The \( \pi^{+} \pi^{+} \) interaction as defined in Eq. (3). The most precise result \( (n = 5) \) is quoted.

Finally, Eq. (4) and its counterparts involving other combinations of energies allow for a determination of residual \( 1/L \) contributions to the quantities we have extracted at N\(^3\)LO. They are all consistent with zero and are \( \lesssim 0.05 \).

Further lattice QCD calculations are required before a definitive statement about the three-pion interaction, \( m_{\pi} f_{\pi} \eta_{3} \), can be made. Whilst at lighter pion masses, there is evidence for a contribution to the various \( n \)-pion energies beyond two body scattering that scales as the three-body contribution in Eq. (1), a number of systematic effects must be further investigated. The extraction of this quantity has corrections that are formally suppressed by \( \pi/L \), however, the coefficient of the higher order term(s) may be large, and the next order term in the volume expansion needs to be computed (for \( n = 3 \), this result is known [8]). It is also possible that the signals seen in Fig. 4 are artifacts of the lattice discretization, but the observed scaling that is consistent with \( \langle n \rangle \) suggests this is not the case. However, calculations at a finer lattice spacings and with different lattice discretizations are required to resolve this issue.

As the lattice QCD study of nuclei is the underlying motivation for this work, it is worth considering difficulties that will be encountered in generalizing the result described here to baryonic systems. Certain difficulties have been discussed in Ref. [2], here we focus on the numerical issues. The ratio of signal to noise scales very poorly for baryonic observables [11], requiring an exponentially large number of configurations to extract a precise result. Also, the factorial growth of the combinatoric factors involved in forming the correlators for large systems of bosons and fermions and the high powers to which propagators are raised (e.g., for the 12-\( \pi^{+} \) correlator, there is a term 43545600 \( \text{tr}[\Pi^{1}]\text{tr}[\Pi^{2}] \)) implies that the propagators used to form the correlation functions must be known to increasingly high precision. There is much room for theoretical advances in this area.

In this work we have numerically studied the ground-state energies of \( n = 2, 3, 4, 5 \) \( \pi^{+} \)'s in a cubic volume with periodic boundary conditions using lattice QCD. We find that the \( \pi^{+} \pi^{+} \) scattering length can be extracted from combinations of these energies that eliminate the three-\( \pi^{+} \) interaction, and agree with previous \( n = 2 \) calculations [10]. In some cases the precision of the extraction is improved. Further, we have found evidence of a repulsive three-\( \pi^{+} \) interaction for \( m_{\pi} \lesssim 350 \) MeV. Future calculations will extend these results to larger \( n \) and to systems involving multiple kaons and pions. Further, calculations must be performed in different spatial volumes to determine the leading correction (\( O(1/L) \)) to the three-\( \pi^{+} \) interaction, and at different lattice spacings in order to eliminate finite-lattice spacing effects, which are expected to be small.

We thank M. Endres and D. B. Kaplan for discussions. Our computations were performed at JLab, FNAL, LLNL, NCSA, and CNdS(Barcelona). We acknowledge DOE Grants No. DE-FG03-97ER4014 (MJS, WD), DE-AC05-06OR23177 (KO), DE-AC52-07NA27344 (TL) and W-7405-Eng-48 (AT), NSF Career Grant No. PHY-0645570 (SB, AT). AP acknowledges EU contract FLAVIANET MRTN-CT-2006-035482, FIS2005-03142 from MEC (Spain) and FEDER and by the Generalitat de Catalunya contract 2005SGR-00343. KO acknowledges the Jeffress Memorial Trust, grant J-813.

[1] M. M. Aggarwal et al. [WA98 Collaboration], Phys. Rev. Lett. 85, 2895 (2000); I. G. Bearden et al. [NA44 Collaboration], Phys. Lett. B 517, 25 (2001); J. Adams et al. [STAR Collaboration], Phys. Rev. Lett. 91, 262301 (2003).
[2] S. R. Beane, W. Detmold and M. J. Savage, arXiv:0707.1670 [hep-lat], to appear in PRD.
[3] K. Huang and C. N. Yang, Phys. Rev. 105, 767 (1957).
[4] T. T. Wu, Phys. Rev. 155, 1390 (1959).
[5] T. D. Lee, K. Huang, and C. N. Yang, Phys. Rev. 106, 1135 (1957).
[6] M. Lüscher, Commun. Math. Phys. 105, 153 (1986).
[7] M. Lüscher, Nucl. Phys. B 354, 531 (1991).
[8] S. Tan, arXiv:0709.2530 [cond-mat.stat-mech].
[9] C. Aubin et al. [MILC Collaboration], Phys. Rev. D 70, 114501 (2004) [arXiv:hep-lat/0407028].
[10] S. R. Beane, et al., arXiv:0706.3026 [hep-lat].
[11] G. P. Lepage, in From Actions to Answers: Proceedings of the TASI 1989, Degrant, T., & Toussaint, D. (1990), Singapore, World Scientific.