Multipion Systems in Lattice QCD and the Three-Pion Interaction

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The ground-state energies of 2, 3, 4, and 5 π^+'s in a spatial volume $V \sim (2.5\ \mathrm{fm})^3$ are computed with lattice QCD. By eliminating the leading contribution from three-π^+ interactions, particular combinations of these n-π^+ ground-state energies provide precise extractions of the $\pi^+\pi^+$ scattering length in agreement with that obtained from calculations involving only two π^+'s. The three-π^+ interaction can be isolated by forming other combinations of the n-π^+ ground-state energies. We find a result that is consistent with a repulsive three-π^+ interaction for $m_\pi \lesssim 352$ MeV.

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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 these interactions. We report on the first lattice QCD calculation of systems comprised of more than two hadrons.

The simplest multihadron systems (both conceptually, and from a numerical perspective) consist of n pseudoscalar mesons of maximal isospin. Interactions among multiple pions are important to explore for phenomenological reasons. Two- and three-pion interferometry is currently being used to determine the coherence of the pion source in heavy-ion collisions [1]. Further, multipion interactions impact the formation of a pion condensate which is energetically favored in systems with large isospin chemical potential and will influence the properties of (hot) pion gases. In this work we perform lattice QCD calculations of the ground-state energies of $\pi^+\pi^+$, $\pi^+\pi^+\pi^+$, $\pi^+\pi^+\pi^+\pi^+$, and $\pi^+\pi^+\pi^+\pi^+\pi^+$ systems in a spatial volume of $V \sim (2.5\ \mathrm{fm})^3$ with periodic boundary conditions and a lattice spacing of $b \sim 0.125$ fm. These systems provide an ideal laboratory for investigating multiparticle 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 multibaryon systems. 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 [2]. Additionally, a result that is consistent with a repulsive three-pion interaction of magnitude expected from naïve dimensional analysis (NDA) is found for $m_\pi \lesssim 352$ MeV.

At finite volume, the ground-state energy of a system of n bosons of mass M is shifted from its infinite-volume value, nM. In a periodic cubic spatial volume of periodicity L, this shift is known to be [3–9]

$$\Delta E_n = \frac{4\pi a}{ML^3}\binom{n}{2}\left\{1 - \frac{a\mathcal{I}}{\pi L} + \left(\frac{a}{\pi L}\right)^2[\mathcal{I}^2 + (2n-5)\mathcal{J}] - \left(\frac{a}{\pi L}\right)^3[\mathcal{I}^3 + (2n-7)\mathcal{I}\mathcal{J} + (5n^2 - 41n + 63)\mathcal{K}]\right\} + \binom{n}{2}\frac{8\pi^2 a^3}{ML^6} r + \binom{n}{3}\frac{\bar{\eta}_3^L}{L^6} + \mathcal{O}(1/L^7), \tag{1}$$

where a and r are the two-boson scattering length and the effective range parameter, respectively, and $\bar{\eta}_3^L$ is the renormalization-group invariant (RGI) three-boson interaction ($\bar{\eta}_3^L$ is renormalization scheme and scale independent, but depends logarithmically on L; in terms of the three-particle interaction defined in Ref. [8], $\bar{\eta}_3^L = \eta_3(\mu) + \frac{64\pi a^4}{M}(3\sqrt{3} - 4\pi)\log(\mu L) - \frac{96 a^4}{\pi^2 M}[2\mathcal{Q} + \mathcal{R}]$). The geometric constants appearing in Eq. (1) are $\mathcal{I} = -8.9136329$, $\mathcal{J} = 16.532316$, and $\mathcal{K} = 8.4019240$. At this order, the energy is only sensitive to a combination of the effective range and scattering length, $\bar{a} = a + \frac{2\pi}{L^3} a^3 r$ and in what follows we replace $a \to \bar{a}$, eliminating r. The above expansion is valid provided a, $r \ll L$ with an additional constraint on n [8].

Various combinations of the energy differences defined in Eq. (1) are particularly useful in what follows. First

$$\frac{L^3 M[\Delta E_n m(m^2 - 3m + 2) - \Delta E_m n(n^2 - 3n + 2)]}{2(m-1)m(m-n)(n-1)n\pi} = \bar{a}\Big(1 - \frac{\bar{a}}{\pi L}\mathcal{I} + \Big(\frac{\bar{a}}{\pi L}\Big)^2[\mathcal{I}^2 - \mathcal{J}] + \Big(\frac{\bar{a}}{\pi L}\Big)^3\{-\mathcal{I}^3 + 3\mathcal{I}\mathcal{J} + [19 + 5mn - 10(n+m)]\mathcal{K}\}\Big), \quad (2)$$

(for $n, m > 2$) is independent of $\bar{\eta}_3^L$ and allows a determination of $\bar{a}$ up to $\mathcal{O}(1/L^4)$ 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 directly determined from

$$\bar{\eta}_3^L = L^6 \binom{n}{3}^{-1}\Big(\Delta E_n - \binom{n}{2}\Delta E_2 - 6\binom{n}{3} M^2 \Delta E_2^3 \Big(\frac{L}{2\pi}\Big)^4 \Big\{\mathcal{J} + \frac{L^2 M \Delta E_2}{2\pi^2}\Big[\mathcal{I}\mathcal{J} - \frac{1}{4}(5n - 31)\mathcal{K}\Big]\Big\}\Big), \quad (3)$$

($n > 2$) with corrections arising at $\mathcal{O}(1/L)$. Additionally, the dimensionless quantity

$$1 - \frac{2}{3}\frac{\Delta E_3}{\Delta E_2} + \frac{1}{6}\frac{\Delta E_4}{\Delta E_2} + \frac{5M^3 L^6 \mathcal{K}}{32\pi^6}\Delta E_2^3 = 0 + \mathcal{O}(1/L^7) \quad (4)$$

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

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

$$C_n(t) = \langle 0|\Big[\sum_{\mathbf{x}} \chi_{\pi^+}(\mathbf{x}, t)\bar{\chi}_{\pi^+}(0, 0)\Big]^n|0\rangle, \quad (5)$$

where $\chi_{\pi^+}(x) = u^a(x)\gamma_5 \bar{d}_a(x)$ is an interpolating operator for the π^+ (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, $S(x; 0)$ (for $n > 12$ additional propagators are required to circumvent the Pauli exclusion principle). As an example, the $n = 3$ correlator can be expressed as

$$C_3(t) = \mathrm{Tr}[\Pi]^3 - 3\mathrm{Tr}[\Pi]\mathrm{Tr}[\Pi^2] + 2\mathrm{Tr}[\Pi^3], \quad (6)$$

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

In this work we have computed $C_{1,2,3,4,5}(t)$ in mixed-action lattice QCD, using domain-wall valence quark propagators from Gaussian smeared sources on the rooted-staggered coarse MILC gauge configurations ($20^3 \times 64$) after hypercubic smearing and chopping (see Refs. [2,10] for details). These are computed at pion masses of $m_\pi \sim 291$, 352, 491, 591 MeV. Details of the propagators used in the correlation functions are given in Table I and can be found in Ref. [2].

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, ΔE_n, the ratios of correlators

$$G_n(t) = \frac{C_n(t)}{[C_1(t)]^n} \overset{t\to\infty}{\sim} A e^{-\Delta E_n t} \quad (7)$$

are formed, where the second relation holds in the limit of infinite temporal extent and infinite number of gauge configurations. Inclusion of the effects of temporal boundaries (here Dirichlet boundary conditions are used) is complicated for multihadron systems, and our analysis is restricted to regions where an effective-mass plot clearly shows that the ground state is dominant.

For the quantities discussed below, both jackknife and bootstrap analyses of the correlators and effective masses (e.g., $\log[G_n(t)/G_n(t-1)]$) are performed for each energy or combination thereof. These are then used in correlated and uncorrelated fits to the t dependence to extract the relevant quantity. Our systematic uncertainties are determined by comparison of our different analysis procedures and variation of the fit ranges. To avoid uncertainties arising from scale setting, we focus on the dimensionless quantities $m_\pi \bar{a}_{\pi^+\pi^+}$ and $m_\pi f_\pi^4 \bar{\eta}_3^L$ ($\bar{\eta}_3^L$ is expected to scale as $m_\pi^{-1} f_\pi^{-4}$ by NDA).

The $\pi^+\pi^+$ scattering length (more precisely, the combination $\bar{a}_{\pi^+\pi^+}$) has been studied repeatedly in lattice QCD using the finite-volume formalism of Lüscher [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 propaga-

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. [2].

m_π (MeV)	N_{cfg}	N_{src}	m_π/f_π
291.3(1.0)(1.0)	468	16	1.990(11)(14)
351.9(0.5)(0.2)	769	20	2.3230(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)

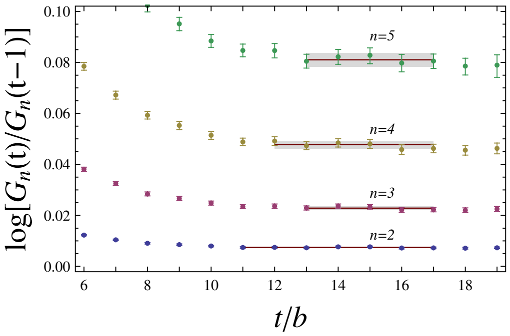

FIG. 1 (color online). Energy shifts, ΔE_n, for $n = 2$, 3, 4, 5 π^+'s for the calculations with $m_\pi \sim 352$ MeV. The statistical and systematic uncertainties of the fits have been combined in quadrature.

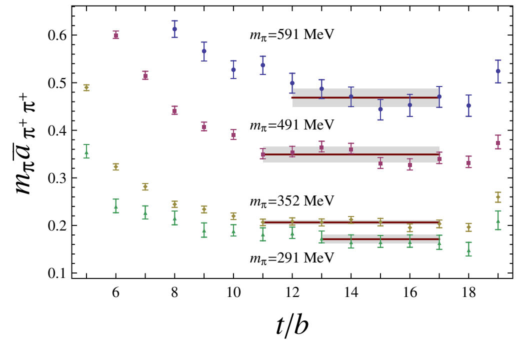

FIG. 3 (color online). Effective $m_\pi \bar{a}_{\pi^+\pi^+}$ plot for $\{n, m\} = \{3, 5\}$ using Eq. (2). The statistical and systematic uncertainties of the fits have been combined in quadrature.

tors as used in this work [2]. Therefore, the utility of multipion energies in extracting the scattering length can be ascertained, as summarized in Figs. 1–3.

In Fig. 1, the energy shifts for $n = 2$, 3, 4, and 5 are displayed for the highest-precision calculation, $m_\pi \sim 352$ MeV. Clear plateaus are visible for each n; indeed, the relative uncertainty decreases with increasing n in the range explored (this is particularly clear for the calculation with $m_\pi \sim 291$ 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 $m_\pi \sim 352$ MeV. For $n > 2$, the next-to-next-to-leading order (NNNLO) ($1/L^6$) extraction is performed using Eq. (2) with the point at $n = 3$ arising from the energy shifts ΔE_4 and ΔE_5, and so on. Significant dependence on n is observed in the lower-order extractions (LO, NLO, and NNLO), indicating the presence of residual finite-volume effects. However, the most accurate extractions using Eq. (2), which eliminates the three-π^+ interaction [Eq. (1) for $n = 2$], are in close agreement for all n. This provides a nontrivial check of the n dependence of Eq. (1), particularly the presence of a term that scales as $\binom{n}{3}$, which can be identified as the three-pion interaction.

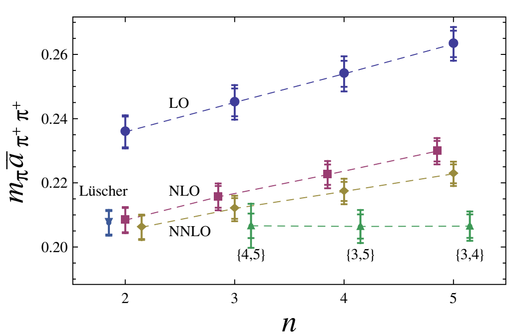

FIG. 2 (color online). Extracted values of $m_\pi \bar{a}_{\pi^+\pi^+}$ at $m_\pi \sim 352$ MeV. LO, NLO, and NNLO correspond to extractions of $\bar{a}$ at $\mathcal{O}(1/L^3, 1/L^4, 1/L^5)$ from Eq. (1), respectively. The NNNLO results for $\{n, m\} = \{3, 4\}, \{3, 5\}$ and $\{4, 5\}$ are determined from Eq. (2). For $n = 2$, the exact solution of the eigenvalue equation [6] is denoted by "Lüscher".

The effective $m_\pi \bar{a}_{\pi^+\pi^+}$ 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 $\{n, m\} = \{4, 5\}$. This agreement suggests that higher-order effects in $1/L$ [such as higher-derivative interactions and four-particle interactions, which occur at $\mathcal{O}(1/L^8)$ and $\mathcal{O}(1/L^9)$, respectively] are small. For the calculations with $m_\pi \sim 291$ MeV, the $n > 3$ effective $m_\pi \bar{a}_{\pi^+\pi^+}$ plots are significantly "cleaner" than for $n = 2$.

To isolate the three-body interaction, we turn now to the combinations defined in Eq. (3), and the effective $m_\pi f_\pi^4 \bar{\eta}_3^L$ plots are shown in Fig. 4. A nonzero value of $m_\pi f_\pi^4 \bar{\eta}_3^L$ is found for $m_\pi \sim 291$ and 352 MeV. Figure 5 and Table II summarize the results for the RGI three-π^+ interaction, $m_\pi f_\pi^4 \bar{\eta}_3^L$, at $L = 2.5$ fm. The magnitude of the result is consistent with NDA. In Table II, we also present $m_\pi f_\pi^4 \eta_3(\mu = 1/b)$, a quantity that has a well-defined infinite-volume limit (unlike $\bar{\eta}_3^L$) but is scale and scheme dependent. Its scale dependence is given below Eq. (1), and we use the minimal subtraction scheme [8].

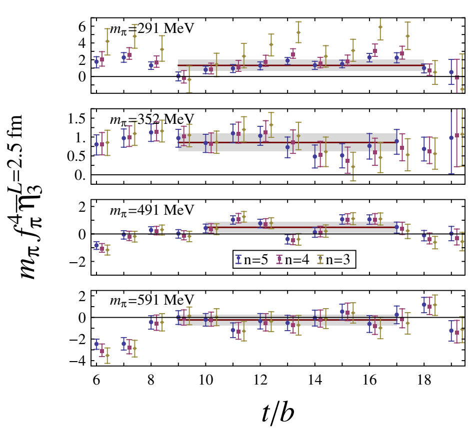

FIG. 4 (color online). Effective $m_\pi f_\pi^4 \bar{\eta}_3^L$ plots extracted from the $n = 3$, 4, and 5 π^+ energy shifts. The fits shown correspond to the $n = 5$ calculation. The statistical and systematic uncertainties have been combined in quadrature.

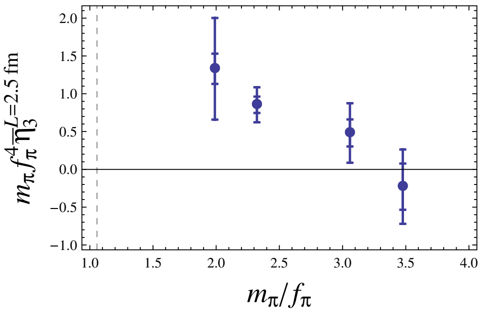

FIG. 5 (color online). Mass dependence of the RGI three-π^+ interaction $m_\pi f_\pi^4 \bar{\eta}_3^L$. The statistical and systematic uncertainties have been combined in quadrature. The vertical dashed line denotes the physical value of m_{π^+}/f_{π^+}.

Finally, Eq. (4) and its counterparts involving other combinations of energies allow for a determination of residual $1/L^7$ contributions to the quantities we have extracted at NNNLO. They are all consistent with zero and are $\lesssim 0.05$.

Further lattice QCD calculations are required before a definitive statement about the physical value of the three-pion interaction, $m_\pi f_\pi^4 \bar{\eta}_3^L$, can be made. While 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 $\bar{a}/L$; 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 [9]). 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 $\binom{n}{3}$ suggests this is not the case. However, calculations at finer lattice spacings and with different lattice discretizations are required to resolve this issue.

As the lattice QCD study of nuclei is an 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. [8]. 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-π^+ correlator, there is a term 435 456 00 $\mathrm{Tr}[\Pi^{11}]\mathrm{Tr}[\Pi]$) 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.

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

m_π (MeV)	291	352	491	591
$m_\pi f_\pi^4 \bar{\eta}_3^{L=2.5\ \mathrm{fm}}$	1.3(2)(7)	0.8(1)(2)	0.4(2)(4)	−0.4(3)(4)
$m_\pi f_\pi^4 \eta_3(\mu = 1/b)$	1.2(2)(7)	0.7(1)(2)	−0.1(2)(4)	−1.3(3)(4)

In this work we have numerically studied the ground-state energies of $n = 2, 3, 4, 5$ π^+'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-π^+ interaction, and we agree with previous $n = 2$ calculations [2]. In some cases the precision of the extraction is improved. We have found evidence of a repulsive three-π^+ interaction for $m_\pi \lesssim 352$ 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 $[\mathcal{O}(1/L)]$ to the three-π^+ interaction, and at different lattice spacings in order to eliminate finite-lattice spacing effects.

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Note added in proof.—The $1/L^7$ contributions to Eq. (1) have been computed recently [13].

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