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HADRON-HADRON AND HADRON-HADRON-HADRON PROPERTIES FROM LATTICE QCD

Silas R. Beane
Department of Physics
University of New Hampshire
Durham, NH 03824-3568

Abstract

While lattice QCD is able to compute some single-hadron properties to few-percent accuracy, only very recently has it become possible to extract precise information about the interactions among hadrons. I will review the methodology for extracting scattering and many-body information from lattice QCD correlation functions in a finite volume, and I will discuss recent progress in computing the $\pi^+\pi^+$ ($I = 2$) scattering length and the $\pi^+\pi^+\pi^+$ interaction using fully-dynamical lattice QCD calculations.

1 Introduction

One of the grand challenges of strong-interaction physics is to make quantitative predictions for the properties and interactions of nuclei directly from Quantum ChromoDynamics (QCD). Recently, Moore's Law, coupled with algorithmic breakthroughs, have allowed pioneering preliminary studies of low-energy nucleon-nucleon (NN) [1] and hyperon-nucleon (YN) [2] scattering in fully dynamical-lattice QCD. While in the context of nuclear physics one may be tempted to focus attention on potentials and wavefunctions rather than on S-matrix elements, these are not fundamental objects in QCD, and they are therefore useful tools only to the extent that they are able to encode information about low-energy scattering [3].

In order to make contact between nuclear physics and lattice QCD, it is essential to understand the mapping between the finite-volume energy levels that one measures in a lattice calculation and the hadronic interactions that give rise to nuclei. The first step in this direction was taken by Lüscher [4, 5] who noted that the two-body elastic S-matrix can be directly related to the energy levels of two particles interacting in a space-time lattice. Analogous relations for the interaction of n particles in the weakly-interacting limit were derived long ago by Huang and Yang and others [6–8]. Only very recently have these relations been extended to include the presence of three-body forces [9, 10].

Current lattice QCD calculations of the interactions among baryons are severely impeded by the exponential decay of the signal/noise ratio [11], and it is clear that, barring theoretical or algorithmic developments that will alleviate the signal problem, significantly more computer power than is now available will have to be brought to bear on nuclear physics before real nuclei can be studied in a quantitative way using lattice QCD. However, it is important to develop and test the technology necessary to extract hadronic interactions from lattice QCD calculations using tractable hadronic systems. In this respect, pions provide the ideal theoretical laboratory for such a study as correlation functions of pions —even arbitrary numbers of them— do not suffer from an exponential decay of the signal/noise ratio. Pions have several additional advantages; they are bosons, and they are guaranteed by the chiral symmetry of QCD to interact weakly.

After we introduce the basic methodology, we will discuss two examples of recent fully-dynamical lattice QCD calculations of pion properties. First we will discuss a lattice measurement of the $I = 2$ $\pi\pi$ scattering length which is now at 1% precision. We will then present recent pioneering work which aims to extract a signal for 3-pion interactions from lattice QCD. Finally we will make some comments about baryons; specifically, why they are difficult.

2 n bosons in a box

The ground-state energy of an n-boson system [9] is calculated with an interaction of the form

$$V(\mathbf{r}_1, \ldots, \mathbf{r_n}) = \eta \sum_{i<j}^{n} \delta^{(3)}(\mathbf{r}_i - \mathbf{r}_j) + \eta_3 \sum_{i<j<k}^{n} \delta^{(3)}(\mathbf{r}_i - \mathbf{r}_k)\delta^{(3)}(\mathbf{r}_j - \mathbf{r}_k) + .., \quad (1)$$

where the ellipsis denote higher-body interactions that do not contribute at the order to which we work (in general, m-body interactions will enter at $\mathcal{O}(L^{3(1-m)})$. For an s-wave scattering phase shift, $\delta(p)$, the two-body contribution to the pseudo-potential is given by $\eta = -\frac{4\pi}{M} p^{-1} \tan\delta(p) = \frac{4\pi}{M} a + \frac{2\pi}{M} a^2 r p^2 + \ldots$, keeping only the contributions from the scattering length and effective range, a and r, respectively. At $\mathcal{O}(L^{-6})$ the coefficient of the three-body potential, η_3, is momentum independent.

As an example, consider the 2-boson energy. The volume dependence of the energy is easily built up using Rayleigh-Schrödinger time-independent perturbation theory. The leading contribution to the perturbative expansion of the energy is given by

$$\Delta E_2^{(1)} \quad = \quad \langle -\mathbf{k}, \mathbf{k} |\, V(\mathbf{r}_1, \mathbf{r}_2) \,| -\mathbf{p}, \mathbf{p} \rangle \ , \tag{2}$$

where $|-\mathbf{p}, \mathbf{p}\rangle$ are the two-body momentum eigenstates in the center-of-mass system. The single-particle wavefunctions in the finite volume are given by: $\langle \mathbf{r}|\mathbf{p}\rangle = \exp(i\mathbf{k}\cdot\mathbf{r})/L^{3/2}$. Inserting two complete sets of position eigenstates in Eq. (2), one easily finds $\Delta E_2^{(1)} = \eta/L^3 = 4\pi\, a/M\, L^3$. It is straightforward to calculate higher-order $1/L$ corrections in this manner.

The volume dependence of the energy of the n-boson (of mass M) ground state in a periodic cubic spatial volume of periodicity L up to $\mathcal{O}\left(1/L^6\right)$ is known to be [4–10]

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

where the geometric constants are $\mathcal{I} = -8.9136329$, $\mathcal{J} = 16.532316$ and $\mathcal{K} = 8.4019240$, and

$$\overline{\eta}_3^L = \eta_3(\mu) + \frac{64\pi a^4}{M}(3\sqrt{3} - 4\pi)\log(\mu\, L) - \frac{96\, a^4}{\pi^2 M}[2\mathcal{Q} + \mathcal{R}] \tag{4}$$

is the renormalization-scheme and scale independent three-boson interaction [9]. Note the logarithmic dependence on L. At this order in the $1/L$ expansion, the energy is only sensitive to a combination of the effective range and scattering length, $\overline{a} = a + \frac{2\pi}{L^3} a^3\, r$ and in what follows we will sometimes replace $a \to \overline{a}$, eliminating r.

While the calculation of ground-state energies described here has been derived in a non-relativistic framework, the results remain valid relativistically. In the two-body case, this has been shown by Lüscher [5]. In the higher-body case, the non-relativistic calculation will not correctly recover a field-theoretic calculation, due to relativistic effects in multiple, two-body interactions involving three or more particles. At $\mathcal{O}\left(L^{-4}\right)$, only two-particle interactions contribute to the n-body ground-state energy and the results of Ref. [5] follow without modification. Since the interaction of three particles due to the two-body interaction first enters at L^{-5}, and relativistic effects in such interactions are suppressed by $(ML)^{-2}$, the first relativistic effects will occur at $\mathcal{O}(L^{-7})$ [9].

3 Hadron-hadron interactions

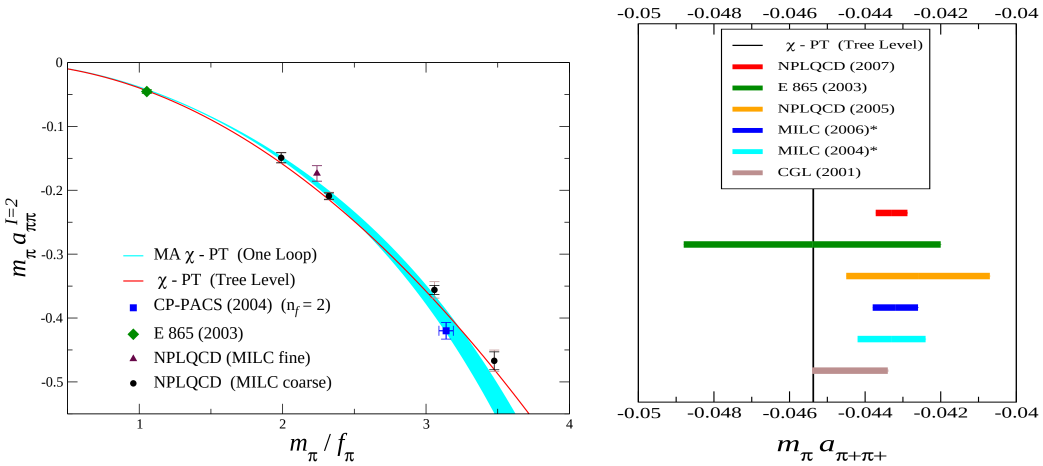

Figure 1: Left panel: $m_\pi\ a_{\pi\pi}^{I=2}$ vs. m_π/f_π (ovals) with statistical (dark bars) and systematic (light bars) uncertainties. Also shown are the experimental value from Ref. [19] (diamond) and the lowest quark mass result of the $n_f = 2$ dynamical calculation of CP-PACS [20] (square). The blue band corresponds to a weighted fit to the lightest three data points (fit B) using the one-loop MAχ-PT formula in Eq. (9) (the shaded region corresponds only to the statistical error). The red line is the tree-level χ-PT result. Right panel: A compilation of the various measurements and predictions for the $I = 2$ $\pi\pi$ scattering length. The prediction made in this paper is labeled NPLQCD (2007), and the Roy equation determination of Ref. [14] is labeled CGL (2001).

As the simplest application of Eq. (3), let us consider recent results for the $\pi\pi$ interaction [12]. Due to the chiral symmetry of QCD, pion-pion ($\pi\pi$) scattering at low energies is the simplest and best-understood hadron-hadron scattering process. The scattering lengths for $\pi\pi$ scattering in the s-wave are uniquely predicted at leading order (LO) in chiral perturbation theory (χ-PT) [13]:

$$m_\pi a_{\pi\pi}^{I=0} \ = \ 0.1588 \ \ ; \ \ m_\pi a_{\pi\pi}^{I=2} \ = \ -0.04537 \quad , \tag{5}$$

at the charged pion mass. While experiments do not provide stringent constraints on the scattering lengths, a theoretical determination of s-wave $\pi\pi$ scattering lengths which makes use of experimental data has reached a remarkable level of precision [14, 15]:

$$m_\pi a_{\pi\pi}^{I=0} \ = \ 0.220 \pm 0.005 \ \ ; \ \ m_\pi a_{\pi\pi}^{I=2} \ = \ -0.0444 \pm 0.0010 \quad . \tag{6}$$

These values result from the Roy equations [16–18], which use dispersion theory to relate scattering data at high energies to the scattering amplitude near threshold. At present lattice QCD can compute $\pi\pi$ scattering only in the $I = 2$ channel as the $I = 0$ channel contains disconnected diagrams. It is of course of great interest to compare the precise Roy equation predictions with lattice QCD calculations.

The lattice calculations that are described in this paper involve a mixed-action lattice QCD scheme of domain-wall valence quarks on a rooted staggered sea. Details of the lattice calculation can be found in Ref. [12]. A $\pi^+\pi^+$ ($I = 2$) correlation function that projects onto the s-wave state in the continuum limit is

$$C_{\pi^+\pi^+}(p,t) = \sum_{|\mathbf{p}|=p} \sum_{\mathbf{x},\mathbf{y}} e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} \langle \pi^-(t,\mathbf{x})\ \pi^-(t,\mathbf{y})\ \pi^+(0,\mathbf{0})\ \pi^+(0,\mathbf{0})\rangle, \quad (7)$$

where $\pi^+(t,\mathbf{x}) = \overline{u}(t,\mathbf{x})\gamma_5 d(t,\mathbf{x})$ is an interpolating field for the π^+. In order to extract the energy difference one forms the ratio of correlation functions, $G_{\pi^+\pi^+}(p,t)$, where

$$G_{\pi^+\pi^+}(p,t) \equiv \frac{C_{\pi^+\pi^+}(p,t)}{C_{\pi^+}(t)C_{\pi^+}(t)} \rightarrow \sum_{n=0}^{\infty} \mathcal{A}_n\ e^{-\Delta E_n\ t} \quad , \quad (8)$$

and $C_{\pi^+}(t)$ is the single-pion correlation function. The arrow in Eq. (8) denotes the large-time behavior of $G_{\pi^+\pi^+}$ in the absence of boundaries on the lattice and becomes an equality in the limit of an infinite number of gauge configurations.

We have computed the energy difference ΔE_n (and via Eq. (3) the scattering length) at pion masses, $m_\pi \sim 290$ MeV, 350 MeV, 490 MeV and 590 MeV, and at a single lattice spacing, $b \sim 0.125$ fm and lattice size $L \sim 2.5$ fm [12]. In order to obtain the physical value of the scattering length, one must extrapolate. In two-flavor mixed-action χ-PT (MAχ-PT) (i.e. including finite lattice-spacing corrections) the chiral expansion of the scattering length at NLO takes the form [21]

$$m_\pi\ a_{\pi\pi}^{I=2} = -\frac{m_\pi^2}{8\pi f_\pi^2}\left\{1 + \frac{m_\pi^2}{16\pi^2 f_\pi^2}\left[3\log\left(\frac{m_\pi^2}{\mu^2}\right) - 1 - l_{\pi\pi}^{I=2}(\mu) - \frac{\tilde{\Delta}_{ju}^4}{6m_\pi^4}\right]\right\}, \quad (9)$$

where it is understood that m_π and f_π are the lattice-physical parameters [21] and

$$\tilde{\Delta}_{ju}^2 = b^2\Delta_I + \dots . \quad (10)$$

where the dots denote higher-order corrections to the meson masses. With domain-wall fermion masses tuned to match the staggered Goldstone pion, one finds (in lattice units) $\tilde{\Delta}^2_{ju} = b^2\Delta_I = 0.0769(22)$ [22] on the coarse MILC lattices (with $b \sim 0.125$ fm and $L \sim 2.5$ fm). Eq. (9), which contains all $\mathcal{O}(m_\pi^2 b^2)$ and $\mathcal{O}(b^4)$ lattice artifacts, reduces to the continuum expression for the scattering length in the QCD limit where $\tilde{\Delta}^2_{ju} \to 0$. Figure 1 (left panel) is a plot of $m_\pi \ a_{\pi\pi}^{I=2}$ vs. m_π/f_π with the lattice results and the fit curves from MAχ-PT.

The final result is:

$$m_\pi a_{\pi\pi}^{I=2} \quad = \quad -0.04330 \pm 0.00042 \quad , \tag{11}$$

where the statistical and systematic uncertainties have been combined in quadrature. Notice that 1% precision is claimed in this result. This result is consistent with all previous determinations within uncertainties (see Figure 1 (right panel)).

4 Hadron-hadron-hadron interactions

It is straightforward to generalize the two-pion correlation function of Eq. (7) to n pions. A non-trivial test of Eq. (3) then results from extracting the two-body scattering length from the n pion correlators. In this respect, one particularly useful combination of the energy differences defined in Eq. (3) is:

$$\begin{aligned}
&\frac{L^3 M(\Delta E_n m(m^2-3m+2) - \Delta E_m n(n^2-3n+2))}{2(m-1)m(m-n)(n-1)n\pi} \\
&= \overline{a}\Bigg\{ 1 - \frac{\overline{a}}{\pi\, L}\mathcal{I} + \left(\frac{\overline{a}}{\pi\, L}\right)^2 \left[\mathcal{I}^2 - \mathcal{J}\right] + \left(\frac{\overline{a}}{\pi\, L}\right)^3 \\
&\quad \times \left[-\mathcal{I}^3 + 3\mathcal{I}\mathcal{J} + (19 + 5m\, n - 10(n+m))\mathcal{K}\right] \Bigg\} ,
\end{aligned} \tag{12}$$

(for $n, m > 2$) which is independent of $\overline{\eta}_3^L$ and allows a determination of $\overline{a}$ 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).

Figure 2 (left panel) presents extractions of the scattering length at all four orders in the $1/L$ expansion in Eq. (3) for $m_\pi \sim 350$ MeV. For $n > 2$, the N^{3}LO ($1/L^6$) extraction is performed using Eq. (12) with the point at $n = 3$ arising from the energy shifts ΔE_4 and ΔE_5, and so on. Significant dependence on n in the lower-order extractions (LO, NLO and NNLO) is observed, indicating the presence of residual finite-volume effects. However the most accurate extractions using Eq. (12), which eliminate the three-π^+ interaction (Eq. (3) for n=2), are in close agreement for all n. This provides a non-trivial check of the n-dependence of Eq. (3), particularly the presence of a term that scales as $\binom{n}{3}$, which can be identified as the three-pion interaction.

To isolate the three-body interaction, we can form a second useful combination of the energy differences defined in Eq. (3):

$$\overline{\eta}_3^L = L^6 \binom{n}{3}^{-1} \Bigg\{ \Delta E_n - \binom{n}{2} \Delta E_2 - 6 \binom{n}{3} M^2 \Delta E_2^3 \times \left(\frac{L}{2\pi}\right)^4 \left[\mathcal{J} + \frac{L^2 M\, \Delta E_2}{2\pi^2} \left(\mathcal{I}\mathcal{J} - (5n-31)\mathcal{K}\right) \right] \Bigg\} , \tag{13}$$

($n > 2$) with corrections arising at $\mathcal{O}(1/L)$. To avoid uncertainties arising from scale setting, we focus on the dimensionless quantity $m_\pi f_\pi^4 \overline{\eta}_3^L$ ($\overline{\eta}_3^L$ is expected to scale as $m_\pi^{-1} f_\pi^{-4}$ by naive dimensional analysis (NDA)). A nonzero value of $m_\pi f_\pi^4 \overline{\eta}_3^L$ is found for $m_\pi \sim 290$ and 350 MeV. Figure 2 (right panel) summarizes the results for the three-π^+-interaction, $m_\pi f_\pi^4 \overline{\eta}_3^L$, at $L = 2.5$ fm. The magnitude of the result is consistent with NDA.

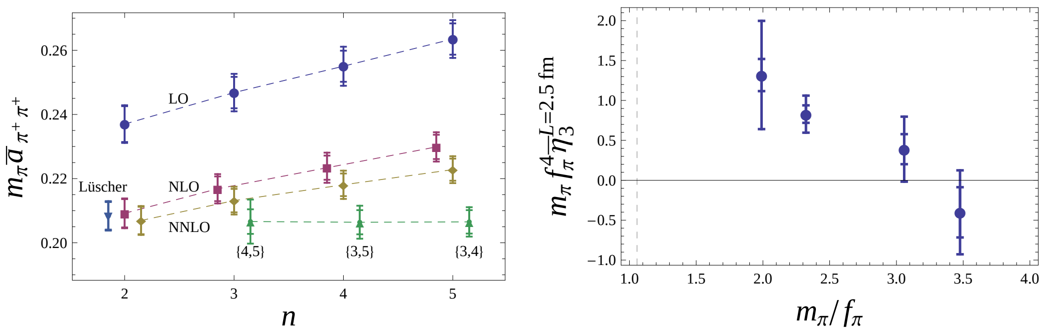

Figure 2: Left panel: extracted values of $m_\pi \overline{a}_{\pi^+\pi^+}$ at $m_\pi \sim 350$ MeV. LO, NLO and NNLO correspond to extractions of $\overline{a}$ at $\mathcal{O}(1/L^3, 1/L^4, 1/L^5)$ from Eq. (3), respectively. The N^{3}LO results for $\{n, m\} = \{3, 4\}, \{3, 5\}$, and $\{4, 5\}$ are determined from Eq. (12). For $n = 2$, the exact solution of the eigenvalue equation [4] is denoted by "Lüscher". Right panel: Effective $m_\pi f_\pi^4 \overline{\eta}_3^L$ 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.

Further lattice QCD calculations are required before a definitive statement about the physical value of the three-pion interaction, $m_\pi f_\pi^4 \overline{\eta}_3^L$, 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. (3), a number of systematic effects must be further investigated. The extraction of this quantity has corrections that are formally suppressed by $\overline{a}/L$, 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 [10]).

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, which are expected to be small.

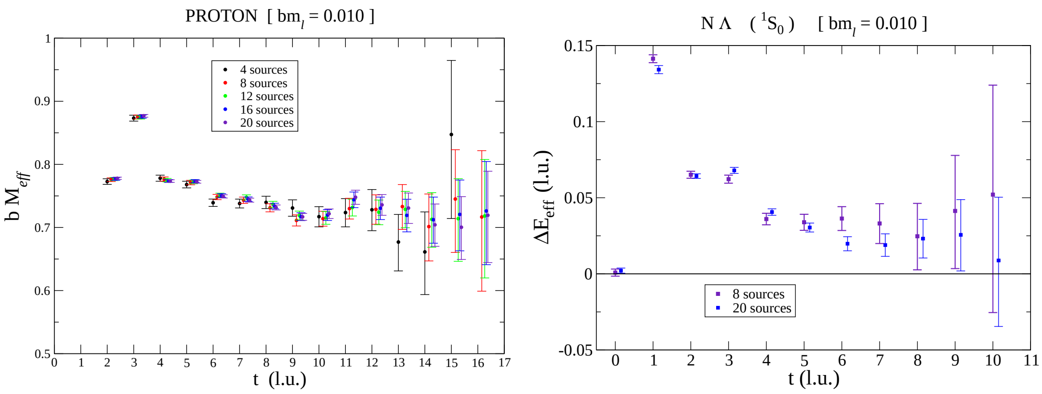

Figure 3: Left panel: effective mass plot for the proton at a pion mass of 350 MeV, with increasing statistics. Right panel: effective mass plot for the ${}^1S_0$ neutron-lambda ground state energy at a pion mass of 350 MeV with increasing statistics.

5 Baryons

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. 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. Several examples are shown in Figure 3. the left panel is an effective mass plot for the proton mass and the right panel is an effective mass plot for the ${}^1S_0$ neutron-lambda ground state energy. The number of sources indicates the number of light (and strange) propagators computed per lattice configuration. While the error bars do decrease more or less as expected, the signal certainly does not improve as it does for the pions. For instance, for the proton, the signal/noise ratio is expected to die exponentially as $\exp(-(M_N - 3m_\pi/2)t)$. And too, 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 43545600 $\mathrm{tr}[\Pi^{11}]\mathrm{tr}[\Pi]$) implies that the propagators used to form the correlation functions must be known to increasingly high precision.

While recent pioneering studies of low-energy NN and YN scattering [1, 2] are clearly plagued by the signal/noise problem discussed above, it is remarkable that the NN s-wave scattering lengths evaluated at pion masses in the range $m_\pi \sim 350 - 600$ MeV are all of natural size, $\sim \Lambda_{QCD}^{-1}$, in sharp contrast with the physical values.

6 Conclusions

Lattice QCD calculations of 2-body pion (and kaon) interactions are now a precision science (for those channels that do not involve disconnected diagrams). The study of multi-pion systems has led to the first lattice QCD evidence of many-body forces. While this result provides an important test of the basic methodology for extracting many-body physics from lattice QCD, it is, of course, somewhat somewhat academic as pions are weakly interacting bosons. The holy grail for this area of research is to see a definitive signal for nuclear physics. Given the current state of lattice QCD calculations involving baryons, it is clear that there is much room for theoretical advances in this area.

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