PROCEEDINGS OF SCIENCE

Spectroscopy and hadron interactions

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Lattice QCD spectroscopy and subsequent determinations of scattering amplitudes are an active line of research with notable advances. In the two-hadron sector there has been significant progress in constraining more complicated scattering amplitudes as well as in controlling systematic uncertainties. A new frontier is the practical application of finite-volume formalisms to treat three-hadron interactions. Some of these recent developments are reviewed.

The 38th International Symposium on Lattice Field Theory, LATTICE2021 26th-30th July, 2021 Zoom/Gather@Massachusetts Institute of Technology

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PoS(LATTICE2021)006

1. Introduction

Spectroscopy is one of the, if not the foundational activity in lattice QCD. Roughly speaking, spectroscopy is concerned with obtaining 'hadron masses' starting from the QCD Lagrangian. Masses of the select number of hadrons which are stable under the strong interaction are precision observables, necessitating the inclusion of the effects of electromagnetism as well as strong isospin breaking. An orthogonal direction in spectroscopy deals with calculations of multi-hadron dynamics to rigorously understand the wealth of hadronic resonances. Resonances manifest themselves as structures in scattering amplitudes and have no direct correspondence with eigenstates of the QCD Hamiltonian in finite volume. Nevertheless, scattering amplitudes can be computed from lattice QCD by exploiting their relationship to Euclidean finite-volume observables. Several approaches to establishing such a connection between lattice QCD observables and scattering amplitudes are available, usually referred to as finite-volume formalisms.

Methods to constrain multi-hadron dynamics from lattice QCD have a breadth of applications beyond unearthing and improving our understanding of hadronic resonances. A prominent recent example is the hadronic-vacuum-polarization (HVP) contribution to the anomalous magnetic moment of the muon, which is dominated by the contribution of two-pion states [1]. Consequently, dedicated studies of this two-pion contribution can greatly benefit lattice QCD determinations of the HVP [2–4]. Further, multi-hadron states are expected to play an important role towards understanding the excited-state contamination in calculations of the structure of the nucleon. A dedicated study using the methods developed for multi-hadron spectroscopy might shed light on how well present nucleon-structure calculations control this important source of systematic uncertainty (see [5] for a discussion at this conference). Finally, the lattice community is uniquely positioned to provide some requisite QCD input towards building an understanding of nuclear physics based on the Standard Model (see e.g. [6, 7]). At least in principle, lattice QCD can provide information which is hard to obtain experimentally, such as interactions of baryons with strangeness and the interaction of three nucleons.

Lattice QCD investigations of multi-hadron physics are a very active line of research with great progress over the last decade or so. Studies of two-meson systems are fairly mature. For simple systems, such as elastic scattering of two pseudoscalars, full control over the usual lattice systematics is becoming feasible. Successful proof-of-principle studies of more complicated systems, for instance involving several coupled channels, corroborate the correctness of the two-body finite-volume formalisms and demonstrate the viability of their practical implementation. Studies of meson-baryon interactions are considerably less advanced, but are picking up pace. Two-baryon systems have received comparatively more attention due to their importance for nuclear physics, but results in the literature show significant disagreement even at heavy pion masses. Furthermore, large discretization effects were recently observed in a study of $\Lambda\Lambda$ interactions, drawing renewed attention to the need to control all sources of systematic uncertainties in order to provide impactful results.

An incomplete subset of the exciting recent developments is reviewed in this contribution.

2. Methods

The approaches to obtaining two-hadron scattering information currently in use fall broadly into two categories.[1] The HALQCD method extracts a potential, which can be determined from the lattice, and solves the resultant Schrödinger equation to obtain two-hadron interactions [12]. Except where noted explicitly, we will focus on results based on the second class of approaches, usually dubbed the Lüscher method, which exploits the connection between the discrete spectrum of QCD confined to a finite box and hadron interactions in infinite volume [13–16]. The central equation, usually referred to as quantization condition, can be written very succinctly as

$$\det\left[\mathcal{M}^{-1}(E_L) + F(E_L, L)\right] = 0, \tag{1}$$

where F is a matrix of known functions and thus the quantization condition, for a given energy-dependent scattering amplitude $\mathcal{M}(E)$, predicts the corresponding spectrum in a box. This relationship is known for all two-body interactions relevant in QCD, including for instance scattering of particles with spin and multiple kinematically open scattering channels (see [17] for a review). Ongoing work concerns the three-body generalization of Eq. (1) [18–45] (reviewed in Refs. [46, 47]), as well as laying the groundwork for and translating to practical use the methods to calculate matrix elements involving multi-hadron initial and final states [48–54].

Clearly, precise determinations of the eigenvalues of the finite-volume QCD Hamiltonian are required for this program, preferably including many energy levels in the kinematic range of interest, i.e. covering nonzero total momentum as well as excited states in addition to the ground state for each total momentum. These spectra $\{E_n\}$ are extracted from the time dependence of a suitable set of Euclidean correlation functions

$$C_{ij}(t) = \langle 0|O_i(t)O_j^\dagger(0)|0\rangle = \sum_n \langle 0|O_i|n\rangle\, \langle n|O_j^\dagger|0\rangle\, \mathrm{e}^{-E_n t}. \tag{2}$$

If the correlation matrix is Hermitean, i.e. if the interpolating operators used to create states at the source time $t = 0$ are conjugates of the operators annihilating states at the sink time t, solutions of a generalized eigenvalue problem can be used to robustly extract not just the lowest-lying energy, but also excited states [55–58]. Furthermore, each decaying exponential in the tower of states is guaranteed to contribute with a positive weight in the diagonal elements of a Hermitean correlation matrix, ensuring a monotonic approach to the ground state. Correlation functions of different creation and annihilation operators on the other hand can suffer from delicate cancellations between terms in the sum over states, which can complicate the accurate extraction of the spectrum [59].

Hermitean correlation matrix or not, the set of interpolating operators must include operators with good overlap onto the states of interest, lest one run the risk of extracting a wrong or incomplete spectrum. Indeed, several such cases are well known in the literature. A classic example arises in the context of string breaking, where one interpolator resembling a pair of a static quark and antiquark connected with a Wilson line as well as one interpolator resembling two static-light mesons are required to resolve the mixing phenomenon underlying string breaking [60–64]. Excluding either of those operators leads to an incomplete spectrum determination. Another recent example concerns finding an interpolator with good overlap onto the finite-volume state related to the $\Lambda(1520)$, where

[1] Alternative approaches are being developed and tested [8–11], which are not discussed further here.

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a three-quark interpolator with nontrivial spatial structure is crucial [65]. Lastly, of relevance to extracting scattering amplitudes through their imprint on the finite-volume spectrum, both a quark bilinear as well as interpolators resembling two-pion states are needed to correctly identify the spectrum in calculations of the ρ resonance [66, 67]. In practice, the best we can do in spectroscopy is to employ a reasonably diverse set of interpolators and monitor the stability of the extracted spectrum under variation of included operators.

Distillation [68, 69] furnishes an economical method to compute correlation functions of such a wide variety of interpolators without requiring additional solutions of the Dirac equation. Indeed the ability to store at moderate cost solutions of the Dirac equation projected into the distillation subspace and reuse them across numerous projects underlies many of the results in the following sections. In particular, distillation generalizes straightforwardly to systems involving more than two hadrons.

A recent addition to the spectroscopy toolbox is the use of sparsened all-to-all propagators [70]. While calculating the full quark propagator is computationally intractable, sampling a sufficiently large subset of source positions on a time slice enables an approximate momentum projection up to mixing with high-frequency modes, which amounts to a modification of the structure of excited states. Like in distillation, correlation functions of a variety of interpolators can then be computed a posteriori. Using this method, the NPLQCD collaboration has recently produced results for the interaction of two nucleons at heavy pion mass, which are discussed in section 5.

3. Meson-meson interactions

Calculations of two-meson interactions from the lattice have a long history and have reached a remarkable level of maturity. The prototypical example of such calculations is $\pi\pi$ scattering in the weakly interacting $I = 2$ channel and the $I = 1$ channel featuring the $\rho(770)$ resonance, with a renewed recent interest [2–4, 71–73] due to its importance for the HVP contribution to $g - 2$ [1, 74]. Numerous determinations of pion-pion scattering amplitudes in those channels exist in the literature [66, 67, 72, 73, 75–93], and more data is becoming available as a byproduct of other calculations, e.g. $K \to \pi\pi$ and from studies of three-body scattering, which offers increased sensitivity to two-body scattering observables. Lattice studies exist also of the isoscalar channel [93–97]. Given that some calculations have started to investigate the pion mass and lattice spacing dependence (see Figure 1), $\pi\pi$ scattering presents another window into the low-energy constants of Chiral Perturbation Theory [98, 99]. Similarly, there is a growing body of results for $K\pi$ scattering [100–105], including at this conference [106, 107].

Beyond elastic scattering, or upon inclusion of higher partial waves, Eq. (1) does not constitute a one-to-one mapping between finite-volume energies and the scattering amplitude at that same energy. Instead, the quantization condition is used to predict the finite-volume spectrum for a given parametrization of the scattering amplitude. If the number of free parameters describing the scattering amplitude (such as effective-range parameters or couplings) is sufficiently smaller than the number of measured energy levels, amplitudes can be obtained from fits to the measured finite-volume spectrum. Implementing those fits becomes more technically challenging as the number of included scattering channels or partial waves increases, because an increasingly dense tower of solutions of the quantization conditions needs to be correctly identified as illustrated in

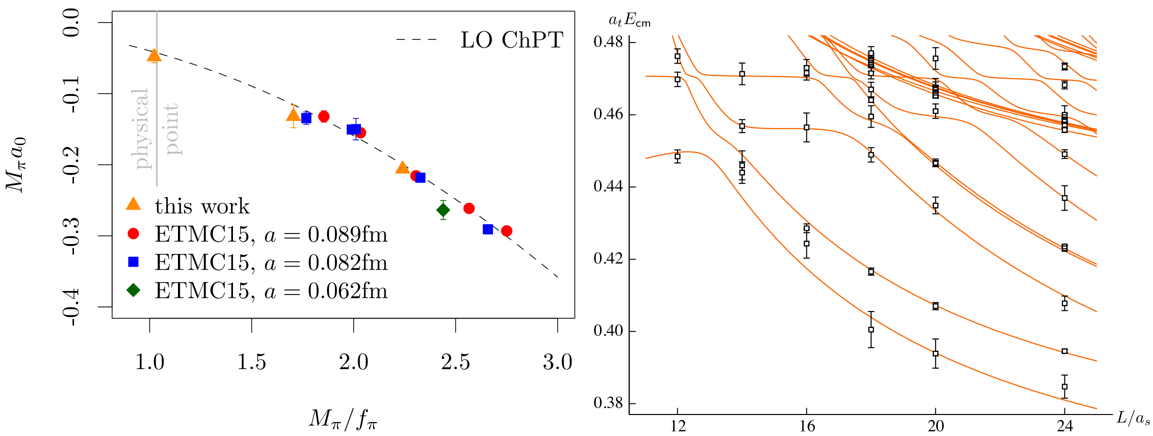

Figure 1: Studies of meson-meson interactions from lattice QCD range from precision calculations to technically challenging exploratory calculations. **Left:** Chiral dependence of the $I = 2$ $\pi\pi$ scattering length, including at different lattice spacings from Ref. [108]. **Right:** Volume dependence of the spectrum in a particular irrep from a recent calculation involving eight coupled scattering channels [109]. The fits of scattering-amplitude parametrizations require finding the solutions of the two-body quantization condition (orange lines) and correctly identifying them with the measured spectrum (open circles).

Figure 1. Some approaches to simplifying those fits are available in the literature [110, 111] and state-of-the-art exploratory studies include up to eight coupled channels [109, 112–114].

4. Meson-baryon interactions

Studies of meson-baryon scattering are considerably less advanced than those in the two-meson sector. Computing the requisite correlation functions suffers from a proliferation of Wick contractions as more valence quark fields are added, and the resulting correlation functions typically have a worse signal-to-noise ratio than their two-meson analogues.

Nevertheless there has been increased recent activity especially in studies of the $\Delta(1232)$ resonance [115, 116] (see also Fig. 2), which is the benchmark system for calculations of baryonic resonances, the 'ρ of baryons', because it decays virtually exclusively into $N\pi$. In addition to being a testbed for lattice QCD studies of baryonic resonances, the $\Delta(1232)$ is phenomenologically important for neutrino-nucleus scattering, and promising results were presented at this conference using both the Lüscher method [117, 118] as well as the HALQCD method [119].

Another low-lying baryonic structure that lattice QCD will soon be able to shed some light on is the $I = 0$, $S = -1$ $\Lambda(1405)$ resonance in the $\Sigma\pi$–$N\bar{K}$ coupled system [120, 121]. Results from a lattice calculation at $m_\pi = 200\,\text{MeV}$ were presented at this conference [118].

5. Baryon-baryon interactions

Baryon-baryon interactions are of fundamental importance to nuclear physics, from the formation of nuclei to being probed in astrophysical systems such as neutron stars. Consequently, two-baryon interactions have been studied for over a decade by several collaborations [122–134]. However, even simulations with pion masses $m_\pi \gtrsim 400\,\text{MeV}$, where the signal-to-noise problem is

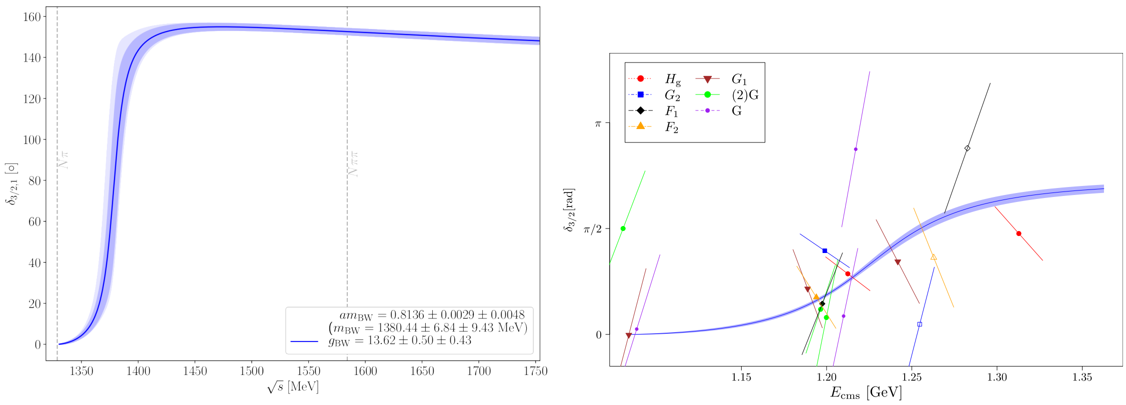

Figure 2: Recent determinations of the $N\pi$ scattering amplitude in the $I = 3/2$ channel showing the Δ resonance at $m_\pi = 255\,\text{MeV}$ (left, from Ref. [116]) and at close to physical pion mass (right, presented at this conference [117]).

much milder than at physical quark masses, have led to conflicting results regarding the existence of two-nucleon bound states at those heavy pion masses [135–137]. In view of the extreme challenges ahead – the deuteron binding is a permille-level effect at physical quark masses, yet accurate determinations of the two-nucleon interaction are a prerequisite for the computation of matrix elements involving two-nucleon states – those discrepancies even at heavy pion masses positively need to be resolved.

At the heart of the disagreement appears to be the question, alluded to in section 2, which set of interpolating operators enables a robust determination of the finite-volume spectrum in two-baryon systems. The calculations pioneered by the NPLQCD collaboration [122–128] employed creation operators resembling a compact six-quark object centered at spatial point $\vec{x}$,

$$\bar{O} \sim \bar{B}(\vec{x})\bar{B}(\vec{x}), \qquad \bar{B} \sim \epsilon_{abc}\, \bar{q}_a(\vec{x})\, \bar{q}_b(\vec{x})\, \bar{q}_c(\vec{x}), \tag{3}$$

where spin and flavor indices have been suppressed. Correlation functions involving such source operators can be computed using point sources[2] and do not require additional solutions of the Dirac equation compared to calculations of single-hadron correlation functions. The CalLat collaboration advocated using creation operators resembling two spatially displaced nucleons [134]

$$\bar{O}_{\vec{\Delta}} \sim \bar{B}(\vec{x})\bar{B}(\vec{x} + \vec{\Delta}), \tag{4}$$

which, through judicious choice of displacement vectors $\vec{\Delta}$, additionally provide improved overlap on sectors of higher partial waves, but require additional solutions of the Dirac equation for each such displacement. As discussed at previous installments of this conference, the spectra obtained using both of those strategies imply the existence of bound states in the $I = 0$ and $I = 1$ flavor sectors of NN scattering, at variance with results reported by the HALQCD collaboration at similarly heavy pion masses [135–137].

More recently, the spectroscopy methods which have proven successful for two-meson systems have been imported to studies of two-baryon systems. A direct comparison of results obtained

[2] *Point source* here refers to a quark source which is localized in a subregion of a time slice and does not preclude the use of smearing.

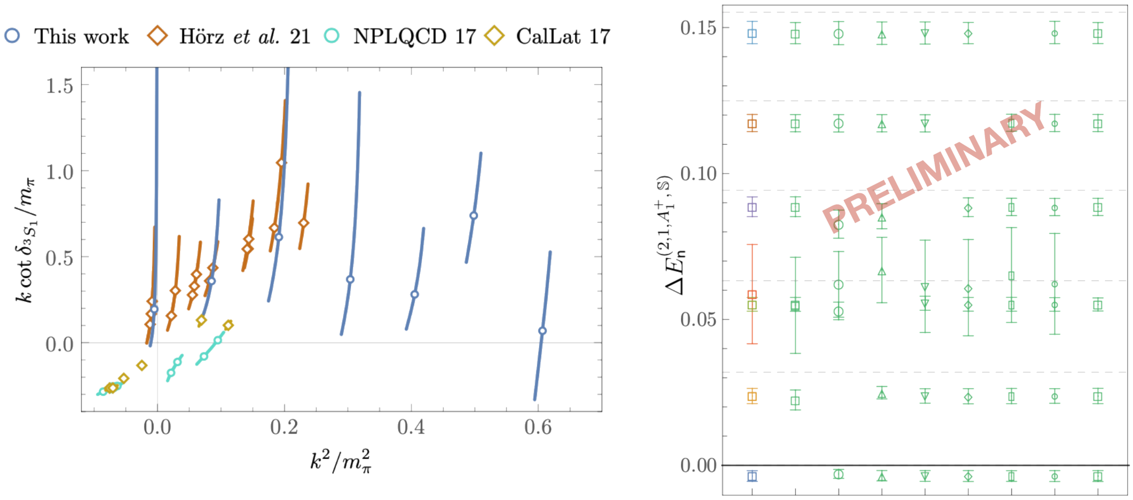

Figure 3: Left: S-wave NN scattering assuming higher partial waves to be negligible, based on nonhermitean correlation matrices (labeled NPLQCD '17 [128], CalLat '17 [134]) and Hermitean correlation matrices (labeled 'This work' and Hörz et al. '21 [138]). The sign of the intercept at $k^2 = 0$ determines whether or not there is a bound state in this system. **Right:** NN spectrum extracted without including operators of the form (3) (rightmost column) and including such operators (all other columns). An additional level is observed when a local six-quark operator is included. Both figures adapted from the talk by M. Wagman at this conference [139].

using either local six-quark source operators or creation operators resembling scattering states, where each baryon is projected to definite momentum individually,

$$\bar{O}_{\vec{p}_1\vec{p}_2} \sim \sum_{\vec{x}} \mathrm{e}^{i\vec{p}_1\vec{x}}\bar{B}(\vec{x}) \sum_{\vec{y}} \mathrm{e}^{i\vec{p}_2\vec{y}}\bar{B}(\vec{y}) \tag{5}$$

was first reported by the Mainz group [140]. Recent results for NN scattering based on Hermitean correlation matrices of such operators disfavor the existence of a bound state in either the deuteron or dineutron sector [138]. Finally, at this conference the NPLQCD collaboration presented new results for two-nucleon scattering using both localized and momentum-projected source operators, which confirm the utility of momentum-projected operators, but find an additional finite-volume state when localized operators are included (see Fig. 3).[3]

In summary, there is mounting evidence that creation operators of the form (5) are practically required to accurately obtain the finite-volume spectrum in the two-baryon sector. The appearance in the NPLQCD results of an additional finite-volume state compared to the number of states expected from enumerating the noninteracting two-baryon states warrants further investigation. A definitive demonstration of consistency between results using the HALQCD method and results based on the Lüscher approach should be achieved and will likely require a concerted effort to perform all flavors of calculations on a single gauge ensemble, such that all but methodological differences are eliminated as sources of systematic uncertainty.

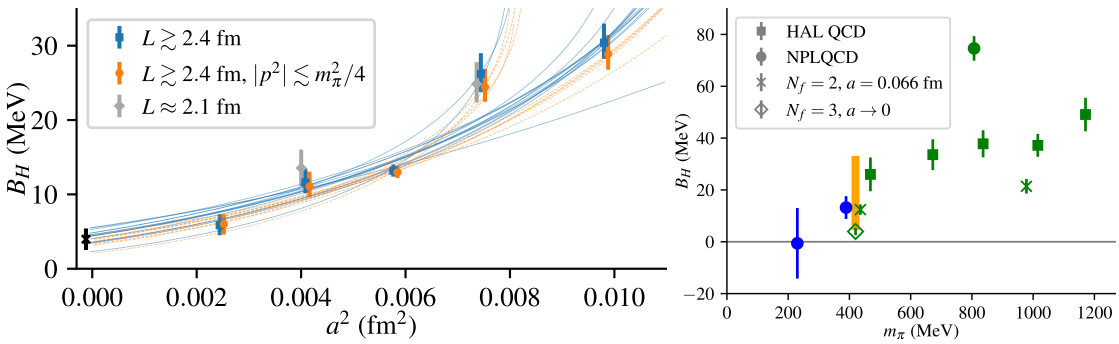

Figure 4: Significance of cutoff effects in the $I = 0$ $\Lambda\Lambda$ system [142]. **Left:** Continuum extrapolation of the H-dibaryon binding energy at $m_\pi = m_K \approx 420$ MeV. The solid curves are obtained from global fits to energy levels from several ensembles and are not fits to the point estimates from each ensemble shown as data points. **Right:** Overview of results for the chiral dependence of the H-dibaryon binding energy. The green diamond and orange band correspond to the binding energy in the continuum and range of binding energies at nonzero lattice spacing, respectively, shown on the left. All remaining data points are at nonzero lattice spacing.

6. Cutoff effects

Recent results by the Mainz group for the H-dibaryon at the SU(3)-flavor-symmetric point with $m_\pi = m_K \approx 420$ MeV highlight discretization effects as a significant source of systematic uncertainty [142]. As shown in Figure 4, the H-dibaryon binding energy in the continuum limit differs by almost a factor of eight from the binding energy obtained at their coarsest lattice spacing $a \approx 0.99$ fm using $O(a)$-improved Wilson fermions.

Such large discretization effects are perhaps somewhat surprising, given that cutoff effects were previously found to be rather mild at least in two-meson scattering amplitudes involving light and strange quarks, from the ρ resonance [85, 115] to the weak interactions of pseudoscalars at maximal isospin [103, 143]. Resonant systems manifest via sizable shifts of finite-volume energies from their noninteracting values, hence it might be reasonable to expect discretization effects to be less pronounced. Even in the weakly-interacting KK system at maximal isospin [143], however, discretization effects only amounted to a 20% effect, a far cry from the variation by a factor of eight observed in the H-dibaryon system.

The key question going forward is whether this enormous lattice-spacing dependence is a unique property of the isoscalar $\Lambda\Lambda$ system, or if other baryon-baryon interaction channels are equally affected. Some level of optimism could derive from baryon-baryon potentials obtained by the HALQCD collaboration, which show a repulsion at small distances for the two-nucleon system, but not for the $\Lambda\Lambda$ system [129]. Colloquially speaking, such a repulsion could prevent enlarged sensitivity to fluctuations near the lattice-spacing scale, and guidance from an effective-field-theory perspective would be desirable. If instead sizable discretization effects turn out to be a general feature of baryon-baryon systems [144], providing reliable QCD input for nuclear physics from lattice QCD will be much more computationally expensive than previously anticipated.

[3] The results have since appeared on the arXiv [141].

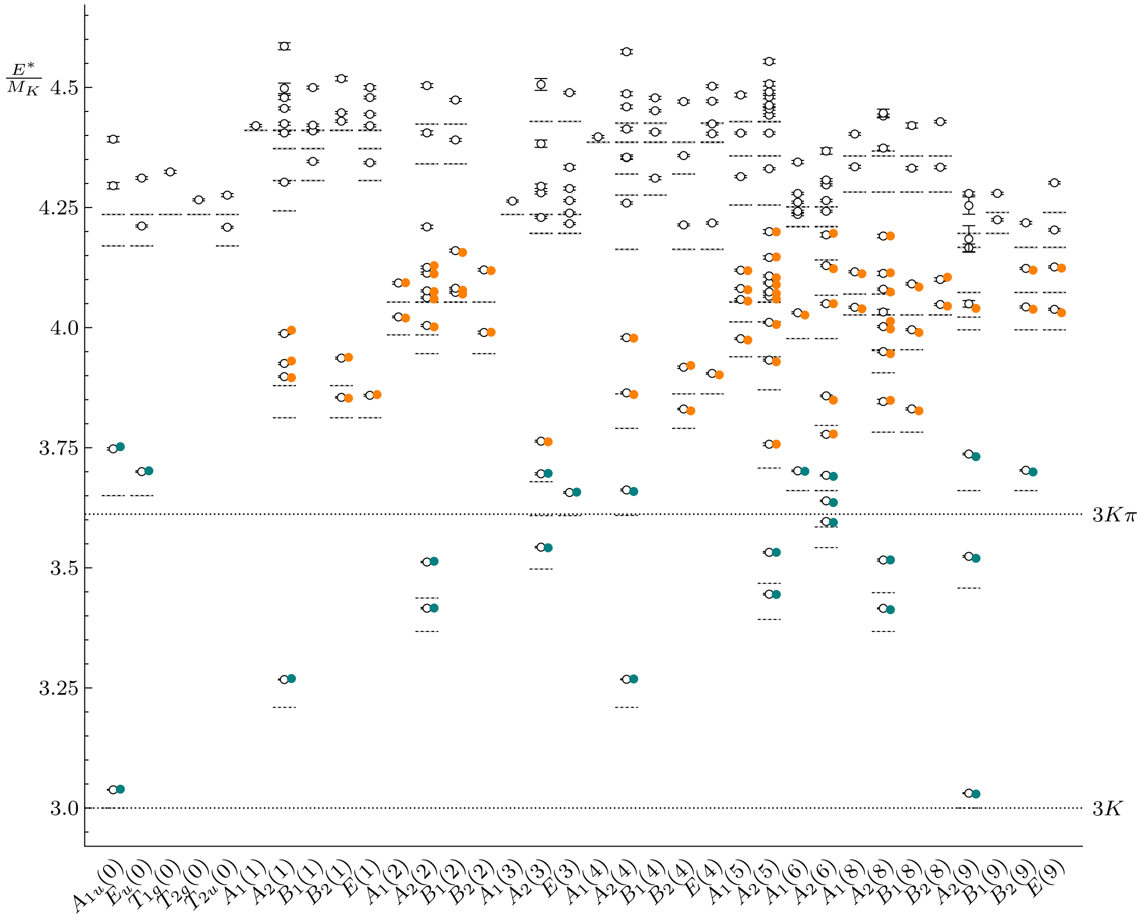

Figure 5: $I = 3/2$ three-kaon spectrum on a single ensemble from Ref. [145]. The irrep labels on the horizontal axis include the total momentum squared in parentheses. Short dashed horizontal lines in each irrep correspond to the expected energy spectrum in the noninteracting theory, white circles show the measured energies. Teal dots show the solutions of the three-hadron quantization condition which were used to fit the measured spectra, and orange dots are its predictions for higher-lying states. Good agreement is observed between measured and predicted energies, confirming to a good approximation the assumed decoupling of the $3K$- and the (four-body) $3K\pi$ sectors.

7. Three-hadron systems

A new frontier in lattice spectroscopy is in calculations of systems with more than two hadrons. Following the successful applications of the two-body formalism, a tremendous amount of work has been done over the last decade to generalize the theoretical foundations to the three-body sector [18–44, 53, 54], reviewed in Refs. [46, 47]. More recently, practical applications of the three-particle formalism have started to appear based on similarly comprehensive finite-volume spectra as are now common in the two-hadron sector.

Mirroring the evolution in the two-hadron sector, the first studies have been focussing on comparatively simple systems, namely the weakly interacting systems of three identical pions and kaons [108, 146–154]. In addition to being computationally tractable due to the high degree of symmetry, these systems present an ideal testbed for structured explorations of the three-body finite-

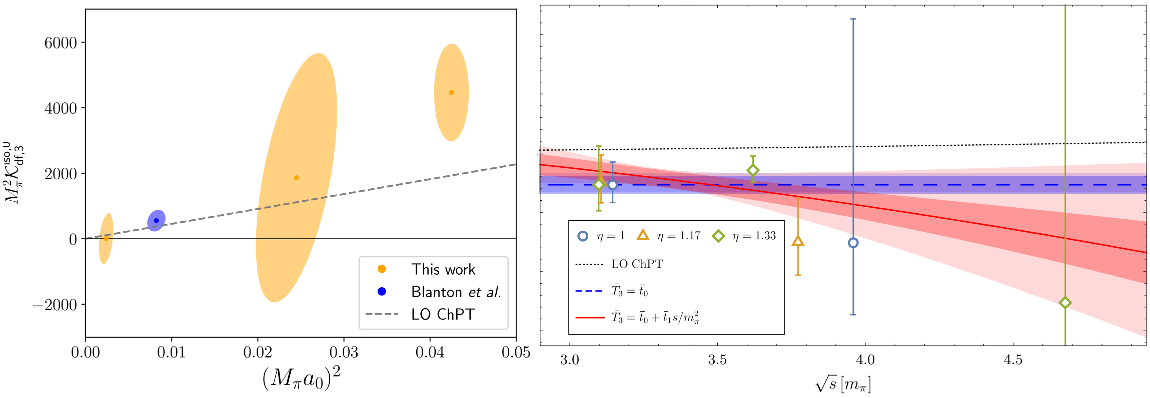

Figure 6: Three-pion interactions – **Left:** Chiral dependence of $\mathcal{K}^{\text{iso},0}_{\text{df},3}$, an intermediate quantity for three-pion scattering at threshold, from Ref. [108]. **Right:** Energy-dependent three-pion contact term on a single ensemble with $m_\pi = 220\,\text{MeV}$ from Ref. [154].

volume formalisms; chiral perturbation theory provides guidance for the pertinent interactions [148, 155], including their chiral behavior, and the weak interactions imply that no energy levels beyond those governed by the degeneracies in the noninteracting theory are expected.

A stringent test of both lattice spectroscopy methods and the three-body formalisms is thus furnished by reproducing the expected number of energy levels as shown in Figure 5 for recent results in the $I = 3/2$ three-kaon system. The three-body quantization conditions correctly predict not only the expected number of levels, but also the shifts from their respective noninteracting values, which are dominated by the effect of pairwise two-hadron interactions (see for instance the $1/L$ expansion in Ref. [34]).

While the two-body dominance complicates the extraction of the three-body interaction [108, 148, 151, 154] (examples shown in Figure 6), conversely three-hadron systems offer an enhanced sensitivity to their contributing two-hadron subchannels. Three-hadron systems may hence turn out to be a very useful tool for precision determinations of two-hadron interactions from the lattice.

Going beyond the weakly interacting systems, which have been used to demonstrate the validity of the three-body formalisms, a first peek at a resonant three-hadron system appeared just before the conference [156]. While this study is based on a relatively small number of energy levels, limiting the ability to constrain all relevant interaction terms, rapid progress in this direction will certainly continue.

8. Summary

Multi-hadron spectroscopy methods are relevant not only for improving our understanding of known and unearthing new hadron resonances, but also power auxiliary calculations for applications ranging from precision tests of the Standard Model to rooting nuclear physics in the fundamental theory. Distillation continues to prove very useful in this space, especially in view of its straightforward generalizability to systems composed of more than two hadrons. Sparsened all-to-all propagators, affording much the same flexibility as distillation, have produced encouraging results as well.

Calculations are performed for a breadth of physics applications. Studies of simple two-meson systems are becoming precision calculations addressing all sources of systematic uncertainty, and exploratory calculations are carried out for complicated meson-meson systems for instance in the context of exotic resonances. Computations of meson-baryon calculations are considerably less advanced, but picking up pace. Investigations of baryon-baryon interactions are progressing towards resolving the discrepant results in the literature, which have been the subject of heated discussions over the last years. The recent observation of large discretization effects in $\Lambda\Lambda$ scattering adds another facet, and an explanation for the (perhaps surprisingly) sizable cutoff effects would be desirable.

Interactions in three-hadron systems are a new frontier with rapid progress over the last two years. The generalization and practical implementation of the three-body finite-volume formalisms is progressing in step with more data becoming available from lattice simulations. While most of the practical results so far focussed on weakly interacting three-meson systems, a first peek at a three-meson resonance appeared very recently, and certainly more to follow suit soon.

Acknowledgments

I would like to thank the organizers for the invitation to present this talk at what has been an exceptionally well-run conference. Discussions with J. Green, A. Hanlon, D. Mohler, F. Romero-López, M. Wagman and A. Walker-Loud are gratefully acknowledged. This work was partially supported by the Laboratory Directed Research and Development Program of Lawrence Berkeley National Laboratory under U.S. Department of Energy Contract No. DE-AC02-05CH11231.

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