Multi-hadron systems in lattice QCD

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Abstract. I present an overview of recent progress in the study of multi-hadron systems in lattice QCD. After reviewing the recent developments that are beginning to enable nuclear physics to be studied from the underlying theory of the Standard Model, I discuss the recent results that have been obtained in multi-hadron systems. I also explore the difficulties particular to lattice QCD calculations of such systems and emphasise the issues that remain to be resolved.

1 Introduction

At a fundamental level, nuclei and nuclear physics arise from the Standard Model of particle physics which describes how matter interacts through Quantum Chromodynamics (QCD) and the electromagnetic and weak (electroweak) forces. For the relatively low energies that are relevant for nuclear physics, only a few parameters of the Standard Model are typically relevant, the light quark and electron masses, the QCD scale $\Lambda_{\text{QCD}}$, and the coupling to electromagnetism, $\alpha_{\text{f.s}}$. Remarkably, from these simple inputs, the whole complexity of nuclear physics, with all its fine-tunings and intricate structure, emerges. Nevertheless calculations involving the strong interaction are enormously challenging, and demonstrating this emergence is beyond our current abilities. To date, the only systematic tool with which to perform the required calculations is lattice QCD (LQCD). In this approach, space-time is discretised and QCD is numerically solved on a space-time lattice; for realistic calculations, this requires highly optimised algorithms and cutting-edge supercomputing resources. LQCD calculations have led to important insights in particle physics and are critical ingredients in the determination of the parameters of the Standard Model.

In recent years the application of LQCD to the intrinsically more complex realm of nuclear physics has begun in earnest. This is a challenging task as nuclei are complicated systems with many important energy scales, ranging from nuclear excitations that can be just a few tens of keV through nuclear bindings of a few MeV per nucleon, to hadronic energies and excitations $\sim A_{\text{QCD}} \sim 300$ MeV, all the way to the total energy of the system (a few hundred GeV). Nevertheless, this is an important endeavour as it will ultimately place nuclear physics on the firm foundation of the Standard Model. Progress over the last few years has been significant, and the goal of this contribution is to highlight this in the context of light nuclei and other multi-hadron systems.

I begin with a discussion of our theoretical understanding of multi-hadron systems and overview recent numerical studies, starting with multi-meson systems, moving to baryon number $B = 2$ bound states, and then to larger $B$ systems. After presenting this overview of the current state of the field, I discuss current issues and future challenges that must be faced in order to provide a truly \textit{ab initio} approach to nuclear physics.

2 Approaching nuclear physics in lattice QCD

Of the various components of the Standard Model, the most challenging piece to deal with in the low-energy regime is the strong interaction, described by QCD. The difficulties arise because of the non-perturbative nature of strong interactions at long distances ($r > 0.1$ fm). For the majority of our discussion, we shall consequently ignore the electroweak interactions and focus on QCD which is defined in Euclidean space by the partition function

$$Z_{\text{QCD}} = \int \mathcal{D}A_\mu \mathcal{D}\bar{q} \mathcal{D}q \exp\{-S_{\text{QCD}}[A, \bar{q}, q]\}$$

$$= \int \mathcal{D}A_\mu \det M[A] \exp\{-S_{\text{g}}[A]\},$$

where $A_\mu$ and $q$ are the gluon and quark fields, respectively, and, defining $D_\mu = \partial_\mu - igA_\mu$ and $F_{\mu\nu} = [D_\mu, D_\nu]$,
\[
S_{\text{QCD}}[A, \eta, q] = \int d^4x \left[ -\frac{1}{2} \text{tr} F^{\mu \nu} F_{\mu \nu} + \eta (iD - m) q \right]
\]  

is the QCD action. In the second line of eq. (1), we have integrated over the fermionic degrees of freedom where \( S_\eta[A] \) is the purely gluonic part of the action and \( M[A] \) is the Dirac operator. The focus of our discussion will be on spectroscopy which is enabled by measurement of two-point correlation functions defined for some set of quantum numbers \( \{Q\} \) by

\[
C_{\{Q\}}(t) = \frac{1}{Z} \int DA_\mu D\eta Dq \tilde{O}_Q(t) O^\dagger_Q(0) e^{-S_{\text{QCD}}[A, \eta, q]} = \frac{1}{Z} \int DA_\mu \tilde{O}_Q(t) O^\dagger_Q(0) \det M[A] e^{-S_\eta[A]},
\]

where the composite operators \( O_Q^\dagger \) and \( \tilde{O}_Q \) create and annihilate states with the quantum numbers \( Q \). For brevity, we have suppressed the spatial structure of such operators which may be used to project to a fixed momentum for example. The Euclidean time behaviour of such correlation functions is determined by the energies of the QCD eigenstates with the requisite quantum numbers and by the specific forms of the operators. By determining \( C_{\{Q\}}(t) \) numerically, we can extract the eigenenergies.

To render the calculation finite, we discretise space-time and impose boundary conditions which we take to be periodic in spatial directions and periodic (anti-periodic) in time for bosons (fermions). The gluon degrees of freedom are implemented through \( SU(3) \)-valued link variables \( U_\mu(x) = \exp[i A_\mu(x)] \); for details of the various discretised forms of the QCD action we refer the reader to the extensive literature (see, for example, ref. [1]). In order to perform the requisite functional integrals over the gluon fields, we use importance sampling, recognising that the factor \( P[U] = \det M[U] e^{-S_\eta[U]} \) can be interpreted as a Boltzmann weight as we work in Euclidean space. By generating an ensemble of configurations of the gluon link variables according to the probability measure that this encodes, we are able to estimate the correlation function \( C_{\{Q\}} \) reliably. For an ensemble of \( N \) configurations, \( \{U_\mu^{[1]}, U_\mu^{[2]}, \ldots, U_\mu^{[N]}\} \),

\[
C_{\{Q\}}(t) = \frac{1}{N} \sum_{c=1}^{N} \tilde{O}_Q(t) O^\dagger_Q(0) \left[ U_\mu^{[c]} \right] + \mathcal{O} \left( N^{-1/2} \right),
\]

with uncertainties that decrease as the size of the ensemble increases.

To generate such ensembles, requires algorithms that efficiently and effectively explore the space of possible gluon configurations and, because of the 4-dimensional nature of space-time and the non-locality of \( P[U] \), this is a challenging problem, requiring supercomputing resources. The necessary machinery has been developed over the last few decades, culminating, for example, in the last few years in increasingly precise determinations of many quantities of importance to particle physics and of the baryon number \( B = 0, 1 \) ground-state hadron spectrum with fully controlled statistical and systematic uncertainties [2] (these results have been nicely reviewed recently in refs. [3,4]). This is an important achievement as, when compared to experimental measurements, it demonstrates that QCD describes the strongly interacting regime of the strong interaction and that lattice QCD provides a systematic and reliable tool for the computation of hadronic contributions to Standard Model observables. It also demonstrates that the field of LQCD is at a point where more computationally challenging problems, such as many of those encompassed by nuclear physics, can begin to be tackled. A number of groups have recently taken up the task of applying LQCD to the nuclear physics of few hadron systems and significant progress has been made. A discussion of this progress, its interconnections to effective field theory, and the issues that still remain is the subject of this review.

Although we are interested in the Minkowski space physics of an infinite volume, lattice calculations are by necessity performed in Euclidean space and in a finite volume. The restriction to Euclidean space places fundamental constraints on the physics that can be extracted [5], or at least constrains the way in which we can access particular physical observables. Similarly, the imposition of boundary conditions to reduce the system to a finite volume modifies the system in the infrared regime and must be accounted for. Nevertheless, for many single hadron observables, the analytic structure of the relevant correlators is such that Wick rotation does not present an obstruction, and for single hadron correlation functions in the low-energy regime, chiral perturbation theory allows a model-independent extrapolation to infinite volume. However, for infinite-volume extrapolations of higher-energy observables, such as form factors at momentum transfers, \( Q > 1 \text{ GeV} \), we must currently rely on more phenomenological approaches.

Multi-hadron systems present a more complex problem, and one in which effective field theory plays an important role. Understanding systems with the quantum numbers of multiple hadrons is, in essence, a matching of QCD correlations onto equivalent correlation functions in an effective hadronic description and this hadronic description is important in defining the observables that can be computed. Hadrons are emergent collective degrees of freedom that arise from QCD dynamics but they are the degrees of freedom that we are necessarily interested in as they define the asymptotic states of the infinite volume theory. QCD correlations that are amenable to an effective hadronic description are those in which it makes sense to consider dominant contributions from a finite, hopefully small, number of hadronic degrees of freedom. Chiral perturbation theory provides such a description at low energy, but the concept is more general. For example, an effective hadronic description of the nucleon matrix element of the vector current at multi-GeV momentum transfer exists, but a chiral expansion of the process is not useful because of the large momentum. In lattice calculations of the three point functions that probe such a matrix ele-
ment, the dominant contribution at large Euclidean times comes from transitions between single-nucleon states at rest and boosted to the high energy scale (we ignore lattice discretisation artifacts here). Contributions from internal excitations of the nucleon and from nucleon+pion multi-hadron states\(^1\) are suppressed in our Euclidean correlation functions by the relevant energy gap and only become important at early times.

For multi-hadron systems, an effective hadronic description allows us to understand the connection between Euclidean space lattice calculations and the Minkowski space hadronic quantities of the real world. Provided an effective hadronic description exists, analytic continuation becomes ambiguous. An example is provided by correlators with the quantum numbers of a minimum of two stable particles; a corresponding two-particle state is not extracted at any value of the Euclidean time. If the hadronic description is too complex to determine cleanly through matching to Euclidean QCD correlations, analytic continuation becomes ambiguous. A number of a minimum of two stable hadrons (for example, \(I = 2\) \(J = 0\), even parity, corresponding most simply to two pion systems). In a finite volume, and at energies far below the inelastic threshold, the long time behaviour of the hadronic theory is dominated by two-body states of the lightest hadrons that can produce the required quantum numbers. In the absence of bound states, the most important contribution at large Euclidean times is from the two-hadron states at rest in the corresponding center-of-mass (CoM) frame, but sub-leading contamination arises from two hadron state moving back to back in the CoM frame and from internal excitations of the hadrons. By careful analysis of multiple different correlators with the given quantum numbers, it is possible to extract information about these states. Crucially, the hadronic description allows us to understand the analytic structure of the two-hadron correlators in this regime and determinations of the energies of these states translate to extractions of the scattering phase shift through the Lüscher formalism [6,7]. At earlier times or with more complicated sets of correlation functions, contributions from higher-energy states of the given quantum numbers begin to be resolved and eventually more complex \(N > 2\) hadron states make significant contributions, resulting in different analytic structure in the correlation function. If we can construct an effective hadronic description in this regime and determine enough information (at high enough precision) about the various contributions by matching to the finite-volume, Euclidean QCD correlators, we can in principle determine infinite-volume Minkowski space information in the inelastic regime. If such an hadronic description is ambiguous, then model dependence necessarily arises. It should be noted that the effectiveness of a hadronic description is volume dependent; as the volume increases, the number of finite-volume states in a given energy range increases making a hadronic description more cumbersome. If one is interested in information about states other than the ground state, this becomes increasingly difficult to reliably extract — an important part of the obstruction discussed many years ago by Maiani and Testa [5].

In what follows, I will focus primarily on bound-state energies and properties, but there has been significant recent progress in constructing generalisations of the so-called Lüscher formalism to deal with scattering states which I shall briefly summarise as it provides a specific realisation of the more abstract discussion of the preceding paragraphs. Following earlier works on quantum mechanical systems, Lüscher showed [6,7] that the spectrum of two-particle states in a Euclidean quantum field theory in a finite volume is connected in a calculable way to the phase shift of the two-particle interaction and can thus be used to determine the phase shift at discrete values of energy up to the inelastic threshold. A particularly simple way to arrive at the eigenvalue equation that defines the Lüscher formalism is to consider the scattering process in terms of a hadronic effective field theory as first proposed in [8], and this approach has been taken up in the analysis of various two-particle channels in refs. [9–15]. The Lüscher formalism has been used extensively to study the scattering phase shifts of many different meson-meson, meson-baryon and baryon-baryon systems.

Eigenstates of the lattice calculation are classified by the irreducible representations of the appropriate symmetry group (for a cubic spatial volume and a spatially isotropic discretisation, this is the octahedral group and its double covering) and are more constrained than in the continuum, infinite-volume limit. Two-particle eigenenergies hence determine a combination of the infinite-volume partial wave phase shifts. The symmetries are further reduced when the eigenstates that are studied are boosted relative to the lattice boundary conditions, or when a rectangular rather than cubic spatial volume is considered (see refs. [16,17] in the latter case). For moving systems, Rummukainen and Gottlieb [18] provided the first analysis and this has been generalised in recent years [19–26]. By performing different boosts of the system, many more energy eigenstates can be accessed in a single lattice calculation, resulting in a more detailed extraction of phases shifts. Boosted systems of unequal mass have been treated in refs. [27,28] and boosted bound states have been investigated in refs. [29,30]. Scattering in the case of multiple channels has been considered in a number of contexts in refs. [23–25,31–34] and a detailed investigation of higher partial waves has been recently presented in ref. [35]. A number of other interesting developments have also been reported recently [36–40].

For three-body systems, investigations based on effective field theory have been presented in refs. [41–47]. In principle, the program developed in these works allows multi-hadron interactions to be extracted from a detailed analysis of the QCD spectra of two- and three-hadron systems at finite volume. However, such an analysis has only been attempted in the case of pion systems [48–51]. Further work in generalising this to higher-body systems is important for our understanding of lattice calculations of such systems.

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1. This is very loose terminology as the ground state should not be thought of as a bare object to which pions are added to get an excited state.
2. At a minimum, stable under the strong interaction.
3 Many-hadron contractions

A major part of the challenge of nuclear physics is in the complexity of the many-body problem that it encompasses. Even at the level of an effective description of nuclei in terms of nucleons, the combinatorics of multi-nucleon systems provide limitations to our ability to perform calculations [52], and for large $A$, techniques that do not explicitly treat the $A$ nucleons are currently necessary. At the fundamental level of QCD, the problem is seemingly even more difficult as each nucleon is made up of a minimum of three quarks.

The machinery of calculating hadronic observables in LQCD begins with the construction of correlation functions as in eq. (3). For simple quantities such as energies, a source and sink are chosen where, by the choice of appropriate combinations of quark and antiquark fields, states with the quantum numbers of the system in question are created and destroyed, respectively. To evaluate this matrix element, the creation and annihilation operators in the quark fields must be paired in all possible ways, forming various different Wick contractions. For a given nuclear system with atomic number $A$ and proton number $Z$, the number of such contractions is $N_{\text{contractions}} = \prod_f N_f! = (2A - Z)!(A + Z)!$ where $N_f$ is the number of quarks of flavour $f$, and the product runs over all such flavours (the second equality only follows for non-strange systems). Their evaluation is consequently an exponentially difficult task for systems with large numbers of particles. The presence of symmetries, Pauli blocking and cancellations amongst contractions means that this counting can be a vast overestimate, but determining the minimal set of contractions is a non-trivial task.

For the case of systems with zero baryon number but large isospin charge, $I_z$ (which naively correspond to large numbers of charged pions), efficient algorithms have been developed to perform the required contractions. The first approach [50] to be developed was recursive and is based on forming partly contracted hadronic blocks which can then be combined sequentially to produce many pion correlation functions. An alternative, more efficient, approach was developed in refs. [53,54] and makes use of modified fast-Fourier techniques. This later approach has been used in numerical calculations of systems with isospin charge up to $I_z = 72$ as discussed below. By constructing appropriate blocks, these approaches can also be applied for more general mesonic systems, including those with $I_z < |I|$, and to calculating three-point multi-meson correlation functions to study multi-meson matrix elements.

In refs. [55,56], algorithms have been developed to perform the more complex contractions that appear in multi-baryon systems with the aim of allowing studies of systems with large numbers of baryons. The fundamental approach used in both of these works is to perform contractions by iterating over a simplified list of indices of quark fields and corresponding weights. Where they differ is in the method used to construct such lists; ref. [55] iterates over the full, factorially large set of possible index values, whereas ref. [56] constructs the index lists recursively by building a multi-baryon system up one baryon at a time.

The former algorithm suffers from a scalability issue and requires supercomputing resources [55] to construct lists even for $A = 4$, and, given this, it is unlikely that the approach can be usefully applied far beyond that point. In contrast, the recursive approach of ref. [56], running on a laptop, has been used to produce contraction code for correlators with the quantum numbers of a large range of nuclei including $^4$He, $^8$Be, $^{12}$C, $^{16}$O and $^{28}$Si, and these codes have been used to compute correlation functions with the quantum numbers of these systems for the first time, as will be discussed below. Very recently, a recursion-based multi-baryon algorithm has appeared in ref. [57] that additionally performs the multiplications of terms in the index lists recursively. In all of these approaches, there is still an intrinsically poor scaling with baryon number implied for all but the simplest choices of multi-baryon operators. For the simplest operators, the cost of contractions in manageable as it scales as $A^3$, but more complex operators require a larger set of terms (in the worst case, growing factorially with $A$) to be considered and there is considerable room for further improvements.

4 Many-meson systems

The many-body nature of nuclei has made their investigation appear to be an almost impossible task for lattice QCD for the reasons that have been discussed above. For this reason significant effort has been devoted to studying simpler multi-hadron systems, those with the quantum numbers of many pseudoscalar mesons [48–51,54] which do not suffer from the statistical noise problems that appear in other cases. These studies have proved useful in a number of regards. They have enabled investigations of the physics of systems at non-zero isospin density (as an example, the ratio of the energy density of isospin charged matter to the Stefan-Boltzmann expectation is shown as a function of the isospin charge density in fig. 1) and allowed the first QCD determination of a
Fig. 2. Summary of the results obtained in $n_f = 2 + 1$ or $n_f = 3$ lattice QCD calculations of the binding energies of the deuteron, di-neutron, $H$-dibaryon and the strangeness $s = -4 \Xi^- \Xi^-$ system. In the case of the deuteron, the red circle corresponds to the experimentally determined binding energy. For the $H$-dibaryon, the results labelled HALQCD and NPLQCD 1206.5219 use three degenerate flavours of quarks and the point at $m_\pi = 230$ MeV (NPLQCD 1103.2821) should be treated with caution as no infinite-volume extrapolation has been performed.

Fig. 3. Effective mass plots for one of the $H$-dibaryon correlators studied in ref. [67] on three different volumes (3.4, 4.5 and 6.7 fm from left to right, respectively) that lead in the infinite-volume limit to the result indicated by the upright triangle in the lower left panel of fig. 2. The horizontal line indicates the two-hadron threshold.

three hadron interaction. In addition, the non-zero isospin density medium created by these correlation functions has been used to investigate its influence on other observables such as quarkonium [58, 59] and pion structure [60].

### 5 Dibaryons

The last few years have seen remarkable progress in lattice calculations of baryon number $B = 2$ systems (dibaryons). In ref. [61], the first calculation of a QCD bound state with $B > 1$ was presented by the NPLQCD Collaboration, albeit at unphysical values of the quark masses corresponding to $m_\pi \sim 390$ MeV. That calculation concerned the so-called $H$-dibaryon postulated many years ago by R. Jaffe [62]. Subsequent works have considered the $H$-dibaryon further and have also looked at the deuteron, di-neutron and other more exotic channels [63–68]. The results of these calculations are summarised in fig. 2 for the deuteron, di-neutron, $H$-dibaryon and the strangeness $s = -4 \Xi^- \Xi^-$ system (for other channels where there are fewer calculations, the reader is referred to the orig-
Fig. 4. Summary of the results obtained in $n_f = 2 + 1$ or $n_f = 3$ lattice QCD calculations of the binding energies of $^3$He, $^3\Lambda$H, $^4$He and $^4\Lambda$He. The red circles correspond to the physical binding energies (for $^4\Lambda$He experimental determinations of both iso-doublet states are shown). For $^3\Lambda$He, both $J^P = 1/2$ and $3/2$ states were extracted, with the higher-spin state being more tightly bound for this $SU(3)$ symmetric quark mass.

In both of the two nucleon channels, it is apparent that these systems become more bound as the quark masses increase and a naive linear fit suggests consistency with the bound deuteron and near-threshold di-neutron system at the physical quark masses. The $H$-dibaryon is predicted to be very close to threshold at the physical masses, but further calculations at lighter quark masses are required to directly ascertain its nature and, as it appears to be a finely tuned system, care must be taken to ensure that the effects of discretisation, isospin breaking and electroweak contributions are correctly accounted for. In the case of the $H$-dibaryon, it is also apparent that there is a significant discrepancy between the $SU(3)_f$ symmetric NPLQCD and HALQCD calculations at $m_\pi \sim 800$ MeV which is further exacerbated by the non-observation of bound deuteron and di-neutron states at this mass by the HALQCD Collaboration [66]. These two sets of calculations have fairly similar lattice discretisations and volumes and the minor differences are unlikely to account for the discrepancy. These calculations also differ in methodology, with NPLQCD (and PACS-CS) performing spectroscopy in multiple volumes (see fig. 3 for representative effective mass plots from the study in ref. [67]) and HALQCD using the “potential method” (see ref. [69] for a review). These differences suggest that there may be systematic effects that are underestimated in one or both approaches and it is important to resolve this discrepancy.

6 Larger nuclei and hypernuclei

The study of baryon number $B > 2$ multi-baryon states began a few years ago with a high-statistics study of the $\Xi^0\Xi^0n$ and triton systems by the NPLQCD Collaboration [70] at light quark masses corresponding to $m_\pi \sim 390$ MeV (in the relatively small volume used in this work, both states were consistent with being unbound). This study was followed up and extended by the PACS-CS Collaboration who have investigated $^3$He and $^4$He first in quenched QCD [71] and very recently in QCD with quark masses corresponding to $m_\pi \sim 500$ MeV [68]. In both later studies, the binding energies of these states were found to be reasonably close to those measured in the experiment despite the unphysical nature of the calculations. After developing new contraction methods discussed above [56], the NPLQCD Collaboration have performed a comprehensive calculation of a large number of phenomenologically relevant nuclei and hyper-nuclei for $A < 5$, albeit at a heavy quark mass corresponding to $m_\pi \sim 800$ MeV [67]. Figure 4 shows a summary of the binding energies of the

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3 We note that the calculations discussed here are performed at essentially one lattice spacing, $a \sim 0.1$–0.12 fm. It is expected that lattice artifacts produce sub-leading modifications to the results discussed herein.
strangeness, \( s = 0 \) and \( s = -1 \) three- and four-body systems that have been investigated, and fig. 5 shows results for these and the other more exotic systems investigated in ref. [67].

The improved contraction methods discussed above also enabled the construction of correlation functions with the quantum numbers of significantly larger nuclei such as \( ^8 \text{Be}, \ ^{12} \text{C}, \ ^{16} \text{O} \) and \( ^{28} \text{Si} \) [56], opening the way for studies of these systems. Examples of these correlations are shown in fig. 6, and while the correlators for \( A < 20 \) show signs of the expected approach to single exponential behaviour, no statistically meaningful binding energies could be extracted at the statistical precision used in this preliminary investigation. Indeed, it appears that the noise is becoming exponentially worse (with a small prefactor) as \( A \) increases for these particular choices of interpolators, which involve multiple lower components of quark fields, and further improvements are required. Even with high-statistics and improved interpolators, the presence of very closely spaced excitations in these complex systems will make extraction of the ground-state energy a challenge as will be discussed below.

From these studies, we can tentatively conclude that light nuclei generically become more deeply bound as the quark masses increase. Clearly there is a long way to go before these calculations make direct contact with experiment, but at least in cases where a trend can be established as a function of quark mass, the trend is towards the experimental result. Even at unphysical quark masses, such as those used in the above studies, it is of broad interest to pursue such calculations as they provide information about possible alternate versions of the Universe. In looking at nuclear physics in a broader context, it is natural to ask how sensitive the structure and evolution of our Universe is to the fundamental parameters (for all but the earliest times, this is the realm of nuclear physics and, as discussed in the introduction, the only relevant parameters are \( \Lambda_{\text{QCD}} \), the fine structure constant \( \alpha_{f.s.} \sim \frac{1}{137} \), and the light quark and electron masses) and it is likely that useful constraints can be determined from \textit{ab initio} studies. For example, Big Bang Nucleosynthesis is determined by a network of reactions of light nuclei that may plausibly be investigated in future LQCD calculations. In addition, such calculations offer the prospect of understanding how finely tuned processes such as carbon production through the triple-\( \alpha \) process are. Studies of smaller \( A \) systems in LQCD (which will be computationally feasible in the near future) also have phenomenological impact as they can be used to constrain effective field theory based approaches and thereby play an important role in predictions for larger systems (see ref. [72] for recent work in this direction). Already, we are gaining surprising insights about such fine-tunings. In ref. [73] the ratios of the scattering lengths to effective ranges of the \( ^3S_1 \) and \( ^1S_0 \) nucleon-nucleon interactions were studied at \( m_\pi \sim 800 \text{MeV} \). There it was shown that in the deuteron channel, the fine-tuning of the system that such a ratio characterises extends from the physical point over a large range of quark masses. It is very interesting to see in which other systems, and for which parameter ranges, such behaviour occurs.

7 Current issues and future challenges

As discussed above, significant progress has been made in the last few years, but the current studies are clearly only the beginning of the application of lattice QCD to nuclear physics. A number of important issues remain to be understood and further improvements in our methods need to be made. In the following, I summarise these challenges as they appear at the present time.

7.1 Statistical precision

Since nuclear physics entails small energies on the scale of QCD, high-precision calculations are important, requiring precise statistical sampling of correlation functions. As discussed in ref. [74], the choice of interpolating operators that are used for a particular set of quantum numbers is critical and can be used to some degree to delay the onset of the noisiest contributions to a given correlation function. It is important to systematise these findings and understand to what extent such noise-reducing optimisations can be implemented.

Statistical noise in many-hadron correlation functions is related, at least indirectly, to the so-called sign problem [75,76] that plagues LQCD calculations at non-zero quark chemical potential. A recent study of the 2+1 dimensional Nambu–Jona-Lasinio model [77] (a model similar in some regards to QCD) has suggested that the noise problem is intimately related to spontaneous chiral symmetry breaking and that the sign problem in QCD at non-zero baryon chemical potential may be ameliorated by formulating the calculations in terms of different degrees of freedom that treat pions explicitly. No specific method to do this is proposed, but it is an intriguing analysis that also has a bearing on the issue of noise.

\[ \text{Fig. 5. Spectrum of light nuclei and hypernuclei studied in ref. [67]. The SU(3)_f flavour symmetry results in unphysical degeneracies. (Redrawn from ref. [67].)} \]
The sampling of configurations representative of the vacuum encoded in eq. (4) is a particularly inefficient way to determine properties of nuclei, states that are very different from the vacuum. It is possible that a reorganisation of the calculation by moving an appropriate part of the multi-nucleon observable into the Boltzmann weight will result in better statistical determination of multi-hadron correlations. However, it is not known how to do this effectively while maintaining positivity of the integration measure, and such a technique would most likely be implemented on an observable-by-observable basis and would therefore be a computationally demanding undertaking.

7.2 Beyond spectroscopy

While most efforts in lattice QCD for nuclear physics currently focus on the spectroscopy of multi-hadron systems, these systems also present a rich set of more complicated observables that are of phenomenological interest. For example, a precise determination of the matrix elements of the axial current in two-nucleon systems would impact our understanding of the pp fusion process that powers the sun and the $\nu d \rightarrow n p$ breakup process used as a neutrino detection mode in the Sudbury Neutrino Observatory. In refs. [17, 78], the problem of determining such matrix elements has begun to be addressed. It is also of interest to determine the matrix elements of unstable states such as the $\Delta$ or $\rho$ resonances (although care needs to be applied in the definition of such matrix elements) and in ref. [79] a possible approach to this problem was discussed. In ref. [60], a first numerical investigation of matrix elements of multi-hadron systems has been presented although it is still a work in progress. Here, the focus has been on determining the first moment of the parton distribution of systems with the quantum numbers of $n = 1, \ldots, 12$ charged pions. Since the operator insertion is local, these results can be interpreted as the modification of the single-pion parton distribution in a medium with varying isospin charge and is a direct analogue of the famous EMC effect in nuclei.

Clearly, many improvements and advances in our theoretical understanding are required to allow QCD calculations of the large range of multi-hadron properties and transitions that are of interest to the experimental and phenomenological nuclear physics communities. It will also be important to understand to what extent we can extract information about more complicated nuclear reactions from lattice calculations.

7.3 How large is a large volume?

In the analysis of two particle systems in finite volume, a requirement for the validity of the Lüscher approach discussed above is that the system size is large compared to the range of the interaction which is typically set by the Compton wavelength of the pion for light pions (at large quark masses, other scales become important [73]). For bound states, the lattice volume must additionally be large compared to the size of the bound state, the scale of which is set by the binding momentum of the system, $\gamma$; this second constraint is more stringent for shallow bound states which can be large even on the scale of the pion Compton wavelength. As discussed in ref. [80], the Lüscher method also requires volumes large enough that the spectrum of
states is dense enough that finite-volume sums provide a good approximation to infinite-volume integrals. Similar constraints will also arise for higher-body systems. There remains a question as to what large means: does \( m_\gamma L \), \( \gamma L > 4 \) suffice? Or are the requirements more stringent? Precise calculations are needed to address this question, both at “large” volumes in the region where asymptotic behaviour can be clearly confirmed, but also in “small” volumes where deviations from theoretical expectations can be demonstrated. For precise results, it is important to mark out the region in which systematics such as these are well controlled.

It is likely that a number of earlier calculations with \( m_\gamma L \sim 4 \) have additional systematic uncertainties from volume dependence that is not controlled by the L"uscher approach (particularly is cases where there is a shallow bound state). For example, in the NPLQCD calculations of bound states at \( m_\pi \sim 390 \) MeV \cite{61,64}, data for \( L = 2.0 \) and 2.5 fm (corresponding to \( m_\pi L = 3.9 \) and 4.9, respectively) were dropped for this reason, and similar exclusions may need to be made elsewhere.

### 7.4 Lattice potentials

The HALQCD Collaboration has pursued a method of extracting inter-hadron potentials for two-baryon and three-baryon systems (see ref. \cite{69} for a recent review). For two hadrons, the approach proceeds by constructing a Nambu-Bethe-Salpeter wave function from correlators that separate the two hadrons at the sink by a distance \( r \) (defined up to an intrinsic uncertainty of \( O(A_{\text{QCD}}^{-1}) \)) \footnote{The method follows that of refs. \cite{80–82}, applied for hadron separations inside the range of the interaction.}. Since the potentials that have been extracted are local, they are by definition, energy dependent and, from an \textit{ab initio} point of view, contain exactly the same information as the phase shift evaluated at the energy of the two hadron system in the lattice calculation. With the assumption of slowly varying behaviour of the phase shift, small extrapolations in energy may be justified; however such assumptions are invalid when the system becomes interesting because of resonance structures and threshold effects. Extrapolations of phase shifts to \( p \sim 300 \) MeV from two-baryon systems calculated essentially at rest (such as those presented in refs. \cite{66,69,83}) should be viewed with caution. The extracted potentials also depend on the sink-interpolating operators used in the calculation \cite{84–86} with significant modifications seen at short hadron separations from different smearings of the quark fields \cite{87}, for example. This is expected as potentials are not observable quantities. Indeed, the use of different interpolating operators results in the construction of different potentials that should be phase-shift equivalent at the given energy, but will produce different phase shifts at other energies. In ref. \cite{86}, M. Birse re-emphasised the ambiguities associated with potentials through the simple example of an attractive square well potential with a repulsive delta function coupling to an excited state at short distance.

### 7.5 Spectral gaps, large volumes and the approach to the chiral limit

At finite volume, multi-hadron two-point correlation functions for large Euclidean times are dominated by exponentials corresponding to a series of poles in energy arising from states is which the two hadrons move with back-to-back momenta in their CoM frame (as discussed above, four- and higher-particle contributions are expected to dominate eigenstates of higher energy). For weakly interacting states, the gaps between these states are approximately given by the difference between \( E_n \) and \( E_{n+1} \) where \( E_n = \frac{2(m_2^2 - \frac{4\pi^2}{n^2})^{1/2}}{m} \) for two identical hadrons (since \( n = |n| \) for integer triplets \( n \), there are some levels that are not allowed, for example, \( n = 7 \)). As \( L \) increases, these gaps shrink rapidly (quadratically in the case of two hadrons) and it becomes hard to isolate the different levels. Variational approaches can help to some degree, but as the states collapse towards each other, they are by definition becoming more and more alike, so diagonalisation of correlator matrices will become an almost degenerate problem. Examples of this increasing level density for increasing volume are given in an appendix of ref. \cite{67} for \(^4\text{He} \). As pointed out in ref. \cite{73}, in the two-body sector this is further manifest in that the poles in the L"uscher eigenvalue equation accumulate at threshold and thus extracted energy levels of a given precision start to straddle these singularities making extraction of phase shifts difficult.

This problem is not unique to the large-volume limit. As the quark masses are decreased toward the chiral limit, pions become lighter and lighter. Consequently, the spectrum becomes denser as, for a given choice of quantum numbers, the energy gap between the ground state and states that include additional pions (see footnote \footnote{The ratio of pion and kaon decay constants, \( f_\pi/f_K \), lattice calculations are attaining the level of precision where electromagnetic effects are important and attempts are being made to include them (see ref. \cite{88} for a recent review). In the future, such effects must also be included in calculations relevant for nuclear physics. Indeed as the number of protons increases, so does the charge and thus the importance of electromagnetic effects, eventually overcoming the smallness of \( \alpha_s f_\pi \sim \frac{1}{17} \), and making inclusion of electromagnetism even more important in nuclei.}) tends to zero. The problem is compounded by the fact that one needs to take the infinite-volume limit before, or at least in combination with, the chiral limit so that finite-volume distortions of individual hadrons remain exponentially small.

This issue is one of the major challenges that must be addressed to open a path towards nuclear physics at the physical quark masses and seems to require a significant conceptual advance.

### 7.6 Electroweak effects

None of the calculations discussed above include the effects of the electroweak interaction. For simple quantities such as the ratio of pion and kaon decay constants, \( f_\pi/f_K \), lattice calculations are attaining the level of precision where electromagnetic effects are important and attempts are being made to include them (see ref. \cite{88} for a recent review). In the future, such effects must also be included in calculations relevant for nuclear physics. Indeed as the number of protons increases, so does the charge and thus the importance of electromagnetic effects, eventually overcoming the smallness of \( \alpha_s f_\pi \sim \frac{1}{17} \), and making inclusion of electromagnetism even more important in nuclei.
8 Conclusion

Over the last decade, lattice QCD has realised its potential and become a precision tool for the calculation of hadronic contributions in particle physics, thereby becoming a crucial part of our understanding of the Standard Model and of the search for physics beyond it. Nuclear physics presents a new frontier for LQCD as it involves intrinsically more complex systems with multiple length scales. As well as providing tests of the Standard Model, it offers exciting opportunities to make reliable predictions in cases that are difficult, or even impossible, to access experimentally. It also presents new challenges, both conceptual and numerical, that we are just beginning to uncover.

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