Nuclear Physics in Box

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Abstract. I provide a short overview of the current status of nuclear physics calculations using lattice Quantum Chromodynamics (LQCD). I demonstrate, at a very high level, how LQCD calculations are performed and how nuclear scattering data are extracted from these calculations, emphasizing the overlap between traditional nuclear many-body theory and LQCD calculations. I look at the $\Omega^-\Omega^-$ system as a concrete example, and in so doing demonstrate the predictive nature of LQCD calculations as applied to nuclear physics.

1. Why Lattice QCD?
It has long been accepted that Quantum Chromodynamics (QCD), the theory governing the behavior of quarks and gluons, is the underlying theory of the nuclear force, and that nuclear physics itself resides in a regime of QCD where the quarks and gluons are strongly interacting. The strongly interacting nature of QCD in this regime is no surprise: the quarks and gluons form bound hadronic states categorized as mesons ($q\bar{q}$) and baryons ($qqq$). The interaction between baryons and mesons, in turn, has its origins from QCD as well. The composite nature of these hadrons, coupled with the strongly interacting behavior of its quark and gluon constituents, makes tracing the lineage of the nuclear force directly from QCD a daunting task.

Fortunately there has been a slew of empirical data related to nucleons and their reactions that have allowed the interaction between nucleons to be constrained to high precision. With all this data, a natural question arises: Is QCD needed for nuclear physics? The answer is, of course, yes. In addition to nucleons and nuclei, the spectrum of QCD includes a diverse range of exotic mesons and baryons with strangeness content. For the former, we will shortly start probing these systems with the upcoming 12-GeV upgrade at the Thomas Jefferson National Accelerator Facility. Having a theoretical understanding of these exotic mesons, coupled with empirical data, will elucidate the nature of confinement. Baryons with non-zero strangeness are difficult to produce terrestrially, yet are known to play significant roles in astrophysical environments. Here QCD offers the means in which to understand the properties and behavior of hyperons and hyper-nuclei without resorting to any model assumptions. Even in the strangeness $S = 0$ sector there are aspects of the nuclear force that are unknown but could be resolved from QCD, such as the three-neutron interaction.

Because of the strongly-interacting nature of QCD, no formal methods are available for calculations of nuclear physics observables. As such, numerical methods must be used to tackle QCD in this regime. To date, lattice QCD (LQCD) offers the only means in which to numerically do this. The promise of LQCD is that, with sufficient high-performance computing (HPC) resources and algorithm development, the properties of few-hadron systems that are poorly...
known or inaccessible by experiments (like the ones mentioned above), will be calculable. As described in later sections, this promise is beginning to come true.

2. Nuclear physics in a box: A primer on LQCD

Lattice QCD is a formulation of QCD in which space and time are discretized on a lattice and the theory is confined to a finite cubic volume with fields subject to periodic boundary conditions. Strictly speaking, the volume is a hyper-cube, as the time extent is also made finite. In this manner the theory becomes amenable to numerical calculations. A lattice QCD calculation is performed using the Monte Carlo method with Markov Chain importance samplings of the QCD vacuum that are generated with a distribution prescribed by QCD, and physical observables are then measured on these samplings. As the measurements are stochastic in nature, there is an inherent uncertainty that is associated with each calculation. However, with increasing number of measurements there is a corresponding smaller statistical uncertainty in the calculation. With sufficient computational resources, and a careful account of the discretization artifacts imposed by the lattice, calculations that are not currently possible with pencil and paper are numerically feasible. Lattice QCD represents the best opportunity for answering longstanding questions in nuclear physics. But because of the diverse scales associated with LQCD calculations of nuclear observables, LQCD is computationally intensive. Because of this, LQCD calculations have historically been done using larger-than-physical quark masses to alleviate the computational demands.

2.1. Working in imaginary time

A central tenet of LQCD is the calculation of propagators using the path-integral formalism, where all possible paths are summed with corresponding weights depending on the path’s particular action. The time-evolution of propagators is dictated by the systems eigen-energies \( E_j \) appearing in the argument of an exponent, \( e^{i E_j t} \), and can be written generically

\[
\text{propagator} = \sum_{j}^{\infty} C_j e^{i E_j t},
\]

where \( C_j \) is some c-number and the tower of eigen-energies \( E_j \) share in common a particular symmetry (usually represented through quantum numbers). The goal of most LQCD calculations is the extraction of the energies \( E_j \) (or at least the lowest few). As the extraction of complex arguments is difficult numerically, LQCD calculations are done in imaginary time where \( t \to it \).

The consequences of working in imaginary time are complex and too numerous to discuss here, but generally speaking LQCD calculations in imaginary time draw strong analogs with statistical mechanics. Propagators are now called correlators, and their time evolution is given by

\[
\text{correlator} = \sum_{j}^{\infty} C_j e^{-E_j t},
\]

\[
\to C_0 e^{-E_0 t} \quad t \gg 1.
\]

The time-evolution is now dictated by a series of decaying exponentials. Given sufficient time, the ground state contribution to the correlator becomes dominant as the higher states have fallen off exponentially faster.

2.2. Interpolators

To impose a specific symmetry on the correlators, lattice QCD practitioners form interpolating operators that have the same quantum numbers as the system in question. These interpolating
operators represent sinks and sources within the lattice, and the probability of propagating from the source to the sink with these operators is given by the correlator that now has the specific symmetries imposed by the interpolating operators. The energies that dictate the time-evolution of this correlator represent the eigen-energies of a system with these same quantum numbers. For example, to determine the lowest eigen-energy of the $\pi^+$ system, interpolating operators representing the up and anti-d quark are formed (e.g. delta-functions at specific lattice sites), and the correlator is calculated using these interpolating operators. The operators themselves do NOT represent a $\pi^+$, but should have sufficient overlap with the true (but not known a priori) $\pi^+$ system\(^1\). After sufficient time the lowest energy $E_0$ is extracted (e.g. by fitting to a single exponential), from which the mass of the pion is determined, $m_\pi = E_0$. Figure 1 shows examples of correlators for the single pion and isospin $I = 2$ two-pion systems. Note that as these calculations are fully relativistic, they include the rest mass of the systems. Therefore the the decay of the two-pion system should be nearly double that of the single pion when plotted on a semi-log scale, as is the case in fig. 1.

2.3. Finite-volumes vs. Continuum physics
The finite-volume nature of LQCD calculations, coupled with its imaginary-time formalism, makes it seem at first sight impossible to extract continuum physics observables, such as scattering phase shifts. L"uscher showed from a field theoretic point of view, however, that there is a simple relation between the finite-volume energies of a two-particle system to the same system’s continuum scattering phase shift\(^2\) [2, 3],

$$q \cot \delta_0 = \frac{2}{\sqrt{\pi L}} Z_{0,0} \left(1; \tilde{q}^2 \right) ,$$

where $Z_{0,0}$ is the generalized zeta function, $\delta_0$ is the s-wave scattering phase shift, $L$ is the length of the cube, $\tilde{q} = qL/2\pi$, and $q$ is related to the energy of the interacting two-particle

\(^1\) The ‘perfect’ overlap would be one where $C_0$ is nonzero and all other $C_j$ are zero.
\(^2\) This relation is only valid below the inelastic threshold.
state, \( E = \sqrt{q^2 + m_1^2} + \sqrt{q^2 + m_2^2} \), which is calculated in LQCD. Equation 3 demonstrates that given the masses \( m \) and two-body energies \( E \) (ground state and excited states) of a system calculated from LQCD at different volumes \( L^3 \), the phase shift \( \delta_0 \) can be mapped out. Analogous finite-volume formulae exists for higher partial waves \([4]\). Figure 2 shows a phase shift example for the \( I = 2 \) two-pion system calculated from LQCD using multiple volumes and energy states. The data was taken from ref. [1]. Other examples of phase shifts, as well as effective range parameters, calculated from LQCD can be found in refs. [5, 6, 7].

Given the phase shifts, one can then extract effective range parameters through the relation

\[
q \cot \delta_0 = -\frac{1}{a_0} + \frac{r_0}{2} q^2 + \ldots,
\]

where \( a_0 \) and \( r_0 \) are the scattering length and effective range, respectively, and higher order terms in the effective range expansion have been dropped. For the \( I = 2 \) two-pion system, the following effective range parameters were found [1]:

\[
m_\pi a_0 = 0.23 \pm 0.019
\]

\[
m_\pi r_0 = 12.9 \pm 3.23
\]

where the statistical and systematic errors have been combined in quadrature.

### 2.4. Recent developments in Nuclear Physics from LQCD

Because of the recent advances in HPC resources, LQCD calculations are constantly pushing the envelope towards calculations using physical quark masses. Recent calculations of single hadron resonances have been performed at the physical point [8], but for multi-hadron systems extrapolations from unphysical masses are made to the physical point. Examples include calculations of certain nucleon-hyperon systems [9], as well as the spectrum of nuclei and hypernuclei at the ‘SU3’ point, where all quark masses are degenerate and set at the strange quark mass [10]. Understanding the interactions of these systems will determine their roles in the nuclear matter equation of state, which ultimately impacts black hole formation, supernova evolution, and neutron star composition. Even without extrapolations, LQCD results at larger-than-physical quark masses provide us with a deeper understanding of the rich nature of QCD in a world where fundamental input parameters are slightly different than what is observed. For example, bound states not observed in nature are prevalent in LQCD calculations where the light quarks (up and down) are larger than physical [11, 12, 13]. Calculations of the nuclear potential have been attempted [14, 15], though these calculations suffer from uncontrolled approximations and are model-dependent.

One of the most promising aspects of LQCD is its power to probe systems and their interactions that are experimentally inaccessible. A prime example is the three-pion interaction, which was found to be slightly repulsive [16]. Studies of the three-nucleon interaction are underway. Also promising is the use of LQCD to calculate nuclear matrix elements. A recent example here involves the first calculation of the neutral current parity violating parameter, \( h_{\pi NN} \), from LQCD [17].

### 3. The \( \Omega^- \Omega^- \) system as a specific example

The strangeness \( S = -6 \) \( \Omega^- \Omega^- \) system is an interesting testbed for nuclear physics. The \( \Omega^- \) particle itself consists of three strange quarks bound with spin=3/2. Typically the \( \Omega^- \) is used to ‘set the scale’ in LQCD calculations, in that the calculated \( \Omega^- \) mass is tuned to its physical value. And because the \( \Omega^- \) has isospin \( I = 0 \), it’s coupling to the light quarks are suppressed. This, in turn, means that the light-quark dependence of the \( \Omega^- \Omega^- \) system is suppressed, and therefore current LQCD calculations of this system should be ‘near’ physical.
Table 1. Angular momentum $J$ designations and their octahedral decompositions $\Gamma$. Parity is also assigned where applicable.

| $J$ | $\Gamma$ |
|-----|----------|
| 0  | $A_1^+$ |
| 1/2 | $G_1$ |
| 1  | $T_1^-$ |
| 3/2 | $H$ |
| 2  | $E^+ \oplus T_2^+$ |
| 5/2 | $H \oplus G_2$ |
| 3  | $A_2^- \oplus T_1^- \oplus T_2^-$ |

The $\Omega^- \Omega^-$ system has been looked at before from a quark model perspective, but calculations have been inconclusive, with results suggesting that the system can be weakly repulsive [18] or strongly bound [19]. This discrepancy can be resolved by LQCD. The results presented below draw off of work presented in ref. [20].

3.1. The $\Omega^-$ interpolating operator

The interpolating operator for the $\Omega^-$ particle is built from linear combinations of the following object:

$$\Omega_{\mu_1 \mu_2 \mu_3} = \epsilon_{abc} s^a_{\mu_1} s^b_{\mu_2} s^c_{\mu_3},$$

where Roman letters refer to color indices, Greek letters refer to spin indices, $s$ are the strange-quark fields, and repeated indices are summed. To build a state with definite spin, appropriate combinations of the spin indices must be made. However, as calculations are done within a cubic volume, standard angular momentum designations no longer apply. Instead of an infinite number of possible spin states (e.g. 1/2, 3/2, 5/2, etc.), within a cubic volume there are only three irreducible representations that, in the continuum limit, connect to odd-half spin: $G_1$, $G_2$, and $H$. These irreps are part of the double cover octahedral point group. Table 1 shows the decomposition of the few lowest lying angular momentum states into the octahedral irreps [21].

The spin-3/2 $\Omega^-$ particle therefore transforms under the $H$ basis within a cubic volume, and the linear combination of spinor indices must account for this. Basak et al. have determined these combinations [22]. For example, the interpolating operator with good $H$ symmetry that most closely transforms as $|3/2, 3/2\rangle$ in the continuum is given by $\Omega_{111}^3$. For a $|3/2, -3/2\rangle$, one would use $\Omega_{222}$.  

3.2. Angular momentum coupling

The two-particle $\Omega^- \Omega^-$ system’s total angular momentum must be made from coupling the individual spin and angular momentum of its constituent parts. As is done in nuclear physics, this is accomplished through standard angular momentum coupling coefficients (i.e. Clebsch-Gordan coefficients). However, as was the case for the spin mentioned above, standard angular momentum designations are different in a cubic volume and are decomposed into five distinct irreps of the octahedral group: $A_1$, $A_2$, $T_1$, $T_2$, and $E$. Table 1 show how these states are decomposed into continuum angular momentum states. The coupling of these irreps utilize analogous Clebsch-Gordan coefficients. The number of Clebsch-Gordan coefficients in this case

\footnote{Spin indices are in the Pauli-Dirac basis.}
Figure 3. Effective mass plots for the single $\Omega^-$ and $\Omega^-\Omega^-A_1^+$ system. Axes are plotted in units of the lattice spacing and are therefore dimensionless. These results show the extracted lowest energies of the single $\Omega^-$ and $\Omega^-\Omega^-$ correlators, as a function of time.

Figure 4. Close-up of the $\Omega^-\Omega^-$ effective mass. Band shows the fit result and range of fit window. The long dashed line corresponds to the two-$\Omega^-$ threshold (i.e. twice the $\Omega^-$ mass), and the short (red) dashed line represents the results if the system were bound by 100 MeV.

are finite, as there are only a finite number of irreps in the octahedral group. The coupling coefficients used in this work were taken from ref. [22].

The $\Omega^-\Omega^-$ system of interest is a s-wave system, and therefore the total angular momentum $J$ of the system is dictated by the coupling of the particle’s individual spins. Antisymmetry dictates that $J$ can be either 0 or 2 in this case, which would correspond to the $A_1^+$ symmetry or $E^+/T_2^+$ symmetry, respectively, in a cubic volume. The s-wave component ($A_1^+$) of the problem is enforced by projecting the individual $\Omega^-$ particles to zero momentum during the LQCD calculation.

3.3. Results
In fig. 3 the effective mass plots are shown for the single-$\Omega^-$ and $\Omega^-\Omega^-A_1^+$ system. These plots essentially show the fitted lowest energy extracted for the corresponding $\Omega^-$ and $\Omega^-\Omega^-$ correlators. Not surprisingly, the value for the $\Omega^-\Omega^-$ mass is nearly twice the value of the single $\Omega^-$ mass. In fig. 4 a close-up of the $\Omega^-\Omega^-$ effective mass is shown, as well as the values of the two-$\Omega^-$ threshold (long black dashed line). The shaded band in the figure provides the fitted energy as well as the time-extent of the fit. As the band falls above the two-$\Omega^-$ threshold, we identify this state as a scattering state with slight repulsion. These results do not see a deeply bound 100 MeV state, as this would have fallen near the short (red) dashed line in the figure.

Using eqs. 3 and 4, the scattering length can be extracted for this interacting system and the following prediction is made,

$$a_0 = .15 \pm .22 \text{ fm},$$

(7)

where the statistical and systematic errors have been combined in quadrature. It is important to note that though these calculations have produced only a scattering state, the presence of a deeply bound state is not completely ruled out, particularly one that is so bound as to not be resolved with the current lattice spacings ($a = .12 \text{ fm}$) used in these LQCD calculations. Future calculations with finer lattice spacings are needed to definitively rule out the presence of a deeply bound state.
4. What’s on the horizon

Much of the recent progress in LQCD calculations of nuclear observables has been enabled, in part, by the recent gains in HPC. This trend is anticipated to continue, with the end result being the seamless coupling of nuclear physics, LQCD, and HPC. As an example of the promise that HPC will bring to LQCD and nuclear physics, fig. 5 shows the weak scaling behavior of an inversion routine (commonly used within LQCD codes) on LLNL’s recently installed 16 Petaflop Sequoia machine. The linear relation between performance and number of cores demonstrates optimal scaling behavior for this code. Because of the large computational power of this machine, LQCD can readily perform calculations at, or near, the physical point. Calculations of the $\Omega^-\Omega^-$ system using Sequoia would reduce current uncertainties by at least an order of magnitude. Anticipated results with petascale (and beyond) resources of nuclear physics observables and their uncertainties have been estimated in ref. [23]

The significance of HPC gains goes beyond just calculating nuclear phenomena at the physical point. It will also allow for seamless integration of nuclear many-body effective theories to couple with LQCD calculations, thereby extending the applicability of LQCD calculations. At the same time, nuclear physics becomes rooted to the fundamental theory of QCD, and answers to longstanding questions about the nuclear force will be addressed. Most importantly, nuclear physics, predominantly data driven historically, becomes a predictive science.
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