

Nuclear Physics with Lattice QCD

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Abstract. We discuss recent progress and future prospects of the application of lattice QCD to the study of hadronic *interactions*. In particular, we review the issues arising in a first principles calculation of the nuclear force.

1. Introduction

The theory of the strong interactions (QCD) has been known for over 30 years. However, the study of the most basic strong interaction process – the force binding nuclei – was very little impacted by the advent of QCD. The root of this problem, of course, is the difficulty in treating the non-perturbative large distance properties of QCD. At this point the only technique available for a first principles attack on QCD is lattice field theory. However, as we will see below, hadronic interactions are usually much harder to compute in the lattice than the more commonly computed observables like masses and decay constants and represent a significant challenge to the current state of technology.

The study of nuclear physics through lattice QCD is a complicated project, likely to last several years. It is important from the outset to understand the relevance of the different goals and stepping stones to be encountered on the way. This program includes the calculation of a large number of observables with different degrees of difficulty and interest. We can roughly divide them in three categories. First there are simplest cases of hadronic interactions. That includes, for instance, meson-meson scattering. They are interesting in their own right since they constrain and test the chiral physics of mesons. But they are also testing grounds for the techniques used in more complicated problems. Then we have observables, like nucleon-nucleon phase shifts, that are central to nuclear physics but empirically well known. A first principle calculation of these observables would mark an important milestone in QCD but, from the point of view of the practicing nuclear physicist, represents little that is new. Even in this case though, we should keep in mind that a calculation of this sort allows us to understand aspects not accessible to experiments (even in principle !) as, for instance, the dependence of the nuclear forces on the value of the quark masses. This kind of information is important from the theoretical point of view (if one hopes to understand the results analytically) and may become of phenomenological importance in the study of fundamental constants variations on cosmological times. Finally, there are observables that are difficult or impossible to be measured like hyperon-nucleon or hyperon-hyperon interactions or certain two-nucleon couplings of electroweak currents. They directly impact the physics of neutron stars, the detection of solar neutrinos, etc... Any information about them obtained through lattice QCD will be of great importance [1].

2. Fundamentals of lattice QCD

Lattice QCD is based on a numerical Monte Carlo-based calculation of the path integral defining n QCD [2]:

$$\langle \mathcal{O} \rangle = \int D\psi D\bar{\psi} DU e^{-S[\psi, \bar{\psi}, U]} \mathcal{O}, \quad (1)$$

where \mathcal{O} is any observable made up of quark ($\psi, \bar{\psi}$) and gluon (U) fields. The quark fields appear quadratically so the integral over the quark fields can be performed analytically resulting in

$$\begin{aligned} \langle \mathcal{O} \rangle &= \int D\psi D\bar{\psi} DU e^{-S_G[U] + \bar{\psi} \mathbf{K}[U] \psi} \mathcal{O} \\ &= \int DU e^{-S_G[U]} \det(\mathbf{K}[U]) \mathcal{O}, \end{aligned} \quad (2)$$

A (large) set of gauge field configurations with the probability distribution $\sim e^{-S_G[U]} \det(\mathbf{K})$ can be used to approximate the value of the integral above

$$\langle \mathcal{O} \rangle \approx \frac{1}{N} \sum_i \mathcal{O}(\mathbf{K}[U_i]). \quad (3)$$

There are two important points to notice. The first is that the set of gauge configurations is independent of the observable \mathcal{O} one is interested in measuring. Second, one can use a different discretization for the fermion operator $\mathbf{K}[U]$ in the determinant (describing the effect of sea quarks) from the discretization of the quark operator appearing in the construction of the observable $\mathcal{O}(\mathbf{K}[U_i])$ (describing the valence quarks).

Lattice calculations are performed in imaginary time. The relation between imaginary time correlators (that can be computed using lattice QCD) and observables is not obvious. For simple observables, like particle masses, this relation is simple. Suppose one is interested in the mass of the π^+ . One can compute the imaginary time correlator $C(t) = \langle \pi^-(\mathbf{r}', \mathbf{t}) \pi^+(\mathbf{r}, \mathbf{0}) \rangle$, with π^+ being *any* operator made up of quarks and gluons with the quantum numbers of the pion like, for instance, $\bar{q} \gamma_5 \tau^+ q$. Using standard quantum mechanics arguments we can arrive at

$$\begin{aligned} C(t) &= \sum_n \langle 0 | e^{Ht} \pi^-(\mathbf{r}', 0) e^{-Ht} | n \rangle \langle n | \pi^+(\mathbf{r}, 0) | 0 \rangle \\ &= \sum_n e^{-E_n t} \langle 0 | \pi^-(\mathbf{r}', 0) | n \rangle \langle n | \pi^+(\mathbf{r}, 0) | 0 \rangle \\ &\rightarrow e^{-m_\pi t} |\langle \text{pion at rest} | \pi^+(\mathbf{r}, 0) | 0 \rangle|^2, \end{aligned} \quad (4)$$

where $|n\rangle$ is the n-th eigenstate of the hamiltonian H with energy E_n . At large times t the sum is dominated by the energy with the smallest energy among those with the quantum numbers of one positive pion (namely, the positive pion at rest). Thus, by measuring the long time behavior of $C(t)$ we can extract the pion mass. It is not so easy to extract scattering information on the lattice. The naive attempt using the two pion correlator leads to

$$C_2(t) = \langle \pi^-(\mathbf{r}', \mathbf{t}) \pi^-(\mathbf{r}', \mathbf{t}) \pi^+(\mathbf{r}, \mathbf{0}) \pi^+(\mathbf{r}, \mathbf{0}) \rangle \rightarrow e^{-2m_\pi t} |\langle 2 \text{ pions at rest} | \pi^+(\mathbf{r}, 0) \pi^+(\mathbf{r}, 0) | 0 \rangle|^2, \quad (5)$$

which does not bring any information about the pion interactions. At infinite volume we find then that the euclidean correlators bring no information about the scattering properties [3]. At

finite volume however, the two particles cannot be well separated and the energy of the ground state of two particles will include the interaction energy [4]

$$C_2(t) = \langle \pi^-(\mathbf{r}', t) \pi^-(\mathbf{r}', t) \pi^+(\mathbf{r}, 0) \pi^+(\mathbf{r}, 0) \rangle \rightarrow e^{-2m_\pi t + \Delta E} |\langle 2 \text{ pions at rest} | \pi^+(\mathbf{r}, 0) \pi^+(\mathbf{r}, 0) | 0 \rangle|^2. \quad (6)$$

The shift in the two-particle energy levels can be related to the phase shift evaluated at the energy ΔE through the Luscher formula [5]

$$\sqrt{M\Delta E} \cot \delta(\Delta E) = \mathcal{S}\left(\frac{M\Delta EL^2}{4\pi^2}\right), \quad (7)$$

where \mathcal{S} is a known function. If one measures the energy levels of two particles in a box with enough precision this formula can be used to learn about the phase shift at that energy. By changing the value of the box size L the phase shift at other energy values can be probed¹. In the case where the scattering length a is much smaller than the lattice size L an approximate formula can be used

$$\Delta E = \frac{4\pi a}{ML^3} \left(1 + c_1 \frac{a}{L} + c_2 \frac{a^2}{L^2} + \dots \right), \quad (8)$$

where c_1, c_2 are known numerical coefficients. The leading term of the formula above can be obtained by a simple use of perturbation theory. It is important to stress however, that the finite energy phase shifts can be obtained even if $a \gg L$. In other words, we can learn about the deuteron using boxes much smaller than the deuteron itself. This is particularly important in nuclear physics as the scattering length in the spin singlet case is very large (of the order of 20 fm) [7]. The condition on the size of the box for the Luscher formula to be valid is that the range of the interaction (in the nuclear case of order $1/m_\pi$) should be much smaller than L . That is a much weaker condition than $a \ll L$ since, in the nuclear case $a \gg 1/m_\pi$.

3. Current results

The Nuclear Physics with Lattice QCD (NPLQCD) collaboration recently performed the calculation of several hadronic scattering observables using the method outlined above. Before discussing the results let me discuss a few details of the simulation. All the calculations discussed here were done using gauge field configurations generated by the MILC collaboration [8] (for different purposes). They are fully dynamical (meaning, the fermion determinant $\det(\mathbf{K})$ is included in the probability distribution). It uses the asqtad action [9] which is improved so the largest discretization errors are of order $\alpha_s a^2$ (a is the lattice spacing and α_s the strong coupling constant). The quark masses for the up and down quarks are chosen so the pion has masses $m_\pi = 294, 348$ and 484 MeV. NPLQCD computed quark propagators for the valence sector moving in these gauge field configurations using a different discretization (domain-wall quarks) of the quark action. Domain-wall quarks were used because, despite being numerically more expensive, they have an almost exact chiral symmetry. In particular, the leading source of discretization errors (of order a), which breaks chiral symmetry, is automatically absent of this formulation. The lattice spacing of these lattices is about 0.125 (extracted from the Sommer scale) fm and the total size of the lattice is about 2.5 fm.

3.1. $I = 2$ $\pi\pi$ scattering length

From the point of view of the lattice, the simplest hadronic interaction to be studied is the isospin $I = 2$ channel of the $\pi\pi$ system. The value of the scattering length extracted at three different

¹ Another, and cheaper, way of measuring the phase shifts at other values of the energy is to change the boundary conditions [6].

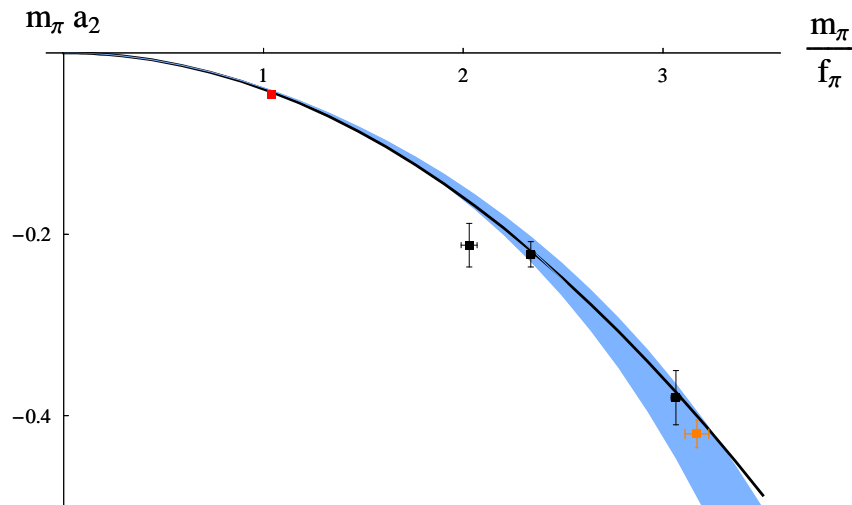


Figure 1. Scattering length (in units of m_π^{-1}) as a function of pion mass (in units of f_π). Black dots represent the NPLQCD calculations, the red point the experimental result from an analysis of K(e4) decays and the orange point at the highest mass to a result of the CP-PACS collaboration. The blue band indicates the result of the chiral extrapolation and its associated uncertainty.

pion masses can be extrapolated to the realistic pion masses using the chiral perturbation theory one-loop result

$$m_\pi a = -\frac{m_\pi^2}{8\pi f_\pi^2} \left[1 + \frac{3m_\pi^2}{16\pi f_\pi^2} \left(\log \left(\frac{m_\pi^2}{\mu^2} + l_{\pi\pi}(\mu) \right) \right) \right], \quad (9)$$

where $l_{\pi\pi}(\mu) = 8(l_1 + l_2) + 2(l_3 - l_4)$ is a combination of Gasser-Leutwyler coefficients parameterizing some short-distance effects and μ is the renormalization scale. Since f_π is also calculated using the same pion masses the formula above can be used to perform a one parameter ($l_{\pi\pi}$) fit to the numerical results. We find $l_{\pi\pi}(4\pi f_\pi) = 3.3(6)(3)$, where the first error is statistical and the second one correspond to the different ways to assign weights to each one of the three numerical points (the chiral perturbation theory formula is supposed to be more accurate at smaller pion masses). The value of $l_{\pi\pi}$ can then be used to compute $m_\pi a$ at the physical value of the pion mass. The result is $m_\pi a = -0.0426(6)(3)(18)$ where the errors are, respectively, statistical, from the uncertainty in $l_{\pi\pi}$ and an estimate of the two-loop contribution to eq. (9). This value is to be compared with the value extracted in an analysis of the K(e4) kaon decays giving $m_\pi a = -0.0454(31)(10)(8)$ where the errors are, respectively, statistical, systematic and theoretical.

The systematic errors in this calculation were not fully explored but can be estimated. The discretization errors are of order $a^2 \Lambda_{QCD} \approx 1\%$ [11]. The finite volume effects (exponentially suppressed and not included in the Luscher formula) can be estimated by chiral perturbation theory are also of the order of a few percent [12]. This indicates that this calculation (before the chiral extrapolation) is still limited by statistical effects. Future work will improve the statistics until to the point where the errors are dominated by systematic effects. It is worthwhile emphasizing the ingredients that allow for such a precise calculation of a scattering observable at the physical value of the pion mass. They are: i) relatively large signal to noise ratio, ii) the existence of an exact result ($m_\pi a = 0$ for $m_\pi = 0$) anchoring the extrapolation down to physical quark masses and iii) a reliable extrapolation formula standing on solid grounds coming from

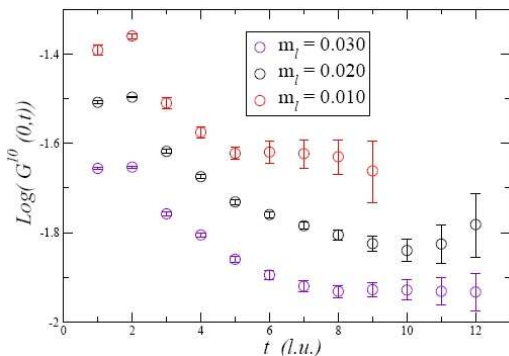


Figure 2. Log of the correlator ratio for the spin singlet nucleon-nucleon channel at three different quark masses.

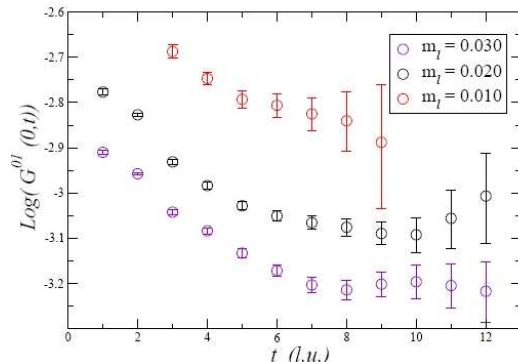


Figure 3. Log of the correlator ratio for the spin triplet nucleon-nucleon channel at three different quark masses.

chiral perturbation theory. Some of these desirable features are unfortunately not present in other scattering observables.

Scattering lengths for π^+K^+ were also calculated with similar level of precision [13].

3.2. Nucleon-nucleon scattering length

At low energies nucleons are non-relativistic and it is useful to describe their interaction through a non-relativistic potential. It should be kept in mind, however, that the non-relativistic potential is a construct belonging to the low-energy effective theory of QCD describing low energy nuclear phenomena and cannot be uniquely defined in QCD. On physical grounds, we don't expect that short distance (high momentum) interaction between two nucleons to be describable by a potential so the nuclear potential at short distances (say, smaller than 0.5 fm) is not well defined. For this reason the study of the nuclear forces from QCD does not pass through the derivation of the nuclear potential (including its short distance piece) but proceeds directly to the calculation of phase shifts. Of course, many potentials, with different short-distance behaviors can be concocted to reproduce the low energy data (experimental or from numerical QCD), as it has been done phenomenologically with great accuracy. But since the short-distance behavior is somewhat arbitrary (in the language of effective field theory, it is "regulator dependent") it cannot be deduced from QCD. This is in contrast to the interaction between two *infinitely* heavy particles where an adiabatic potential is well defined at all distances. Any attempt at a lattice QCD calculation of the nuclear potential will be plagued, at short distances, by the arbitrariness in the choice of interpolating fields for the nucleons. The phase shifts, as we argued above, are related to energy levels and are independent of this choice.

On figures 2 and 3 [14] we show the results for the correlator ratio

$$\frac{\langle N(t)N(t)N^\dagger(0)N^\dagger(0) \rangle}{\langle N(t)N^\dagger(0) \rangle^2} \xrightarrow{t \rightarrow \infty} e^{-\Delta E t}, \quad (10)$$

whose long time behavior directly measures the energy shift ΔE , for the two spin channels (singlet and triplet) in the nucleon-nucleon system. Compared to the $\pi\pi$ case one outstanding feature is the decreasing signal-to-noise ratio for large t . This can be understood from simple arguments [15] that indicate that

$$\text{signal to noise ratio} \sim e^{-(2M-3m_\pi)t}, \quad (11)$$

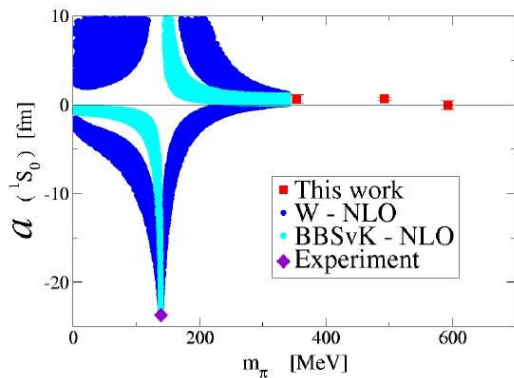


Figure 4. Interpolation/extrapolation between the lattice QCD and the experimental results in the spin singlet channel.

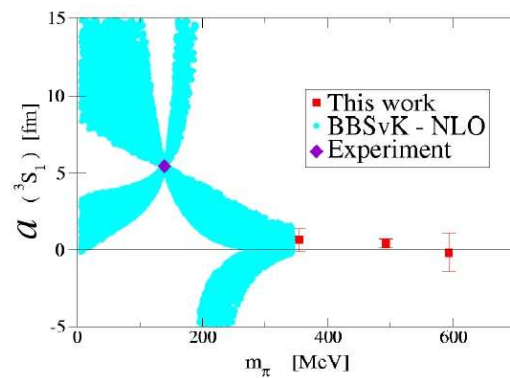


Figure 5. Interpolation/extrapolation between the lattice QCD and the experimental results in the spin triplet channel.

where M is the nucleon mass. Consequently, the uncertainty in the extraction of the scattering length is much larger. Nucleon-nucleon scattering lengths however, are very large, at least for physical pion masses. Thus even upper bounds on the value of the scattering lengths contain non-trivial information. The values found are shown in table 1.

Table 1. Scattering lengths for the two nucleon-nucleon spin channels. The numbers in parentheses indicate the time range used in the fit.

$m_\pi (MeV)$	$a(^1S_0) (fm)$	$a(^3S_1) (fm)$
353.7 ± 2.1	$0.63 \pm 0.50(5 - 10)$	$0.63 \pm 0.74(5 - 9)$
492.5 ± 1.1	$0.65 \pm 0.18(6 - 9)$	$0.41 \pm 0.28(6 - 9)$
593.0 ± 1.6	$0.0 \pm 0.5(7 - 12)$	$-0.2 \pm 1.3(7 - 12)$

The effective theory describing nucleon-nucleon scattering contains, at next-to-leading order, two undetermined constants [16]. One (C_0) is the leading short-distance quark mass independent interaction. The other (D_2) describes the leading short-distance quark mass dependence. Unfortunately, the regime of applicability of the nuclear effective theory is smaller than the chiral perturbation theory in the meson sector and only the lowest value of the pion mass falls (at the edge) of this range. With only one data point both C_0 and D_2 cannot be determined and a prediction for the scattering length at the physical point is not possible. However, we can use the measured value of the scattering length at the physical point and predict what the scattering length would be at different values of the quark mass. The result of these calculations are shown in figures 2 and 3. The shaded area correspond to results obtained with values of C_0 and D_2 fitting both the lowest pion mass point and the experimental datum and also conforming with the expectations of naive dimensional analysis. Two power counting schemes were used, the one advocated by Weinberg [17] and the one discussed in reference [18]. Their predictions are not significantly different and their difference suggests what the errors in this extrapolation is.

Like in the $\pi\pi$ system, the systematic errors in this calculation were not fully explored. The error arising from the formally exponentially suppressed corrections to the Luscher formula, were estimated in [20] and, for the pion masses used, are smaller than the statistical errors. In

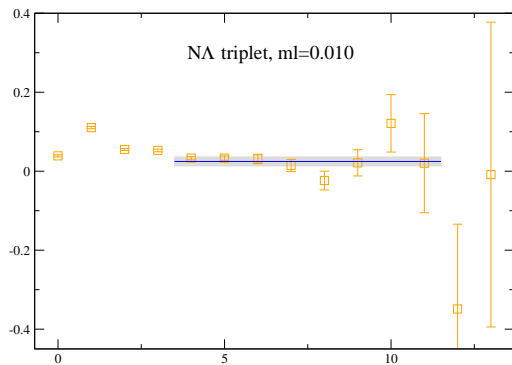


Figure 6. Effective mass plot for the spin singlet Λ -nucleon system and $m_\pi = 353$ MeV. The straight line and the shaded band indicate the result of the fit.

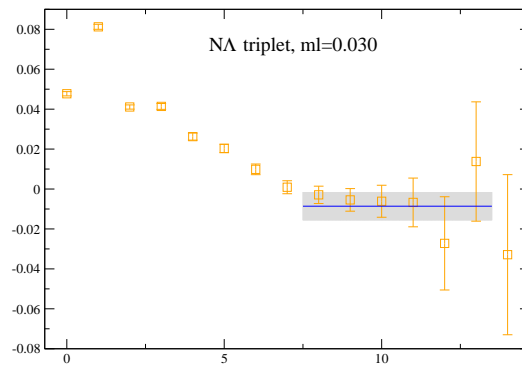


Figure 7. Effective mass plot for the spin singlet Λ -nucleon system and $m_\pi = 593$ MeV. The straight line and the shaded band indicate the result of the fit.

this reference it is pointed out that the most naive finite volume correction – the fact that the two nucleons can interact in a direct way and also through pions exchanged “around the lattice” – in fact vanish at leading order in perturbation theory.

4. Hyperon-nucleon scattering

The same method used in the nucleon-nucleon calculation was employed in the hyperon-nucleon sector. Here again the statistical noise is a problem but some non-trivial results were obtained in several pion mass/spin channel combinations. The full set of results can be found in reference [19]. Here, as an example, we show in figures 6 and 7 the effective mass plots for the Λ -nucleon system in the triplet with the pion mass $m_\pi = 353$ and $m_\pi = 593$ MeV.

5. Future prospects

This calculation of the baryon-baryon scattering lengths obviously would benefit of higher statistics. The strategy followed by NPLQCD is to compute quark propagators on the same gauge field configurations generated by MILC, but with different initial points. Each set of MILC configurations has of the order of 500 configurations and in excess of 10 propagators per configurations have been generated and showed to be statistically independent. Other approaches to the noise problem are also being pursued. One is the use of anisotropic (improved Wilson) lattices that were successful in the somewhat related problem of determining the glueball spectrum.

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