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Hadron-Hadron Interactions from Lattice QCD

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We discuss the status of our project concerned with the determination of hadron-hadron interactions from lattice Quantum Chromodynamics. In addition, we discuss our optimisation efforts for current and future supercomputer architectures.

1 Introduction

The Standard Model (SM) of particle physics is extremely successful in describing nature as we observe it in experiment. With the Higgs boson, only in 2012 found at the Large Hadron Collider at CERN, it might seem that even the last missing jigsaw piece was found.

However, most physicists believe the SM not to be the final answer. The reason for this are fundamentally not understood questions in the SM. For instance, there are six quarks interacting mainly via the strong force. To our current knowledge quarks are elementary particles. The six flavours appear to have very similar properties, apart from their coupling to the Higgs boson (i.e. their mass), which differs by orders of magnitude. The SM does neither predict the values for these coupling nor does it explain the large differences in their values.

This and other fundamentally open questions are nowadays attacked by considering the SM as an effective theory of some other, more general theory. This comes along with an experimental and theoretical effort trying to identify possible discrepancies between experiment and theory.

On the theory side this requires to compute as many quantities as possible with as much precision as feasible. This concerns in particular the strong force, called Quantum Chromodynamics (QCD), the strongest of the three forces described by the SM. Because QCD is strongly coupled and the coupling constant is large at low energies, it cannot be solved by perturbation theory, which would mean an expansion in a coupling constant with a value small compared to one. QCD must be solved applying non-perturbative methods.

The only known non-perturbative method to investigate QCD, which is systematically improvable, is called Lattice QCD. In Lattice QCD, space-time is discretised with a lattice spacing a. Moreover, only a finite volume box is considered. This setting allows one to apply numerical methods and in particular Markov Chain Monte Carlo statistical methods to Lattice QCD. This approach makes it possible to solve QCD up to statistical uncertainties exactly, once the limits $a \to 0$ and volume to infinity are taken appropriately. Still, since we are interested in the strong coupling region of QCD, the corresponding numerical calculations require formidable computer resources.

In this proceeding contribution we will touch on two aspects of our work. One is our efforts to optimise our software for current and future high performance computing

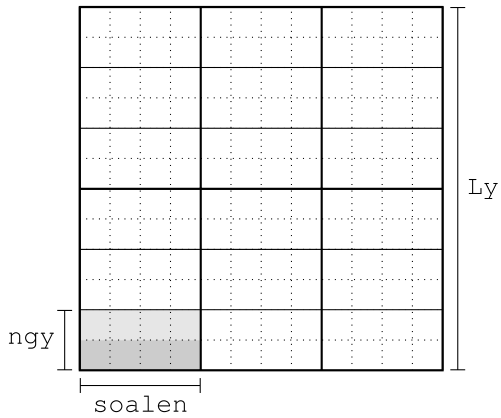

Figure 1. The division of lattice points into tiles and blocks, as explained in the text.

architectures. The second aspect will cover our physics results concerning the interaction of hadrons.

2 Optimising Code for Current and Future Architectures

Current and very likely also near future high performance computing architectures have different levels of parallelism. First of all, there is the fast network interconnect connecting different nodes. Second, each node has typically several CPUs, connected via shared memory. Third, every CPU has a number of cores, giving rise to a number of hardware and/or software threads. Finally, each core has a floating point unit (FPU) with a certain vector length. Such an FPU allows one to perform an number of operations, e.g. eight, in a single instruction in a SIMD fashion (single instruction, multiple data). An efficient usage of such high performance systems is only possible if all levels of parallelism are optimally handled.

We are maintaining and developing a software suite for lattice QCD simulations, called tmLQCD[1]. It supports all modern computing architectures, including NVIDIA GPUs, Intel and Bluegene. In this proceeding we will concentrate on our optimisation efforts for Intel based machines like JURECA.

The kernel of most of our computations is the so-called Wilson twisted mass Dirac operator. It represents a very large, but also extremely sparse matrix, which must be applied repeatedly to vectors, in particular in iterative solvers such as the conjugate gradient (CG) iterative solver. It is at the core of our efforts to make this matrix-vector multiplication as fast as possible. This makes it necessary to exploit the SIMD vector unit optimally, including the challenge that every new chip exhibits a different vector length. On the next level, the available core must be fed with a sufficient amount of data to keep it busy.

In the software package QPhiX[3] a particular approach was implemented to tackle all these challenges, however for a different Dirac operator. We have extended the package for our Dirac operator. The idea is illustrated in Fig. 1 and the following: assume we work in $d = 2$ dimensions. One of the directions, say the x-direction is divided into pieces of

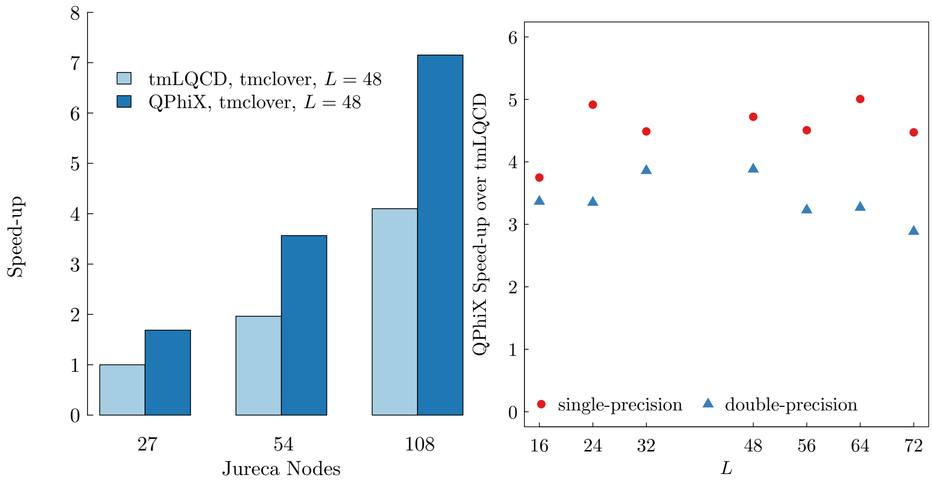

Figure 2. Speedup observed with our implementation of the QPhiX software package over the tmLQCD plain C implementation on JURECA (left) and KNL (right).

length `soalen`, which is a divisor of the vector length `veclen`. `ngy` of such pieces are combined into a tile, with `ngy`·`soalen`=`veclen`. Tiles then have length `veclen` and can be used in a SIMD operation. Tiles are indicated by the thin continuous lines in Fig. 1.

A number `nt` of such tiles is grouped into what we call a block. Those are loaded into cache one at a time. They are then distributed evenly on the available cores. Blocks are indicated by the thick continuous lines in Fig. 1. Both, `soalen` and `nt` are parameters which can be optimised for maximal performance. The idea can be generalised for higher dimensions.

In order to implement this approach for adjustable parameters `veclen`, `soalen` and `nt`, a code generator has been implemented. This code generator takes care of the intrinsic functions needed for a certain architecture and generates the data layout and C++ code for the Wilson twisted mass Dirac kernel. At the level of internode communication MPI is used.

In Fig. 2 we compare our `QPhiX` implementation of our Wilson twisted mass Dirac operator with the plain tmLQCD implementation in a CG solve with fixed problem size. In the left panel we show the speedup. The `QPhiX` implementation gives rise to a factor 1.6 improvement in speed. This speedup is independent on the number of the nodes used. The strong scaling of our code appears to be close to optimal on JURECA. On the KNL architecture the speedup is more impressive, as shown in the right panel of Fig. 2 as a function of the spatial lattice extent.

3 Hadron-Hadron Interactions from Lattice QCD

3.1 Motivation

As mentioned in the introduction, lattice QCD is the non-perturbative tool to investigate QCD from first principles. Lattice QCD is very well suited to determine masses of stable particles. However, most of the states described by QCD are unstable, i.e. they decay into two or more finite state particles. It was shown several decades ago by Maiani and Testa that – due to a technical complication – properties of unstable particles are not directly accessible in lattice QCD.

Therefore, a detour needs to be taken which was first invented by Martin Lüscher[2]. Lüschers approach is based on the following idea: suppose we consider two particles in a box with extent much larger than the extent of the single particles. In such a box the probability of interaction between the two particles can safely be set to zero. Hence, the energy of the two particles is given by the sum of the two single particle energies.

Now reduce the extent of the box. At a certain point, the probability of interaction between the particles will become significant. This interaction will cause an energy shift in the two particle energy. This implies that the energy of the interacting two particle system is no longer the sum of the two single particle energies. Of course, the energy shift is a finite volume effect. However, it turns out that – besides being a finite volume effect – this energy shift is directly related to the infinite volume scattering properties of the two particles.

This connection allows one, circumventing the Maiani-Testa no-go theorem, to extract properties of unstable particles in lattice QCD by studying finite size effects. The approach is well understood theoretically for particles decaying into only two final states. And it is currently being worked out for three particles in the final state, however, with increasing complexity.

Also, in practical simulations results for more and more two particle systems become available. If we restrict ourselves to two interacting bosons, the quantity of interest here is the scattering phase $\delta_\ell(k^2)$ for given partial wave ℓ and scattering momentum k^2. The phase shift fully parametrises the interaction, because the asymptotic incoming and outgoing wave functions far away from the interaction region differ only by a phaseshift. And in most of the cases the lowest partial wave dominates the process, which further simplifies the calculation.

At small scattering energies more is known about the phase shift: one can perform a so-called finite-range expansion and finds

$$k^{2\ell+1}\cot\delta_\ell(k^2) \;=\; \frac{1}{a_\ell} + \mathcal{O}(k^2)\,.$$

The parameter a_ℓ is called scattering length. It already contains important information on the strength of the interaction by its modulus. Its sign indicates whether the interaction of the two particles is attractive or repulsive.

3.2 Pion-Pion Scattering with Isospin $I = 2$ and $I = 0$

As a first example we have computed the scattering length of two pions. Two pions can appear with different isospin I. Here we show results for $I = 2$ and $I = 0$, starting with the former.

Pions are the lightest hadrons in the spectrum, because they are pseudo Goldstone bosons of spontaneously broken chiral symmetry. Due to this special role they are particularly interesting for testing chiral perturbation theory (ChPT), the low energy effective theory of QCD. ChPT predicts the quark mass dependence of the product of pion mass

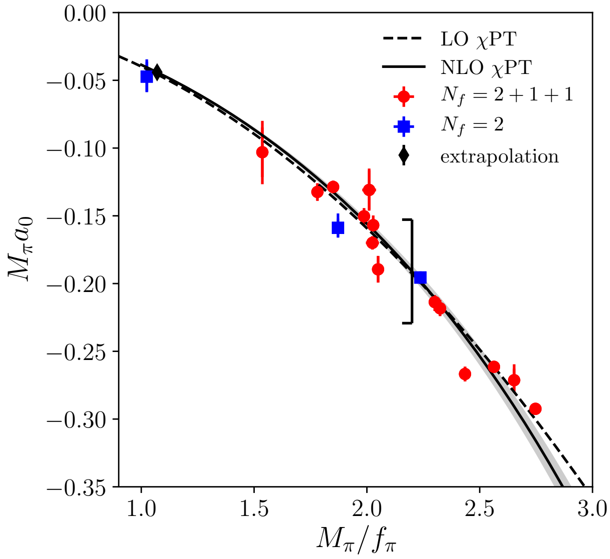

Figure 3. $I = 2$ pion-pion S-wave scattering length a_0 in units of the pion mass M_π as a function of M_π/f_π. Red symbols correspond to results obtained from three different lattice spacing values with $N_f = 2+1+1$ dynamical quark flavours[6]. Blue symbols represent $N_f = 2$ results at a single lattice spacing, but including the physical point. The bracket indicates the fit range.

with scattering length $M_\pi a_0$ at second order with only a single parameter, a so-called low energy constant.

We have obtained results on ensembles generated by the European Twisted Mass Collaboration (ETMC) with $N_f = 2+1+1$, i.e. up/down, strange and charm dynamical quarks with pion masses larger than what is found in nature[4]. Moreover, we have used $N_f = 2$ ensembles by ETMC[5] including a physical point ensemble, i.e. an ensemble where the pion mass assumes its physical value found in nature.

The results are shown in Fig. 3: we plot $M_\pi a_0$ as a function of M_π/f_π, with f_π the pion decay constant. Red symbols correspond to results obtained from three different lattice spacing values on the $N_f = 2+1+1$ ensembles[6]. Blue symbols represent the $N_f = 2$ results. In addition we show the leading order, parameter free ChPT prediction as dashed line and the second order (NLO) ChPT prediction fitted to our $N_f = 2+1+1$ data. The extrapolation to the physical point using the NLO fit of the $N_f = 2+1+1$ results is shown as a black diamond.

For the $N_f = 2+1+1$ case we find that lattice artefacts are actually negligible. Moreover, the NLO correction turns out to be very small, leading to a tiny correction of the physical value of $M_\pi a_0$ at the physical value of the pion mass. Consistent with nature our result indicates that the interaction is repulsive. Our result is in excellent agreement with other lattice and phenomenological determinations, but currently the most precise one, see the original publication[6] for more details.

Even if the $N_f = 2$ ensembles are at a single lattice spacing value only, they are still very valuable: the simulation directly at the physical point allows us to control our

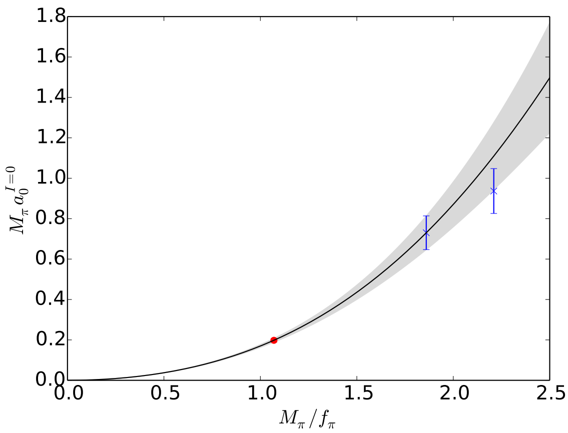

Figure 4. Pion-pion S-wave scattering length in the isospin 0 channel as a function of M_π/f_π. The solid line represents a fit of the NLO ChPT prediction to our data. The red square is our extrapolation to the physical point.

(long) chiral extrapolation in M_π/f_π. And we find very good agreement, even though the statistical uncertainties are still too large to be fully conclusive.

The expected behaviour in the isospin $I = 0$ channel is different: the interaction should be larger and of opposite sign compared to $I = 2$. In addition, the $I = 0$ case is technically much more difficult to compute: so-called fermionic disconnected diagrams contribute, which are very noisy. For this reason there are only three lattice estimates of the $I = 0$ S-wave scattering length available from lattice QCD, one of which could be obtained by us with the computer resources available to us at Forschungszentrum Jülich.

We have carried out this calculation on the aforementioned $N_f = 2$ ensembles, but at unphysically large pion masses[7]. The result is displayed in Fig. 4. The solid line with shaded error band represents again an NLO ChPT fit to the data, with again one degree of freedom. The value at the physical point is indicated by the red square.

Disconnected contributions lead, as visible from the figure, to significantly larger statistical uncertainties. However, within the statistical errors we agree to other lattice and phenomenological determinations. In particular, we find a strong and attractive interaction, compared to the $I = 2$ case. For more details we refer to the corresponding original publication[7].

3.3 Kaon-Kaon Scattering with Isospin $I = 1$

Kaon-kaon scattering with isospin $I = 1$ is to some extend very similar to pion-pion scattering. In principle only one of the light quarks is replaced by a strange quark. However, in contrast to the pion-pion case, there is no experimental result available for the scattering length. However, this quantity is important input for experiments, such as STAR or ALICE, where numerous light hadrons are created. Since kaons carry on average much lower momenta than pions, due to their lower mass value, kaons are much more likely to interact elastically than pions. Such interaction is described by the scattering length. Here a lattice

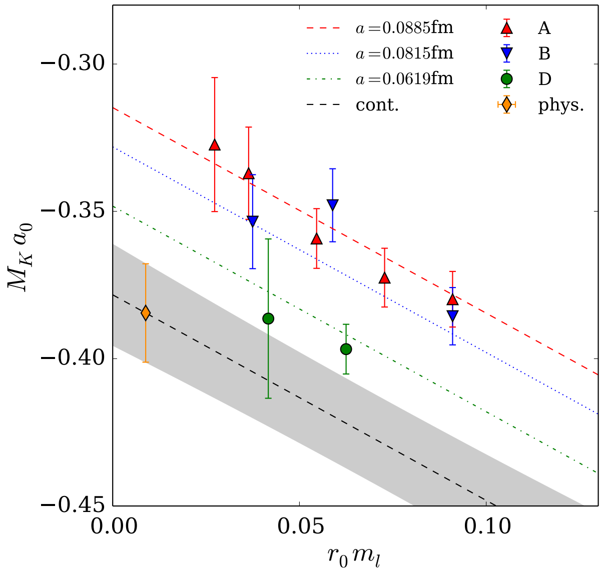

Figure 5. Kaon-kaon scattering length in the isospin $I = 1$ channel. Colour coded are the data at three values of the lattice spacing a and the extrapolated value in the continuum and at the physical point (in orange). The lines represent the light quark mass dependence at each lattice spacing value.

calculation of kaon-kaon scattering properties is valuable input.

Moreover, it is much less clear to what extent ChPT works for kaons, since ChPT is an expansion in the momenta and the quark masses. The strange quark mass value is a factor of ten to 20 larger than the ones of the light quarks. Therefore, it is interesting to investigate the quark mass dependence using lattice QCD and compare to ChPT.

We have computed the kaon-kaon S-wave scattering length using the $N_f = 2 + 1 + 1$ ETMC ensembles mentioned above. In these ensembles the strange quark mass was off its physical value by about 10%. In order to correct for this we use three valence strange quark masses and tune the strange quark mass value to its physical value using the combination of kaon and pion masses $M_K^2 - 1/2M_\pi^2$.

At fixed strange quark mass value, the extrapolation must still be performed in the light quark mass m_l. Looking at our data in Fig. 5, it seems we cannot include more than the leading order term proportional to m_l. In contrast to the pion-pion $I = 2$ case, we observe significant lattice artefacts for the kaon-kaon case. We include those in our fit to the data. The fitted curves at separate lattice spacing values are displayed as lines in the figure. The dashed line with error band is the continuum curve, which one can follow down in m_l to the physical point.

Lattice artefacts represent a significant correction to the measured data, suggesting that systematic uncertainties are not fully controlled yet. Also, we cannot finally exclude that the extrapolation is m_l is sufficient. Upcoming studies with smaller light quark masses will shed light on this point. However, our investigation represents the first of this quantity with more than one value of the lattice spacing and is, hence, a significant progress.

4 Summary

In this proceeding we have presented a part of the results that were only possible with the computer resources available to us from NIC and Forschungszentrum Jülich. We have discussed the significant improvements we could make in the performance of our code by programming explicitly for the Intel chip architecture.

Moreover, we have shown the progress in our computation of hadron-hadron interaction we could make thanks to the NIC resources. As examples we showed results obtained for pion-pion and kaon-kaon scattering, including one of the very few lattice QCD results for $I = 0$ pion-pion scattering.

Currently we are working on pion-kaon as well as pion-nucleon scattering. There we hope to have results for the Δ resonance available soon.

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