One Flavour QCD as an analogue computer for SUSY

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We numerically study QCD with a single quark flavour on the lattice probing predictions from effective field theories that are equivalent to minimal super-symmetric Yang-Mills theory in the large $N_c$ limit. The hadronic spectrum including excited states is analysed using one gauge coupling and several physical volumes and fermion masses. We use the LapH method and also compute disconnected diagrams. Lattice simulations with an odd number of Wilson fermions give rise to regions of configuration space with a negative fermionic weight entailing a sign problem. We perform a detailed analysis on the spectrum of the Wilson-Dirac operator and report on observed cases of a negative fermion determinant in our ensembles.
1. Introduction

In these proceedings we report on our ongoing efforts to study supersymmetry (SUSY) via lattice computations of the hadronic spectrum of $N_f = 1$ QCD. The relation between supersymmetric Yang-Mills theory and QCD with a single quark flavour can be seen as follows. The Lagrangian

$$L = \frac{1}{2g^2} F_{\mu\nu}^a F_{\mu\nu}^a + \bar{\psi}(m_0 + \gamma_\mu D_\mu)\psi,$$  \hspace{1cm} (1)

describes a QCD-like theory containing a single Dirac fermion in the two-index anti-symmetric representation of the gauge group $SU(N_c)$ whereas the gluons are in the adjoint representation. Note that $\psi^{ij} = \psi^b (i^b)^{ij}$, $i, j = 1, \ldots, N_c$, $a = 1, \ldots, N_c^2 - 1$, $b = 1, \ldots, \frac{N_c(N_c-1)}{2}$. Historically, this theory was studied in a technicolour extension to QCD at large $N_c$ by Corrigan and Ramond [1], who named the fermion field in the two-index anti-symmetric representation a lark (merging the words quark and large). Moreover, it was shown that the lark theory (1) and $N = 1$ super-Yang-Mills (SYM) theory are equivalent in the limit $N_c \rightarrow \infty$ with regard to the bosonic sector of the spectrum [2, 3]. Note also that the number of fermionic degrees of freedom scales as $N_c^2$ as $N_c \rightarrow \infty$ in both the lark theory and in SYM signalling their equivalence.\footnote{This can be seen from a simple counting of dimensions. For the lark theory there are 2 Dirac spinors with 4 components each and the dimension of the anti-symmetric representation scales as $N_c^2 / 2$ for large $N_c$ whereas for SYM there are 2 Majorana spinors with 2 components each and the adjoint representation scales as $N_c^2$ for large $N_c$.} For $N_c = 3$ the two-index anti-symmetric representation coincides with the conjugate representation, i.e. a lark is equivalent to an anti-quark, hence (1) describes $N_f = 1$ QCD.

In SYM the even and odd parity mesons are degenerate. Deviations from the degeneracy have been studied in the lark theory in the large $N_c$ limit in [4] and [5]. Both works use planar equivalence to predict the lightest pseudo-scalar meson to be lighter than the lightest scalar meson. In particular, the former work takes into account the explicit SUSY breaking due to the finite fermion mass studying low-energy effective Lagrangians of the lark theory and making use of exact SUSY results at the effective action level. The lark theory by Corrigan and Ramond has led to a plethora of applications including investigations of meson scattering [6], a study on (super-) glue balls in comparison to QCD mesons and glue balls [7], investigations of the conformal window [8, 9] as well as works in phenomenology [10, 11].

In this work we simulate $N_f = 1$ QCD on the lattice to probe the mentioned prediction and to study relics of SYM for $N_c = 3$. This also comes with the advantage of lower simulation costs compared to direct lattice simulations of SYM, the latter being hard because massless fermions need to be handled. However, it should be emphasised that $N_f = 1$ QCD should be regarded if at all as a proxy for SUSY.

A few years back a lattice study probing the planar equivalence prediction was presented at the Lattice conference by the Münster group and collaborators [12]. Our work at hand can be regarded as an update in an advanced setup using tree-level $O(a)$-improved Wilson fermions. In addition, we also extract excited states of the mesonic spectrum.

Unlike in the continuum formulation where the fermion determinant is guaranteed to be positive in the lattice formulation with Wilson fermions there are regions of configuration space with a negative fermionic weight. This gives rise to a sign problem. We present a detailed analysis...
on the sign of the fermion determinant on our gauge field ensembles. This account is organised as follows: In Section 2 we summarise our lattice setup, followed by the sign problem analysis in Section 3. In Section 4 we show the results on the hadronic spectrum and we conclude this work in Section 5.

2. Lattice setup

The lattice action considered in this work contains the tree-level Symanzik improved gauge action and the tree-level $O(a)$-improved Wilson clover fermion action ($c_{SW} = 1$). We restrict ourselves to a single gauge coupling corresponding to $\beta = 4.5$. To simulate the single quark flavour the RHMC algorithm [13, 14] is used. $N_f = 1$ QCD comes with two main challenges. (i) The scale setting cannot be carried out in the usual way as in e.g. $N_f = 2 + 1$ QCD by using an experimentally known (low-energy) quantity such as a hadron mass. (ii) chiral symmetry is absent which excludes comparisons with chiral perturbation theory. Addressing challenge (i), we obtain an approximation to the scale by setting the lattice spacing using the Wilson flow in the pure gauge theory following [15] which results in $a \approx 0.06$ fm. Regarding challenge (ii) it is noteworthy that even in the absence of chiral symmetry it is possible to guarantee (at least approximately) a well-defined extrapolation to zero quark mass. To that end the mass of the lightest pseudo-scalar meson, called the fake pion, is measured in the partially quenched extension of the single flavour theory obtained by adding an additional valence quark, see [12] for details and references. Simulating $N_f = 1$ QCD amounts to navigating in unknown territory in parameter space for the various mentioned reasons. To our knowledge neither chiral perturbation theory nor the method put forward in [16, 17] for estimating finite volume effects have been worked out for the lark theory in general. However, we consider these effects to be sub-leading at the level of precision we are interested in. Therefore we have produced and analysed gauge field ensembles for several physical volumes $L/a \in \{12, 16, 20, 24, 32\}$, $T/a = 64$ and hopping parameters\textsuperscript{2} $\kappa \in \{0.1350, 0.1370, 0.1390, 0.1400, 0.1405, 0.1410\}$. All configurations for this project have been generated with the openQCD software package [18].

3. Sign problem

As mentioned above in a setup of a single flavour of Wilson fermions at finite lattice spacing there exist regions of configuration space on which the fermion determinant is negative. This can also occur in multi-flavour QCD and has been subject to a recent study in $N_f = 2 + 1$ flavour QCD [19]. Since we are generating our gauge field ensembles with respect to the sign quenched fermionic weight we need to monitor the sign of the fermion determinant on configurations we measure observables on and in case a negative determinant is detected it has to be accounted for by reweighting. Since a direct computation of the sign of the fermion determinant is numerically too expensive, we infer it indirectly from the low-lying eigenvalue spectrum of the Wilson Dirac operator $D$. $\gamma_5$-hermiticity of $D$ guarantees the eigenvalues to come either in complex conjugated pairs or to be real. This entails that only real eigenvalues can produce a sign change of the determinant. Hence,

\textsuperscript{2}The hopping parameter is defined as $\kappa = \frac{1}{\pi(4+m_0)}$. 

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on a given configuration it remains to check if there is an odd number of negative real eigenvalues of $D$. 

In practice it is more convenient to consider the Hermitian matrix $Q := \gamma_5 D$. Because $\det(Q) = \det(D)$ and since a zero eigenvalue of $D$ is also a zero eigenvalue of $Q$ we can thus reduce the sign computation to analysing the behaviour of the low eigenvalues $\lambda_i(m_0)$ of $Q$ as a function of the bare mass $m_0$. Monitoring the sign and counting the zero crossings of the low eigenvalues of $Q$ when varying $m_0$, the change in the number of negative real eigenvalues of $D$ can be inferred.

Technically, we proceed in two stages: (i) For a given configuration simulated with a bare mass $m_0^*$ we compute the lowest lying eigenpairs $(\lambda_i, \phi_i)$ of $Q$. In addition, the chirality $\chi_i = d\lambda_i/dm_0|_{m_0=m_0^*} = (\phi_i, \gamma_5\phi_i)$ being the slope of the eigenvalue function [19, 20] is computed. Hence from the sign of the chirality we can infer if a given eigenvalue moves towards or away from zero as $m_0$ is increased infinitesimally. A showcase for stage (i) of the analysis is displayed in the left panel of Figure 1.

(ii) Configurations giving rise to low eigenvalues of $Q$ that might cross zero are further analysed using the tracking method presented in [19]. On a given configuration we measure the lowest $N_{ev}$ eigenpairs $(\lambda_i, \phi_i)$ of $Q$ for several bare masses $m_0$ around the simulation mass. The measurements were carried out using the PRIMME package [21, 22] combined with openQCD. Assuming that $\text{span} (\{\phi_i\})$ changes slowly and continuously as $m_0$ is varied in steps of $\Delta m_0$ allows to extract the

Figure 1: \textit{Left:} Showcase of stage (i) of the determinant sign analysis. The 12 lowest eigenvalues and their corresponding chiralities of $Q$ are computed on a subset of ca. 40 configuration from the $L/a = 24$ ensemble at $\kappa = 0.1410$. It is visible that there are a few points in the second and fourth quadrant signalling that the corresponding eigenvalues at this bare mass move towards zero as the mass is infinitesimally increased. These configurations are further checked in stage (ii) of the analysis with regard to whether and how many sign changes of the eigenvalue functions appear.

\textit{Right:} Showcase of stage 2 of the determinant sign analysis. Displayed is the partially quenched computation of the lowest 20 eigenvalues of $Q$ on a fixed gauge configuration in the ($L/a = 24, \kappa = 0.1410$) ensemble for a range of values for the bare mass around the simulation mass $m_0^* \approx -0.453$ indicated by the pink vertical line. This configuration is safe in the sense that the fermion determinant is positive as there are no sign changes of the eigenvalue functions $\lambda_i(m_0)$. 

In this context, it is important to note that the bare mass $m_0$ is a quantity that is determined by the lattice spacing $a$ and the lattice spacing $\Lambda$ through the relation $m_0 = \Lambda/a$. This relationship is crucial in understanding the role of the bare mass in the analysis of the fermion determinant.
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| bare mass $m_0$ | 0.000 | 0.025 | 0.050 | 0.075 |
|------------------|-------|-------|-------|-------|
| eigenvalue function $\lambda_i(m_0)$ | 0.075 | 0.050 | 0.025 | 0.000 |

Figure 2: Showcase of stage 2 of the tracking analysis where the occurrence of a negative fermionic determinant can be deduced from a single sign change in one of the low eigenvalues of $Q$ above the simulation mass $m_0^*$. From this we can also conclude that $D$ must have an odd number of negative real eigenvalues at the simulation mass.

4. Hadron spectroscopy

We are interested in the massless limit of the mesonic spectrum of $N_f = 1$ QCD. We are using the LapH method [23, 24] which provides a suitable framework to include quark-disconnected pieces, which are vital to correctly extract the spectrum. It furthermore allows to cheaply construct different operators $\hat{O}_i$ inducing the same quantum numbers and hence the same spectrum but differing in the approach to the ground state. We are interested in the masses of the pseudo-scalar (P), scalar (S), and vector (V) mesons. In principle a scalar glueball can be present, so in addition to operators of the type $\bar{q} \Gamma q$ we also use a purely gluonic operator that is expected to...
predominantly couple to the glueball (G). We extract the spectrum by performing simultaneous correlated three-exponential fits to several correlation functions using the ansatz

\[ C_{ij}(t) = \sum_n \langle 0 | \hat{O}_i | n \rangle \langle n | \hat{O}_j^\dagger | 0 \rangle e^{-m_n t}. \]  

(2)

In Figure 3 the result for the spectrum of the pseudo-scalar meson is shown. As a measure of stability we perform each for different subsets of the operators in the basis, shown by the different symbols (circles, squares, diamonds). In the left panel the bare quark mass dependence is shown at fixed volume \( L/a = 16 \). As expected the ground state is strongly mass dependent. In the right panel we investigate the volume dependence of the spectrum at fixed bare quark mass corresponding to \( \kappa = 0.1390 \). At this value of \( \kappa \), we find the ground state to be volume independent, but with sizable finite size effects being displayed for the smallest volume.

For the scalar-glueball channel the extracted spectrum looks qualitatively different as shown in Figure 4. The left panel shows the mass dependence at the same fixed volume. Looking at the ground and first excited state, the lightest observed state is mass-insensitive at fixed volume whilst the first excited state displays a clear mass dependence. In the right panel of the same figure we again investigate the volume dependence of these states at fixed mass. For this value of \( \kappa \), there appears to be one volume dependent state and one volume independent state with a cross-over somewhere between \( L/a = 16 \) and \( L/a = 20 \). We repeat this comparison for each volume and in each case identify the mass-sensitive state with a scalar meson. This identification is guided by monitoring the behaviour of the overlap factors, for example whether the correlation function purely built from the gluonic operators couples more strongly to the ground or the first excited state. The resulting data points are shown in the left hand panel of Figure 5. From the right hand panel of Figure 5 we find that the remaining lowest state is strongly volume dependent, getting heavier as the volume increases. This is inconsistent with the expected behaviour for a glueball state, so we identify this state to be a finite volume state possibly resulting from flux tubes around the periodic lattice, also called a torelon state [25]. However, in the study at hand we have not further investigated the
Figure 4: Left: Spectrum of the scalar meson for the various bare masses $m_0$ at fixed volume $L/a = 16$. Right: Spatial volume dependence of the spectrum of the scalar meson at fixed $\kappa = 0.139$.

Figure 5: Categorisation of the spectrum of the scalar meson into a mass-dependent (left) and a remaining lowest state (right). In the right-hand side plot the strong volume dependence is inconsistent with what is expected for a glueball state. A possible interpretation is that this state is a finite volume torelon state.

character of these states and whether they are torelon states. In principle this could be done by computing correlators of spatial Wilson loops.

Figure 6 shows the mass ratio of the (mass-dependent) pseudo-scalar to scalar meson. Disregarding the smallest volume which appears to show strong finite size effects the results for the different volumes are in agreement in the range between large and intermediate masses. Our data confirms that the pseudo-scalar meson is lighter than the scalar one. For a robust comparison with the low-energy effective theory prediction from [4] we need to perform an extrapolation to vanishing
Figure 6: Ratio of the pseudo-scalar to scalar meson mass as a function of the various bare masses $m_0$.

quark mass. This is subject to ongoing work and we are currently producing more statistics at the largest volumes and hopping parameters.

5. Conclusion and perspectives

We have presented an analysis on the hadronic spectrum of $N_f = 1$ QCD in the mesonic sector. By including excited states we have extracted the mass dependency of the scalar and pseudo-scalar state. The next step of performing the extrapolation to zero quark mass is subject to ongoing work. From this, comparisons with the predictions from low-energy effective theories for the deviation from the even-odd parity degeneracy can be made. Loosely speaking, this will also show what remnant SUSY is contained in the $N_c = 3$ lark theory. Moreover, we have shown that the sign problem due to the use of Wilson fermions is mild but must be monitored. We emphasise the relevance of this aspect also in multi-flavour QCD simulations.

Future work will be devoted to investigating the lark theory on the lattice for larger number of colours $N_c > 3$. To that end we are working on code development and the use of GPU accelerators.

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