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Hadron spectrum of QCD with one quark flavor

Federico Farchioni*, **Gernot Münster, Tobias Sudmann, Jaïr Wuilloud**
Universität Münster, Institut für Theoretische Physik,
Wilhelm-Klemm-Strasse 9, D-48149 Münster, Germany
E-mail: farchion@uni-muenster.de

István Montvay

Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, D-22603 Hamburg, Germany

Enno E. Scholz

Physics Department, Brookhaven National Laboratory, Upton, NY 11973, USA

The latest results of an ongoing project for the lattice simulation of QCD with a single quark flavor are presented. The Symanzik tree-level-improved Wilson action is adopted in the gauge sector and the (unimproved) Wilson action for the fermion. Results from new simulations with one step of Stout-smearing ($\rho = 0.15$) in the fermion action are discussed. The one-flavor theory is simulated by a polynomial hybrid Monte Carlo algorithm (PHMC) at $\beta = 4.0$ corresponding to $a = 0.13\,\mathrm{fm}$, on $16^3 \cdot 32$ and $24^3 \cdot 48$ lattices; the box-size is $L \simeq 2.1\,\mathrm{fm}$ and $L \simeq 3.1\,\mathrm{fm}$, respectively. At the lightest simulated quark mass the (partially quenched) pion mass is ~ 300 MeV. The masses of the lightest bound states are computed, including the flavor singlet scalar and pseudoscalar mesons σ_s and η_s, the scalar glueball 0^{++}, and the Δ^{++} baryon. Relics of SUSY in the mass spectrum, expected from a large N_c orientifold equivalence with the $\mathcal{N}$=1 supersymmetric Yang-Mills theory, are discussed.

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1. Introduction and motivation

The low-energy dynamics of QCD with a single quark flavor ($N_f = 1$ QCD) strongly differs from the one of the multi-flavor theory since chiral symmetry, and its spontaneous breaking, is absent. Nevertheless, several open questions of the physical theory may be better understood in the theory with minimal number of fermionic degrees of freedom [1, 2, 3]. For example [2], whether setting to zero just one quark mass produces physical effects; in the one-flavor model, due to the lack of a chiral symmetry, even the definition of the quark mass is non-trivial [1]. Another question [3] is whether spontaneous breaking of CP is possible for special combinations of the light quark masses (negative quark mass for one flavor).

Another intriguing aspect of one-flavor QCD, emerging from string theory, is the connection with the $\mathcal{N}$=1 supersymmetric Yang-Mills theory (SYM), also investigated by our collaboration [4]. The equivalence of the two theories in the bosonic sector can be proved at the planar level of an "orientifold" large N_c limit [5]. Relics of SUSY are therefore expected in $N_f = 1$ QCD (with $N_c = 3$) where approximately degenerate scalars with opposite parity should be observed. These two particles can be identified in the single-flavor theory with the singlet scalar and pseudoscalar mesons which we denote with σ_s and η_s.

As we have argued in [6], some chiral symmetry can be recovered in $N_f = 1$ QCD by embedding the theory in a larger partially quenched (PQ) theory with additional valence quark flavors. This allows to build pions and obtain a possible definition of the quark mass by the PCAC relation.

We present here the latest results of an ongoing computation of the low-lying hadron spectrum of $N_f = 1$ QCD in the Wilson formulation [6], obtained from $16^3 \cdot 32$ and $24^3 \cdot 48$ lattices at lattice spacing $a \simeq 0.13\,\text{fm}$ ($L = 2.1$ and $3.1\,\text{fm}$). The lightest simulated pion mass is $M_\pi \simeq 300\,\text{MeV}$.

2. Partial quenching

The definition of a quark mass is not immediate in one-flavor QCD due to the lack of chiral symmetry (even in the continuum). For example a PCAC quark mass cannot be defined. More generally, the bilinear quark operator $\bar{q}q$ is not protected against scheme-dependent additive renormalizations and the concept of vanishing quark mass could be devoid of physical meaning [1]. In our approach we take $N_V = 2$ valence quarks degenerate with the (single) sea quark. With the $N_V \geq 2$ valence quarks plus the sea quark, all mesons and baryons of QCD can be build, appearing in degenerate multiplets due to the exact $\mathrm{SU}(N_V + 1)$ flavor symmetry. A PCAC quark mass can be defined in the PQ theory by the non-singlet axial-vector chiral current $A^a_{x\mu}$

$$m_{\text{PCAC}} \equiv \frac{\langle \partial^*_\mu A^+_{x\mu} \, P^-_y \rangle}{2\langle P^+_x \, P^-_y \rangle} \ . \tag{2.1}$$

Relation (2.1) should be considered here just as a possible definition of the quark mass in $N_f = 1$ QCD (a possible physical meaning of this definition is not claimed at this stage).

In [6], validity of the GMOR relation for the pions in the PQ extension of the one-flavor theory was confirmed: the masses of the pions can be made to vanish by suitably tuning the bare quark mass on the lattice; in this situation the quark mass (2.1) vanishes, too. This scenario is confirmed by a study of the chiral Ward identities [7].

Table 1: Summary of the runs: the bar indicates runs with Stout-link in the fermion action (see text).

	L	β	κ	$N_{\rm conf}$	plaquette	$\tau_{\rm plaq}$	r_0/a
a	12	3.80	0.1700	5424	0.546041(66)	12.5	2.66(4)
b	12	3.80	0.1705	3403	0.546881(46)	4.6	2.67(5)
c	12	3.80	0.1710	2884	0.547840(67)	7.6	2.69(5)
A	16	4.00	0.1600	1201	0.581427(36)	4.3	3.56(5)
B	16	4.00	0.1610	1035	0.582273(36)	4.1	3.61(5)
C	16	4.00	0.1615	1005	0.582781(32)	3.3	3.73(5)
$\overline{A}$	16	4.00	0.1440	5600	0.577978(23)	9.7	3.74(3)
$\overline{B}$	16	4.00	0.1443	5700	0.578167(28)	11.3	3.83(5)
$\overline{B}_{24}$	24	4.00	0.1443	3900	0.578182(10)	5.8	3.83(4)

Although pions do not belong to the unitary sector of the theory, their properties and the PCAC quark mass can be used for a characterization of the one-flavor theory. In particular the low-energy coefficients of the chiral Lagrangian can be extracted by an analysis in PQ chiral perturbation theory [6].

3. Simulation

The gauge action is discretized by the tree-level improved Symanzik (tlSym) lattice action [8] including planar rectangular (1×2) Wilson loops. We apply the (unimproved) Wilson formulation in the fermionic sector. Previous results [6] were presented for simulations with the original Wilson formulation; with the goal of improving stability of the Monte Carlo evolution at small quark masses, we now apply Stout-smeared links [9] in the hopping matrix (one step of isotropic smearing with coefficient $\rho_{\mu\nu} = \rho = 0.15$).

The update algorithm is a Polynomial Hybrid Monte Carlo algorithm with a two-step polynomial approximation (TS-PHMC) [10]. A correction factor $C[U]$ in the measurement is associated to configurations for which the eigenvalues of the (squared Hermitian) fermion matrix lie outside the validity range of the polynomial approximation. See [6] for more details on the algorithmic setup. The sign of the determinant associated to one (light) Wilson quark can become negative on some configurations, even for positive quark masses. Since the sign cannot be taken into account at the update level, it must be computed "off-line" and included in the correction factor; the expectation value of a generic quantity A is therefore given by

$$\langle A \rangle = \frac{\int [dU]\, \sigma[U]\, C[U]\, A[U]}{\int [dU]\, \sigma[U]\, C[U]} \;, \tag{3.1}$$

where $\sigma[U]$ is the sign of the one-flavor determinant. For the computation of the sign we study the (complex) spectrum of the non-Hermitian matrix concentrating on the lowest real eigenvalues: sign changes are signaled by negative real eigenvalues. We applied the ARPACK Arnoldi routines on a transformed Dirac operator. The (polynomial) transformation was tuned such that the real eigenvalues are projected outside the ellipsoidal bulk containing the whole eigenvalue spectrum [11]. This allows an efficient computation of the real eigenvalues [12].

Table 2: Results for hadron observables in $N_f = 1$ QCD (lattice units).

	aM_{η_s}	aM_{σ_s}	aM_{Δ_s}	am_{PCAC}	aM_π	af_π	aM_N
a	0.462(13)	0.660(39)	1.215(20)	0.0277(5)	0.3908(24)	0.1838(11)	1.044(5)
b	0.403(11)	0.629(29)	1.116(38)	0.0195(4)	0.3292(25)	0.1730(15)	0.956(3)
c	0.398(28)	0.584(55)	1.204(57)	0.0108(12)	0.253(10)	0.156(10)	1.01(5)
A	0.455(17)	0.607(57)	1.006(15)	0.04290(36)	0.4132(21)	0.1449(9)	0.902(4)
B	0.380(18)	0.554(52)	0.960(15)	0.02561(31)	0.3199(22)	0.1289(10)	0.798(5)
C	0.344(21)	0.576(53)	0.971(30)	0.01681(33)	0.2622(19)	0.1190(17)	0.762(9)
$\overline{A}$	0.347(16)	0.538(41)	0.855(50)	0.01651(27)	0.2471(19)	0.0983(20)	0.733(13)
$\overline{B}$	0.286(18)	0.485(46)	0.848(70)	0.01094(23)	0.2028(35)	0.0913(24)	0.670(20)
$\overline{B}_{24}$	0.261(11)	0.496(22)	0.900(24)	0.01047(17)	0.1958(15)	0.0920(11)	0.672(10)

The updating has been performed by applying determinant break-up by a factor of two (that is, two half-flavors were considered instead of one). The update sequence consisted of two PHMC trajectories followed by an accept-reject step by the second (precise) polynomial approximation. The precision of the first polynomial approximation was tuned such that an acceptance of about 90% was obtained. The same acceptance was required for the Metropolis test at the end of every individual PHMC trajectory by tuning the trajectory length (0.4-0.5). This resulted in a high total acceptance rate of about 80%. The gauge configurations were stored after every accept-reject step by the precise polynomial. Relatively short trajectories were chosen in order to have many configurations for the glueball mass determination. Optimization of the parameters of PHMC turned out to have a substantial impact on the integrated autocorrelation times of the average plaquette. Information about the sets of configurations generated up to now can be found in Table 1. New results presented in this Contribution concern runs $C, \overline{A}, \overline{B}, \overline{B}_{24}$.

We fix the lattice scale by the Sommer scale parameter r_0 [13]. For the conversion into physical units we assume the conventional value $r_0 = 0.5\,\mathrm{fm}$. As in ordinary QCD, r_0/a grows with the hopping parameter κ; consistently with a massless scheme the value of r_0/a should be extrapolated to the critical value $\kappa = \kappa_c$ where the PCAC quark mass (2.1) vanishes. The number of quark masses at our disposal are however not sufficient for an extrapolation and we rely on the value at the highest κ for given β. We obtain in this way $a(3.8) \simeq 0.19\,\mathrm{fm}$ and $a(4.0) \simeq 0.13\,\mathrm{fm}$. This corresponds to a roughly constant volume $L = 2.1\,\mathrm{fm}$. In order to check finite volume effects, a run on a larger $24^3 \cdot 48$ lattice has been started, see Table 1, corresponding to $L = 3.1\,\mathrm{fm}$.

We observe that, for a fixed quark mass (in lattice units), the Stout-smearing leaves r_0/a essentially unchanged (as can be seen by comparing runs C and $\overline{A}$). On the basis of this observation, we will assume approximate equality of the lattice spacing for the $\beta = 4.0$ runs with and without smearing; therefore data from both sets will be included in analyzes at fixed lattice spacing.

4. Hadron spectrum

The disconnected diagrams of the η_s and σ_s correlators (with usual interpolating fields) were computed by applying for each configuration 20 stochastic sources with complex Z_2 noise and spin

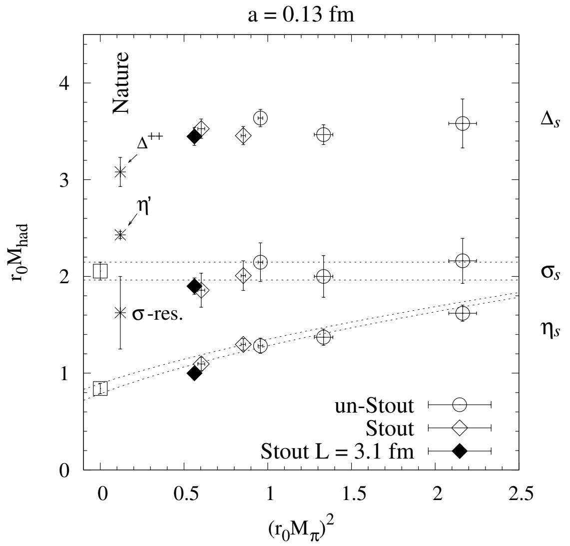

Figure 1: The mass of the lightest physical particles in one-flavor QCD as a function of the squared pion mass in units of the Sommer scale. The hadron masses are multiplied by the value of r_0/a at the given κ.

dilution. In consideration of autocorrelations, we analyzed every 10th, 16th or 32th configuration according to κ. The resulting statistics vary between 400 and 600.

In the case of the baryon, we take the interpolating field $\Delta_i(x) = \varepsilon_{abc}[\psi_a(x)^T C\gamma_i \psi_b(x)]\psi_c(x)$. The low-lying projected state is expected to be a spin $3/2$ parity-positive particle which we denote with Δ_s (the desired spin 3/2 component is extracted by spin-projection). It corresponds to the $\Delta^{++}(1232)$ baryon of QCD if the single quark is identified with the *u*-quark.

In the PQ sector we measure the pion observables, $M_\pi, f_\pi, m_{\rm PCAC}$, in which case correlators trivially coincide with the connected parts of the corresponding η_s correlators; the nucleon mass is determined by applying the standard projecting operator [6].

No smearing was applied for the extraction of the masses. It turns out however that this is necessary in the baryon sector where the approach to the asymptotic behavior is slow. The optimization of the overlap with the ground state by Jacobi smearing is in plan.

Results. The results for the hadron observables in lattice units including new runs with Stout-smearing are reported in Table 2. The lightest pion mass corresponds to $\sim$ 300MeV. From the comparison between runs $\overline{B}$ and $\overline{B}_{24}$ ($L = 2.1\,\mathrm{fm}$ and $L = 3.1\,\mathrm{fm}$, respectively) finite volume effects can be estimated. These are below the statistical accuracy ($\sim$ 10%) for the particles in the unitary sector. In the pion sector, they exceed statistical accuracy in the case of the pion mass and of the PCAC quark mass, however they are relatively small ($\sim$ 4% in both cases). Observe that the sign of the finite size scaling agrees with what is observed in standard QCD.

In Fig. 1 the hadron masses in the unitary sector are reported in physical units as a function of the squared pion mass. The σ_s and the Δ_s masses are (surprisingly) near to the values observed in nature for the corresponding particles or resonances. In contrast, the η_s meson is much lighter than the QCD flavor-singlet η'; this can be understood [6] in terms of the Witten-Veneziano formula. The η_s mass, which shows a clear quark mass dependence, can be extrapolated to zero quark

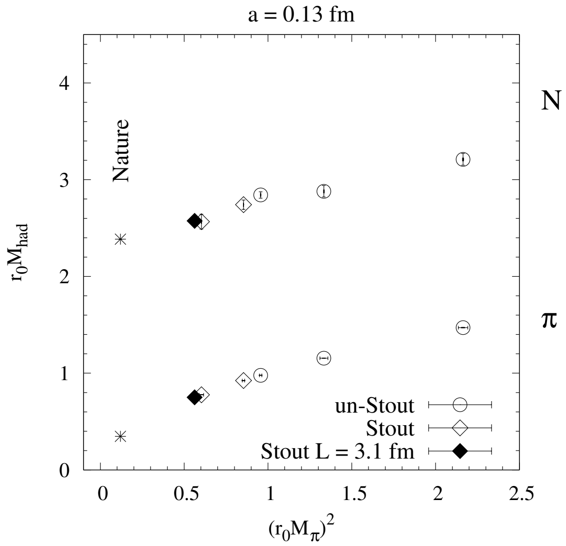

Figure 2: The PQ sector of one-flavor QCD: the nucleon mass as a function of the square pion mass in units of the Sommer scale. The pion mass is also reported for comparison.

mass by applying the LO chiral perturbation theory formula [14, 6] $M_{\eta_s}^2 = (M_\phi^2 + M_\pi^2)/(1+\alpha)$, with M_ϕ and α constants. The result is: $r_0 M_{\eta_s}(m_q = 0) = 0.84(5)$ [330(20) MeV]; the error also includes a rough estimate of the extrapolation uncertainty, obtained by comparing results including or excluding the heaviest quark mass. It is interesting to compare this result for the η_s mass with the one obtained by our collaboration for the corresponding particle in SU(2) SYM, the *adjoint* η' (a-η'): $r_0 M_{a\text{-}\eta'} = 1.25(5)$ [499(20) MeV] [4]. Since the quark mass dependence of the σ_s mass cannot be seen with our statistical accuracy, we simply apply a fit to a constant; the result is: $r_0 M_{\sigma_s} = 2.05(9)$ [810(35) MeV].

We can now check our results against the prediction from the orientifold planar equivalence [15]: $M_{\eta_s}/M_{\sigma_s} = (N_c - 2)/N_c \times (1+\delta)$, where the correction $\delta = O(1/N_c, 1/N_c^2)$ is expected to be suppressed. We obtain:

$$\frac{M_{\eta_s}}{M_{\sigma_s}} = 0.410(32)(25)\,, \quad \delta = 0.23(10)(7)\ . \tag{4.1}$$

(the second error comes from the extrapolation, only data from the $L = 2.1$ fm volume are included). The relatively small value of δ seems to confirm suppressed $O(1/N_c)$ corrections, as expected on theoretical grounds [15]. Small deviations from the leading orientifold prediction were also observed for the fermion condensate, in numerical simulations [16], and in an analytical computation for free staggered fermions [17]. The inclusion in the analysis of smaller quark masses and larger volumes could further lower the ratio (4.1) and therefore the deviation δ.

Purely gluonic operators, the glueballs, project onto Spin 0 states, too. We investigate here the 0^{++} state, which is expected to mix with the σ_s. We neglect for the moment possible mixings with the mesonic state and consider diagonal correlators only. Since the computational load is low, we analyze in this case each configuration; this allows to obtain a decent signal for the case of the Stout-runs, where fluctuations are reduced. We obtain $r_0 M_{0^{++}} = 1.94(25)$ for run $\bar{A}$ and $2.43(35)$ for run $\bar{B}$; these results are in the ballpark of the σ_s mass in accordance with strong mixing.

The behavior of the nucleon mass as a function of the pion mass squared is reported in Fig. 2; for comparison, we also report the pion mass. Also in the case of the nucleon we observe a surprising agreement with the expectations from the physical world.

5. Conclusions and perspectives

New data from simulations of lighter quark masses in sufficiently large volumes allowed first quantitative estimates for the hadron spectrum of $N_f = 1$ QCD. Results for the σ_s and η_s masses could be compared with the predictions from the orientifold equivalence; the deviation from the leading formula for the ratio of the masses turns out to be relatively small, in accordance with observations for the fermion condensate [16, 17]. With the exception of a lighter η_s, no other striking deviation from the physical (multi-flavor) picture is observed for the measured quantities. The simulation of additional lighter quark masses in view of an analysis in chiral perturbation theory is planned for the future. The search for the expected CP-violating phase transition is ongoing.

The computations were carried out on Blue Gene L/P and JuMP systems at JSC Jülich (Germany).

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