Full QCD with Wilson Fermions: Recent Results from the SESAM Collaboration

SESAM-Collaboration

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We present recent results of SESAM’s large scale lattice simulation of QCD with two dynamical flavours of Wilson fermions.

1 Introduction

As was pointed out by Gottlieb simulations with dynamical Wilson fermions at weak coupling on large lattices and at light quark masses are still lacking. In an effort to improve on this situation, SESAM (Sea-Quark Effects on Spectrum and Matrix Elements) and T$\chi$L (Towards the Chiral Limit) have been producing dynamical gauge configurations (with Wilson fermions) at a total of 4 sea-quark mass values, on two lattice volumes and working at a coupling which - as we shall show below - corresponds to a quenched coupling in the scaling regime. In this short note, we summarize some of SESAM’s recent findings; more details can be found in [3, 4, 5, 6, 7].

2 Status of Simulation

We work with two dynamical Wilson fermions on a lattice of dimensions $16^3 \times 32$ and at a strong coupling of $\beta = 5.6$. SESAM is now close to completing its QH2 ($4 \times 8 \times 8$ nodes) run-time of approx. 350 days and in this time we have produced, after thermalisation, 5000 trajectories of unit length ($100 \pm 20$ molecular dynamics steps with $dt = 0.01$ - see [3] for details) at sea quark values $\kappa_{\text{sea}} = \{0.156, 0.157, 0.1575\}$. A half-time analysis was presented at Lattice 96 where we analysed $\{100, 160, 100\}$ configurations per sea-quark taken at intervals of 25 units. This interval size is motivated from clean signals in the autocorrelation function which emerge once the ensembles become larger than approx. 2000 trajectories. As an example we quote the integrated autocorrelation times of the plaquette $\tau_{\text{pla}}^{\text{int}} = \{3.3(5), 4.1(3), 7.1(5)\}$ and - as a “worst case” - that of the average number of iterations in the HMC (using BiCGStab) $\tau_{\text{int}}^{N_{\text{it}}} = \{20(1), 27(3), 31(4)\}$.

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$^a$Talk given by H. Hoeber
3 Spectrum

For each sea-quark mass we calculate hadron masses with valence quarks \( \kappa_{\text{val}} = \{0.1555, 0.1560, 0.1565, 0.1570, 0.1575\} \). Gauge invariant smearing (50 iterations and smearing parameter \( \alpha = 4 \)) is applied to obtain smeared sources and smeared/local sinks. We use uncorrelated single-exp. fits to SL and SS data (simultaneously). Least-\( \chi^2 \) fits favour (linear + quadratic) chiral parametrizations for pseudoscalar and vector mesons as well as the nucleon (for vector particle and nucleon, a term \( \propto m^{3/2} \) does equally well). The lattice spacing is determined using the rho mass at \( \kappa_c \); using instead \( \kappa_{\text{light}} \) reduces \( a^{-1} \) by no more than 1%. The values for \( \kappa_{\text{light}} \) and \( \kappa_{\text{strange}} \) are obtained by interpolating to the mass ratios \( m_\pi^2/m_\rho^2 \) and \( m_\rho^2/m_\pi^2 \) and can be used to extract the quark masses. From table 1 we note that our lattice spacings correspond to a quenched \( \beta \) of around 6.0, one that is at the onset of the scaling regime. These values of \( a^{-1} \) are in agreement with those extracted from the interquark-force

| \( \kappa_{\text{sea}} \) | \( \kappa_c \) | \( a m_\rho \) | \( a_\rho^{-1}[\text{GeV}] \) | \( \kappa_{\text{light}} \) | \( \kappa_{\text{strange}} \) |
|-----------------|--------|---------|-----------------|-------------|-------------|
| 0.156           | 0.16065(8) | 0.359(8) | 2.14(5)         | 0.16058(8) | 0.1576(2)   |
| 0.157           | 0.15987(6) | 0.341(8) | 2.23(7)         | 0.15980(5) | 0.1569(2)   |
| 0.1575          | 0.15963(11) | 0.316(10) | 2.44(8)        | 0.15944(7) | 0.1544(1)   |
| quenched        |         |         |                 |             |             |
| \( \beta = 6.0 \) | 0.15718(6) | 0.330(8) | 2.33(6)         | 0.15709(4) | 0.1544(1)   |

Table 1: Lattice spacings and \( \kappa \)-values.

An alternative way of taking the chiral limit is to use only data with \( \kappa_{\text{sea}} = \kappa_{\text{val}} \) in the extrapolation of mass ratios. We postpone this discussion until higher statistics are reached and an additional \( \kappa_{\text{sea}} \) from T\( \chi \)L becomes available.

4 The \( \pi \)-Nucleon \( \sigma \) term

Over the past years there has been significant computational progress in the calculation of flavour singlet matrix elements (see and references therein). It was shown, in particular, that the noisy-estimator technique with a random \( Z_2 \) noise is a promising method to calculate the amplitude of the disconnected contribution to \( \sigma_{\pi N} \), where the term “disconnected” refers to:

\[
\sigma_{\pi N} = m_q \langle N | \bar{u}u + \bar{d}d - 2\bar{s}s | N \rangle + 2m_q \langle N | \bar{s}s | N \rangle = \sigma_{\pi N}^{\text{connected}} + \sigma_{\pi N}^{\text{disconnected}}. \tag{1}
\]
Here, $|N\rangle$ is a nucleon state and $m_q$ denotes the current quark mass of the $u$ and $d$ (taken to be equal).

Pioneering attempts to calculate the disconnected amplitude in full QCD have not led to overly clear signals. Quenched (high-statistics) calculations have produced rather more promising data (see [11] for a review and [13], [14], [15]), however, it is unclear, a priori, what meaning can be attributed to disconnected amplitudes for gauge configurations which disregard the effects of dynamical quarks. In addition, quark masses are found to be much smaller in full lattice QCD adding a significant uncertainty to the quenched calculations.

Algorithmic Investigation
We have carried out an extensive algorithmic investigation for the calculation of the disconnected diagram using our full QCD configurations to check whether - and if so, at what cost - a decent signal can be obtained on a sample of maximally 200 configurations. The matrix element of the nucleon with $\bar{q}q$ insertions is obtained on the lattice from the following ratio:

$$R(t) = \frac{\sum_x \langle N(\vec{x}, t) | \sum_z \bar{q}q(z) | N(0) \rangle}{\sum_x \langle N(x) | N(0) \rangle} = -\frac{\partial}{\partial m} \ln \Delta^{-1}(t) \rightarrow \text{constant} + t \langle N | \bar{q}q | N \rangle,$$

(2)

where $\Delta(t)$ is the nucleon propagator. The hadron correlator is calculated in a standard fashion (using smearing as above). The disconnected contribution to the three-point function in the numerator is given by the correlation of the nucleon propagator and the disconnected insertion $\sum_x (\text{Tr} \Delta_{xx})$. In the following we present the results of our numerical investigation for the most efficient calculation of such disconnected diagrams.

Noisy Estimator Techniques: The noisy estimator technique uses complex random sources with the property $\lim_{N_E \to \infty} \frac{1}{N_E} \sum_{i=1}^{N_E} \eta_i(E, C)\eta_j(E, C) = \delta_{i,j}$ to calculate $(\eta_i M^{-1}\eta_j) N_E$ times per configuration $C$. Using 157 configurations at our intermediate sea quark mass (i.e. $\frac{m_\pi}{m_\rho} = 0.76(1)$ and $m_q \simeq 1.3 m_s$) we have first compared Gaussian and $Z_2$ noise sources to calculate the chiral condensate $\chi \propto \text{Tr}(M^{-1})$. Monitoring the standard deviation of $\chi$ versus the number of estimates $N_E$ we found $Z_2$ to outdo Gaussian noise by a near factor of 2; we pushed $N_E$ all the way up to 300 in this investigation. Next, we varied the accuracy of the inversion residual $r = \frac{\|Mr - \phi\|}{\|\phi\|}$ which, obviously, we wish to relax as much as possible. Monitoring the quantity $\delta \chi = \chi(r = 10^{-5}) - \chi(r)$ we find that we can choose $r \simeq 10^{-4}$ and be safely within the $1 \sigma$ error margin of the $Z_2$ technique ($N_E = 300$). We now turn to the quality of the signal for $R(t)$ which can be obtained with our 157 dynamical configurations and to the dependence of the signal-quality on the number of estimates applied; recall
that so far, we have chosen $N_E = 300$, a number suggested by the authors of ref.\[15\]. In figure 1 we show $R(t)$ measured on 100 and 157 configurations. With more than 100 configurations the signal becomes acceptable and the error starts to display a $1/\sqrt{N_E}$ behaviour. For comparison we show a plot from a quenched simulation with the same number of configurations (157); note that the signal is much worse, indicating that the determinant in the probability density with which configurations are sampled has a smoothing effect. Since a decent signal emerges, we monitor in figure 2 the chiral condensate and its variance as a function of $1/\sqrt{N_E}$. Whereas the mean value of $R(t)$ is unaffected when varying $N_E$, figure 2 shows clearly that it does not pay to increase $N_E$ beyond 10-20. This drastically reduces the cost of the calculation. An analogous study using the volume source technique\[14\], where $M(C)x = \phi$ is solved for a volume source vector $\phi_i = 1$, shows a much worse signal. Our method of choice is therefore the stochastic estimator technique with about 20 $Z_2$ sources per configuration and a relaxed residual $r = 10^{-4}$. The results of our simulation, where we calculate connected and disconnected amplitudes in full and
Figure 2: $\text{Tr}M^{-1}$ and its variance as a function of $1/N_Z$ (157 gauge configurations).

quenched QCD will be presented in a forthcoming paper.

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