Results on improved KS dynamical configurations: spectrum, decay constants, etc.

Steven Gottlieb

Department of Physics, Indiana University, Bloomington, IN 47405, USA

The MILC Collaboration has been producing ensembles of lattice configurations with three dynamical flavors for the past few years. There are now results for three lattice spacings for a variety of light and strange quark masses, ranging down to \( m_l = 0.1 m_s \), where \( m_s \) is the dynamical strange quark mass and \( m_l \) is the common mass of the \( u \) and \( d \) quarks. Recently, the Fermilab, HPQCD, MILC and UKQCD collaborations have presented a summary of results obtained using these lattices. Compared with quenched results, these new calculations show great improvement in agreement with experiment. This talk addresses the technical improvements that make these calculations possible and provides additional details of calculations not presented in the initial summary. We demonstrate that a wide range of hadronic observables can now be calculated to 2–3% accuracy.

1. INTRODUCTION

The past several years have seen a marked improvement in our ability to do realistic calculations in Lattice QCD (LQCD). Improved actions have better scaling properties thus allowing us to more quickly approach the continuum limit than with the simplest actions. For staggered quarks, these improved actions also allow us to perform simulations (on current computers) with small enough up and down quark masses that we can use chiral perturbation theory to extrapolate to the physical quark masses. Further, the use of improved actions has greatly reduced the “flavor” symmetry violations, that we now call “taste” symmetry violations. Without this improvement, many of the non-Goldstone pion states are as heavy as the lightest kaon state. However, with the improvement in taste symmetry, the splitting between pions and kaons is more clear, and one expects to be better able to discern the effects of a dynamical strange quark. These improvements, and the general increase in available computer power have made it attractive to embark on a large scale calculation of QCD with three dynamical quarks.

Generation of the gauge ensembles has been going on for four years. MILC has been sharing dynamical configurations through the Gauge Connection and informally for some time. The Fermilab, HPQCD, MILC and UKQCD collaborations have all been using the MILC configurations to calculate a variety of quantities with both light (\( u, d \) or \( s \)) and heavy (\( c \) or \( b \) ) quarks. Taken together, we find that these calculations result in a compelling picture. LQCD with three flavors agrees with experiment with errors of 2–3% for a wide variety of quantities, whereas quenched QCD has errors as large as 15–20%.

In the rest of this article, I shall briefly discuss some of the issues that arise when dealing with staggered quarks. I will then give an introduction to the parameters set in lattice calculations, and some details of the MILC ensembles. After an explanation of high precision observables, we go on to discuss a variety of calculations such as the light meson decay constants, the heavy quark spectrum, the light quark spectrum and topological susceptibility. We conclude with a discussion of future prospects.

2. ALGORITHM ISSUES

Staggered quarks are fast compared to other discretizations, but one must take a fourth root to deal with the so-called fermion doubling problem. This leads to a potential loss of locality, and we don’t know how to construct a transfer matrix. Nevertheless, there are positive things one can say.
If one considers a formal perturbative expansion of the theory, the fractional root causes no problems in the expansion.

It is known that the CP violation that should occur when \( m_u + m_d < 0 \) does not happen with staggered quarks, but this deficiency is not obviously relevant to the real world.

The taste singlet axial current is only partially conserved so the chiral anomaly is preserved. We now understand how to modify chiral perturbation theory in the presence of taste changing interactions [1,2].

An important part of recent progress in LQCD is the use of improved actions. The MILC collaboration uses the “Asqtad” action [3–7].

The gauge action includes the plaquette, the 1 \times 2 rectangle and a bent parallelogram 6-link term. The quark action includes paths up to seven links long as shown below and the 3-link Naik term.

Each diagram in Fig. 1 represents a term in the quark action of the form \( \bar{\chi}(x) V(x, x + \hat{\mu}) \chi(x + \hat{\mu}) \), where \( V \) is the product of links along the path.

The “fat-link” contributions help to suppress taste symmetry breaking. The final 5-link path was introduced by Lepage [5] to correct the small momentum form factor. The result is an action that has leading errors of order \( a^2 \alpha \) and \( a^4 \).

The decision to base our calculations on the Asqtad action is based not on a fondness for fractional powers, but on the expectation that we can get to the correct chiral physics more easily this way. The chiral extrapolation for the \( u \) and \( d \) quarks has been a challenge for LQCD throughout its history.

To generate ensembles of gauge configurations, we must select certain physical parameters: the lattice spacing (\( a \)) or gauge coupling (\( \beta \)), the grid size \( (N_s^3 \times N_t) \), and the quark masses \( (m_u, d, s) \).

To control systematic errors, we must take the continuum limit, take the infinite volume limit and extrapolate to light quark mass for the \( u \) and \( d \) quarks. However, we can work at the physical \( s \) quark mass.

In the Table 1 we give some of the details of the MILC ensembles. We are able to go closer to the chiral limit than we did with unimproved staggered quarks in the mid-90s. This can be seen in Fig. 2, where the pion and nucleon masses are plotted in lattice units. The straight line corresponds to the physical pion to nucleon mass ratio. Approaching this line corresponds to the chiral limit. As the plot is a log-log plot, approaching the lower left corner (and going beyond) corresponds to the continuum limit. Note the three octagons to the left of the lowest left-most diamond. At this lattice spacing, with 2+1 flavors we have gone closer to the chiral limit. One also sees fancy plus symbols at smaller lattice spacing and comparable or smaller \( m_\pi/m_N \).

![Figure 1. Some of the products of links used in the Asqtad action. The Naik term is not shown.](image)

Table 1

<table>
<thead>
<tr>
<th>( a ) = 0.12 fm; 20(^3) × 64 (coarse)</th>
<th>( am_u,d ) / ( am_s )</th>
<th>( 10/g^2 )</th>
<th># conf.</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.40 / 0.40</td>
<td>7.35</td>
<td>332</td>
<td></td>
</tr>
<tr>
<td>0.20 / 0.20</td>
<td>7.15</td>
<td>341</td>
<td></td>
</tr>
<tr>
<td>0.10 / 0.10</td>
<td>6.96</td>
<td>340</td>
<td></td>
</tr>
<tr>
<td>0.05 / 0.05</td>
<td>6.85</td>
<td>425</td>
<td></td>
</tr>
<tr>
<td>0.04 / 0.05</td>
<td>6.83</td>
<td>351</td>
<td></td>
</tr>
<tr>
<td>0.03 / 0.05</td>
<td>6.81</td>
<td>564</td>
<td></td>
</tr>
<tr>
<td>0.02 / 0.05</td>
<td>6.79</td>
<td>485</td>
<td></td>
</tr>
<tr>
<td>0.01 / 0.05</td>
<td>6.76</td>
<td>608</td>
<td></td>
</tr>
<tr>
<td>0.007 / 0.05</td>
<td>6.76</td>
<td>447</td>
<td></td>
</tr>
<tr>
<td>0.005 / 0.05</td>
<td>6.76</td>
<td>137</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>( a ) = 0.09 fm; 28(^3) × 96 (fine)</th>
<th>( am_u,d ) / ( am_s )</th>
<th>( 10/g^2 )</th>
<th># conf.</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.031 / 0.031</td>
<td>7.18</td>
<td>336</td>
<td></td>
</tr>
<tr>
<td>0.0124 / 0.031</td>
<td>7.11</td>
<td>583</td>
<td></td>
</tr>
<tr>
<td>0.0062 / 0.031</td>
<td>7.09</td>
<td>583</td>
<td></td>
</tr>
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3. RESULTS FOR HIGH PRECISION OBSERVABLES

Certain quantities are intrinsically easier to calculate on the lattice than others. For example, a ground state mass is much easier to calculate than an excited state mass in the same channel. Also, a stable particle mass is much easier to calculate accurately than an unstable particle mass. The Fermilab, HPQCD, MILC and UKQCD collaborations have been working together to confront a variety of experimental results, and to make predictions that can be tested. So far, we have mainly been concentrating on high precision observables. If we fail to reproduce well known experimental results, after having controlled the chiral, continuum and finite volume extrapolations, we are left with little wiggle room. That is, we can no longer blame the quenched approximation. We would either conclude that staggered quarks are flawed, or that there is a problem with (L)QCD. On the other hand, if we are able to demonstrate good agreement with a variety of measured quantities, it would give us confidence that we are also able to make predictions, many of which are crucial for accurate determination of standard model parameters such as quark masses and CKM mixing matrix elements.

Our results depend on four input masses and the gauge coupling (equivalently the lattice spacing). The lattice spacing is determined from the $\Upsilon' - \Upsilon$ mass difference, a quantity with little dependence on the $b$ quark mass [8]. The common mass of the $u$ and $d$ quarks can be determined from $m_\pi$, while $m_s$ is determined from $2m_K^2 - m_\pi^2$, or a simultaneous fit to $m_\pi$ and $m_K$ determines $m_{u,d}$ and $m_s$. The charm quark mass $m_c$ is determined from $m_D$, and $m_b$ is determined from $m_\Upsilon$.

The results that follow are mainly the work of the following people and collaborations [9]:


The work on the topological susceptibility was done by MILC including T. DeGrand, A. Hasenfratz and A. Hart [10].

4. $\pi$, K MASSES AND DECAY CONSTANTS

In our latest calculations, we have a greatly improved understanding of chiral extrapolation due to five factors: 1) inclusion of taste symmetry breaking, 2) improved action, 3) more and lighter quark masses, 4) partial quenching and 5) simultaneous fit to mass and decay constant results.

In MILC’s prior work with two flavors of unimproved KS quarks, we had five dynamical quark masses at several fixed values of $\beta$. With no consideration for taste symmetry breaking, we tried seven combinations of powers and logs to try to fit the pion masses, but our best fits had only a combined confidence level of 0.1. In that work, the
valence light quark mass was the same as the dynamical mass, so there were only five data points for each \( \beta \) value. (In the current work with partial quenching, we have over 100 points for each lattice spacing.)

In Fig. 4 we plot some of our data for the five ensembles with the lightest \( m_{u,d} \) on the coarse lattice [11]. Quark propagators for nine different valence quark masses were calculated. The octagons correspond to equal mass quark and antiquark. The crosses have the antiquark fixed at the dynamical strange quark mass. Many additional points with different combinations of the valence masses are not plotted. The bursts include results from ensembles with heavier quarks than those listed in the legend.

The leading order formula from chiral perturbation theory for pion mass and decay constant depends on four combinations of the Gasser-Leutwyler constants.

\[
\frac{M_\pi^2}{2\mu m_1} = 1 + \frac{1}{96\pi^2f^2}[3M_\pi^2\log(M_\pi^2) - M_\eta^2\log(M_\eta^2)] \\
+ (2L_5 - L_3)\frac{f^2}{4\pi M_\pi^2} \\
+ (2L_6 - L_4)\frac{f^2}{4\pi}(M_\pi^2 + M_\eta^2) 
\] (1)

\[
f_\pi/f = 1 + \frac{(\gamma - 1)}{2\pi f^2} [M_\pi^2\log(M_\pi^2) - \frac{1}{4}(M_\pi^2 + M_\eta^2)\log(\frac{1}{4}(M_\pi^2 + M_\eta^2))] 
\]

However, with staggered quarks there are taste symmetry violations that modify these formulae to take into account the fact that all the pion states are not degenerate with the Goldstone pion. These formulae are quite complicated and may be found in Ref. [12]. They involve new couplings \( \delta'_V \) and \( \delta'_A \) from the taste symmetry breaking part of the effective Lagrangian. The formulae also involve the chiral log function, \( \ell \), given by

\[
\ell(m^2) = m^2 \left( \ln \frac{m^2}{\Lambda_c^2} + \delta_1(mL) \right) , 
\] (3)

with \( \Lambda_c \) the chiral scale, \( \delta_1 \) the known finite volume correction and \( L \) the spatial size.

In Figs. 5 and 6, we show results for \( r_1m_\pi^2/(m_x + m_y) \) and \( f_\pi r_1 \) with \( m_x \) and \( m_y \) the two valence quark masses, and \( r_1 \) a scale set from the heavy-quark potential. Only some of the data points are plotted. The curves correspond to partially quenched results on ensembles with the light quark mass indicated in the legend. Coarse (fine) lattice results are plotted with dia-

Figure 3. Ratio of lattice result to experimental value for nine quantities. Quenched (dynamical) results on the left (right).

Figure 4. Some of the results for \( r_1m_\pi^2/(m_x + m_y) \) on some of the coarse ensembles. There are too many partially quenched results to plot all available data.
mons (squares). The confidence level of the fit is 0.72, ignoring the contribution of the Bayesian constraints and 0.73 including them. The points are plotted after taking into account finite volume corrections that are sometimes as large as 1%. In Fig. 5, a vertical bar shows the value of \(m_u + m_d\), determined from the physical pion mass. The extrapolated value for \(f_\pi\) and the experimental result are shown in the lower left of Fig. 6. Note the close agreement. The systematic error includes variations in which points are included in the fit, variations in assumptions about how rapidly the taste-violating terms and non-taste violating terms are changing with lattice spacing, and, most important, the scale error of 2.2%. In Fig. 7, a similar plot is shown for \(f_K\). The difference here is that more heavy valence mass points are included in the \(f_K\) fits. One can see that the Bayesian constraints contribute more to \(\chi^2\) here. Agreement with experiment is also acceptable. The dynamical strange quark mass used in these ensembles is 10–20% higher than the result obtained for the valence \(m_s\). Additional coarse ensembles are being generated with \(am_s = 0.03\).

Figure 8 shows the continuum limit of \(f_\pi\) and \(f_K\). For these decay constants, the leading correction is linear in \(\alpha_s a^2\). Values for the coarse and fine results are also shown with taste symmetry violating terms set to zero. When this is done, there is very little difference between the two lattice spacings, supporting the contention that taste violations are the major source of difference.

4.1. Gasser-Leutwyler Parameters

We now have preliminary results for several combinations of Gasser-Leutwyler parameters using \(m_\eta\) as the chiral scale. We find

\[
2L_6 - L_4 = 0.5(2)(^{+1}_{-3}) \times 10^{-3} \tag{4}
\]

\[
2L_8 - L_5 = -0.1(1)(^{+3}_{-4}) \times 10^{-3} \tag{5}
\]

\[
L_4 = 0.3(3)(^{+7}_{-2}) \times 10^{-3} \tag{6}
\]

\[
L_5 = 1.9(3)(^{+9}_{-2}) \times 10^{-3} \tag{7}
\]

where the first error is statistical and the second is systematic. The systematic errors are dominated by differences over various acceptable chiral fits.

In the continuum, it is expected that \(L_5 = 2.3(2) \times 10^{-3}\) and \(L_4 \approx L_6 \approx 0\) [13].
The result for $2L_8 - L_5$ of $-0.1(1)^{+1}_{-3} \times 10^{-3}$ is well outside the range that allows for $m_u = 0$ [14] which is (approximately)

$$-3.4 \times 10^{-3} \leq 2L_8 - L_5 \leq -1.8 \times 10^{-3}.$$  \hspace{1cm} (8)

Thus, if MILC’s preliminary result holds up, it would rule out the $m_u = 0$ possibility. This result seems likely to be robust under changes in treatments of higher order terms.

5. HEAVY QUARK SPECTRUM

The most stringent tests of LGT come from hadrons that require no chiral extrapolation for the valence quarks, are stable to strong decay, and far from threshold. For example, $J/\Psi$, $\Upsilon$, $D_s$ and $B_s$ meet these conditions. The HPQCD and UKQCD collaborations have used a non-relativistic QCD (NRQCD) [15] action accurate to order $v^4$ to study bottomonium on MILC configurations. The Fermilab collaboration has used clover quarks with the Fermilab interpretation [16] to study charmonium states.

The spin averaged bottomonium splittings are shown in Fig. 9 for the 1P, 2P and 3S differences from the 1S level [17]. (Recall, the 2S-1S splitting is used to set the scale.) Three coarse dynamical ensembles have been used. The experimental results (without error bars) are plotted near the left edge of the diagram. On the right hand side of the diagram, the quenched values are plotted. The corresponding values in Fig. 3 come from the quenched results and lightest dynamical mass results shown here.

Several fine and hyperfine splittings are shown in Fig. 10 which contrasts results in the quenched approximation with results on one dynamical ensemble with $m_{u,d} = 0.2m_s$. There are significant differences for the hyperfine splittings of $\Upsilon$ and $\Upsilon'$. However, the corresponding $\eta$ states have not been observed. The fine structure in the $\chi$ states is improved on the dynamical ensemble.

Another quantity in the ratio plot is $2m_B - m_\Upsilon$. Using NRQCD, this quantity has been calculated on three of the ensembles ($m_{u,d} = 0.01, 0.02$ and
Figure 9. Spin averaged Υ splittings using NRQCD.

Figure 10. Several fine and hyperfine splittings in the Υ system using NRQCD. Experimental results indicated with dashed lines; open circles denote quenched approximation, filled circles are from the coarse ensemble with $a m_{u,d} = 0.01, m_s = 0.05$.

Figure 11. $2 m_B - m_{\Upsilon}$ in units of GeV vs. $m^2$. The experimental values for $B_{u,d}$ and $B_s$ are shown as bursts.

6. LIGHT QUARK SPECTRUM

Hadrons containing up or down valence quarks require chiral extrapolation before they can be...
compared with experiment. We have seen how this can be done including taste symmetry breaking terms for the pseudoscalars. For the nucleon, there is not yet a corresponding formula. In Fig. 14, we show $m_N r_1$ for the coarse and fine ensembles as well as some ensembles with $a \approx 0.20$ fm. The figure contains a phenomenological chiral perturbation theory curve, which is not a fit to the data. Although this figure may be suggestive that the lattice results will approach the experimental result in the chiral and continuum limit, more work is needed. The nucleon is not yet a high precision lattice quantity.

For the nucleon, we need to consider finite size effects carefully. All our previous studies were done with two dynamical flavors and with much larger taste symmetry breaking. This case may have smaller finite size effects. For $m_{u,d} = 0.2 m_s$ we are studying $28^3 \times 64$ to complement the $20^4 \times 64$. Preliminary results shows about a 1% decrease in mass on the larger volume. More statistics are needed. Another critical need is a chiral fit to the nucleon masses including taste violations.

With the additional caveat that the $\rho$ can decay and the lattice fits take no particular account of this possibility, I present MILC’s current APE plot in Fig. 15.

7. TOPOLOGY

At Lattice 2002 there was a concern that the dynamical quarks were not sufficiently suppressing topological susceptibility at light quark mass [19]. Since then, the fine lattice runs have been extended [10]. This has resulted in smaller errors, and the 3-flavor point that was so high previously has come down. Figure 16 shows an extrapolation to the continuum limit in the quenched approximation and for the three fine lattice ensembles. We see in Fig. 17 that the continuum extrapolations are in reasonable agreement with the leading order theory.
Figure 14. Nucleon mass vs. $(m_\pi/m_\rho)^2$.

Figure 15. APE plot for Asqtad improved KS quarks, with 0, 2 and 3 flavors.

8. PROSPECTS

We feel that with the Asqtad action and 2+1 dynamical quarks, we are making excellent progress. Most notably, the ratio plot is much improved compared with the quenched approximation. This is particularly true for the $b$-quark spectrum. Much other work is in progress that could not be discussed in this talk, and much additional work remains:

- Control chiral limit better on fine lattice
- Study possible finite size effects further
- Reduce lattice spacing to demonstrate control of continuum limit
- Complete physics measurements on more ensembles, $f_B$, form factors, etc. [20]
- Use a highly improved FNAL-type heavy quarks [21]
Develop new techniques for unstable particles and excited states

Complete additional perturbative calculations for renormalization and matching [22]

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