SCRI Results With the Tadpole-Improved Clover Action

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I discuss a study performed by the SCRI lattice gauge theory group which compared light hadron spectroscopy using the Wilson and Clover fermionic actions. We showed that a Clover coefficient chosen using tadpole-improved tree-level perturbation theory effectively eliminates the $O(a)$ discretization errors present in the Wilson action. We found that discretization errors in light spectroscopy for both the Wilson and Clover actions are characterized by an energy scale $\mu$ of about 200-300 MeV, indicating that these errors can be reduced to the 5% level by using the Clover action at an inverse lattice spacing of about 1.3 GeV.

1. INTRODUCTION

In this talk, I will discuss the results of an ongoing project at SCRI to understand the systematic errors in lattice light spectroscopy calculations. The short term goal of our program has been to determine the value of the lattice spacing at which the Clover lattice fermion action reduces discretization errors to the 5% level. Once this lattice spacing is known, we can perform dynamical simulations on a large physical volume and attempt to match our results to experiment.

To determine this lattice spacing, we have concentrated on two sub-projects. First, we have performed a detailed comparison of light spectroscopy using the Wilson and Clover discretizations on a pre-existing gluonic ensemble, generated by the HEMCGC collaboration, which has an inverse lattice spacing of about 2 GeV and includes the effects of two flavors of (staggered) light quarks. The purpose of this study was to see if, at typical lattice spacings, the Clover discretization significantly improved the discrepancies with experiment found in Wilson simulations, particularly in ratios of observables which probe different energy scales (such as the ratio of bottomonium splittings to the proton mass). Second, we have used an improved gluonic action on coarse lattices to determine the size of the scaling violations directly where they are large.

This talk is organized as follows. In section 2, I discuss technical details of our calculations. In section 3, I discuss the techniques we used in the scaling analysis of our quenched spectroscopy data, while in section 4, I present the results of these calculations. In section 5, I present the results of our comparison of Wilson and Clover spectroscopy, including the effects of two flavors of dynamical fermions, at an intermediate lattice spacing. In section 6, I summarize our conclusions.

2. THE SIMULATIONS AND FITTING PROCEDURES

We used two different types of gluonic ensemble in this study. To determine the size of discretization effects, we generated quenched ensembles using a one loop $O(a^2)$ improved gluonic action\footnote{\label{footnote1}Speaker at the Workshop.} at six values of $\beta$. The inverse lattice spacing of these ensembles ranged from 1.3 to 0.5 GeV, corresponding to lattice spacings between $0.25$ and $0.4$ fermi (see table \ref{table1}). The ensemble at each $\beta$ consisted of 100 configurations of size $16^3 \times 32$. For the dynamical runs, we used $16^3 \times 32$ gauge configurations generated by the HEMCGC collaboration\footnote{\label{footnote2}}, with $\beta = 5.6$ and 2 flavors of staggered fermions at a mass of $am = 0.01$. The inverse lattice spacing for this ensemble has previously been...
determined to be roughly 2 GeV.

Table 1
Values of $O(a^2)$ improved $\beta$ and corresponding inverse lattice spacings for quenched study.

| $\beta$   | 7.9 | 7.75 | 7.6 | 7.4 | 7.1 | 6.8 |
|-----------|-----|------|-----|-----|-----|-----|
| $a^{-1}$ (GeV) | 1.3 | 1.1  | .96 | .78 | .59 | .48 |

On all ensembles, both quenched and dynamical, we calculated light hadron correlation functions using both Wilson and tadpole improved Clover quark propagators. In all cases we used methods involving multi-state fits to multiple correlation functions to extract hadron masses, the technical details of which are discussed in [4].

The main focus of this work, especially of the quenched portion, was to determine the size of scaling violation effects rather than to attempt to reproduce or predict experimental results. Since discretization errors should get worse with increasing quark mass (because the typical energy scales should grow), we did not devote much effort to chiral extrapolations. Most of the quenched results I will present here used a lowest order (quadratic in $M_{PS}$) chiral fit ansatz, while the dynamical results were analyzed using both quadratic and cubic ansätze. Gottlieb has already presented a detailed discussion of this extremely important (and ill-controlled) source of systematic errors in his talk [5], so I will not discuss chiral extrapolations here, other than to say that our results agree qualitatively with his.

2.1. Low Quark Masses on Coarse Lattices

I would like to make two technical comments concerning coarse lattices before proceeding to the bulk of the talk. First, for a particular dimensionful value of $M_{PS}$, going to a coarse lattice does not seem to improve the speed of convergence of the fermion inversion algorithm. In other words, the condition number of the fermion kernel seems to be controlled by $m_q/\Lambda_{QCD}$, the quark mass over the QCD scale, rather than $a m_q$, the dimensionless quark mass. This is a very reasonable behavior, but it means that the gains to be found in going to a coarse lattice might be smaller than one might think.

The other comment involves exceptional configurations. We had originally planned to perform our quenched coarse lattice runs using $8^3 \times 16$ configurations. At low values of $\beta$, however, we found many exceptional configurations. This forced us to increase the lattice size to $16^3 \times 32$, which suppressed the effect. This method of increasing the volume to reduce exceptional configurations, can, however, result in an unacceptable increase in computational cost (which scales linearly with the lattice volume in the regime where finite volume effects are unimportant) unless one is careful. This is because each inversion of a localized hadronic source will only sample a roughly $(1\text{fm})^3$ volume of the lattice, so there is no gain in statistics when one increases the lattice volume. The solution is to smear the hadron around multiple origins (separated by some multiple of the hadron’s radius) on the initial timeslice. Naively this would increase the computational cost by the number of origins used, but one can invert the quark propagators from all origins simultaneously by superposing them with a random $Z(3)$ phase [6]. When using this method the computational cost of inverting from multiple origins is the same as the cost to invert from a single origin.

In practice, this means that one can double the spatial extent of the lattice (decreasing both finite volume and exceptional configuration effects) without increasing the computational cost of achieving equal statistics! This is because, although each inversion will be eight times as expensive, it will also yield eight times as many statistically independent measurements. This means that (ignoring memory limitations, thermalization times, and the reduction of HMC acceptance rates on larger volumes) one can always effectively eliminate finite volume effects from one’s simulations at no additional CPU cost by increasing the lattice volume and using the superposition trick. Although the superposition trick is vital on coarse lattices (where the lattice volume must be large), it should also be used to eliminate finite volume effects on fine lattices.
3. SCALING FITS

The main idea in performing extrapolations to the continuum limit, as well as in attempting to reduce discretization errors through improvement programs, is to Taylor expand dimensionless physical ratios around $a = 0$. For example,

$$
\frac{M(a\sqrt{\sigma})}{\sqrt{\sigma}} = M(0) \left[ 1 + \frac{M'(0)}{M(0)} (a\sqrt{\sigma}) + \frac{M''(0)}{M(0)} (a\sqrt{\sigma})^2 + \ldots \right]
$$

$$
= M(0) \left[ 1 + C^{(1)} a + C^{(2)} a^2 + \ldots \right], \quad (1)
$$

where $M(0)$, $M'(0)$, $\ldots$ are the continuum limits of the ratio and its derivatives (note that I will work in units of the string tension $\sigma$ when discussing scaling, even though it is not an experimental observable). Continuum extrapolations attempt to truncate the expansion at some order (usually first) and fit to data obtained at different $a$'s to determine $M(0)$. Improvement programs modify the action so as to reduce or eliminate the low order coefficients such as $C^{(1)}$ and $C^{(2)}$. For the (non-perturbatively tuned) Clover action, the leading discretization error is $C^{(2)} a^2$. Our strategy in this project has been to determine $C^{(2)}$ by running on coarse lattices with large $a$. Once we have determined $C^{(2)}$, we can choose a value of $a$ for our production runs at which the discretization errors are comparable to the other errors in our simulation. In particular, it is a waste of computational effort to run at values of $a$ where the attainable statistical errors are an order of magnitude larger than the discretization errors; higher statistics can be obtained for the same effort on coarser lattices, while the discretization errors will still be negligible.

3.1. $\mu$

Discretization errors in lattice calculations are caused by irrelevant, higher dimension operators appearing in the cut-off action. In general, physical observables will have some characteristic infra-red energy scale, $\mu$, which is the typical energy scale of the quantum fluctuations important to the observable. For light hadronic observables, we expect this scale to be set by $\Lambda_{QCD}$ or the constituent quark mass, i.e. $\mu$ should be several hundred MeV.

If we rewrite the dimensionful coefficients of equation $[3]$, $C$, in terms of dimensionless coefficients $D$, i.e. $C^{(n)} = D^{(n)} \mu^n$, then a reasonable discretization should have $D$'s which are $\mathcal{O}(1)$. If we assume that this is the case (i.e. set $D = 1$), then each coefficient in equation $[3]$ gives us an independent estimate of $\mu$:

$$
\mu_n \equiv |C^{(n)}|^{1/n}. \quad (2)
$$

If the different estimates $\mu_n$ are in rough agreement, then it is reasonable to estimate the higher order $\mathcal{O}(a^N)$ corrections to be about $(\mu_n a)^N$. Conversely, if the estimates $\mu_n$ wildly disagree, then we know that the coefficients of the $a$ expansion are not very well behaved, and we should be very cautious in inferring the size of higher order (unmeasured) discretization errors. In our quenched study, we found that $\mu_n$'s for the $\rho$, the nucleon, and the $\Delta$ were all in the region 200-300 MeV, for both the Wilson and Clover discretizations. This means that one can expect discretization errors of about 1-2% when using the Clover action at a lattice spacing of .1 fm. If one wants discretization errors to be about 5%, as is reasonable for a first effort at reproducing the physical spectrum using dynamical fermions, then a lattice spacing of about .2 fm appears to be the best choice.

Note that $\mu$ is closely related to the perturbative $q^*$ of Lepage and Mackenzie $[4]$. In particular, one might consider equation $[2]$, for a particular $n$, to be a non-perturbative definition of $q^*$. It is not necessary, however, that the physical scale $\mu$ be close to our estimates $\mu_n$; a particularly bad discretization of the action, for example, would yield discretization errors much worse than the expected $(\mu a)^n$, leading to spuriously large values of $\mu_n$. For example, one might expect the $\mu_n$'s in calculations using Staggered fermions to be about twice those of Wilson or Clover calculations because of the two hop nature of the Staggered derivative operator. It is likely, however, that $\mu$ is a (rough) lower bound on $\mu_n$, since it is hard to imagine an action with spuriously small values of the $D$'s.
3.2. Scaling Fit Ansätze

We used linear and quadratic ansätze for our scaling fits of Wilson and Clover data. We called these ansätze 1, 2, and 12, corresponding to pure linear (1), pure quadratic (2), or mixed linear plus quadratic (12). All of our scaling fits are done in units of the string tension; for physical predictions we must take ratios of extrapolated values (to remove the string tension, which is not experimentally measurable).

The first question we attempted to answer was whether the Clover action with a tadpole improved tree level coefficient is effective in removing the linear discretization errors of Wilson fermions. If the Clover coefficient, \( C_{SW} \) is non-perturbatively tuned, then the lowest order discretization errors will be quadratic. In our calculations, however, we used tadpole-improved tree level perturbation theory to set \( C_{SW} \), so we expect \( O(\alpha(a)a) \) errors in addition to \( O(a^2) \). Since \( \alpha(a) \) runs fairly slowly, we treated it as a constant over the range of lattice spacings in our calculation, i.e. we included it in our fit ansätze as a linear term with a coefficient which we expect to be small (\( O(\alpha) \)).

Table 2 contains the values of the confidence level, \( Q \), for scaling fits of the vector mass at all six \( \beta \) values, using the 1, 2, and 12 ansätze. Both Wilson and Clover results are shown for vector masses corresponding to the \( \rho \) (i.e. \( M_{PS}/M_V = M_{\pi}/M_{\rho} \)) and to a benchmark value agreed to at the recent Seattle workshop \( 6 \), for which chiral extrapolations are not required (\( M_{PS}/M_V = 0.7 \)). For the Wilson fits it is clear, as expected, that a linear term is necessary; the pure quadratic ansatz is clearly ruled out by the small \( Q \) values. For the Clover fits, however, one cannot draw a definitive conclusion from these \( Q \) values alone; both the linear and quadratic fits to the \( \rho \) have acceptable \( Q \), although the linear \( Q \)'s (especially .04 for the \( V \)) are low. The message to be drawn from Table 2 is that it is extremely difficult to distinguish between analytic functional forms to be used in extrapolations by looking at confidence levels for fits to a single curve; roughly 2 Gflops-yr of CPU time were required to generate the Clover data yet these fits still are unable to distinguish linear from quadratic behavior. This observation is important not only when doing lattice spacing extrapolations, but also when doing chiral extrapolations. I will show later that simultaneous fits to both Wilson and Clover data do rule out the pure linear Clover ansatz; unfortunately we do not know how to apply this technique to chiral extrapolations.

Although the linear and quadratic ansätze cannot be distinguished by \( Q \), they result in significantly different continuum extrapolations. Figure 1 shows the results of the three different fits to the Clover \( M_{\rho} \) data, along with the continuum extrapolations. It is obvious that the linear and quadratic extrapolations differ by many standard deviations. This is a serious problem, since it shows that there is a systematic error associated with choice of fit ansatz which can be many (statistical) \( \sigma \).

Our analytic knowledge tells us that the (perturbatively tuned) Clover action should reduce but not eliminate the \( O(\alpha) \) errors. The mixed ansatz permits both the large quadratic and suppressed linear terms to appear in the extrapolation. As can be seen from figure 1, the linear coefficient is consistent with zero but the extrapolated value has a much larger statistical uncertainty. This is because (as in all other cases in table 2) the mixed fit is underdetermined; an ansatz with fewer parameters (linear for Wilson or quadratic for Clover) fits the same data with good \( Q \). We expect the true uncertainty of the Clover extrap-
olation to fall somewhere between the quadratic and mixed error bars. In presenting extrapolated values I will quote both estimates of the uncertainty.

3.3. Joint Fits

Until now, I have presented the Clover and Wilson results separately. The zeroth order coefficient in both cases, however, is just the continuum limit of the quantity being fit. This value should not depend on the discretization scheme used, so we can obtain more constrained fits by simultaneously fitting Clover and Wilson data:

\[ M_W(a \sqrt{\sigma}) = M(0) \left[ 1 + (\mu_1^W a) + (\mu_2^W a)^2 \right] \]
\[ M_C(a \sqrt{\sigma}) = M(0) \left[ 1 + (\mu_1^C a)^2 \right], \tag{3} \]

where \( M \) is the quantity being fit (i.e. \( aM_V/a\sqrt{\sigma} \)) and the subscript indicates data from Wilson (W) or Clover (C) discretizations. In this example, I have used the 2 ansatz for the Clover data, and the 12 ansatz for Wilson. Although the Wilson and Clover data at a particular value of \( a \) are correlated, we have not included these correlations in our joint fits. This could lead us, in principle, to overestimate the confidence levels of our fits, but we expect this effect to be small.

Table 3 presents the \( Q \)'s for joint fits using all three ansätze for Clover and the linear and mixed ansätze for Wilson data. The quadratic Wilson ansatz is not considered because it has already been ruled out in table 2. It is now obvious that the pure linear ansatz for Clover is also ruled out; its extrapolated value cannot be made to agree with that of any of the Wilson ansätze. Although the 12 \( \text{mixed} \) (mixed Clover, linear Wilson) fits have reasonable \( Q \), they are unstable when more parameters are added; the parameters differ from those in the 12 \( \text{linear} \) fits by \( \pm 2 \) standard deviations for the \( \rho \) and \( \pm 3 \) for the \( V \) (using the underdetermined 12 \( \text{mixed} \) error bars). As we saw when comparing the Clover fits in table 2, this is an indication of an incorrect ansatz. This behavior should be compared with that of the 2 \( \text{linear} \) fits, all of whose parameters agree with those in the 12 \( \text{linear} \) fits. This is entirely consistent with our analytic expectations; we are at a coarse enough lattice spacing that we can resolve the quadratic errors in Wilson fermions in addition to the leading linear errors, which the Clover term suppressed sufficiently to allow a pure quadratic ansatz. When an additional linear term is included (i.e. 12 \( \text{12} \) rather than 2 \( \text{12} \) ansatz), the parameters are essentially unchanged, albeit with larger error bars, while the linear term is consistent with zero.

In presenting the scaling results that follow, I will use central values from the 2 \( \text{12} \) fits and quote error bars from both the 2 \( \text{12} \) and 12 \( \text{12} \) fits as “best case” and “worst case” uncertainties.

Table 3

| State | Ansatz       | Wilson | Clover |
|-------|--------------|--------|--------|
|       | linear       | \( \approx 10^{-26} \) | .016   | .69    |
|       | mixed        | .002   | .85    | .78    |
| \( \rho \) | linear       | \( \approx 10^{-72} \) | \( \approx 10^{-12} \) | .16    |
|       | mixed        | .001   | .98    | .96    |

Figure 1. Results of different scaling fits to the \( \rho \) mass.
4. SCALING RESULTS

Figure 2. Joint scaling fit to the benchmark vector mass, using a pure quadratic ansatz for Clover(+) and mixed ansatz for Wilson(○) data.

Figure 2 shows the results of a joint 2+12 fit to the benchmark vector mass, with the string tension used to set the scale. The most striking feature is that, at reasonable $\beta$, the Clover term has succeeded in eliminating most of the discretization effects, even though its coefficient was set using tree-level (tadpole-improved) perturbation theory. Note that the two highest $\beta$ values correspond to an inverse lattice spacing of about 1 GeV; a 6 GeV inverse lattice spacing would be required before the Wilson discretization errors are reduced to the same level. The slope parameters from the fit, $\mu_C^2$, $\mu_W^1$, and $\mu_W^2$, as defined in equation 3, are 240, 300, and 180 MeV, respectively, where we have taken $\sqrt{\sigma}$ to be 440 MeV. The fact that all three estimates are about the same size is an indication that the discretization scale $\mu$ is roughly 200-300MeV.

Overall, we conclude that the $\mu$ for light hadron spectroscopy, using Wilson-type actions, is roughly 200-300MeV. If we take a worst-case estimate of 300MeV and assume pure quadratic errors for the Clover action, this implies that lattice spacings of $2.1$ and $1.3$ GeV are required to obtain discretization errors of 2% and 5%, respectively. To obtain the same errors with the Wil-
son action, one would need corresponding lattice spacings of 15 and 6 GeV, respectively!

Figure 3. World scaling data for the $\rho$ mass. IG indicates an improved gluonic action (our results), while NP uses the chiral ward identity to tune the Clover parameter.

To illustrate the effectiveness of using the Clover action at intermediate lattice spacings, figure 3 shows a sample of world data for the $\rho$ mass. The discretization errors in our Clover point at $\beta = 7.9$ (corresponding to an inverse lattice spacing of about 1.3 GeV) are about the same size as the statistical errors, and are comparable to the statistical errors of other calculations.

Although it was not the main goal of this project, we have obtained the quenched continuum values of the $\rho$, nucleon, $\Delta$, and 0.7 benchmark vector masses in units of $\sqrt{\sigma}$, as well as the nucleon-$\rho$ mass ratio from our joint fits. These results are presented in table 5 with best and worst case error bars shown. The benchmark $V$ was chosen to be in the vicinity of computationally accessible quark masses; it is unlikely to be sensitive to chiral extrapolation uncertainties. The physical hadrons, however, required a large extrapolation (using an ansatz linear in $M_{PS}^2$); these results are susceptible to (undetermined) systematic errors arising from other terms in the chiral expansion. The only value which can be compared directly to experiment is the nucleon-$\rho$ mass ratio. We obtain 1.297(17)(81), which is consistent with the experimental value of 1.22 if one uses the worst case uncertainty.

| Observable | Value ($\sqrt{\sigma}$) |
|------------|--------------------------|
| $M_V$      | 2.122(11)(56)            |
| $M_\rho$   | 1.758(11)(46)            |
| $M_N$      | 2.30(3)(12)              |
| $M_\Delta$ | 2.93(5)(15)              |
| $M_N/M_\rho$ | 1.297(17)(81)        |

5. DYNAMICAL RESULTS

Our dynamical runs were intended to investigate whether Clover results on a fine lattice with dynamical fermions (partially) included would resolve discrepancies with the experimental spectrum found in Wilson studies, and to check how large the differences between Wilson and Clover spectroscopy are on a fine lattice. The most important of these discrepancies is the disagreement between the lattice spacings obtained from light spectroscopy and those obtained from $\Upsilon$ splittings [4]. Previous Wilson calculations on this ensemble [10] found inverse lattice spacings of about 2 GeV. Spin-independent bottomonium splittings calculated on the same ensemble using the NRQCD formalism, however, obtained values near 2.4 GeV - a 20% discrepancy. It is unlikely that this would change if three flavors of dynamical fermion were used, since quenched results at
similar lattice spacing show roughly the same discrepancy. The good news is that the differences between Wilson and Clover spectroscopy on the dynamical ensemble are entirely consistent with the $\mu$ value of about 200 MeV that we found in the quenched study. In all observables we studied, the relative change upon inclusion of the Clover term was less than or approximately 10%, i.e. $(\mu a)$. In fact, in comparing chiral intercepts and slopes of the vector, nucleon, and $\Delta$, we were only able to resolve a difference between the Clover and Wilson values of the vector intercept, i.e. the mass of the $\rho$. This can be seen by examining figures 4, 5, and 6, in which Wilson and Clover chiral plots of the masses of these three states as a function of pseudoscalar mass are superposed. The $\rho$ plot is the only one in which there is a clear separation between the Clover and Wilson data. More good news is that we found consistency with experiment at the 5-10% level in the light hadron spectrum, since the Clover $a^{-1}$'s we obtained from different light observables ranged from 1.8-2.1 GeV.

The bad news is that these inverse lattice spacings are still inconsistent with $\Upsilon$ spectroscopy; the 20% discrepancy has not been removed by the Clover discretization. Since it is not a discretization effect, this discrepancy is probably due to some other systematic error. The most likely culprit is finite volume effects; the spatial extent of our lattice is only 16, which corresponds to a 1.6-1.3 fm box depending on which lattice spacing one uses. This is much larger than bottomonium, but probably too small for light hadrons. Squeezing the light hadronic states would raise their masses, resulting in spuriously low inverse lattice spacings. Systematic errors in the chiral extrapolation could also be causing the problem - adding a term linear in $M_{\pi}$ (which might be induced by partial quenching effects) to the chiral ansatz can significantly reduce the extrapolated mass values. Another possibility is that the dynamical fermions are not light enough to act as true up and down quarks. Whatever the reason for the discrepancy, higher quality dynamical calculations, especially at larger volumes, are needed. It would be a tremendous accomplishment if the community could demonstrate that lattice QCD can simultaneously reproduce the spectra of both heavy and light hadron systems.
6. CONCLUSIONS

We have shown that a Clover term, with the coefficient chosen using tree-level tadpole-improved perturbation theory, eliminates the bulk of the linear discretization errors in the Wilson action. At any value of $\beta$, tadpole-improved Clover calculations will be much closer to the continuum value than the corresponding Wilson calculation.

We have shown that the $\mu$'s for light hadron spectroscopy using the Wilson or Clover actions seem to be roughly 200-300 MeV, with the vector meson discretization errors slightly larger than those of the baryons. This means that inverse lattice spacings no harder than $1.3$ GeV should be required to reduce discretization errors to the 5% level when using the Clover action. This determination of $\mu$ can be used by other groups to estimate the discretization errors they will face at a particular value of $\beta$ and can also be used to determine the lattice spacings where further improvements of the Clover action should be attempted.

Finally, we found that it was very difficult to numerically rule out a dominant linear behavior in the Clover data in the range of lattice spacings studied. These fits indicated that the coefficient of any sub-dominant $O(a)$ behavior (due to higher order or non-perturbative corrections to the perturbative Clover coefficient) is small.

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