

# Reweighting towards the chiral limit

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We propose to perform fully dynamical simulations at small quark masses by reweighting in the quark mass. This approach avoids some of the technical difficulties associated with direct simulations at very small quark masses. We calculate the weight factors stochastically, using determinant breakup and low mode projection to reduce the statistical fluctuations. We find that the weight factors fluctuate only moderately on nHYP smeared dynamical Wilson-clover ensembles, and we could successfully reweight  $16^4, (1.85 \text{ fm})^4$  volume configurations from  $m_q \approx 20 \text{ MeV}$  to  $m_q \approx 5 \text{ MeV}$  quark masses, reaching the  $\epsilon$ -regime. We illustrate the strength of the method by calculating the low energy constant  $F$  from the  $\epsilon$ -regime pseudoscalar correlator.

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## I. INTRODUCTION

The steady progress of simulation techniques over the last decade (see e.g. [1–5]) as well as new insights into the reasons for algorithmic failures [6] have profoundly altered the status of lattice QCD: With the latest generation of supercomputers, essentially all  $p$ -regime points, including the point of physical quark masses, have become accessible to direct simulation. However, in the small quark mass regime the challenges are still considerable:

- (i) Large volumes are needed for the stability of the algorithms when Wilson fermions are used [6].
- (ii) Autocorrelation times increase dramatically towards the chiral limit [7].
- (iii) Statistical fluctuations of fermionic correlators become difficult to estimate since configurations with large contributions become rare as small Dirac modes are more and more suppressed.

A possible solution to evade these problems is to avoid generating an ensemble with the fermionic weight of the small target quark mass, but instead simulate a heavier quark and reweight to the desired ensemble.

This approach solves all of the above-mentioned issues: The algorithm is more efficient at the larger mass, and smaller volumes will be sufficient from the algorithmic point of view. At a larger quark mass the region of small Dirac eigenvalues is oversampled with respect to the target distribution, and thus observables that receive large con-

tributions there (e.g. pseudoscalar correlators) will be better estimated. Previously, the polynomial hybrid Monte Carlo algorithm [8] has been used as an alternative way to achieve such an oversampling [9,10].

Since the variance of an observable  $O$  is a field theoretical observable, its statistical error on an importance sampled ensemble depends only on the autocorrelation of  $O$ . On the other hand, when reweighting is employed the error is not given by the quantum mechanical variance  $\langle O^2 w \rangle - \langle O w \rangle^2$ , with  $w$  being the normalized reweighting factor, but rather the statistical variance  $\langle O^2 w^2 \rangle - \langle O w \rangle^2$  which depends on the variance of the reweighting factor itself as well as its correlation with the observable of interest. If  $O$  and  $w$  are (strongly) anticorrelated, this controls and limits the statistical error on the reweighted ensemble.

Nevertheless, if the overlap (in configuration space) of the generated and desired ensembles is insufficient, reweighting will break down due to the fluctuations of the reweighting factor. This limits the range of quark mass values that can be bridged by reweighting.

In this paper we work with two degenerate flavors of Wilson-type fermions, though generalization to other fermionic actions is straightforward. If we have an ensemble of configurations  $\{U_i\}$  generated at bare mass  $m_1$  with the Dirac operator  $D_1 = D(U; m_1)$ , we can reweight it to the ensemble that corresponds to bare quark mass  $m_2$  by assigning to each configuration a weight factor

$$w_i \propto \det \frac{D_2^\dagger[U_i] D_2[U_i]}{D_1^\dagger[U_i] D_1[U_i]}, \quad (1)$$

and calculating expectation values as

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$$\langle O \rangle_2 = \frac{\sum_i w_i O[U_i]}{\sum_i w_i}. \quad (2)$$

Since the reweighting factors and their fluctuations will increase with the volume, reweighting becomes inefficient on very large lattices. In practice, we find that the fluctuations can be controlled and quite large volumes can be reweighted. Nevertheless, reweighting is a technique that is most useful at small quark masses and moderate volumes—like in  $\epsilon$ -regime calculations.

There are two sources of fluctuations for the weights. One is due to the small eigenmodes of the Dirac operator. These physical infrared eigenmodes contribute to the weight factor as

$$\log(w_i)|_{\text{low modes}} = (m_2 - m_1) \sum_{\lambda} \frac{1}{\lambda + m_1} + O((m_2 - m_1)^2). \quad (3)$$

The suppression of configurations due to the small eigenvalues is physical. The weight factors control exceptionally large contributions to quark propagators that arise on configurations with small eigenmodes. Reweighting in fact reduces the statistical fluctuations of many observables when compared to the partially quenched case. The ultraviolet, large eigenvalue modes are not physical, but due to their large number they can dominate the fluctuations. Some of these fluctuations can be removed by smoothing, and with nHYP smeared Dirac operators [5] reweighting is possible also in bigger volumes. However, even on an nHYP smeared gauge background, the UV fluctuations are still large. They are also closely correlated with the fluctuations of the nHYP smeared plaquette, giving us yet another option to reduce the noise by absorbing it into the gauge action: Including a term proportional to the smeared plaquette in the Lagrangian reduces the UV fluctuations of the weight factors. This latter reduction is not essential, especially at smaller mass shifts, but extends the reach of the method at the expense of introducing a (very) small pure gauge term to the action.

Calculating the determinant in Eq. (1) to any reasonable accuracy can be very costly. Fortunately it is not necessary to do that; a stochastic estimator is sufficient. In Sec. II we describe the stochastic reweighting, and several of its improvements. Section III describes the numerical tests and efficiency of the reweighting technique, and in Sec. IV we present physics results using reweighted configurations.

## II. STOCHASTIC REWEIGHTING

When the Dirac operator corresponds to Wilson or clover fermions it has the form<sup>1</sup>

<sup>1</sup>Here  $M$  is a suitable combination of the hopping and clover terms.

$$D[U] = 1 - \kappa M[U], \quad (4)$$

where  $\kappa$  is the hopping parameter  $\kappa = (2m + 8)^{-1}$ . Reweighting a configuration from  $\kappa_1$  to  $\kappa_2$  requires a weight factor

$$w = \det \frac{D_2^\dagger D_2}{D_1^\dagger D_1} = \det^{-1}(\Omega), \quad \Omega = D_2^{-1} D_1 D_1^\dagger (D_2^\dagger)^{-1}. \quad (5)$$

The determinant can be calculated as an expectation value

$$w = \frac{\int \mathcal{D}\xi e^{-\xi^\dagger \Omega \xi}}{\int \mathcal{D}\xi e^{-\xi^\dagger \xi}} = \langle e^{-\xi^\dagger (\Omega - 1) \xi} \rangle_\xi,$$

but obtaining a reliable estimate for  $w$  is expensive, especially when  $\Omega$  is not close to 1.

An alternative way is to calculate only a stochastic estimator of the true weight factor and do the average over the  $\xi$  fields together with the configuration average. A similar approach is used in the stochastic global Monte Carlo update [11–13]. We start by writing the expectation value of an operator  $O[U]$  at mass  $m_2$  as

$$\begin{aligned} \langle O \rangle_2 &= \frac{1}{Z_2} \int \mathcal{D}U e^{-S_g} \det(D_2^\dagger D_2) O[U] \\ &= \frac{1}{Z_2} \int \mathcal{D}U e^{-S_g} \det(D_1^\dagger D_1) \det^{-1}(\Omega) O[U] \\ &= \frac{Z_1}{Z_2} \langle O[U] e^{-\xi^\dagger (\Omega - 1) \xi} \rangle_{1, \xi}, \end{aligned} \quad (6)$$

where

$$\frac{Z_2}{Z_1} = \frac{\int \mathcal{D}U e^{-S_g} \det(D_2^\dagger D_2)}{\int \mathcal{D}U e^{-S_g} \det(D_1^\dagger D_1)} = \langle e^{-\xi^\dagger (\Omega - 1) \xi} \rangle_{1, \xi} \quad (7)$$

and the expectation value is with respect to both the  $U$  and  $\xi$  fields at  $m_1$ . If we consider the configuration ensemble  $\{U_i, \xi_i\}$ , with the gauge configurations from the original sequence and  $\xi_i$  generated independently with weight  $e^{-\xi_i^\dagger \xi_i}$ , the expectation value becomes

$$\langle O \rangle_2 = \frac{\sum_i O[U_i] e^{-\xi_i^\dagger (\Omega[U_i] - 1) \xi_i}}{\sum_i e^{-\xi_i^\dagger (\Omega[U_i] - 1) \xi_i}}, \quad (8)$$

i.e. the weight factors are replaced by a single estimator

$$s_i = e^{-\xi_i^\dagger (\Omega[U_i] - 1) \xi_i}. \quad (9)$$

The obvious advantage of the stochastic approach is that the averages of the noise sources and the gauge fields commute. Without introducing any systematic error, we therefore need only one estimator of the weight on each configuration. The disadvantage is that a single estimator might fluctuate too much and introduce large statistical errors in Eq. (8). Fortunately there are several methods that can reduce the fluctuations of  $s_i$  to acceptable levels.

### A. Improving the stochastic estimator

In this section we describe two methods, the determinant breakup [14,15] and the low mode subtraction that we use in calculating the stochastic weight factors. Both methods were used in [13] in a different context. It will be useful for the discussion to rewrite Eq. (5) as

$$\Omega = ((1-x)(D_2^\dagger)^{-1} + x)((1-x)D_2^{-1} + x), \quad (10)$$

where  $x = \kappa_1/\kappa_2$ . We consider reweighting to smaller quark masses so  $x < 1$ , though everything works for  $x > 1$  as well. At leading order  $(1-x) \propto (m_1 - m_2)$ , i.e. apart from a gauge field independent additive constant  $x^2$ ,  $\Omega \propto (m_1 - m_2)$ . The exponent of the stochastic estimator in Eq. (9) now can be written as

$$\begin{aligned} \xi^\dagger(\Omega - 1)\xi &= (1-x)^2 \xi^\dagger (D_2^\dagger)^{-1} D_2^{-1} \xi \\ &+ x(1-x) \xi^\dagger ((D_2^\dagger)^{-1} + D_2^{-1}) \xi \\ &+ (x^2 - 1) \xi^\dagger \xi, \end{aligned} \quad (11)$$

which requires one inversion of the Dirac operator  $D_2$  on  $\xi$ .

#### 1. Determinant breakup

The determinant breakup is based on Ref. [15] and has been used extensively in dynamical simulations. The idea is to break up the interval  $(\kappa_1 \rightarrow \kappa_2)$  to  $N$  sections  $\kappa_1 \rightarrow \kappa_1 + \Delta\kappa \rightarrow \dots \rightarrow \kappa_1 + N\Delta\kappa = \kappa_2$ , and write the determinant as the product of  $N$  terms, each on a  $\Delta\kappa$  interval. Thus the stochastic estimator takes the form

$$\exp\left(-\sum_{n=1}^N \xi_n^\dagger (\Omega_n - 1) \xi_n\right), \quad (12)$$

where  $\Omega_n$  is the analogue of Eq. (5) on the  $\kappa_n \rightarrow \kappa_{n+1}$  interval. Since the operators  $\Omega_n$  are much closer to 1 than the original  $\Omega$ , the estimator in Eq. (12) has reduced fluctuations. Calculating it on  $N$  intervals requires  $N$  applications of  $D^{-1}$ , so it is expensive. On the other hand, it predicts a stochastic weight factor for the configuration at any intermediate  $\kappa_n$  value, so the same calculation can be used to reweight to many different mass values.

#### 2. Separating the low eigenmodes

Equations (3) and (11) clearly show that the low eigenmodes of the Dirac operator not only give large contributions to the reweighting factor, but they can dominate the stochastic fluctuations as well. This latter problem can be reduced by explicitly calculating the low eigenmodes and removing them from the stochastic estimator. It is not necessary to work with the exact eigenmodes of  $\Omega$ ; subtracting approximate eigenmodes works as well.

Assume that  $P$  is an arbitrary but Hermitian projection operator, i.e.  $P^2 = P$ ,  $P^\dagger = P$ , and  $\bar{P} = 1 - P$  is the complementary projector. Any operator can be decomposed as

$$\Omega = \begin{pmatrix} P\Omega P & P\Omega\bar{P} \\ \bar{P}\Omega P & \bar{P}\Omega\bar{P} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ T & 1 \end{pmatrix} \begin{pmatrix} P\Omega P & 0 \\ 0 & Q \end{pmatrix} \begin{pmatrix} 1 & R \\ 0 & 1 \end{pmatrix}$$

with  $T = \bar{P}\Omega P(P\Omega P)^{-1}$ ,  $R = (P\Omega P)^{-1}P\Omega\bar{P}$ , and

$$Q = \bar{P}\Omega\bar{P} - \bar{P}\Omega P(P\Omega P)^{-1}P\Omega\bar{P}. \quad (13)$$

Now the determinant can be written as

$$\det\Omega = \det(P\Omega P) \det Q, \quad (14)$$

so the sectors projected by  $P$  and  $\bar{P}$  are separated. If the projection operator  $P$  is built from the eigenvectors of  $\Omega$ , the second term in Eq. (14) vanishes and  $Q = \bar{P}\Omega\bar{P}$ . If  $P$  is built only from approximate eigenmodes, both terms in  $Q$  are present but the second term gives only a small correction. We will refer to it in the following as the correction term.

*Separating Dirac eigenmodes.*—Because of the  $\gamma_5$  Hermiticity of the Wilson Dirac operator, the eigenvalues of  $D$  come in complex conjugate pairs and the eigenvectors are  $\gamma_5$  orthogonal. The eigenvectors of the massless operator  $D_0|v_\lambda\rangle = \lambda|v_\lambda\rangle$  are the eigenvectors of the massive one as well, with eigenvalues  $\lambda + m$ . The  $\gamma_5$  orthogonality implies that one can normalize the eigenvectors such that  $\langle v_{\lambda'}|\gamma_5|v_\lambda\rangle = \delta_{\lambda'\lambda}$  and the operator

$$P_\lambda = |v_\lambda\rangle\langle v_\lambda^*|\gamma_5$$

is a projector. Since  $P_\lambda$  is not Hermitian, the discussion of the previous paragraph does not apply. Nevertheless, if  $P_\lambda$  is built from the eigenvectors of the Dirac operator, Eq. (15) is valid with a vanishing correction term. If  $P$  projects to a few low energy modes of  $D_2$ , the first term,  $\det(P\Omega P)$ , can be calculated explicitly, and the second one,  $\det(\bar{P}\Omega\bar{P})$ , can be estimated stochastically using Eq. (11). Since the eigenvectors of the massless Dirac operator can be used at all mass values, the overhead of the low mode subtraction is a one-time calculation of the eigenmodes. If those modes are subtracted during the inversion, some of the additional cost can be recouped by the improved convergence as well.

*Separating Hermitian eigenmodes.*—An alternative approach is to construct the projection operator from the eigenmodes of the Hermitian operator

$$H = \gamma_5 D.$$

Equations (5) and (10) in terms of the Hermitian operator become

$$\begin{aligned} \Omega &= H_2^{-1} H_1^2 H_2^{-1} \\ &= (1-x)^2 H_2^{-2} + x(1-x)(\gamma_5 H_2^{-1} + H_2^{-1} \gamma_5) + x^2. \end{aligned} \quad (15)$$

Now the projector is Hermitian, but it is not constructed from the eigenmodes of  $\Omega$  so the correction term in Eq. (13) is necessary.

Working with  $n$  normalized eigenvectors of  $H_2|w_i\rangle = \eta_i|w_i\rangle$ , the projector is  $P = \sum_{i=1}^n |w_i\rangle\langle w_i|$ , and

$$P\Omega P = \omega_{ij}|w_i\rangle\langle w_j|$$

is an  $n \times n$  matrix with coefficients

$$\omega_{ij} = (1-x)^2 \frac{\delta_{ij}}{\eta_i^2} + x(1-x)\langle w_i|\gamma_5|w_j\rangle(\eta_i^{-1} + \eta_j^{-1}) + x^2 \delta_{ij}. \quad (16)$$

Both the determinant and the inverse of  $P\Omega P$  are easily calculable. The leading term of the stochastic estimator,  $\bar{P}\Omega\bar{P}$ , requires the evaluation of  $H_2^{-1}\bar{P}|\xi\rangle$ . Since the inversion is done on the subspace that is orthogonal to the low eigenmodes, this can be considerably faster than calculating  $H_2^{-1}|\xi\rangle$ . The correction term does not require a new inversion if one uses the identity  $H_2^{-1}|w_i\rangle = 1/\eta_i|w_i\rangle$ .

The eigenmodes of  $H_2$  have to be recalculated for every  $\kappa$  interval. While the initial calculation of the eigenmodes is usually expensive, changing  $\kappa$  by a small amount does not affect the eigenmodes much, and starting from nearly correct eigenmodes the calculation converges fast. An alternative is to use the eigenmodes of  $H$  of the first interval throughout, but then one needs to calculate  $H_2^{-1}|w_i\rangle$  on every interval. The inversion on the low modes is expensive, and we found recalculating the eigenmodes on each interval is a better option.

### III. NUMERICAL TESTS

We have tested the reweighting on a set of  $16^4$  configurations generated with a 2-flavor nHYP clover action. At the original parameter values,  $\beta = 7.2$ ,  $\kappa_1 = 0.1278$ , the lattice spacing is  $a = 0.115(3)$  fm and the axial vector current quark mass (PCAC mass) is  $m_{\text{PCAC}} \approx 20$  MeV. We have 180 thermalized configurations separated by 5 trajectories. The topological charge, as measured by an overlap operator based on nHYP Wilson fermions ( $R_0 = 0.6$  and no clover term [16]), fluctuates evenly, suggesting that the autocorrelation of these lattices is small even for this traditionally slowly changing quantity (Fig. 1).

Figure 2 shows the Hermitian gap, i.e. the histogram of the absolute value of the lowest Hermitian eigenmode of the configurations [6]. Direct simulations are safe when the left edge of the gap is far from zero. In our case one could probably lower the quark mass to about  $am_q = 0.009$ , but not much more. With reweighting, on the other hand, one can go to much lower quark masses. Configurations with near zero eigenvalues will be suppressed, just as they should be, so exceptional configurations do not cause problems. Of course at some point one has to worry about the chiral symmetry breaking lattice artifacts of such actions.

We reweighted the ensemble up to  $\kappa_2 = 0.1281$ , or  $m_{\text{PCAC}} \approx 5$  MeV. At this value there is one configuration in the ensemble with negative eigenvalues, and a few with very small real (Dirac) eigenvalues. Reweighting to such a small mass is interesting, not necessarily for its physical

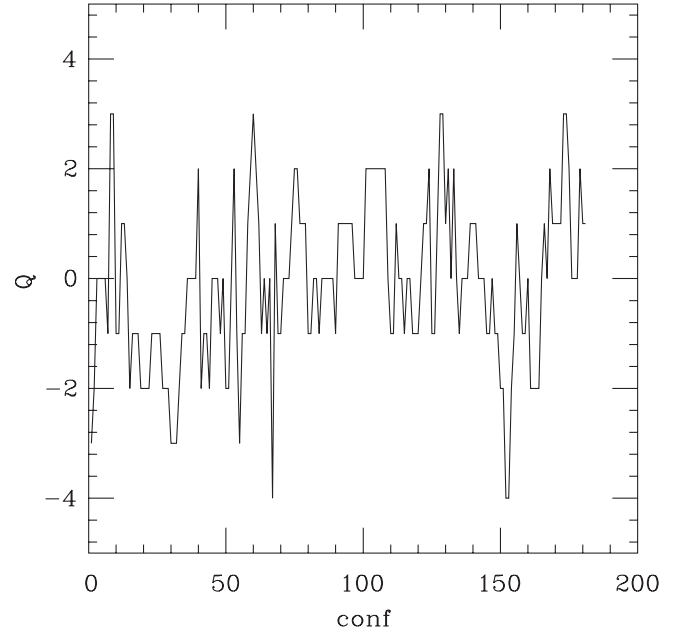


FIG. 1. The topological charge of the original configurations.

importance, but rather to see the suppression of the determinant at work. Since the stochastic reweighting automatically gives the weights at intermediate mass values, we have done weighted spectrum calculations at  $\kappa = 0.1279$  and  $\kappa = 0.1280$  as well. These values do not cut into the gap and give physically more reliable results.

Our goal with these configurations is to probe the  $\epsilon$ -regime with Wilson fermions. Already, the configura-

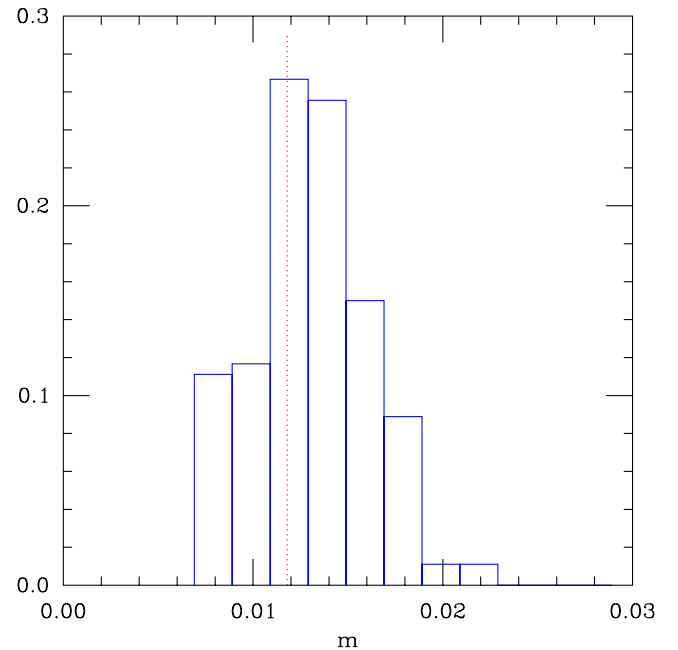


FIG. 2 (color online). The gap of the Hermitian Dirac operator of the original  $16^4$ ,  $\kappa = 0.1278$ ,  $\beta = 7.2$  configurations. The dashed line indicates the PCAC quark mass.



tions at  $\kappa = 0.1278$  are controlled by the finite volume. From the PCAC quark mass and the pseudoscalar correlator on these runs, and from our previous  $16^3 \times 32$  dynamical runs [17,18], we estimate  $m_\pi L \approx 2.8(1)$  on these  $16^4$  lattices. In the  $\epsilon$ -regime the eigenmodes of both the Dirac and Hermitian Dirac operators are pushed away from zero, while the finite volume has little effect on the PCAC quark mass. The ratio of the median of the gap,  $\bar{\mu}$ , and  $m_{\text{PCAC}}$  increases as one approaches the  $\epsilon$ -regime. In infinite volume the ratio is the renormalization factor  $Z_A$ , which we expect to be near 1 with nHYP fermions. On large but finite volume the ratio might not have any physical meaning, but there is indication that, in practice, it remains close to  $Z_A$  [6]. Our large volume runs give  $\bar{\mu}/m_{\text{PCAC}} \approx 0.82$ , while the ratio here is 1.1, showing the effect of the finite volume. (In [5] we quoted  $\bar{\mu}/m_{\text{PCAC}} \approx 0.91$ . Those runs on  $12^3 \times 24$  lattices with  $La = 1.5$  fm also have strong finite volume effects even with the relatively heavy  $m_q = 70$  MeV quark mass.)

### A. Reweighting with Hermitian eigenmodes

With Hermitian subtraction one has to balance the cost of calculating the low energy eigenmodes with the improved convergence of the conjugate gradient iteration. The cost of the latter is proportional to the number of intervals between the starting and ending  $\kappa$  values, which in turn determines the statistical fluctuations of the stochastic estimator due to the ultraviolet modes.

We have found that removing more than 6 eigenmodes did not substantially increase the convergence of the inversion, nor did it decrease the fluctuations of the estimator. Subtracting only 3 eigenmodes resulted in a significantly more expensive inversion that quickly overtook the cost of calculating the eigenmodes. Therefore we have settled on subtracting 6 Hermitian eigenmodes. Next we considered the optimal number of steps in the determinant breakup. This should be such that the stochastic fluctuations of the weight factors are small compared to the fluctuations between the weight factors of the different configurations. We found that 99 intervals between  $\kappa = 0.1278$  and  $\kappa = 0.1281$  were more than sufficient to achieve that. Reducing the number of intervals further might have worked, but at some point the startup cost of the eigenmode calculations dominate the cost.

For the computation of the eigenvalues and eigenvectors of the Hermitian Dirac operator, we use the PRIMME package of McCombs and Stathopoulos [19,20].

### B. Reweighting with Dirac eigenmodes

We have also tested reweighting with Dirac eigenmodes. Using the ARPACK package we calculated 20 eigenmodes and separated  $\approx 16$  real or complex conjugate pairs. While these eigenmodes work on every  $\kappa$  interval, the conjugate gradient inversion is still expensive (we project on  $D_2$  modes but invert the operator  $D_2^\dagger D_2$ ), and we found this

approach more expensive than removing Hermitian eigenmodes. Our tests were done with single precision Dirac eigenmodes, and it is quite possible that with better eigenmodes the Dirac eigenmode separation becomes competitive.

### C. Reweighting factors

In this section we present results obtained using Hermitian eigenmode separation.

Figure 3 shows the reweighting factors at three different  $\kappa$  values starting from the original  $\kappa = 0.1278$ . As expected, they fluctuate more and more as we reweight to smaller and smaller masses, and the last case,  $\kappa = 0.1281$ , is just barely acceptable. At that point there are several configurations that have very small Hermitian eigenvalues, and the extreme suppression of those configurations is evident.

There is another source for the large fluctuations, the ultraviolet noise. The fluctuation of the nHYP plaquette is a good representative of the UV noise, and it correlates closely with the UV part of the weight factor (top panel of Fig. 4). We define the UV part as the weight factor without the explicitly calculated low eigenmodes, i.e. the value determined by the stochastic process. While this definition is not unique, it captures the correlation with the nHYP plaquette and suggests that at least some of the UV noise can be removed by introducing an nHYP plaquette term in the new action by reweighting from  $S_1 = S_g - \text{Indet}(D_1^\dagger D_1)$  to

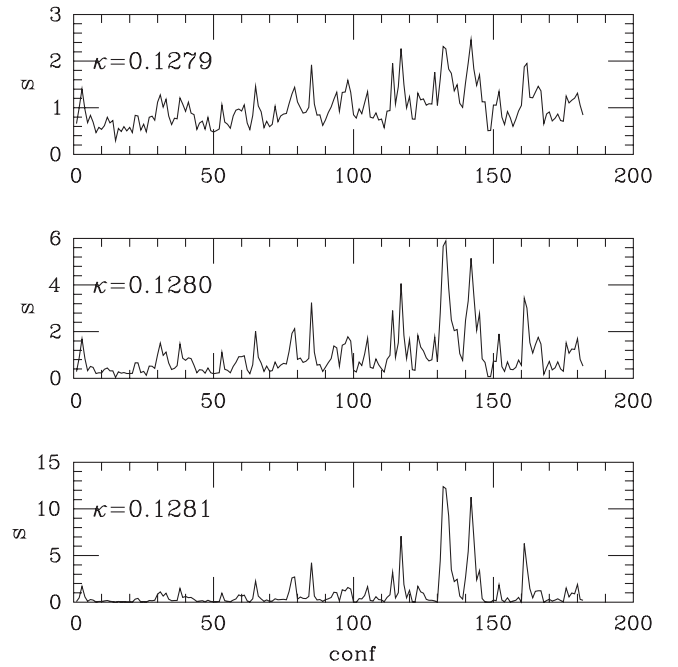


FIG. 3. Reweighting factors at  $\kappa = 0.1279$ ,  $0.1280$ , and  $0.1281$  on 180  $16^4$  configurations. The reweighting factors are normalized such that their average is  $\langle s \rangle = 1$ .

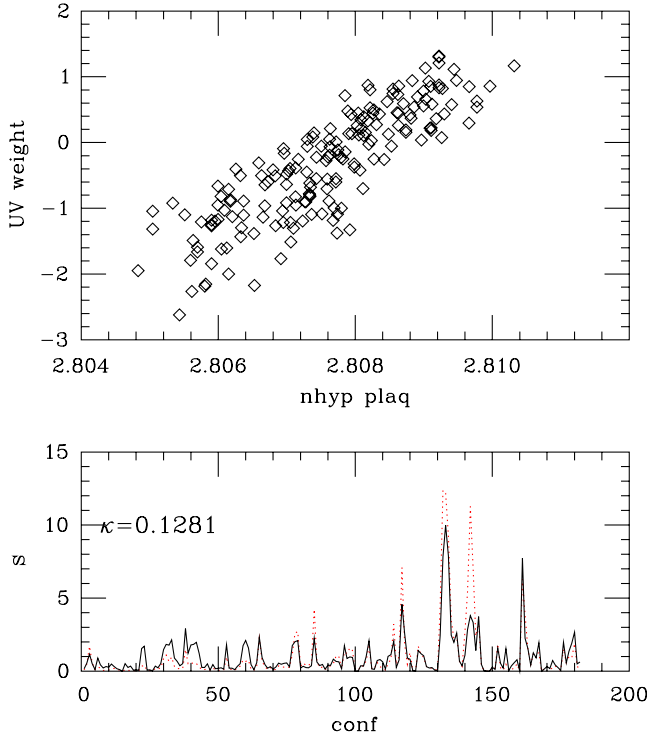


FIG. 4 (color online). The logarithm of the UV part of the reweighting factor versus the smeared nHYP plaquette (top panel), and the reweighting factors after the observed correlation is removed by an nHYP plaquette term in the action (lower panel). The dashed red line in the lower panel is the original reweighting factor. The data are for  $\kappa = 0.1281$ .

$$S_2 = S_g - \text{Indet}(D_2^\dagger D_2) + \frac{\tilde{\beta}}{3} \sum_p (3 - \text{Re Tr} U_{p, \text{nHYP}}). \quad (17)$$

The correlation shown in Fig. 4 can be captured by an nHYP plaquette term with a  $\tilde{\beta} = -0.00133$  coefficient at  $\kappa = 0.1281$ , or  $\tilde{\beta} = -0.00116$  at  $\kappa = 0.1280$ . The new term is a local, pure gauge term with a very small coefficient. While such a term is not necessary, it does help in reducing the fluctuations. The lower panel of Fig. 4 shows the reweighting factors at  $\kappa = 0.1281$ , both with (solid line) and without (dotted line) an nHYP plaquette term in the action.

Of course the variance of the reweighting factor is only one aspect. The real test is how they combine with observables to give fully unquenched results. We present two examples here, both for reweighting to  $\kappa = 0.1280$ .

Figure 5 shows the scalar correlator for the partially quenched, reweighted and nHYP reweighted ensembles. The partially quenched data show that the correlator becomes negative, a well-known “artifact” of partial quenching. This disease is cured by reweighting. On the fully dynamical ensembles the propagator is positive with both kinds of reweighting. In fact, the two reweighted ensem-

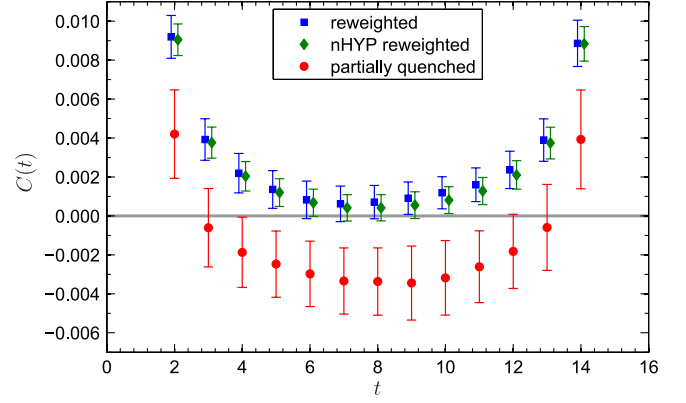


FIG. 5 (color online). The scalar correlator at  $\kappa = 0.1280$  for the partially quenched, reweighted and nHYP reweighted ensembles. The reweighted data points are slightly offset for clarity.

bles are hardly distinguishable, though the errors on the nHYP ensemble are about 25% lower.

In our second example we look at the pseudoscalar correlator at  $t = n_t/2 = 8$ , estimated from point-to-point propagators at a single time slice on the individual configurations. Figure 6 shows the partially quenched and reweighted values,  $C_{\pi\pi}(n_t/2)$  and  $s_i C_{\pi\pi}(n_t/2)$ , with weight factors  $s_i$  corresponding to a new action  $S_2$  both

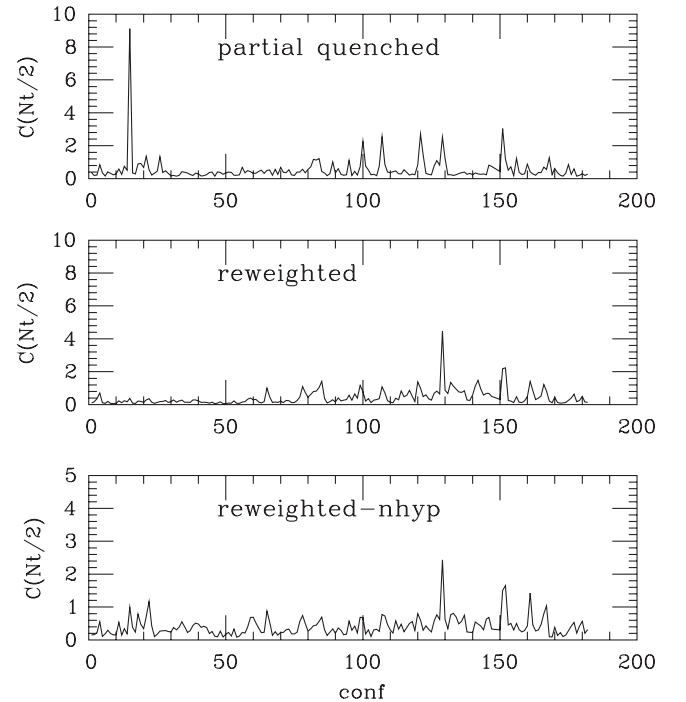


FIG. 6. The pseudoscalar correlator at  $t = n_t/2$  without reweighting and with reweighting. The third panel shows the correlator with reweighting that includes an nHYP plaquette term. Observe the scale difference for the last panel. All data are for  $\kappa = 0.1280$ .

with and without the nHYP plaquette term [see Eq. (17)]. Reweighting removes the very large spike (corresponding to a configuration with a nearly zero eigenmode), and reweighting with the nHYP plaquette term reduces the fluctuations by an additional factor of 2 (observe the scale difference). The reweighted data have considerably smaller statistical fluctuations than the partially quenched data.

#### IV. PHYSICAL RESULTS

Our goal in this paper is to illustrate the effectiveness of the reweighting method. The physical results we present in this section are preliminary; they merely serve to illustrate the power of the reweighting technique.

As we have mentioned in Sec. III, the original ensemble consists of  $180 \cdot 16^4$  configurations generated with 2 degenerate flavors of nHYP clover fermions at coupling  $\beta = 7.2$ ,  $\kappa = 0.1278$ . The lattice spacing is  $a = 0.115(3)$  as calculated from the Sommer parameter  $r_0/a = 4.25(10)$  [21,22] using  $r_0 = 0.49$  fm, and the PCAC quark mass is  $am_{\text{PCAC}} = 0.0119(5)$ , translating to  $m_{\text{PCAC}} \approx 20$  MeV. From the quadratic time dependence of the axial correlator [23], on our volume of  $V = (1.87 \text{ fm})^4$  we estimate  $m\Sigma V \approx 2.1$ , in or close to the  $\epsilon$ -regime.

Reweighting has no observable effect on the lattice spacing, both with standard and with nHYP reweighting  $r_0/a = 4.25$  at every  $\kappa$  value, though the error increases to 0.15 at  $\kappa = 0.1281$ . One reason for the relatively large error is the short time extent of the lattices.

Table I lists the PCAC quark mass as obtained on the reweighted ensembles. These values correspond to quark masses between 5 and 20 MeV.  $m_{\text{PCAC}}$  shows a linear dependence on the bare quark mass with  $\kappa_{cr} = 0.1282$ , as shown in Fig. 7. With reweighting we were able to decrease the quark mass by a factor of 4.

In the  $\epsilon$ -regime next-to-leading-order chiral perturbation theory predicts a quadratic form for the meson correlators. For the pseudoscalar meson the prediction to  $\mathcal{O}(\epsilon^4)$  is [24–26]

$$\begin{aligned} G_P(t) &= \frac{1}{L_s^3} \int d^3x \langle P(x)P(0) \rangle \\ &= a_p + \frac{L_t}{L_s^3} b_p h_1\left(\frac{t}{L_t}\right) + \mathcal{O}(\epsilon^4), \end{aligned} \quad (18)$$

TABLE I. The PCAC quark mass and the low energy constant  $F$  on the original and reweighted ensembles. The first error of  $F$  is statistical; the second is systematic, due to the uncertainty of the parameter  $m\Sigma V$ .

$\kappa$	$am_{\text{PCAC}}$	$F$ (MeV)
0.1278	0.0119(5)	79(3)(4)
0.1279	0.0090(3)	79(4)(4)
0.1280	0.0062(3)	81(8)(3)
0.1281	0.0027(5)	78(10)(1)

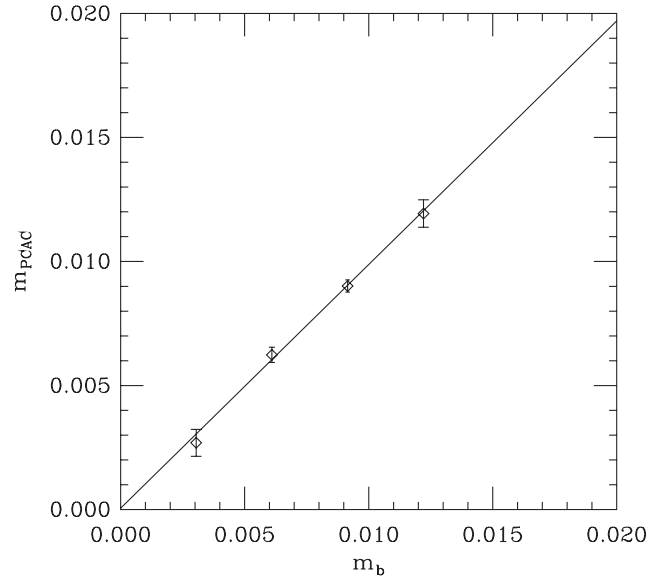


FIG. 7. The  $m_{\text{PCAC}}$  quark mass as a function of the bare mass,  $m_q = (1/\kappa - 1/\kappa_{cr})/2$  with  $\kappa_{cr} = 0.1282$ .

where

$$\begin{aligned} a_p &= \frac{\Sigma^2 \rho^2}{8} I_1(2m\Sigma V\rho), \\ b_p &= \frac{\Sigma^2}{F^2} \left(1 - \frac{1}{8} I_1(2m\Sigma V\rho)\right) \end{aligned} \quad (19)$$

are related to the chiral low energy constants  $\Sigma$  and  $F$ , while

$$\rho = 1 + \frac{3\beta_1}{2F^2\sqrt{V}}$$

is the shape factor with  $\beta_1 = 0.14046$  for our symmetric geometry [24].  $I_1$  can be expressed in terms of Bessel functions,  $I_1(u) = 8Y'(u)/(uY(u))$ . The function

$$h_1(\tau) = \frac{1}{2} \left[ \left( \tau - \frac{1}{2} \right)^2 - \frac{1}{12} \right] \quad (21)$$

describes the quadratic time dependence. Our data follow this expected functional form in the region  $t \in [4, 12]$ . Figure 8 shows the pseudoscalar correlator on the original as well as on the reweighted data sets with the corresponding quadratic fits.

The fit gives the constant term  $a_p$  with 6%–8% error, predicting  $\Sigma^{1/3}$  with 1% accuracy, while the ratio  $a_p/b_p$  has 8%–30% errors, predicting  $F$  at the 4%–15% level. The large errors are not surprising as the quadratic term measures only finite size effects, and our lattices are not small. The errors are particularly large at  $\kappa = 0.1281$  where the configuration overlap with the original ensemble

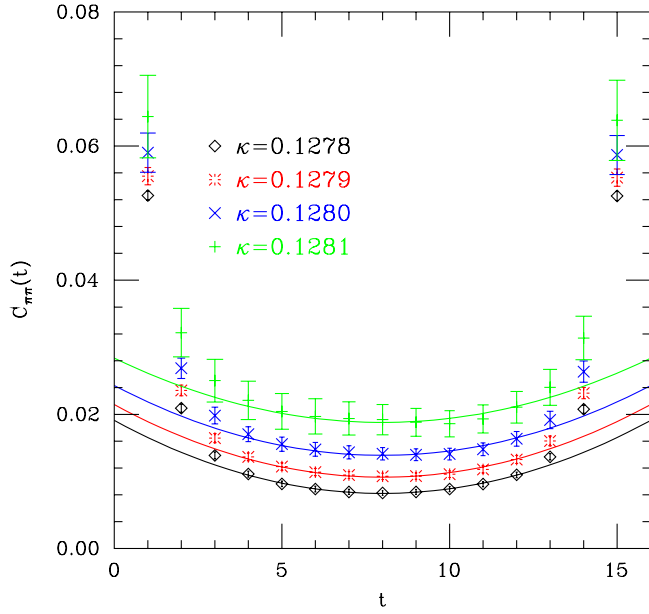


FIG. 8 (color online). The pseudoscalar correlator on the original and nHYP reweighted data sets.

is getting small. Nevertheless, we chose to present results based on the ratio  $a_p/b_p$  as it is free of renormalization factors. To predict the low energy constant  $\Sigma$  we would need the renormalization factor of the pseudoscalar density. This calculation is in progress and we will report the results in a forthcoming publication [23]. In Table I we list the predictions for  $F$  as obtained from the pseudoscalar correlator. The first error is statistical; the second is systematic from the uncertainty of the quantity  $m\Sigma V$ . The central values correspond to  $m\Sigma V = 2.1$  at  $\kappa = 0.1278$ , and at the other  $\kappa$  values we rescaled this according to the PCAC quark mass. It is satisfying that the values we obtain are consistent with each other, suggesting that all four data sets are governed by the  $\epsilon$ -regime predictions. The value is also consistent with recent  $p$ -regime overlap action calculations, though somewhat smaller than overlap  $\epsilon$ -regime calculations [27–29]. It is possible to determine  $F$  from the eigenvalue distribution of the Dirac operator at imaginary chemical potential, giving consistent results, though with large finite volume corrections [30]. Other meson correlators can be used in a similar way to predict the low energy constants of the chiral Lagrangian.

The advantage of using Wilson-clover fermions is that it is relatively inexpensive to create even large volume configurations. With the reweighting technique it is possible to probe a whole range of mass values and approach the  $\epsilon$ -regime without independent simulations. At present, we are running simulations on  $24^4$  volumes at the same lattice spacing ( $L = 2.8$  fm) at approximately 8 MeV quark masses. Our tests indicate that reweighting to 2–3 MeV quarks does not introduce large statistical errors; therefore we will be able to test the finite volume dependence of the low energy constants.

## V. CONCLUSION

Dynamical simulations with light quarks are still computationally expensive and have to overcome technical difficulties due to large autocorrelation time, algorithmic instability, and statistical fluctuations. In this paper we presented an alternative to direct simulations, suggesting that reweighting in the quark mass to reach the desired light mass value might be a better alternative. We described stochastic reweighting and presented several improvements.

The gain from reweighting is largest, once large autocorrelation times make it difficult to generate independent configurations directly. The relatively cheap simulation at a larger quark mass makes it easier to keep the decorrelation under control. Then, one can space the measurements (including the reweighting factors) sufficiently far apart. The computation of the reweighting factors themselves is not particularly expensive, maybe of the same order as generating the ensemble in the case at hand. However, once the autocorrelations become more prominent, this relative cost is expected to decrease. It would have been interesting to directly simulate one of the smaller quark masses. However, our measurement of the spectral gap indicates that those simulations are no longer safe with the hybrid Monte Carlo algorithm by the criterion given in Ref. [6].

Our numerical tests show that with reweighting one can easily approach the  $\epsilon$ -regime with Wilson-clover quarks, and we presented preliminary data for the low energy chiral constant  $F$ . Reweighting can also provide an alternative to partially quenched studies in the  $p$ -regime, since the statistical fluctuations of the reweighted dynamical lattices can be considerably smaller than the partially quenched data. As an example we showed how the scalar correlator, known to become negative in partially quenched simulations, becomes positive and follows the expected theoretical form on the reweighted (and therefore fully dynamical) ensembles.

Reweighting might not be efficient in large volumes, or it might be limited to small mass differences. Our experience indicates that this is not a problem on  $(1.87 \text{ fm})^4$  volumes between 20 and 5 MeV quarks or  $(2.8 \text{ fm})^4$  volumes between 8 and 3 MeV quarks with nHYP smeared Wilson-clover fermions.

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