technique can be efficient even on large lattices. This improvement arises from the new update scheme in accord with about 20% probability. This implies that the determinant ratio is still close to one and with the improved stochastic estimator the proposed method is still effective on large lattices. We also show the ratio of the Fermionic determinants on the new and original configurations. We study the ratio as a function of the number of lattices that are changed in the last batch update. We find that even after the update of a large number of lattices the determinant ratio is close to one.

Results that are essentially the same for a recent proposed update method of smeared link dynamical fermions. This is essential for a recent proposed update method of smeared link dynamical fermions.

We propose and study an improved method to calculate the Fermionic determinant of dynamical configurations.

Abstract

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Evolution of the Fermionic Determinant of Dynamical Configurations

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I. INTRODUCTION

The use of smeared or fat links in staggered fermion actions has gained popularity in recent years due to the improved flavor symmetry these actions possess \cite{1,2,3}. Smeared links are naturally part of most systematic improvement programs and many overlap fermion formulations as well \cite{4,5}. The main difficulty that limits the use of smeared link fermions is their potential complexity in dynamical simulations. Unless the smeared links are linear combinations of the original thin links the explicit form of the fermionic force needed for standard molecular dynamics simulations is very complicated, making the HMC or R algorithms impractical or even impossible. A recently proposed update for smeared link dynamical fermions\cite{6,7} avoids this problem by creating a sequence of configurations by updating a subset of the gauge links by a pure gauge heat bath or over relaxation step. The proposed configuration is accepted or rejected according to the change in the fermionic determinant. In fact one does not even have to evaluate the change in the determinant, a stochastic estimator can be used instead. That requires no more than the evaluation of the inverse fermion matrix on a Gaussian random source vector.

The above outlined algorithm can fail in two ways. First, if the ratio of the fermionic determinants is small, the acceptance rate is small. The algorithm can also fail if the stochastic estimator gives a poor approximation of the determinant, making the autocorrelation time of the simulation (i.e. the number of independent Gaussian random sources needed to get a good estimate for the determinant) very large. In this paper we discuss systematic ways to improve the stochastic estimator. With the improved estimator we calculate the ratio of fermionic determinants as the function of the number of links updated with a heat bath step, and show that it remains close to one even if the updated volume is large. We illustrate and test the method using staggered fermions with HYP smeared gauge links though the generalization to any other smeared link action is straightforward.

II. THE HYP ACTION AND ITS DYNAMICAL UPDATE

In this section we define the HYP action and briefly summarize the partial-global updating technique. We consider a smeared link action of the form

\[ S = S_g(U) + \tilde{S}_g(V) + S_f(V) \]  

(1)
where $S_g(U)$ and $\bar{S}_g(V)$ are gauge actions depending on the thin links $\{U\}$ and smeared links $\{V\}$, respectively, and $S_f$ is the fermionic action depending on the smeared links only. The updating method and all its improvements that we discuss in this paper would work with any kind of smeared links $\{V\}$, though the efficiency suffers if the smeared links are not smooth enough. In our work we use HYP smeared links with staggered fermions. The HYP links are optimized non-perturbatively to be maximally smooth. The construction and properties of HYP smearing are discussed in detail in Ref. [1].

We use a plaquette gauge action for $S_g(U)$

$$S_g(U) = -\frac{\beta}{3} \sum_p \Re \text{Tr}(U_p).$$

We choose $\bar{S}_g(V)$ to improve computational efficiency and we will discuss our specific choice in Sect. III.C. The staggered fermionic matrix is defined in the usual way

$$M(V)_{i,j} = 2m\delta_{ij} + \sum_\mu \eta_i\mu(V_i\mu\delta_{i,j}\cdot\bar{\mu} - V_{i,\bar{\mu}}\cdot\bar{\delta}_{i,j}\cdot\bar{\mu}.)$$

The matrix $M^d(V)M(V)$ is block diagonal on even and odd lattice sites. In the following we will denote the even block by $\Omega$

$$\Omega(V) = (M^d(V)M(V))_{\text{even, even}}$$

and define the fermionic action as

$$S_f(V) = -\frac{n_f}{4} \text{Tr} \ln \Omega(V)$$

to describe $n_f$ flavors of staggered fermions. In the following we consider $n_f = 4$ flavors but we will briefly describe the generalization to arbitrary flavors at the end of Sect. III.B.

In Refs. [6, 7] a partial-global heat bath and over relaxation updating method was proposed to simulate the system described by Eq. 1. In this paper we are not concerned about the update itself, but to motivate our interest in calculating the fermionic determinant ratios we briefly summarize the main points of the method. In the first step of the update one changes a subset of the thin links $\{U\}$ to propose a new thin gauge link configuration $\{U'\}$. The new links are chosen with a heat bath or over relaxed update that satisfies the detailed balance condition with the thin link gauge action $S_g(U)$. The smeared links $\{V\}$ and $\{V'\}$ are unique once the thin links are defined. Next the proposed configuration is
accepted with the probability

\[ P_{\text{acc}} = \min\{1, \exp(-\delta_s(V') + \delta_s(V)) \frac{\det(\Omega(V'))}{\det(\Omega(V))}\}. \]  

(6)

The ratio of the determinants can be written as

\[
\frac{\det(\Omega(V'))}{\det(\Omega(V))} = \frac{\int d\xi^* \exp(-\xi^*\Omega^{-1}(V')\Omega(V)\xi)}{\int d\xi^* \exp(-\xi^*\xi)}
= \langle \exp(-\xi^*[\Omega^{-1}(V')\Omega(V) - 1]\xi) \rangle_{\xi^*\xi}. \]

(7)

The expectation value can be evaluated stochastically where on every gauge configuration pair \{U\} and \{U'\} only one random source \(\xi\) is used to estimate the determinant ratio and the expectation value is taken together with the configuration ensemble average. That leads to the stochastic acceptance probability

\[ P_{\text{stoch}} = \min\{1, e^{-\delta_s(V') + \delta_s(V)} e^{-\xi^*[\Omega^{-1}(V')\Omega(V) - 1]\xi}\}. \]  

(8)

III. IMPROVING THE PARTIAL-GLOBAL UPDATE

The success of the partial-global updating algorithm depends on two things. First, on the ratio of the determinants of the new and old links, and next on the effectiveness of the stochastic estimator. If the stochastic estimator fluctuates wildly, it can reduce the acceptance rate to practically zero even if the change in the determinant is actually small. In the following we will discuss improving the stochastic estimator first.

A. Improving the stochastic estimator

To calculate the acceptance probability we have to calculate the ratio of the determinants

\[
\frac{\det^{-1}(A)}{\det \Omega} = \langle \exp(-\xi^*[A - 1]\xi) \rangle_{\xi^*\xi} = \langle \exp(-\Delta S_f) \rangle
\]

where \(\Omega = \Omega(V), \Omega' = \Omega(V')\) denote the old and new fermionic matrix, \(A = \Omega'^{-1}\Omega\) and \(\xi\) is a Gaussian random source vector. The standard deviation of this stochastic estimation can be written as

\[
\sigma^2 = \langle \exp(-2\xi^*[A - 1]\xi) \rangle_{\xi^*\xi} - \langle \exp(-\xi^*[A - 1]\xi) \rangle_{\xi^*\xi}^2
= \det^{-1}(2A - 1) - \det^{-2}(A).
\]  

(10)
Eq. 10 is valid only if the matrix $2A - 1$ is positive definite. If the matrix $A$ has even one eigenvalue that is less than or equal to 1/2, the formula in Eq. 10 is not valid, the standard deviation is infinite. There is no a priori reason to assume that the matrix $A$ has no small eigenvalues. This is a very serious problem that could make the stochastic estimator useless in dynamical calculations. If the fermionic matrices $\Omega$ and $\Omega'$ are close, i.e. only a few links are changed in the update, $A = \Omega'^{-1} \Omega \approx 1$ and consequently $\det(A) \approx 1$ and $\det(2A-1) \approx 1$ as well. However for an effective updating method we would like to change the configuration at as many links as possible, which makes the occurrence of a small eigenvalue likely. In the following we propose a 2-step solution that can always be used to handle the small eigenvalues in $A$.

First we follow the program of Refs. [6, 7, 8] and replace $\Omega$ and $\Omega'$ by reduced matrices

$$\Omega_r = \Omega e^{-2f(\Omega)} , \quad \Omega'_r = \Omega' e^{-2f(\Omega')} ,$$

with $f$ a yet to be determined polynomial. We can rewrite eq. 9 as

$$\frac{\det \Omega'}{\det \Omega} = \frac{\det \Omega'_r}{\det \Omega_r} \exp(2 \text{Tr}(f(\Omega') - f(\Omega)))$$

$$= <\exp(-\xi^* [\Omega'^{-1} \Omega_r - 1] \xi) >_{\xi^*} \exp(2 \text{Tr}(f(\Omega') - f(\Omega))) .$$

(12)

Since $\text{Tr} f$ can be calculated exactly, only the first factor of the last expression is evaluated stochastically. Its fluctuations are minimized if $A_r = \Omega'^{-1} \Omega_r \approx 1$. It is difficult to optimize the polynomial $f$ both for $\Omega$ and $\Omega'$ at the same time, instead we choose $f$ such that $\Omega'^{-1} \approx 1$. That also guarantees $\Omega_r \approx 1$. Since for staggered fermions the eigenvalues of the matrix $\Omega$ can vary between $4m^2$ and $16 + 4m^2$, we choose the polynomial $f$ such the the function $e^{2f(x)/x}$ is close to one in that range. In practice we use a third order polynomial

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3$$

(13)

and choose the coefficients $a_i$ by minimizing the function

$$\Delta = \int_{4m^2}^{16 + 4m^2} \left( \frac{1}{x} e^{2f(x)} - 1 \right)^2 \rho(x) dx .$$

(14)

The weight function $\rho(x)$ should approximate the eigenvalue density distribution of the fermionic matrix. We used a linear approximation for $\rho$

$$\rho(x) = x, \quad x \in (4m^2, 8 + 4m^2)$$

$$= 16 + 8m^2 - x, \quad x \in (8 + 4m^2, 16 + 4m^2)$$

(15)
and considered mass values \( m = 0.01 - 0.1 \). We have also tried more complex forms for the eigenvalue density that included higher order terms, all motivated by free field calculations. The results were not very sensitive to the specific choice of \( \rho \). We do not want to change the \( \alpha \) parameters depending on the quark mass of the simulation so we decided to use the following values in all cases

\[
\begin{align*}
\alpha_0 &= -0.34017 \\
\alpha_2 &= 0.35645 \\
\alpha_4 &= -0.030379 \\
\alpha_6 &= 0.000937.
\end{align*}
\]

(16)

The eigenvalues of the reduced matrix \( \Omega_r \) span a smaller range than the original fermionic matrix. At mass \( am = 0.1 \) the smallest eigenvalue is increased from \( 4m^2 = 0.04 \) to about 0.08, while the ratio of the largest to smallest eigenvalue is reduced from \( (16 + 4m^2)/4m^2 \approx 400 \) to about 14. At \( am = 0.04 \) the increase in the smallest eigenvalue is from 0.0064 to 0.0125, while the reduction in the ratio of the largest to smallest eigenvalue is from 2,500 to about 95.

When expressed in terms of the reduced matrices the acceptance probabilities of Eqs. 6,8 contain a new gauge-action like term

\[
\begin{align*}
P_{\text{acc}} &= \min\{1, \exp(-\Delta \xi_g + 2\Delta f) < \exp(-\xi^* \Omega_{r^{-1}} \Omega_r - 1) > \xi \xi^* \} \\
P_{\text{stoch}} &= \min\{1, \exp(-\Delta \xi_g + 2\Delta f) \exp(-\xi^* \Omega_{r^{-1}} \Omega_r - 1) \xi \}
\end{align*}
\]

(17)

with \( \Delta \xi_g = \xi_g(V') - \xi_g(V) \) and \( \Delta f = \text{Tr}(f(\Omega') - f(\Omega)) \). To calculate the expression \( \xi^* \Omega_{r^{-1}} \Omega_r - 1 ) \xi \) requires multiplications with \( \Omega, \Omega^{-1}, \) and with the reduction factors \( \exp(-2f(\Omega)) \) and \( \exp(2f(\Omega')) \). The exponentials can be expanded in a Taylor series and approximated with a few terms. In [7] we found that it was sufficient to keep only 15 terms. Later we will argue that it is better to replace \( \Omega_r \) and \( \Omega_{r^{-1}} \) themselves with a finite order polynomial.

To complete the evaluation of the determinant and acceptance probabilities we still have to calculate the trace of \( f(\Omega) \). \( \text{Tr}(f(\Omega)) \) can be expressed as the combination of the plaquette and the three 6-link loops of the smeared links \( V \). It is a fairly straightforward calculation giving

\[
\text{Tr} f(\Omega) = (-8\beta_4 + 336\beta_6) \sum_n \text{Re} \text{Tr} \Omega_n +
\]

6
\[12\beta_0 = -\sum_n \text{Re Tr} \sum_n \text{Re Tr} \sum_n \delta_{N,6} \sum_n \text{Re Tr} P_n + \text{const}, \tag{18}\]

where the summation is over all distinct objects in the lattice. \(P_n\) is the Polyakov line that gives a contribution on lattices of size \(N = 6\). Lattices that are smaller than \(N = 6\) in any direction would have additional contribution of length-6 overlapping loops. Eq. 18 is not valid in that case. The coefficients \(\beta\) are related to the quark mass and the optimized \(\alpha\) parameters of Eq. 16 as

\[
\beta_0 = \alpha_0 + \alpha_2 \cdot 4m^2 + \alpha_4 \cdot (4m^2)^2 + \alpha_6 \cdot (4m^2)^3 \\
\beta_2 = -\alpha_2 \cdot 2 \cdot 4m^2 - \alpha_6 \cdot 3 \cdot (4m^2)^2 \\
\beta_4 = \alpha_4 + \alpha_6 \cdot 3 \cdot 4m^2 \\
\beta_6 = -\alpha_6. \tag{19}\]

In Ref. [6] we used a similar reduction using a second order polynomial for \(f\). There we determined the \(\alpha_0\) and \(\alpha_4\) coefficients by trial and error attempting to maximize the acceptance rate in Eq. 6. The values we obtained there are consistent with what we would determine now with the minimization procedure. Increasing the order of the reduction polynomial further gives only slight improvement but would require the evaluation of \(\text{Tr} \Omega^4\) and higher order terms in \(\text{Tr} f\), a considerable computational task.

The polynomial reduction of the fermionic matrix results in considerable improvement in the evaluation of the determinant ratio but it is not sufficient to guarantee that the standard deviation of the stochastic estimator is finite or small. To achieve that we now proceed to rewrite the reduced fermionic determinant ratio as

\[
\det^{-1} A_r = \det^{-n} A_r^{1/n} = \left< \exp\left( -\sum_{j=1}^n \xi_j [A_r^{1/n} - 1] \xi_j \right) \right>_{\xi_j \xi_j}, \tag{20}\]

with \(n\) an arbitrary positive integer. The expectation value is evaluated with \(n\) independent \(\xi_j\) random vectors and the standard deviation becomes

\[
\sigma^2 = \det^{-n} (2A_r^{1/n} - 1) - \det^{-2} (A_r). \tag{21}\]

\(\sigma^2\) is finite if none of the eigenvalues of the matrix \(A_r\) is smaller than or equal to \(2^{-n}\). This is a much easier condition to satisfy than the one before. With the reduced matrix, assuming
that the smallest eigenvalue of $A_r$ is not smaller than the product of the smallest eigenvalues of $\Omega_r$ and $\Omega'_r^{-1}$, $n = 4$ is sufficient to guarantee the finiteness of the standard deviation at $am = 0.1$, and $n = 8$ is sufficient at $am = 0.04$. For small standard deviation one might need to use larger $n$ values, but with any mass $am \neq 0$ and matrix $A_r$, it is possible to choose $n$ such that the standard deviation is finite and small. The cost of this improvement is that we have to evaluate the expression $\xi^* (A_r^{1/n} - 1) \xi^n$ times for one estimate of the determinant.

The $n$th root of the matrix $A_r$ can be approximated with polynomials to arbitrary precision [9, 10]. Since the order of the matrices in the determinant are irrelevant, we write the $n$th root of the matrix as

$$A_r^{1/n} = \Omega_r^{-1/2n} \Omega_r^{1/n} \Omega'_r^{-1/2n}.$$  \hspace{1cm} (22)

We found that breaking up $\Omega'_r^{-1/n}$ to two identical terms and separating them with the less singular $\Omega_r^{1/n}$ improves the stochastic estimator. The terms $\Omega_r^{1/n}$ and $\Omega'_r^{-1/2n}$ are approximated with polynomials

$$\Omega_r^{-1/2n} = \Omega_r^{-1/2n} \exp(f(\Omega')/n) = P_l^{(2n)}(\Omega'),$$

$$\Omega_r^{1/n} = \Omega_r^{1/n} \exp(-2f(\Omega)/n) = Q_k^{(n)}(\Omega),$$  \hspace{1cm} (23)

where $P_l^{(2n)}$ and $Q_k^{(n)}$ are $l$ and $k$ order polynomials of the fermionic matrices $\Omega$ and $\Omega'$. To reduce the errors of the polynomial approximation we write the exponent in the stochastic estimator as

$$\xi^* [A_r^{1/n} - 1] \xi = \xi^* P_l^{(2n)}(\Omega') Q_k^{(n)}(\Omega) P_l^{(2n)}(\Omega') \xi - \xi^* P_l^{(2n)}(\Omega') Q_k^{(n)}(\Omega') P_l^{(2n)}(\Omega') \xi.$$  \hspace{1cm} (24)

The necessary order for the polynomials $P$ and $Q$ vary with the quark mass but we found that in most cases fairly low orders are sufficient.

At this point the generalization of the partial-global updating method to arbitrary flavor numbers is straightforward. To describe $n_f$ flavors we have to replace the determinant ratio in Eq. 6 by its $n_f/4$th power. That can be easily done by summing up to $\frac{n_f}{4} n$ only in Eq. 20. The polynomials $P$ and $Q$ do not have to be changed and smaller $n$ will be sufficient for the same standard deviation of the determinant.

### B. Calculating the determinant ratio

To illustrate the improved estimator, in this section we calculate the ratio $\det(\Omega') / \det(\Omega)$ for a specific configuration pair. We chose $\{U\}$ from a configuration set that was generated
Figure 1: The stochastic estimator for $\det(\Omega')$ using a) the naive estimator with $f = 0$, b) the estimator with improved $f$ given in Eqs. 13, 16 and c) the form of Eq. 20 with $n = 8$ and improved $f$.

with the HYP dynamical action at $\beta = 5.2$, $am = 0.1$, and $\bar{s}_p(V) = 0$. The scale at these parameter values is $r_0/a = 3.0(1)$ and $m_\pi/m_\rho \approx 0.8$ [7]. We updated 300 random links of $\{U\}$ with a heat bath step corresponding to a $\beta = 5.2$ plaquette gauge action to create the $\{U'\}$ configuration. To calculate the determinant ratio we use Eq. 12 with $f = 0$, with the improved $f$ given in Eqs. 13, 16, and also using the formula of Eq. 20 with $n = 8$ and the improved $f$. We calculate the expectation value using 500-1500 random vectors. Figure 1 shows the stochastic estimator for the three cases. One could not guess from the figure that the three estimators describe the same quantity. The naive $f = 0$ estimator is 15 orders of magnitude smaller than the improved ones. How is that possible? The average $<e^{-\Delta S_f}>$ will be the same for all three estimators, but for the naive one the average will come from many almost zero values and an occasional large one. That occasional large value is so rare
that we did not even encounter it in 500 samples. The improved estimator with \( n = 1 \) looks much more reliable and it predicts

\[
\frac{\det(\Omega')}{\det(\Omega)} = 0.81(12), \quad n = 1.
\] (25)

The estimator with \( n = 8 \) is even better. With only a third of the statistics of the \( n = 1 \) case it predicts the determinant ratio as

\[
\frac{\det(\Omega')}{\det(\Omega)} = 0.77(2), \quad n = 8.
\] (26)

That does not mean that the acceptance rate of the partial-global update is close to 80% if we update 300 links at a time. The acceptance rate is better described by the expectation value

\[
< \min\{1, e^{-\Delta s_i}\} >_{\xi, \pi} = 0.32(1), \quad n = 1,
\]

\[
= 0.65(1), \quad n = 8.
\] (27)

One should remember that the above values correspond to a specific pair of configurations. Before calculating the determinant ratio on an ensemble of configurations we first discuss a modification of the gauge action.

C. Choosing the gauge action \( \tilde{S}_2(V) \)

In the previous chapter we showed how to remove the most singular part of the inverse fermion matrix by multiplying it with a factor \( \exp(2f(\Omega)) \). The change in the fermion determinant is compensated by the additional term \( \exp(2 \text{ Tr}(f(\Omega') - f(\Omega))) \) in the stochastic estimator that can be calculated exactly. With \( f(\Omega) \) a third order polynomial \( \text{Tr} f(\Omega) \) is a combination of the plaquette and 6-link loops of the smeared links as given in Eq. 18. While it is straightforward to evaluate \( f(\Omega) \), it is not a completely negligible computational cost. On the smeared link lattice the plaquette and the 6-link loops are very correlated and \( \text{Tr} f(\Omega) \) can be approximated by the plaquette term only, thus reducing the computational overhead. In general we choose the gauge action \( \tilde{S}_2(V) \) as

\[
\tilde{S}_2(V) = 2 \text{ Tr} f(\Omega) - 12\beta_0 \delta_{N,6} \sum_n \text{ Re} \text{ Tr} P_n - \frac{\gamma}{3} \sum_n \text{ Re} \text{ Tr} \square_n.
\] (28)

Here we have included the Polyakov line term explicitly, i.e. \( \tilde{S}_2(V) \) is the combination of the 4 and 6-link gauge loops only, it contains no loops closed because of the periodicity of the
lattice. Like before, this action should not be used if in any direction the lattice is smaller than 5. With this choice for $\tilde{S}_g(V)$ the gauge term in the acceptance probability in Eq. 17 simplifies to

$$-\Delta \tilde{S}_g + 2\Delta f = 12\beta_0 \delta_{N,6} \sum_n (\text{Re Tr} \, P'_n - \text{Re Tr} \, P_n) + \frac{\gamma}{3} \sum_n (\text{Re Tr} \, \square, - \text{Re Tr} \, \square, \gamma).$$  \hspace{1cm} (29)

We can choose the coefficient $\gamma$ to account for the $2 \text{Tr} \, f(\Omega)$ term, or even better, we can choose it to maximize the determinant ratios and the acceptance rate. Then we not only avoid the computation of the term $\exp(2 \text{Tr} (f(\Omega') - f(\Omega)))$ in Eq. 17 but can also increase the efficiency of the updating algorithm.

When we write the gauge action as $S_g(U) + \tilde{S}_g(V)$, we break up the gauge term into two pieces. We use the first term $S_g(U)$ in the heat bath update and include the second one, $\tilde{S}_g(V)$, in the accept-reject term. Such a break-up usually lowers the acceptance rate, especially if the second term fluctuates considerably. With the choice of Eq. 28 $\tilde{S}_g(V)$ actually cancels another fluctuating term, $2\Delta f$, and the algorithm should get more efficient. The introduction of the plaquette term proportional to $\gamma$ could compromise the efficiency. Since the smeared plaquette term does not fluctuate much, a small $\gamma$ coefficient does not harm the acceptance rate much. How should we choose the coefficient $\gamma$? According to Ref. [7] the HYP action with $\tilde{S}_g(V) = 0$ at $\beta = 5.2$, $am = 0.1$ has lattice spacing $a \approx 0.17$ fm. In the global heat bath update the links of the configurations are updated with a pure gauge action of gauge coupling $\beta = 5.2$. The pure gauge configurations at this coupling are very different form the dynamical configurations. The correlation length that characterizes the large distance behavior is much smaller on the pure gauge configurations. At short distances the average plaquette on the dynamical configurations is $<\text{Re Tr} \, \square>_{\text{dyn}} = 1.45$ while on the pure gauge configurations the average plaquette is much smaller, $<\text{Re Tr} \, \square>_{\beta=5.2} = 1.30$.

The gauge action that we use to create new configurations does not match the dynamical action neither at long nor at short distances. One would expect that the partial-global update is most effective when the pure gauge configurations of the heat bath step are close to the dynamical configurations. This suggests that in order to maximize the efficiency of the partial-global update we can try to match the short and/or long distance fluctuations of the heat bath and dynamical actions. To match the short distance fluctuations we can require that the average plaquette of the heat bath update action and the dynamical action are close. This condition requires different $\gamma$ coupling at different quark masses and gauge
coupling values but choosing
\[ \gamma = -0.1 \] (30)
offers a good compromise. The choice \( \gamma = 0.0 \) is not much worse and leads to a somewhat simpler action, but in the following we will use \( \gamma = -0.1 \). By construction now the small scale fluctuations of the pure gauge heat bath action and of the dynamical action are about the same. The modification also improves the matching of the large distance correlations.

With the new action, in order to reproduce the lattice spacing \( a = 0.17\text{fm} \) of the \( \beta = 5.2 \), \( am = 0.1 \), \( S_\beta(V) = 0 \) action, we have to choose the gauge coupling \( \beta = 5.65 \) while keeping \( am = 0.1 \). The lattice spacing of the pure gauge model at \( \beta = 5.65 \) is almost \( 0.17\text{fm} \), a very good agreement. At smaller quark masses the same lattice spacing requires a smaller gauge coupling \( \beta \) suggesting that a slightly larger \( \gamma \) value would be the optimal one. At this point we feel that the difference is not significant to justify a quark mass dependent coupling.

By choosing the gauge action \( S_\beta(V) \) according to Eq. 28 we modify the dynamical action. This modification will not affect the perturbative properties of the smeared link action as the terms in \( S_\beta(V) \) are independent of the thin link gauge coupling and will become negligible in the continuum limit. At finite lattice spacing the new terms could change the scaling behavior of the system and their effect should be investigated.

IV. DETERMINANT RATIOS WITH THE MODIFIED ACTION

In this chapter we investigate the fermionic determinant ratios on configurations generated with the modified action of Eqs. 28, 30. We will use two sets of configurations. Both sets contain about 100 \( 8^3 \times 24 \) lattices. The first one was created at \( \beta = 5.65 \), \( am = 0.1 \) and has lattice spacing \( a = 0.17 \text{fm} \) \( (r_0/a = 2.95(5)) \) and \( m_\pi/m_\rho \approx 0.70 \). The second set is at couplings \( \beta = 5.55 \), \( am = 0.04 \) with lattice spacing \( a = 0.17 \text{fm} \) \( (r_0/a = 2.88(6)) \) and \( m_\pi/m_\rho \approx 0.55 \). On both sets we created pairs of configurations by updating a random subset of the original thin links with a heat bath step corresponding to the thin link pure gauge couplings, i.e. \( \beta = 5.65 \) and \( \beta = 5.55 \). On each pair we calculated the modified determinant ratio \( \exp(-\Delta S_\beta) \det^{-1}(\Omega \Omega^{-1}) \) using Eqs. 7, 20, 24 with 400\( (800) \) random source vectors with \( n = 4(8) \) break-up of the determinant, i.e. we estimated the determinant value from 100 independent measurements on each configuration pair. We calculated the determinant both with relatively small order polynomials (order 16 to 32) and higher order polynomials (order
Figure 2: The distribution of the modified fermionic determinant ratios on configuration set I. a) $t_{HB} = 3000$ links are updated with a heat bath step and the determinant ratios are calculated with $n = 4$ (dotted lines) and $n = 8$ (solid lines) determinant break-up. b) all links of a given direction and parity ($t_{HB} = 6144$) are updated at once and the determinant ratio is calculated with $n = 8$ break-up.

64 to 128) to monitor possible systematical errors. The difference between the small and higher order approximations is small and well within the errors of the final results. The numbers we present here were obtained with the higher order polynomials.

Figure 2 shows the distribution of the modified determinant ratios on 80 configuration pairs from set I. The histogram of figure 2/a corresponds to determinant ratios on configuration pairs that differ at 3000 links. The solid lines shows the distribution measured with $n = 8$, the dotted lines with $n = 4$ determinant break-up. The two measurements are consistent predicting

\[ <e^{-\Delta S_z \det^{-1}(\Omega \Omega^{-1})}>_{\tau=1} = 0.80(13), \quad t_{HB} = 3000 \quad (31) \]

for the determinant and

\[ <\min\{1, e^{-\Delta S_z \det^{-1}(\Omega \Omega^{-1})}\}>_{\tau=1} = 0.54(5), \quad t_{HB} = 3000 \quad (32) \]

for the acceptance rate as defined in Eq. 6. While the $n = 4$ and $n = 8$ measurements
Figure 3: The configuration average of the stochastic acceptance rate $< P_{\text{stoch}} >_U$ on the configuration set 1 as the function of the number of links touched in the heat bath update. Bursts correspond to $n = 8$, octagons to $n = 4$ break-up of the determinant. The crosses correspond to the acceptance rate using the determinants as defined in Eq. 6.

agree in their prediction of the determinant ratios, they differ considerably in their standard deviation. The average standard deviation as defined in Eq. 21 of the $n = 4$ calculation is $\sigma_{n=4} = 3.5(8)$ while for $n = 8$ it is $\sigma_{n=8} = 1.8(3)$. The standard deviation of the determinant measurement can influence the autocorrelation time of a simulation as that depends both on the effectiveness of the gauge update and on the error of the stochastic estimator. A factor of two increase in the standard deviation of the determinant could require up to a factor of four increase in the number of stochastic estimators, increasing the autocorrelation time accordingly. The extra computational cost of breaking the determinant up to $n = 8$ instead of $n = 4$ parts could be easily compensated with the reduced autocorrelation time. Whether it is worth using even larger number of terms should be investigated at different quark masses separately.

With the heat bath update we change a random set of links of given direction and parity. On an $8^3 24$ configuration a maximum of 6144 links can be changed at once. In figure 2/b we show the modified determinant ratio distribution when we update all 6144 links of a
randomly chosen direction and parity. This result was obtained with $n = 8$ break-up. The average of the determinant ratios

$$< e^{-\Delta S_2} \det^{-1}(\Omega \Omega'^{-1}) >_{\text{set} I} = 0.71(10), \quad t_{HB} = 6144,$$

and the acceptance rate as defined in Eq. 6

$$< \min\{1, e^{-\Delta S_2} \det^{-1}(\Omega \Omega'^{-1})\} >_{\text{set} I} = 0.44(4), \quad t_{HB} = 6144$$

are not much different from the previous $t_{HB} = 3000$ values, though the average standard deviation is worse, $\sigma_{n=8} = 2.7(6)$. To us this is a surprising result: on a 10fm$^4$, 8$^3$24 lattice we can perform a heat bath update on all the links in a given direction and parity, the maximum that can be updated on this volume simultaneously, and accept this change with close to 50% probability. The configuration average of the stochastic acceptance rate $< P_{\text{stoch}} >_U$ of Eq. 8 is not that high. Figure 3 compares the average stochastic acceptance rate as the function of the links touched in the heat bath update both for $n = 4$ and $n = 8$ determinant break-up and the acceptance rate from the determinant as defined in Eq. 6. With $n = 8$ the stochastic acceptance rate is close to 20% if $t_{HB} = 6144$ and about 30% if $t_{HB} = 3000$. The stochastic acceptance rate with $n = 4$ is somewhat lower. Even though these values are smaller than the maximal ones predicted by the determinants themselves, they are still quite large. What parameters would provide the best choice in an actual simulation depends on many things: the number of links that effectively change in an update step, the cost of increasing the breakup of the determinant, and on the autocorrelation time of the simulation.

The study of these questions is beyond the scope of the present paper and we will return to them in a future publication.

Figures 4 and 5 are the same as figures 2/a and 3 but for configuration set II. Most fermionic methods lose some efficiency at smaller quark masses and the stochastic estimator is no exception. While the average of the determinant ratios

$$< e^{-\Delta S_2} \det^{-1}(\Omega \Omega'^{-1}) >_{\text{set} II} = 0.8(2), \quad t_{HB} = 3000,$$

is not much different from the set I configurations, the acceptance rate as defined in Eq. 6 is smaller

$$< \min\{1, e^{-\Delta S_2} \det^{-1}(\Omega \Omega'^{-1})\} >_{\text{set} II} = 0.35(7), \quad t_{HB} = 3000.$$
Figure 4: The distribution of the modified fermionic determinant ratio on configuration set II. $t_{HB} = 3000$ links are updated with a heat bath step and the determinant ratios are calculated with $n = 4$ (dotted lines) and $n = 8$ (solid lines) break-up.

Whether this decrease is due to the smaller quark mass or reflects the fact that the pure gauge heat bath action does not match the dynamical action well is worth further investigation. To match the stochastic acceptance rate of set I with $n = 4$ determinant break-up we have to use $n = 8$ on set II as figure 5 shows.

V. CONCLUSION

In this paper we proposed an improved method to calculate the fermionic determinant of dynamical configurations. The method is very general but relies on the smoothness of smeared gauge links. To test the method we considered dynamical configurations, updated a large subset of their links with a pure gauge heat bath step, and calculated the ratios of the fermionic determinants on the old and new configurations. We found that even if all the links of a given direction and parity of an $8^3 24, 10 fm^4, m_s/m_w = 0.7$ configuration are updated at once, (6144 links in all), the fermionic determinant ratio is still fairly large and such a change would be accepted by a Metropolis accept-reject step with about 50% probability.
Figure 5: The configuration average of the stochastic acceptance rate $< P_{\text{succ}} >_U$ on the configuration set II as the function of the number of links touched in the heat bath update. Bursts correspond to $n = 8$, octagons to $n = 4$ break-up of the determinant. The cross corresponds to the acceptance rate using the determinants as defined in Eq. 6.

Using only a single stochastic estimator for the determinant reduces the acceptance rate to 20% but still offers an effective update. On configurations with smaller quark masses the stochastic estimator loses some efficiency. When $m_q/m_\pi = 0.55$ only about half that many links can be updated at one time with 20% stochastic acceptance rate though the determinants stay about the same as with larger quark masses.

We have not used the fully improved method in dynamical simulations yet, nor did we optimize all its parameters. The optimization requires tuning the parameters of the action and calculating autocorrelation times with different determinant break-up and updating steps. This work is in progress and the results will be reported in a forthcoming publication.

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