Fermilab FERMILAB-Pub-00/306-T January 2001

FERMILAB-Pub-00/306-T
Nov 2000

arXiv:hep-lat/0011076 v2 4 Dec 2000

String Breaking in Four Dimensional Lattice QCD

A. Duncan[1], E. Eichten[2], and H. Thacker[3]

[1]Dept. of Physics and Astronomy, Univ. of Pittsburgh, Pittsburgh, PA 15260

[2]Fermilab, P.O. Box 500, Batavia, IL 60510

[3]Dept.of Physics, University of Virginia, Charlottesville, VA 22901

Abstract

Virtual quark pair screening leads to breaking of the string between fundamental representation quarks in QCD. For unquenched four dimensional lattice QCD, this (so far elusive) phenomenon is studied using the recently developed truncated determinant algorithm (TDA). The dynamical configurations were generated on an Athlon 650 MHz PC. Quark eigenmodes up to 420 MeV are included exactly in these TDA studies performed at low quark mass on large coarse (but $O(a^2)$ improved) lattices. A study of Wilson line correlators in Coulomb gauge extracted from an ensemble of 1000 two-flavor dynamical configurations reveals evidence for flattening of the string tension at distances $R \gtrsim$ 1 fm.

1 Introduction

The behavior of the static energy of a quark-antiquark pair at large distance provides perhaps the most striking qualitative difference between quenched and full QCD. In the quenched theory virtual quark-antiquark pairs unconnected to external sources are neglected and the string tension rises indefinitely at large distance, whereas the full theory automatically screens the quark-antiquark potential at large distances by populating the vacuum with dynamical quark pairs. It is therefore not surprising that the demonstration of string breaking has long been regarded as a classic bellwether for testing the efficacy of dynamical QCD algorithms. Unfortunately, despite numerous studies [1] and the expenditure of a large amount of computational effort, the direct observation of string breaking in zero-temperature 4-dimensional unquenched QCD, in which the string tension is seen to become essentially flat at large distances, has not yet been clearly established. On the other hand, the phenomenon has been seen quite convincingly in lower dimensional gauge theories such as QED2 [2], QCD3 [3], or in QCD4 at finite temperature [4]. The expected softening (though not flattening) of the potential due to sea-quarks has also been seen in recent work on three flavor QCD [5].

The reasons suggested for the failure to observe a clear signal of string breaking in zero temperature 4-dimensional QCD range from the inability to decouple the lowest energy string states at the still rather small Euclidean time extents of the measured Wilson loops [3, 6] to the existence of a completely new phase of the string in which breaking is completely invisible [7]. In the former case, it has been suggested that use of an improved string operator which suppresses appropriately the coupling of higher energy string states as the breaking point is approached is a prerequisite for exposing the desired flattening of the string tension . The results that we present in this paper confirm that string breaking only appears in Wilson line correlators at sufficiently large Euclidean times, but demonstrate the breaking directly at the level of unsmeared Wilson lines and without explicitly mixing in two-meson

states [8] in the initial string state.

The three major differences between the simulations described here and previous studies of stringbreaking are

1. We measure the static energy of Wilson lines in Coulomb gauge rather than the large area behavior of Wilson loops. The Wilson line operator in Coulomb gauge has a larger overlap with the lowest energy states of a static quark-antiquark source pair than the Wilson loop. (In the case of abelian gauge theory, the overlap for the Wilson line operator is perfect.)

2. We work on physically large coarse lattices, which allows us to go to large Euclidean time (up to 1.2 fm) in order to project out the lowest state, which for large distance corresponds to a meson-antimeson pair.

3. We work at relatively small quark mass (pion mass about 195 MeV). As emphasized previously [2], the truncated determinant algorithm works perfectly well at arbitrarily small quark masses, as the convergence rate of the Lanczos algorithm used to extract the low eigenvalues depends only on the density of the infrared spectrum and does not dramatically deteriorate as we lower the quark mass.

The dynamical fermion algorithm used in this paper has been described in considerable detail elsewhere [2] so we will merely summarize the basic features. The hermitian quark Dirac operator has a completely gauge invariant spectrum which can therefore be gauge-invariantly split into a set of infrared modes (up to some momentum cutoff large enough to encompass the desired infrared virtual quark physics), while the ultraviolet modes are very accurately modelled by a local gauge-invariant pure-gauge action [9] which for large distance physics mainly results in a coupling renormalization. In the truncated determinant algorithm (TDA), we perform a simulation of the theory including *exactly* all the infrared eigenvalues in the quark determinant up to the chosen cutoff (for a detailed description of this approach see [2]). The Lanczos technique used to extract the low eigenvalues does not

suffer from rapidly increasing convergence time even at very low quark masses (in contrast to HMC algorithms, where the quark inversions become prohibitively expensive in this limit), so we are able to work essentially at kappa critical. Of course, string breaking is expected to set in earlier for light dynamical quarks, so the TDA approach has a natural advantage over other dynamical QCD schemes for this problem. The other important feature of the calculations described in this paper is the use of large coarse lattices with an $O(a^2)$ improved gauge action to restore the rotational invariance of the measured static energies. Specifically, we give results for simulations performed on 6^4 lattices with the improved action $S = 3.7[1.0(\mathrm{plaq}) + 1.04(\mathrm{trt})]$, using the notation of [10]. Although there is considerable scale uncertainty on such a course lattice, we estimate the lattice spacing for this theory is about 0.4 fm. We have performed the simulations at κ=0.2050 corresponding to $m_\pi \simeq 195$ MeV. Preliminary results from these simulations have been reported earlier [11].

In Section 2 we describe the computational and statistical issues underlying our results. Some further details of the computational load required by the TDA method are discussed. We describe the equilibration of our configurations in the TDA simulations, and the autocorrelation data underlying our error analysis are given. In Section 3 results for the correlators of Wilson lines at Euclidean times 0.4, 0.8, and 1.2 fm (1,2 and 3 lattice spacings) are reported. The flattening of the static energy associated with string breaking is finally visible for T$\simeq$ 1 fm. In Section 4 we summarize our conclusions and indicate ongoing calculations.

2 TDA Simulations on large coarse lattices

In the TDA approach to dynamical QCD, the quark determinant $\mathcal{D}(A) = \det(\gamma_5(\not{D}(A) - m)) \equiv \det(H)$ is gauge-invariantly split into infrared and ultraviolet parts

$$\mathcal{D}(A) = \mathcal{D}_{IR}(A)\mathcal{D}_{UV}(A) \tag{1}$$

by introducing a cutoff $\Lambda_{\rm cut}$ on the absolute magnitude of the eigenvalues λ_i of the hermitian Dirac operator H. These eigenvalues are gauge-invariant generalizations of the quark offshellness (i.e. for $A \to 0$, $\lambda_i \to \pm\sqrt{p^2 + m^2}$)) and the cutoff is chosen to include as much as possible of the low energy structure of the unquenched theory while leaving the fluctuations of $\ln\mathcal{D}_{IR}(A)$ (which is included *exactly* in the Boltzmann measure of the simulation) of order unity after each sweep updating all gauge links. Fortunately, this choice is possible on lattices of large physical size as well as for light quark masses close to the critical value. In the simulations reported in this paper, the cutoff $\Lambda_{\rm cut}$ is chosen at about 420 MeV. On the lattices generated this corresponds to including the lowest 840 eigenvalues of H. These eigenvalues are extracted by a Lanczos procedure for each trial gauge configuration generated using an improved gauge action and the new configuration is then subjected to a Metropolis accept/reject step based on the change in $N_{\rm flav}\ln\mathcal{D}_{IR}(A)$ (we have used $N_{\rm flav}$=2 flavors of degenerate light quarks in the simulations). Detailed balance in this procedure is ensured by using a random link choice procedure in the pure gauge update step. We have stored gauge configurations after ten combined gauge-update + metropolis determinant accept/reject steps. (The metropolis step had a typical acceptance rate of 50%.)

The computational load in these simulations is completely dominated by the extraction of the infrared quark eigenmodes (typically to seven or eight place accuracy). For example, on a 6^4 lattice, the gauge update takes a few seconds while the calculation of $\mathcal{D}_{IR}$ takes about 9 minutes on an Athlon 650-MHz processor. The string breaking results reported in Section 3 were performed on such a processor and required about 2.0 processor-months to accumulate 1000 configurations once equilibration is reached.

As mentioned previously, we work on coarse 6^4 lattices but with $O(a^2)$ improved gauge action. Following Alford et al [10], we improve the gauge action with a single additional operator, with coefficients tuned to optimize rotational invariance of the string tension

$$\begin{aligned} S(U) &= \beta_{\rm plaq} \sum_{\rm plaq} \frac{1}{3} {\rm ReTr}(1 - U_{\rm plaq}) \\ &+ \beta_{\rm trt} \sum_{\rm trt} \frac{1}{3} {\rm ReTr}(1 - U_{\rm trt}) \end{aligned} \tag{2}$$

where "trt" refers to a 8 link loop of generic structure (+x,+y,+x,-y,-x,+y,-x,-y) (the "twisted rectangle" of Ref[10]). With the choices $\beta_{\rm plaq}$=3.7, $\beta_{\rm trt}$=1.04$\beta_{\rm plaq}$, the quenched static quark potential becomes a smooth function of lattice radial separation [10] even on these very coarse lattices, with lattice spacing $a \simeq 0.4$ fm (for the unquenched theory). As we do not improve the quark action, the lattice spacing quoted here is determined by matching the initial linear rise of the string tension to a physical value. The results given below show that the restoration of rotational invariance survives reasonably well the introduction of the quark determinant, so that we have not found it necessary to retune the pure gauge action.

To maximize our chances of seeing string breaking within the spatial limitations of the lattices being used we have chosen a kappa value corresponding to a rather light pion, namely κ=0.2050, corresponding to a pion mass of about 195 MeV (or 0.39 in lattice units). This does not seem to result in a serious loss of acceptance at the level of individual Monte Carlo steps, but the equilibration process (starting from a quenched initial configuration) is definitely slower in comparison to TDA simulations performed with heavier quarks on lattices of smaller physical size [2]. The sequence of infrared determinant values (specifically, $\ln\mathcal{D}_{IR}(A)$) generated in a TDA simulation starting from a quenched configuration is shown in Fig.1. It appears that about 7000 Monte Carlo sweeps were needed to reach equilibrium (corresponding to about 1.5 650-MHz Athlon processor months). The results reported in the next section were based on the 1000 saved configurations between sweeps 7000 and 169900 (see Figure 1).

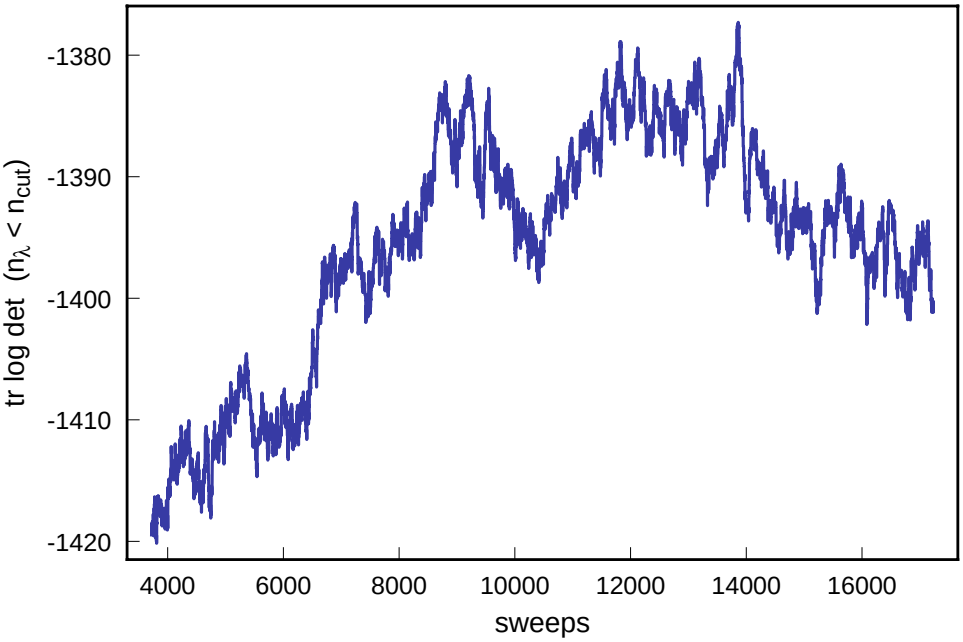

Figure 1: Equilibration of the quark determinant in TDA simulation of a coarse 6^4 lattice

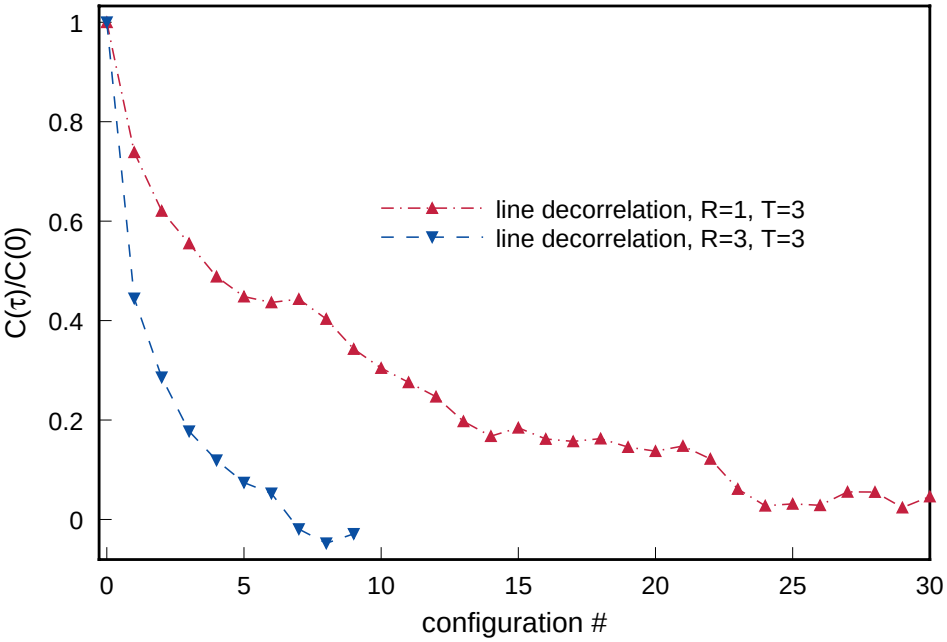

Figure 2: Typical autocorrelation curves of Wilson line correlators (R=1,3; T=3)

Given the rather long times needed for equilibration, the issue of autocorrelation of measured quantities in the post-equilibrium configurations naturally assumes great importance. We have performed a careful study of the decorrelation rate of all the Wilson line correlators used to extract the static energy plots given in Section 3 below. Thus, if $W(\tau)$ is a Wilson line correlator measured for the τ'th saved configuration, an autocorrelation function can be computed as the ensemble average

$$C(\tau) \equiv \sum_n (W(n+\tau)W(n) - < W >^2) \tag{3}$$

The autocorrelation time can then be read off from the exponential decay of $C(\tau)$. Typical autocorrelation curves are shown in Figure 2, which shows the decorrelation of Wilson line correlators spatially separated by 1 or 3 lattice units and of Euclidean time extent 3, measured on an ensemble of 300 successive saved configurations. For $R = 1$, an exponential fit gives an autocorrelation time of 7.9 (in units of 10 Monte Carlo steps), while the area under the autocorrelation curve gives 8.4 for the same quantity. For $R = 3$, the autocorrelation time is of order unity (1.5, from an exponential fit). In general, autocorrelation times range from about unity for the largest loops to on the order of 20 for the smallest. We have therefore assumed that line correlators from successive bins of 20 (or more) saved configurations are effectively decorrelated for all relevant R and T.

We have calculated the standard light meson and baryon spectrum, the eta prime, and the heavy-light mesons. We will report on these results in a future paper. The ground state heavy light meson mass is relevant to the static energy analysis. As shown in Figure 3, a consistent mass value was obtained for all the various fitting time windows. The mass fit using $T = 1 - 5$ was $m_{HL} = 0.811 \pm .007$.

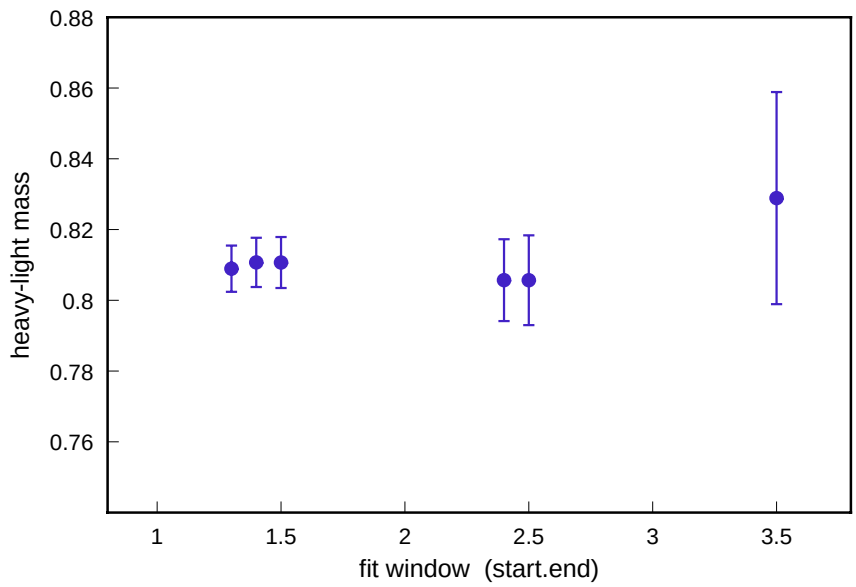

Figure 3: Various fits to ground state heavy-light meson mass. The start time and end time are represented as the decimal start.end

.

3 Static Energy Results

The static energy of a quark-antiquark pair is calculated using the Euclidean time evolution of a color-singlet pair in Coulomb gauge. The relevant correlator is

$$W(\vec{R},T) =< \bar{\Psi}(0,T)\Psi(\vec{R},T)\bar{\Psi}(\vec{R},0)\Psi(0,0) >_{\rm coul} \tag{4}$$

where Ψ is an infinitely massive quark field and the correlator is evaluated in Coulomb gauge. The static energy $V(\vec{R})$ is then defined as the energy of the lowest state coupled by $\bar{\Psi}(\vec{R},0)\Psi(0,0)$ to the vacuum, i.e.

$$W(\vec{R},T) \to C\exp\left(-TV(\vec{R})\right), \quad T\to\infty \tag{5}$$

or equivalently

$$V(\vec{R}) \equiv \lim_{T\to\infty} \ln \frac{W(\vec{R},T-1)}{W(\vec{R},T)} \tag{6}$$

On the lattice the correlator (4) is evaluated as an ensemble average of $\mathrm{Tr}(L(0,T)L^\dagger(\vec{R},T))$, where $L(\vec{R},T)$ is a Wilson line- i.e. a product of T adjacent link matrices in the temporal direction at spatial location $\vec{R}$. As mentioned previously, there is a distinct advantage to the use of Coulomb gauge Wilson line correlators over Wilson loop expectations in the study of stringbreaking effects. The Wilson loop necessarily involves additional contributions from intermediate states containing transverse gluons which are absent in the Coulomb gauge Wilson line correlators. In perturbation theory these states correspond to diagrams in which gluons are exchanged between the top and bottom horizontal (i.e. fixed time) portions of the Wilson loop. In quenched abelian theory, for example, the correlator (4) is a pure exponential $W(\vec{R},T) \propto e^{-V(R)T}$, whereas the corresponding Wilson loop expectation is proportional to $e^{-(V(R)T+V(T)R)}$ implying the presence of excited states. It is therefore reasonable to expect that stringbreaking in unquenched QCD will emerge more rapidly (i.e. at smaller Euclidean times T) if the Coulomb gauge correlator (4) is used.

Since the calculation is done on symmetrical 6^4 lattices, we actually obtain four sets of correlators for each gauge configuration, obtained by successively gaugefixing to Coulomb gauge with the time direction chosen as each of the four original Euclidean spacetime directions. Exploiting this degeneracy provides a valuable increase in the statistics, as we effectively have an ensemble of 4000 correlators from the original set of 1000 gauge configurations. The autocorrelation times described in the preceding section were obtained however by preaveraging the four correlator sets coming from each configuration.

In Figure 4 the static energy at $T = 2$ (circles) is compared with the similar results for two other theories. First, we show (down triangles) the $T = 2$ static energy for the quenched theory (with identical improved gauge action (2) but with the determinant contribution switched off), obtained from an ensemble of 8000 configurations, but otherwise analysed identically to the dynamical configurations (the untuned quenched theory). Both a shift in scale at short distances and the deviation at longer distances are clearly observed. Second, the static energy at $T = 2$ for the original Alford et. al. [10] unquenched action is plotted

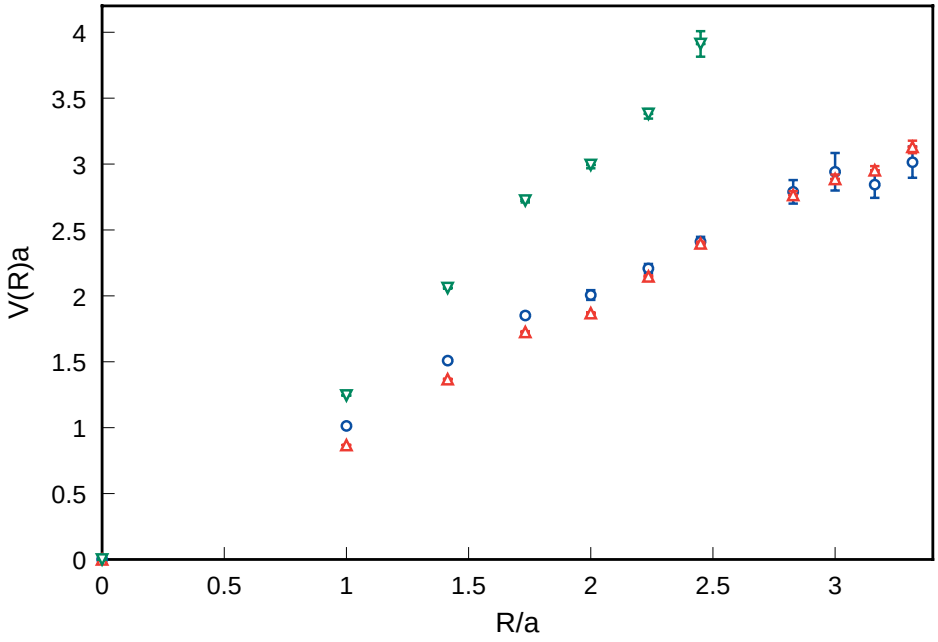

Figure 4: Static energy from Wilson line correlator (T=2) for unquenched QCD and quenched (untuned and tuned) QCD.

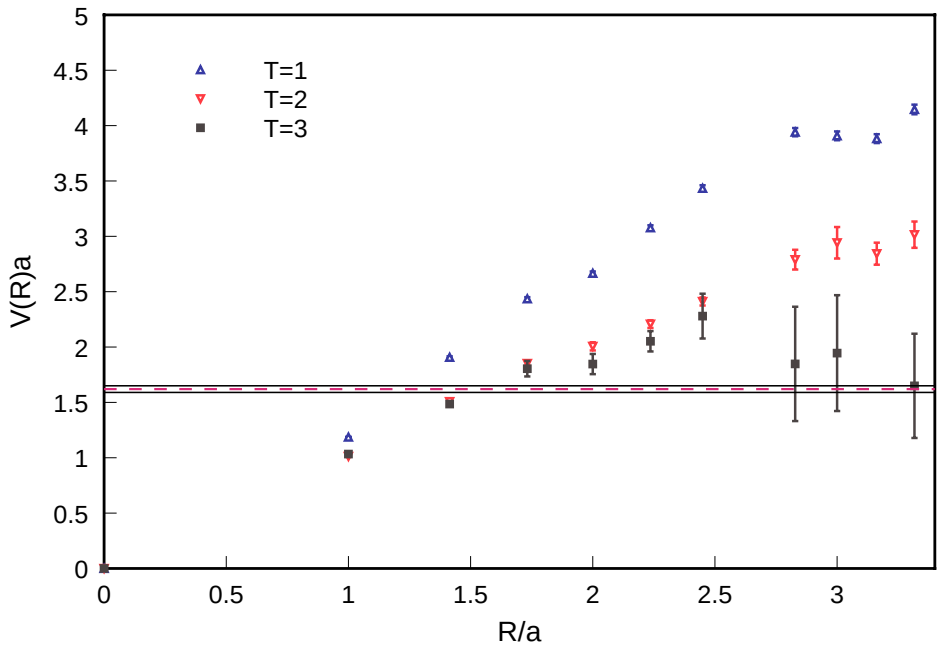

Figure 5: Static energy from unquenched QCD Wilson line correlators (T=1,2,3). The calculated heavy-light meson pair threshhold is also indicated.

(up triangles). This curve was used to tune our action to obtain an approximately equal initial slope.

In Figure 5 we show the static energy curves for T=1,2 and 3 in (6) respectively. For comparison the heavy-light meson pair production threshhold is also shown. As we are working on a large coarse lattice (lattice spacing a $\simeq$0.4 fm) 3 temporal lattice spacings already represents a fairly large Euclidean time $T \simeq$ 1.2 fm and the signal to noise ratio at larger spatial distances has clearly deteriorated substantially at T=3. The shortest time evolution, T=1 shown in Fig(3), on the other hand is still contaminated by higher energy states and the flattening of the string tension is certainly not visible. However, at T=3 the string tension appears to flatten out convincingly for distances $R \gtrsim$ 1 fm (=2.5a). (Further simulations are in progress to substantially reduce the statistical errors in this regime.) Moreover, the smoothness of the potential curve within the statistical errors suggests that

the improved action terms are doing a good job of restoring rotational invariance on this very coarse lattice.

The errors in the static potential are obtained most simply by computing a separate error on the line correlators $W(\vec{R}, T)$ and $W(\vec{R}, T-1)$ in (6), using the measured standard deviation and an autocorrelation time extracted separately for every loop size R, T. The errors for the log ratio in (6) can then be obtained by combining the numerator and denominator errors in quadrature. This approach however almost surely yields an overestimate of the true errors, as $W(\vec{R}, T)$ and $W(\vec{R}, T-1)$ tend to be *positively* correlated, reducing the variance in the ratio. Line correlators extracted from individual configurations on a small lattice tend to be extremely noisy (especially for the large loops of interest here) so to examine this correlation we have performed the error analysis by binning the 1000 configurations into 40 sets of 25 consecutive configurations. The average line correlators in each bin are then essentially decorrelated and a straightforward jackknife analysis can be performed on the ratios in (6). This is the approach used to obtain the errors displayed in Figure 5.

4 Conclusions

The analysis of dynamical two-flavor configurations on large coarse lattices obtained by the truncated determinant simulation method provides evidence for string breaking in zero temperature 4-dimensional QCD. One clear advantage of the method essential for its success in this case is the ability to generate a sufficient number of equilibrated and decorrelated dynamical configurations even for light quark mass on a physically large lattice, where standard HMC simulations would encounter computational problems. Evidently, as is the case for QED2 [2], the infrared quark modes included in the determinant in the TDA contain all the essential physics of string breaking.

Simulations on larger coarse lattices (8^4 lattices with the same action (2)) as well as at different kappa values for the two light quark flavors are in progress. In particular, we hope to study in detail the hairpin amplitudes relevant to the eta-prime mass. Here also, the essential physics should be obtainable from amplitudes measured in a TDA simulation [11].

5 Acknowledgements

The work of A. Duncan was supported in part by NSF grant PHY00-88946. The work of E. Eichten was performed at the Fermi National Accelerator Laboratory, which is operated by University Research Association, Inc., under contract DE-AC02-76CHO3000. The work of H. Thacker was supported in part by the Department of Energy under grant DE-FG02-97ER41027. The numerical work was performed on a 9 node Beowulf system at the University of Pittsburgh.

References

[1] For a review of recent work, see K. Schilling, hep-lat/9909152 (review talk at Lattice99, Pisa).

[2] A. Duncan, E. Eichten and H. Thacker, Phys. Rev. D59 (1998) 014505.

[3] H.D. Trottier, Phys.Rev. D60 (1999) 034506.

[4] E. Laermann, C. DeTar, O. Kaczmarek, F. Karsch, Nucl. Phys. Proc. Suppl. 73 (1999) 447.

[5] C. Bernard et al, "The Static Quark Potential in Three Flavor QCD", hep-lat/0002028.

[6] F.D.R. Bonnet, D.B. Leinweber, A.G. Williams and J.M. Zanotti, "Towards String breaking in the Static Quark Potential",hep-lat/9912044.

[7] F. Gliozzi and P. Provero, Nucl. Phys. B556 (1999) 76.

[8] C. DeTar, U. Heller and P. Lacock, hep-lat/9909078; P. Pennanen and C. Michael, hep-lat/0001015; and C. Bernard, et.al. (MILC Collaboration), "Zero Temperature String Breaking with Staggered Quarks", hep-lat/0010066.

[9] A. Duncan, E. Eichten, and H. Thacker, hep-lat/9908057 (talk of A. Duncan, Lattice99, Pisa).

[10] M. Alford, W. Dimm, G. P. Lepage, G. Hockney, and P.B. Mackenzie, Phys. Lett. B361 (1995) 87.

[11] A. Duncan, E. Eichten and H. Thacker, hep-lat/9909123 (talk of E. Eichten, Lattice99, Pisa).