QCD $\beta$ Function with Two Flavors of Dynamical Wilson Fermions

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Abstract
We test the asymptotic scaling behavior of state-of-the-art simulations of QCD with two flavors of light Wilson fermions. This is done by matching $\pi$ and $\rho$ masses on lattices of size $16^3 \times 32$ and $8^3 \times 16$. We find that at $\beta = 6/g^2 = 5.3$ matching is not possible over a range extending down to $\beta = 3.5$. The large lattice data at $\beta = 5.5$ matches the small lattice values at $\beta = 4.9(1)$ leading to a shift $\Delta \beta = 0.6(1)$, considerably larger than the perturbative prediction of 0.45. In both cases we conclude that the simulations are very far from the asymptotic scaling region.

1 Introduction
Assuming that a universal continuum limit of lattice QCD exists, measurements of some physical observable $\Omega$, such as a hadron mass, in a Monte Carlo computation will not depend on the details of the lattice discretization if the lattice spacing $a$ is small enough. The value of the observable, $\Omega = a^\delta f(g, \kappa)$, obtained by numerical calculation in lattice QCD with Wilson fermions, depends only on the parameters appearing in the lattice action: the gauge coupling $\beta = 6/g^2$ and the hopping parameter $\kappa$. The dimensionless quantity $f$ has been related to the dimensionful observable $\Omega$ by multiplying by the appropriate power of the lattice spacing $a$. As we approach the continuum limit $a \to 0$ the fact that $\Omega$ is independent of $a$ is expressed by the renormalization group equation

$$a \frac{d\Omega}{da} = a^{\delta} \left( \delta f - \beta \frac{\partial f}{\partial g} - \beta' \frac{\partial f}{\partial \kappa} \right) = 0$$

where

$$\beta = -a \frac{dg}{da}, \quad \beta' = -a \frac{d\kappa}{da}.$$

The derivatives with respect to $a$ are taken at "constant physics." As we have two independent relevant parameters we require two independent physical observables to use as
renormalization conditions to fix these parameters; \( \beta \) and \( \beta' \) should, of course, be independent of the choice of renormalization conditions.

In a perturbative expansion of \( \beta \) about \( g = 0 \) only the first two terms are independent of the details of the lattice regularization scheme. When the higher order terms are negligible one generally speaks of being in the asymptotic scaling regime. The aim of this work is to determine, for the realistic case of QCD with two flavors of light Wilson fermions, how close present simulations are to this asymptotic scaling regime.

In numerical simulations it is impractical to determine the \( \beta \)-function, which correspond to an infinitesimal change of scale, directly. Rather we work with a finite change of scale. We consider two lattices, \( \Lambda_1 \) with \( L_1 \) sites in each direction and with lattice spacing \( a_1 \), and \( \Lambda_2 \) with \( L_2 \) sites in each direction and lattice spacing \( a_2 \). By fiat we assert that \( \Lambda_1 \) and \( \Lambda_2 \) represent the same physical volume, thus \( L_1 a_1 = L_2 a_2 \).

If we select some set of physical observables \( \Omega_i \), we have

\[
\Omega_i = a_j^{\delta_i} f_i(g(a_j), \kappa(a_j)),
\]

where \( \delta_i \) is the dimension of \( \Omega_i \) and \( f_i \) is the corresponding dimensionless function measured on the lattice. In the continuum limit all these observables must become independent of the lattice, so for the two different lattices

\[
f_i(g(a_1), \kappa(a_1)) a_1^{\delta_i} = f_i(g(a_2), \kappa(a_2)) a_2^{\delta_i}.
\]

We define the quantities

\[
\Delta \beta \equiv \frac{6}{g^2(a_2)} - \frac{6}{g^2(a_1)}, \quad \Delta \kappa \equiv \kappa(a_2) - \kappa(a_1)
\]

to be the change in the couplings needed to compensate for this change in the cutoff.

\section{The \( \beta \)-function}

We expect the \( \beta \)-function to become independent of \( \kappa \) in the continuum and chiral limits\footnote{If we use continuum perturbation theory with dimensional regularization and the minimal subtraction renormalization scheme, then the BRS identities insure that all divergences are logarithmic, and thus must be independent of the quark mass. From this we may conclude that in the vicinity of the chirally symmetric continuum limit any \( \kappa \) dependence of the \( \beta \)-function must arise from irrelevant lattice operators and be suppressed by some power of the lattice spacing.}

The \( \beta \)-function at fixed \( \kappa \) is defined by \( \beta(g) = -a \, dg/da \), and the two universal terms from perturbation theory are \( \beta(g) = -b_0 g^3 - b_1 g^5 + O(g^7) \) where

\[
\begin{align*}
b_0 &= \frac{33 - 2n_f}{48\pi^2} \\
b_1 &= \frac{153 - 19n_f}{384\pi^4}
\end{align*}
\]

for QCD with \( n_f \) flavors of light fermions.
The solution of these equations, expressed in terms of $\beta = 6/g(a_2)^2$, is

$$\ln \left( \frac{a_2}{a_1} \right) = \frac{\sqrt{6}}{2} \int_{\beta-\Delta\beta}^\beta \frac{dx}{x^{3/2} \beta \left( \sqrt{6/x} \right)};$$

after evaluating the integral we find that

$$\Delta\beta_{\text{perturbative}} \approx -12 \left( b_0 + \frac{6b_1}{\beta} \right) \ln \left( \frac{a_2}{a_1} \right)$$

which is the perturbative prediction for the change in $\beta$ needed to effect a change in scale by a factor $a_2/a_1$.

$\Delta\beta$ has been thoroughly studied for pure gauge theory with the Wilson action (see [1] and references therein) and exhibits the well-known dip around $\beta = 6.0$. For QCD with dynamical fermions we are unaware of recent studies of $\Delta\beta$. For staggered fermions, Blum et al. [2], determined the $\beta$-function, needed for the computation of the equation of state for finite temperature QCD, from fits to hadron masses obtained at different couplings, and hence different lattice scales. They found significant deviations from asymptotic scaling that again would lead to a dip in $\Delta\beta$.

### 3 Results

The $\beta$-function for two flavors of Wilson fermions was computed earlier by some of us [3, 4]. The physical observables used for that purpose were $m_\pi$ and several Creutz ratios of Wilson loops.

The main conclusion then was that perturbative scaling was only expected to occur for $\beta > 6.0$. In those simulations the $\pi$-like object was heavy, and it was thought at the time that this may have hidden the effects of the dynamical fermions in the system. Simulations with smaller $m_\pi$ are thus needed to clarify the issue.

In this work we concentrated on data available on lattices of size $16^3 \times 32$ with two flavors of Wilson fermions with parameters and results shown in Table 1 [5, 6]. These were matched using $8^3 \times 16$ lattices with the parameters and results for the interesting parameter region shown in Table 2.

A preliminary report on this work was presented in [7].

The values of $\beta$ were chosen for hadron spectrum and other calculations largely based on the assumption that the presence of two fermion flavors renormalizes $\beta$ downwards by about 0.5 from its quenched value, and thus we may not be far from the perturbative scaling regime at these parameter values.

For our test of scaling we used two hadron masses, $m_\pi$ and $m_\rho$, as observables for matching with similar data generated on lattices of size $8^3 \times 16$ at values of $\beta$ ranging from 5.1 down to 3.5 and many $\kappa$ values.

The $8^3$ simulations used step sizes from 0.015 to 0.025 to insure a reasonable acceptance rate. The conjugate gradient residual used for the molecular dynamics steps was $10^{-6}$. Hadron measurements were made every 5 trajectories. We found integrated autocorrelation times were typically of this order.
Table 1: Parameters and masses on $16^3 \times 32$ lattice [5, 6]. # is the number of measurements made, each separated by $\Delta$ trajectories.

| $\beta$ | $\kappa$ | #   | $\Delta$ | $am_\pi$ | $am_\rho$ | $am_N$ | $m_\pi/m_\rho$ | $m_\pi/m_N$ |
|---------|----------|-----|-----|--------|--------|--------|-------------|-------------|
| 5.3     | 0.1670   | 484 | 5   | 0.4540(20) | 0.6350(20) | 0.9620(40) | 0.715(5)    | 0.4719(29)  |
| 5.3     | 0.1675   | 417 | 3   | 0.3120(40) | 0.5230(40) | 0.7660(90) | 0.596(15)   | 0.4073(71)  |
| 5.5     | 0.1596   | 400 | 5   | 0.3754(27) | 0.4947(78) | 0.7644(48) | 0.759(11)   | 0.4911(36)  |
| 5.5     | 0.1600   | 400 | 5   | 0.3262(17) | 0.4606(28) | 0.7106(91) | 0.708(4)    | 0.4591(57)  |
| 5.5     | 0.1604   | 669 | 3   | 0.2666(20) | 0.4208(55) | 0.6326(56) | 0.634(8)    | 0.4215(48)  |

Table 2: Parameters and masses for the matching region on $8^3 \times 16$ lattices. # is the number of measurements made.

| $\beta$ | $\kappa$ | #   | $am_\pi$ | $am_\rho$ | $am_N$ | $m_\pi/m_\rho$ | $m_\pi/m_N$ |
|---------|----------|-----|--------|--------|--------|-------------|-------------|
| 4.8     | 0.1890   | 130 | 0.6681(41) | 0.964(12) | 0.964(12) | 0.678(16)   | 0.4038(51)  |
| 4.8     | 0.1900   | 170 | 0.5814(35) | 0.897(7)  | 1.522(26) | 0.6480(54)  | 0.3820(64)  |
| 4.8     | 0.1905   | 109 | 0.5110(48) | 0.896(28) | 1.362(26) | 0.571(19)   | 0.3753(65)  |
| 4.9     | 0.1840   | 189 | 0.7826(28) | 1.013(5)  | 1.783(36) | 0.7722(36)  | 0.4390(88)  |
| 4.9     | 0.1845   | 190 | 0.7520(23) | 0.988(5)  | 1.714(20) | 0.7609(33)  | 0.4388(49)  |
| 4.9     | 0.1850   | 110 | 0.6808(46) | 0.928(5)  | 1.549(13) | 0.7334(44)  | 0.4396(40)  |
| 4.9     | 0.1855   | 272 | 0.6491(40) | 0.930(7)  | 1.660(57) | 0.6982(63)  | 0.391(13)   |
| 4.9     | 0.1860   | 200 | 0.5636(47) | 0.872(10) | 1.451(31) | 0.6467(88)  | 0.3886(88)  |
| 4.9     | 0.1865   | 150 | 0.5018(59) | 0.852(20) | 1.55(11)  | 0.590(13)   | 0.324(22)   |
| 4.9     | 0.1870   | 70  | 0.4981(65) | 0.816(20) | 1.395(23) | 0.611(15)   | 0.3572(81)  |
| 4.95    | 0.1815   | 80  | 0.8083(37) | 1.003(6)  | 1.693(19) | 0.8059(44)  | 0.4775(47)  |
| 5.0     | 0.1800   | 30  | 0.7734(85) | 0.990(14) | 1.690(36) | 0.781(11)   | 0.4578(95)  |
| 5.0     | 0.1810   | 150 | 0.6321(53) | 0.875(7)  | 1.462(19) | 0.7228(53)  | 0.4325(65)  |
| 5.0     | 0.1815   | 270 | 0.5145(83) | 0.814(9)  | 1.342(19) | 0.632(12)   | 0.3834(77)  |
Quark propagators with wall sources and point sinks were computed in Coulomb gauge on time slices 0 and $L_t/2$. We determined the meson masses by a correlated single state cosh fit to two correlation functions with interpolating fields $\bar{\psi}\Gamma_i\psi$ and $\bar{\psi}\gamma_0\Gamma_i\psi$; our baryon correlation functions used only one interpolating field. The covariance and errors were determined via the bootstrap method. Fits were made through the center of the lattice with a starting time slice determined by the criterion $\max N_{\text{dof}} Q \delta m/m$, where $N_{\text{dof}}$ is the number of degrees of freedom for a fit of mass $m$. In all cases $Q$, the 1 standard deviation confidence level, was greater than 10%.

### 3.1 Non-Matching at $\beta = 5.3$

Our first result is the unmatchability of the data at $\beta = 5.3$. We find that $\Delta \beta$ must be larger than 1.8. Figure 1 shows the two points obtained at $\beta = 5.3$ on the larger lattice (with $m_\pi$ appropriately scaled by a factor of 2) and the corresponding data for $m_\pi$ and $m_\pi/m_\rho$ on the smaller volume for $\beta = 3.5$. Data points obtained at larger $\beta$ values lie to the left of those from $\beta = 3.5$ (see figure 1).

![Figure 1: Non-matching of $m_\pi/m_\rho$ at $\beta = 5.3$.](image-url)
3.2 Matching at $\beta = 5.5$

Our second result is that at $\beta = 5.5$ matching is possible. Figure 2 shows the matching with $\beta = 4.9$ on the smaller lattice. It is interesting to note that all three points, at different values of $\kappa$, match with corresponding points at the same value of $\beta$. For comparison similar points obtained at $\beta = 4.8$ and 5.0 on the smaller lattice are shown. For $\beta = 4.8$ $m_\pi/m_\rho$ tends to be lower than the values at $\beta = 5.5$, whereas at $\beta = 5.0$ they are higher. Two conclusions follow from this data: the first is that the data at $\beta = 5.5$ is consistent with a value of $\Delta \beta = 0.6(1)$, and second that this matching is the same for all three different values of $\kappa$ used, indicating a $\kappa$ independence of the $\beta$-function.

At the central matching $\beta$ value ($\beta = 4.90$) we find $\Delta \kappa = -0.0249(1)$, $-0.0253(2)$, and $-0.0258(2)$ for large lattice values $\kappa = 0.1596$, 0.1600, and 0.1604 respectively, thus giving an estimate of the integrated $\beta'$-function.

On the other hand, figure 3 shows that the system is not in the scaling region because the pion-nucleon mass ratio does not match for the same values of $\beta$ and $\kappa$.

Another set of observables which we can match to determine $\Delta \beta$ are appropriate ratios of Wilson loops, just as was done for pure gauge theories [8]. We computed space-like planar Wilson loops on all our lattice configurations and evaluated ratios $R$ of two or four Wilson loops arranged such that the corner and perimeter singularities cancel between numerator

![Figure 2: Matching of $m_\pi/m_\rho$ at $\beta = 5.5$](image-url)
and denominator,

$$R(\beta, \kappa, \{r_1, r_2, r_3, r_4\}, L_s, L_t) = \frac{W(r_1, r_2)}{W(r_3, r_4)}, \quad r_1 + r_2 = r_3 + r_4;$$

$$R(\beta, \kappa, \{r_1, r_2, r_3, r_4, r_5, r_6, r_7, r_8\}, L_s, L_t) = \frac{W(r_1, r_2)W(r_3, r_4)W(r_5, r_6)W(r_7, r_8)}{\sum_{i=1}^{4} r_i = \sum_{i=5}^{8} r_i}.$$ 

We then determined $\Delta \beta$ from the condition

$$R(\beta - \Delta \beta, \kappa', \{r\}, 4L_s, 4L_t) = R(\beta, \kappa, \{2r\}, L_s, L_t).$$

$\kappa'$ on the smaller lattice was tuned such that the $\pi$ mass on the smaller lattice was twice that on the larger lattice. In practice we interpolated (or extrapolated) linearly from two simulations on the smaller lattice with slightly different values of $\beta'$. Unfortunately, with our statistics the errors on the larger Wilson loops grew quickly and they were not useful for the ratio matching. With smaller Wilson loops dominating the ratios lattice artefacts in the matching become important. We tried to avoid this by considering tree level and one-loop improved ratios [3]. For the matching of the $\kappa = 0.16$ data, for example, depending on various “cuts” imposed on the ratios considered, such as the minimum perimeter and area of the Wilson loops and the maximum relative error, we obtained average $\Delta \beta$ values between 0.36 and 0.55. This is somewhat smaller than the preferred value from the matching of $m_\pi/m_\rho$, 

Figure 3: Non-matching of $m_\pi/m_N$ at $\beta = 5.5$. 

We then determined $\Delta \beta$ from the condition

$$R(\beta - \Delta \beta, \kappa', \{r\}, 4L_s, 4L_t) = R(\beta, \kappa, \{2r\}, L_s, L_t).$$
indicating again that we are not yet in the regime of a unique, observable independent $\beta$-function.

The static quark potential provides us with another matching condition between the large and small lattices. We computed finite $t$ approximations to the static quark potential using time-like Wilson loops $W(\vec{r}, t)$ which were constructed using “APE”-smeared spatial links $\mathcal{R}_1, \mathcal{R}_2$. On- and off-axis spatial paths were used with distances $r = n, \sqrt{2}n, \sqrt{3}n,$ and $\sqrt{5}n$, with $n$ a positive integer. The “effective” potentials

$$V(\vec{r}, t) = \ln \frac{W(\vec{r}, t)}{W(\vec{r}, t + 1)}$$

were fitted using a correlated $\chi^2$ procedure with the spatial covariance estimated using the bootstrap method. The potential on the large lattice was fitted to the form

$$V(\vec{r}) = V_0 + \sigma r - e\frac{r}{r} - e'(G_L(\vec{r}) - \frac{1}{r})$$

the last term takes account of the lattice artifacts at short distance. Here, $G_L(\vec{r})$ denotes the lattice Coulomb potential for the Wilson gluonic propagator.

In figure 4, we plot the potential for the $16^3 \times 32$ lattice with $\beta = 5.5$ and $\kappa = 0.1600$ scaled to a spatial lattice of length 8. Also plotted are the potentials for the $8^3 \times 16$ lattices with $\beta = 4.80$ and $\kappa = 0.1890$, and $\beta = 5.0$ and $\kappa = 0.1810$: the latter point only has the on-axis values shown. These points have nearly matching pion-rho ratios.

We can see that the $8^3 \times 16$ potentials do not match the $16^3 \times 32$ lattice. While we do not expect the constant $V_0$ to match between the fine and coarse lattices, it is clear that the slopes of the coarse lattice potentials are too large. The slope decreases with increasing $\beta$, indicating that the shift $\Delta \beta$ required for matching the potential is smaller than that required for matching $m_\pi/m_\rho$ and closer to that of the Wilson loops ratios. We also see large violations of rotational symmetry in the coarse lattice potential compared to the finer lattice potential, indicating that the coarse lattice is at relatively strong coupling.

### 3.3 Parameter reduction at strong coupling

A third result is an approximate parameter reduction in the theory at strong coupling ($\beta = 3.5$ to $\beta = 4.7$). Figure 5 includes all our data in this range of $\beta$ on the smaller lattice and shows that for $3.5 \lesssim \beta \lesssim 4.9$ the data is essentially a function of only a single parameter. Any change in $\beta$ may be compensated for by a change in $\kappa$. This is consistent with the large $N$ strong coupling result of Kawamoto and Smit [10], which for $N = 3$ and $r = 1$ gives

$$m_\pi^2 = 4.8m, \quad m_\rho = 0.984 + 1.97m.$$

### 4 Conclusions

Combining the present results with those obtained earlier on smaller lattices [3] we find the $\beta$-function shown in figure [6]. It is similar to that found for pure $SU(3)$ lattice gauge.

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[1] We note that we never observed string breaking.
Figure 4: Non-matching of the $q\bar{q}$ potential. The line shows the “effective” potential fitted to the $16^3 \times 32$ lattice potential at $\beta = 5.5$, with the solid part of the line indicating the range of $r$ values used in the fitting procedure. The best fit gives $V_0 = 0.748(4)$, $\sigma = 0.0585(6)$, $e = 0.340(6)$, and $e' = 0.33(1)$ with $\chi^2 = 8.7$ for 14 degrees of freedom.

theory with the Wilson gauge action. We are led to the conclusion that current dynamical simulations are being done at strong coupling.

Indeed, not only do we find that for $\beta \lesssim 5.5$ the $\beta$-function does not agree with the perturbative predictions (asymptotic scaling), but that different renormalization conditions give different estimates for the $\beta$-function: the shift $\Delta \beta = 0.6(1)$ which gives satisfactory matching for $m_\pi$ and $m_\pi/m_\rho$ fails to match $m_\pi/m_N$, ratios of Wilson loops, or the $q\bar{q}$ potential. In other words we do not even observe a universal but non-perturbative $\beta$-function (scaling).

One therefore may need to reassess estimates for parameters and hence the cost of future computations with dynamical Wilson fermions accordingly.

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Figure 5: Cumulative data for $3.5 \leq \beta \leq 5.1$ on an $8^3 \times 16$ lattice. The line shows the large $N$ strong coupling result.

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Figure 6: The QCD $\beta$-function for $m_\pi/m_\rho \approx 0.6$. The previous data is from reference [1].

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