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Measuring the derivatives of couplings with respect to lattice spacing for dynamical Wilson fermions

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In finite temperature QCD, the calculation of thermodynamic quantities requires the derivatives of the couplings with respect to lattice spacings in different directions. A method of calculating these derivatives from measurements of long distance observables on a set of three lattices with symmetric and asymmetric couplings is presented. Our simulations at $\beta = 5.3$ and $\kappa = 0.158$ indicate that an asymmetric change in the gauge couplings does not produce an asymmetric lattice, within statistical errors, while changing κ asymmetrically does produce different lattice spacings. This indicates that the derivatives of the gauge couplings with respect to different lattice spacings are large and their perturbative values should not be used in the calculation of nonperturbative thermodynamic quantities.

1. INTRODUCTION

The derivatives of couplings with respect to lattice spacing (see ref [1,4,2,3,5]) are important quantities in lattice QCD since they appear in the definitions of the energy, pressure, and entropy and also in the renormalization group equation. Presently, most lattice simulations of QCD are done at large coupling, far from the continuum limit (especially dynamical fermion simulations), so the nonperturbative values of these derivatives are required to accurately calculate thermodynamic quantities. Presently, perturbative values (or none at all) have been used. In fact, not even perturbative estimates of the hopping parameter derivatives for Wilson quarks have been available previously.

We have performed simulations employing symmetric and asymmetric lattices to determine the nonperturbative derivatives of the couplings with respect to lattice spacing for two flavors of Wilson quarks. The use of asymmetric lattices is only an intermmediate step which allows the calculation of derivatives in different directions in Euclidean space. The final results are for symmetric lattices.

2. Theory

The QCD action on the lattice is

$$S = \sum_{x,\mu>\nu} \beta_{\mu\nu} P_{\mu\nu} + \frac{n_f}{2} \mathrm{Tr} \log M^\dagger M, \qquad (1)$$

with the fermion matrix

$$M = 1 - \sum_\mu \kappa_\mu \not{D}_\mu, \qquad (2)$$

and where $P_{\mu\nu}$ is the real part of the trace of the product of link matrices around the elementary plaquette in the $\mu\nu$ plane normalized to one. We introduce a gauge coupling, $\beta_{\mu\nu}$, for each of the six planes in Euclidean space and a hopping parameter, κ_μ, for each direction. Euclidean invariance gives four independent derivatives of these couplings with respect to lattice spacing which are defined as:

$$\begin{aligned} B_\tau &= a_\nu \frac{\partial \kappa_\mu}{\partial a_\nu} \ (\mu = \nu), \\ B_\sigma &= a_\nu \frac{\partial \kappa_\mu}{\partial a_\nu} \ (\mu \neq \nu), \\ C_\tau &= -6 a_\lambda \frac{\partial g_{\mu\nu}^{-2}}{\partial \alpha_\lambda} \ (\lambda = \mu, \nu), \\ C_\sigma &= -6 a_\lambda \frac{\partial g_{\mu\nu}^{-2}}{\partial \alpha_\lambda} \ (\lambda \neq \mu, \nu). \end{aligned} \qquad (3)$$

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The energy and pressure are obtained by differentiating the partition function. Since we are interested in infinitesimally varying one lattice spacing while holding three fixed and varying three together while holding one fixed, only two different gauge couplings and two different hopping parameters are required. These are denoted β_{st}, β_{ss}, κ_t and κ_s where s is any of the spatial directions and t is the time direction. In this study the π and ρ masses in the t and z directions were chosen as the four independent observables to determine the asymmetry coefficients B_τ, B_σ, C_τ and C_σ. A matrix equation is written to express the total change in the observables when the couplings are changed by a small amount:

$$d\,ln(ma) = M\,dc. \tag{4}$$

Explicitly,

$$\begin{bmatrix} d\,ln(m_\pi a_t) \\ d\,ln(m_\pi a_z) \\ d\,ln(m_\rho a_t) \\ d\,ln(m_\rho a_z) \end{bmatrix} =$$

$$\begin{bmatrix} 3A_\pi & 3B_\pi & C_\pi & 3D_\pi \\ A_\pi + 2B_\pi & 2A_\pi + B_\pi & D_\pi & C_\pi + 2D_\pi \\ 3A_\rho & 3B_\rho & C_\rho & 3D_\rho \\ A_\rho + 2B_\rho & 2A_\rho + B_\rho & D_\rho & C_\rho + 2D_\rho \end{bmatrix} \times$$

$$\begin{bmatrix} d\,\beta_{st} \\ d\,\beta_{ss} \\ d\,\kappa_t \\ d\,\kappa_z \end{bmatrix}, \tag{5}$$

where the elements of M are found using Euclidean invariance and the definitions

$$\begin{aligned} A_\pi &= \frac{\partial ln(m_\pi a_\lambda)}{\partial \beta_{\mu\nu}}\ (\lambda = \mu, \nu), \\ B_\pi &= \frac{\partial ln(m_\pi a_\lambda)}{\partial \beta_{\mu\nu}}\ (\lambda \neq \mu, \nu), \\ C_\pi &= \frac{\partial ln(m_\pi a_\mu)}{\partial \kappa_\nu}\ (\mu = \nu), \\ D_\pi &= \frac{\partial ln(m_\pi a_\mu)}{\partial \kappa_\nu}\ (\mu \neq \nu). \end{aligned} \tag{6}$$

The derivatives of $ln(m_\rho a)$ are defined similarly. Inverting Eq (4), the changes in the couplings are obtained:

$$dc = M^{-1} d\,ln(ma). \tag{7}$$

Now, the desired coefficients as well as the β function can be obtained by choosing $d\,ln(ma)$ properly. For example, C_τ is obtained by setting $d\,ln(ma) = (\delta, 0, \delta, 0)$ where δ is arbitrarily small. Likewise, the β function is found by setting $d\,ln(ma) = (\delta, \delta, \delta, \delta)$. A small bit of algebra reveals that this procedure keeps m_π/m_ρ constant (and therefore the quark mass) while changing only the desired lattice spacing(s).

3. SIMULATIONS

The elements of M can be measured directly from three simulations with slightly different couplings. The simulations include one with symmetric couplings ($\beta = 5.3, \kappa = 0.158$), one with $\beta_{zx} = \beta_{zy} = 5.3265$ and all others equal to those in the symmetric case, and one with $\kappa_t = 0.15642$ and all others equal to those in the symmetric case. For the asymmetric β simulation, we used the fact that

$$\frac{\partial ln(m_{\pi,\rho} a_\mu)}{\partial \beta_{zx}} = \frac{\partial ln(m_{\pi,\rho} a_\mu)}{\partial \beta_{zy}}$$

to get a larger change in mass while keeping the change in coupling small. Each simulation used the hybrid Monte Carlo algorithm on lattices of size 20 slices in the t and z directions and 8 slices in the x and y directions. Each simulation contained over 1300 molecular dynamics trajectories after discarding thermalization runs, and propagators were measured every other trajectory. The integrated autocorrelation time for the long distance elements of the propagator was roughly 24 trajectories. The acceptance rate was roughly 85% for the symmetric and asymmetric β simulations and 55% for the asymmetric κ simulation.

4. RESULTS

4.1. Masses

The measured π and ρ masses from each simulation are given in Table 1. The errors shown are from fits using the full covariance matrix where the propagators were blocked over 24 trajectories. The suprising result is that the masses measured in the t and z directions for the asymmetric β lattice are the same, within errors, even though

Table 1
Masses. The t direction propagators for the symmentric lattice were fit from time slices $6-8$ and $7-9$ for the π and ρ, respectively. All other fits were over the range 7-10.

particle	dir	mass	χ^2/dof	cl
		symmetric		
π	t	1.2643(15)	1.5/1	0.22
π	z	1.2649(16)	0.35/2	0.84
ρ	t	1.3342(16)	3.0/1	0.08
ρ	z	1.3344(21)	0.82/2	0.66
		asymmetric β		
π	t	1.2376(21)	1.6/2	0.44
π	z	1.2394(18)	3.5/2	0.17
ρ	t	1.3081(24)	2.2/2	0.34
ρ	z	1.3087(19)	1.4/2	0.51
		asymmetric κ		
π	t	1.2857(17)	0.79/2	0.79
π	z	1.2772(19)	0.79/2	0.67
ρ	t	1.3544(17)	3.3/2	0.20
ρ	z	1.3449(22)	0.02/2	0.99

they differ from the symmetric values by many standard deviations. Changing only β_{zx} and β_{zy} did not produce an asymmetry in the masses, and therefore in the lattice spacings, but did produce an overall change in the scale. It will be shown below that this means M has a zero eigenvalue. Contrary to the asymmetric β case, changing κ in the time direction while holding the spatial κ's fixed did produce an asymmetry in the masses of several standard deviations. The masses also differ from the symmetric values.

4.2. Derivatives

For either asymmetric lattice, if $m_\pi a_t = m_\pi a_z$ and $m_\rho a_t = m_\rho a_z$, then M has a zero eigenvalue with eigenvector $(-\sqrt{2}/2, \sqrt{2}/2, 0, 0)$ which can be seen easily by setting $A_\pi = B_\pi$ and $A_\rho = B_\rho$ in Eq (5) and operating with M on the above eigenvector. We expect then that our M will have an eigenvalue close to zero since there was no asymmetry, within errors, on the asymmetric β lattice. This is indeed the case. The elements of M were calculated as outlined above. Errors were computed using a jackknife procedure where one tenth of the data were omitted and the rest were used to compute M. The result is

$$-\begin{bmatrix} 1.16(15) & 1.18(15) & 10.0(2.1) & 17.9(5.5) \\ 1.17(13) & 1.17(13) & 6.0(1.9) & 22.0(4.9) \\ 1.09(16) & 1.04(13) & 9.2(2.0) & 14.2(5.1) \\ 1.06(12) & 1.07(13) & 4.7(1.7) & 18.7(4.6) \end{bmatrix}.$$

It has eigenvalues (-26.29, 0.024, 0.21, -4.17) with the eigenvector corresponding to 0.024 equal to (-0.67, 0.75, -0.01, -0.001). Obviously, a small change in the smallest eigenvalue will produce a large change in M^{-1}. If we continue with the jackknife procedure to compute M^{-1}, we find a large spread in the elements, since some of the estimates of M^{-1} in our ensemble have eigenvalues two or three orders of magnitude closer to zero than the average given above. The error is also sensitive to the number of blocks used in the jackknife estimate.

4.3. Asymmetry coefficients

Because changing the gauge couplings asymmetrically did not produce different masses (within errors) in the t and z directions, the coefficients C_τ and C_σ cannot be determined from our simulations. However, this result implies they must be large, since a large change in the couplings is required to produce different lattice spacings. On the other hand, changing κ asymmetrically did produce different masses, so there is some hope of extracting B_τ and B_σ from the data. We cannot simply invert M as described above since the near zero eigenvalue allows an arbitrary component in dc along the zero eigenvector which dominates the change in the couplings. However, setting $d\beta_{st} = d\beta_{ss} = 0$ in Eq (5) gives two sets of two equations for $d\kappa_t$ and $d\kappa_s$. If the two sets are solved independently, each with a right hand side equal to (δ,0) to fix the quark mass, two estimates for B_τ and B_σ are obtained. Of course, the values should be the same. A jackknife estimate using ten blocks gives $B_\tau = -0.197(98), -0.182(78)$ and $B_\sigma = 0.054(33), 0.046(27)$ which are the same within errors. A jackknife estimate of the averages gives -0.19(9) for B_τ and 0.05(3) for B_σ. These estimates remained essentially unchanged when the number of blocks was increased to

twelve. Plugging this solution into Eq (5) and using the value of M above gives $dln(ma) = (1.02, 0.03, 0.98, -0.02)$. If the zero eigenvector with the normalization given above is added to the solution, the right hand side becomes (1.00, 0.04, 0.98, -0.02).

4.4. Beta function

The β function is calculated by requiring a symmetric change in the gauge couplings. We proceed by summing the first two and last two equations in Eq (5). This results in a two by two matrix equation. Inverting, the symmetric change in β and κ is obtained. The almost zero eigenvector of M is eliminated by adding the first two equations. However, M has a second small eigenvalue which is not eliminated by adding the equations since its eigenvector is symmetric in $d\beta_{st}$, $d\beta_{ss}$ and $d\kappa_t$, $d\kappa_s$. Our jackknife procedure is again too sensitive to this small eigenvalue to produce a reasonable result. However, since at this value of β and κ $m_\pi/m_\rho = constant$, within errors, when only β is changed (see Table 2), $d\beta_{\mu\nu}/dln(a)$ can be estimated by solving the first line in Eq (5) independently. Taking $A_\pi = B_\pi = A_\rho = B_\rho$, four estimates of the β function are obtained: -0.43(6), -0.42(6), -0.46(7), and -0.48(6). This result is about 3/5 the perturbative result of -0.73 [3].

Table 2
Mass ratios. The errors are from a jackknife estimate using ten blocks.

	sym	asym β	asym κ
$m_\pi a_t/m_\rho a_t$	0.9468(6)	0.9459(10)	0.9494(6)
$m_\pi a_z/m_\rho a_z$	0.9475(5)	0.9466(10)	0.9495(8)

5. CONCLUSION

A method was outlined to calculate the derivatives of the gauge couplings and the hopping parameters with respect to lattice spacing, in particular when the lattice spacings were changed symmetrically and when only the time direction lattice spacing was changed. The method was implemented for the case of two flavors of Wilson quarks at $\beta = 5.3$ and $\kappa = 0.158$. The presence of a near zero eigenvalue in M, the matrix of derivatives, prevented the calculation of the asymmetry coefficients C_τ and C_σ. The zero eigenvalue arose because changing the gauge couplings asymmetrically did not produce asymmetric lattice spacings, contrary to expectations. This may be caused by too small a change in the gauge couplings to resolve the difference in masses outside statistical errors. However, an overall symmetric change in the masses of several standard deviations was obtained with this change. In any case, our simulations indicate that these two asymmetry coefficients are large. Thus, nonperturbative thermodynamic quantities should not be calculated using their perturbative values.

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