

Probing the chiral limit of M_π and f_π in 2+1 flavor QCD with domain wall fermions from QCDOC

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We present results for the pseudoscalar meson masses and decay constants on 2+1 flavor DWF configurations with different sea quark masses and an inverse lattice spacing of 1.6(1) GeV, with a focus on chiral fits at small quark masses. The calculation is done on $16^3 \times 32 \times 8$ lattices generated with the DBW2 gauge action.

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1. Introduction

Lattice calculations allow us to study hadronic properties from first principles. One of the great challenges of lattice QCD, however, is that the physical light quark masses, in particular the physical up and down sea quark masses, are numerically inaccessible with present hardware. We thus rely on (partially quenched) chiral extrapolations to get to the physical light quark regime from simulations with unphysically heavy quarks. We can also determine the low energy constants (LECs) [1], *aka* Gasser-Leutwyler coefficients, which appear in the chiral Lagrangian, from these partially quenched simulations provided the systematic errors are treated properly and the correct number of fermion flavors are used [2].

Domain wall fermions (DWF) have the advantages of nearly exact chiral symmetries with a moderate extent in the fifth dimension and a continuum-like chiral perturbation theory. The residual chiral symmetry breaking of DWF, quantified as m_{res} [3], comes in as an additive constant to the quark masses at the lowest order approximation. The employment of the rational hybrid Monte Carlo (RHMC) technique [4], free of finite step-size errors, also gives us better control over systematic errors. It thus makes possible a direct comparison of our numerical results with the predictions of chiral perturbation theory. This proceeding focuses on a set of $N_f = 2 + 1$ DWF simulations on $16^3 \times 32 \times 8$ lattices with a lattice spacing of 1.6(1) GeV. After detailing the simulation parameters, I present results for the masses and decay constants of the pseudoscalar mesons. Preliminary chiral fits up to next-to-leading order (NLO) on these quantities are then given. A rough investigation of the effect of nondegeneracy is also described.

2. Simulation details

The gauge action used in our simulation can be written in the general form [5]:

$$S_G[U] = -\frac{\beta}{3} \left((1 - 8c_1) \sum_{x,\mu,\nu} P[U]_{x,\mu\nu} + c_1 \sum_{x,\mu \neq \nu} R[U]_{x,\mu\nu} \right) \quad (2.1)$$

We generated three sets of $16^3 \times 32 \times 8$ gauge configurations with the DBW2 action, in which $c_1 = -1.4069$, at $\beta = 0.72$. Two light sea quarks with equal mass m_l and one strange quark with mass m_s were included in the fermion determinant. The RHMC algorithm was used to update the gauge fields. All the data was generated on QCDOC machines at Columbia, the RBRC and Edinburgh.

Valence measurements with two degenerate quarks of up to 8 different masses m_V were performed on these lattices. Nondegenerate valence measurements with light quark masses of 0.005, 0.01, 0.015, 0.02 and a heavy quark mass of 0.04 were also done for $m_l = 0.01$ and 0.02. We skipped the first 1000 trajectories for thermalization and measured *point-point* meson correlators thereafter. Table 1 shows the relevant parameters for evolution and measurements. The integrated autocorrelation time was determined to be on the order of 50 to 100 trajectories. Thus we binned the data into blocks of 100 trajectories prior to statistical analysis to account for the autocorrelations in a robust fashion. All the quantities are in lattice units unless noted.

The residual chiral symmetry breaking turns out to be quite large at this coupling. When extrapolated to the dynamical chiral limit ($m_l = 0$),

$$m_{\text{res}} = 0.0106(1) \quad (2.2)$$

Table 1: Simulation parameters. $\delta\tau$ is the step size in molecular dynamics integration and τ is the total length in one trajectory. Data for the $m_l = 0.01$ and 0.02 ensembles used in this proceeding reflects twice as much statistics as that in the talk given at the conference.

(m_l, m_s)	L_s	M_5	$\delta\tau$	τ	$\frac{N_{acc}}{N_{tot}}$	# traj.	m_V	# meas.(deg;nondeg)
(0.01,0.04)	8	1.8	0.02	0.5	66%	6000	0.005 \rightarrow 0.04	500; 250
(0.02,0.04)	8	1.8	0.0185	0.5	70%	6000	0.005 \rightarrow 0.04	1000; 500
(0.04,0.04)	8	1.8	0.02	0.5	65%	3395	0.02, 0.03, 0.04	479; –

which is comparable to the input light sea quark mass. Noting that the coupling is fairly large and L_s is rather small, it is not surprising to have a large m_{res} . For hadronic observables like meson masses and decay constants, we treat m_{res} as a shift to the input quark masses and neglect other possible higher-order effects.

3. Preliminary Results

The pseudoscalar masses and decay constants can be extracted from both the pseudoscalar and axialvector correlators [3]. Here emphasis will be given to the results from the pseudoscalar channel, since they give smaller statistical errors than the axialvector correlators.

M_π and the chiral fits. The next-to-leading order (NLO) quark mass dependence of the pseudoscalar masses in PQ χ PT with N flavors of sea quark has been computed generally [2]. With 2+1 flavors of sea quark and two degenerate valence quarks, the formula simplifies to

$$\begin{aligned}
M_\pi^2 = \chi_V \left\{ 1 + \frac{16N}{f^2} (2L_6 - L_4) \bar{\chi} + \frac{16}{f^2} (2L_8 - L_5) \chi_V \right. \\
+ \frac{1}{8f^2 \pi^2 N} \left[\frac{2\chi_V - \chi_l - \chi_s}{\chi_V - \chi_\eta} \chi_V \log \chi_V - \frac{(\chi_V - \chi_l)(\chi_V - \chi_s)}{(\chi_V - \chi_\eta)^2} \chi_V \log \chi_V \right. \\
\left. \left. + \frac{(\chi_V - \chi_l)(\chi_V - \chi_s)}{\chi_V - \chi_\eta} (1 + \log \chi_V) + \frac{(\chi_\eta - \chi_l)(\chi_\eta - \chi_s)}{(\chi_V - \chi_\eta)^2} \chi_\eta \log \chi_\eta \right] \right\} \quad (3.1)
\end{aligned}$$

where $\chi_x = 2Bm_x$, $x = V, l, s$, or η , $\chi_\eta = \frac{1}{3}(\chi_l + 2\chi_s)$ and $\bar{\chi} = \frac{1}{3}(2\chi_l + \chi_s)$. Here we have explicitly taken the chiral scale to be 1 GeV. For DWF, the masses should all be shifted by m_{res} . Thus to leading order in the valence quark masses, $M_\pi^2 = 2B(m_V + m_{res})$.

As a consistency check, we fit our results for M_π^2 to the linear form

$$M_\pi^2 = 2B(m_V + m_{res}) + C \quad (3.2)$$

where m_{res} is the residual mass at the valence chiral limit ($m_V \rightarrow 0$), *i.e.*, 0.0111(1), 0.0113(1) and 0.0122(1) for $m_l = 0.01$, 0.02 and 0.04 respectively. We would expect C to vanish if the lowest-order approximation is good enough. Independent linear fits for the pion masses with different sea quarks are shown in the left panel of Figure 1. The two heaviest masses were excluded from the fit except for $m_l = 0.04$ where all the available data were used. In all the cases, M_π^2 is quite close to zero when $m_V = -m_{res}$. The larger deviation from 0 for $m_l = 0.02$ may be due to higher order corrections from χ PT or $\mathcal{O}(a^2)$ violations of chiral symmetry, which need to be further investigated.

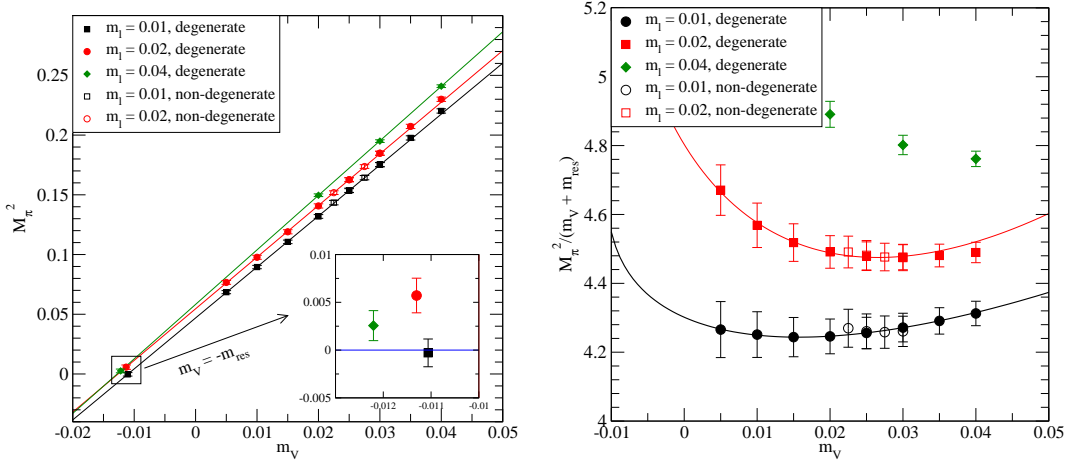


Figure 1: LEFT: M_π^2 vs. m_V in the pseudoscalar channel; RIGHT: $M_\pi^2/(m_V + m_{\text{res}})$ vs. m_V . The lines are fits to the mass range [0.005,0.03]. Filled symbols and open symbols represent data from measurements with degenerate and nondegenerate quarks, respectively. m_V is the average of two valence quark masses.

We also show $M_\pi^2/(m_V + m_{\text{res}})$ as a function of m_V in the right panel of Figure 1. Nonlinearities are evident in all the datasets. The solid lines are the partially quenched NLO fit to Eq. 3.1 with sea quark mass fixed. We chose the fitting range to be [0.005,0.03]. In the fit, the value of f_π at $m_l = m_V = -m_{\text{res}}$ from the dynamical linear extrapolation was used as the input for f , while in principle the limit of $m_s \rightarrow -m_{\text{res}}$ should also be taken to obtain the value for f . As can be seen, for $m_l = 0.01$ the curve does go through all the data. For $m_l = 0.02$ the NLO fit represents the data well, for all but the heaviest valence masses, where differences of about one standard deviation are seen. As will be shown later, the NLO fit to f_π also has the same problem.

f_π and the chiral fits. We use the definition of f_π in which its physical value is about 130 MeV. When two degenerate valence quarks are used, the NLO mass dependence of f_π can be simplified to [2, 6]

$$f_\pi = f \left\{ 1 + \frac{8}{f^2} (NL_4 \bar{\chi} + L_5 \chi_V) - \frac{1}{16\pi^2 f^2} \left[(\chi_V + \chi_l) \log \frac{\chi_V + \chi_l}{2} + \frac{\chi_V + \chi_s}{2} \log \frac{\chi_V + \chi_s}{2} \right] \right\} \quad (3.3)$$

We show the results for f_π from the pseudoscalar correlators in Figure 2. The data points have obvious curvatures, especially for $m_l = 0.02$. The straight lines fit the data poorly. We also fit the $m_l = 0.01$ and $m_l = 0.02$ data independently to Eq. 3.3 using the values of B from the NLO fit of M_π^2 as an input. Two fitting ranges were used: [0.005,0.025] and [0.005,0.03]. For $m_l = 0.01$, the fitting results do not depend on the fitting range we choose. Even a fit to the first five points reproduces the data at heavier quark masses quite well. However, this is not the case for $m_l = 0.02$, where the fit curve misses the data points at heavier masses. It is especially obvious for the fit to the range [0.005,0.025]. Similar behaviors were observed in $N_f = 2$ DWF simulations [7], where, instead of fitting data with different sea quarks independently, simultaneous fits to f_π from different sea quarks were performed.

Remarks. We cannot conclude here that we have found a signal of chiral logs. The nonlinearities we see for both M_π^2 and f_π may also be attributed to finite-volume corrections, zero-mode

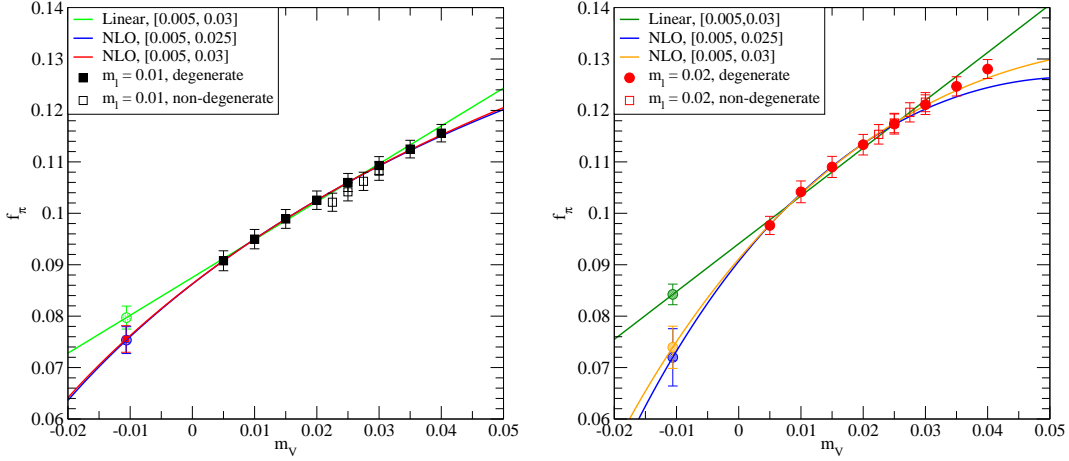


Figure 2: f_π with linear and NLO fits to mass range [0.005,0.025] and [0.005,0.03] for $m_l = 0.01$ (left) and $m_l = 0.02$ (right) datasets. Filled symbols and open symbols represent data from measurements with degenerate and nondegenerate quarks, respectively. m_V is the average of two valence quark masses.

effects or uncertainties in the residual mass. For the large quark masses we used, NNLO contributions may already be important, especially for f_π . More thorough investigations of these systematic effects are needed to justify our NLO fits.

4. Effect of nondegeneracy

We also explored the possible effects of nondegenerate quarks in the pseudoscalar masses and decay constants. Suppose we have two sets of valence measurements on the same lattices. One uses two degenerate quarks ($m_A = m_B = m_V$) and the other uses two nondegenerate quarks ($m_A \neq m_B$, $m_V = \frac{m_A + m_B}{2}$). Leading order χ PT predicts, for the pseudoscalar masses, $M_\pi^2 = B(m_A + m_B)$. If we take the nondegenerate dynamical points ($m_A = m_l$, $m_B = m_s$) and the matching degenerate points ($m_V + m_{\text{res}} = \frac{m_s + m_{\text{res}}}{2}$) to extrapolate to the light sea quark limit ($m_l \rightarrow -m_{\text{res}}$), we would expect the results to be the same assuming the higher order corrections are small. This gives us rough estimates of the kaon mass from both the degenerate and nondegenerate valence quarks. The same comparison can also be done for the pseudoscalar decay constants. We show the comparisons in Figure 3. The two extrapolations gave quite consistent results within errors.

5. Summary and Outlook

Our present data are still statistically limited. Further improvements are needed to reduce the statistical uncertainties in the determinations of M_π and f_π . In the meanwhile, better estimates of the systematic effects coming from finite volume, finite lattice spacing and residual chiral symmetry breaking are necessary to justify our chiral fits and determine LECs. For the work reported here, the smallest $M_\pi L$ is 4.2, which should make the finite volume corrections few percent effects. The ongoing $24^3 \times 64 \times 16$ simulations with 2+1 dynamical flavors of DWF on QCDOC will provide us better opportunities to probe the chiral limit of various physical quantities.

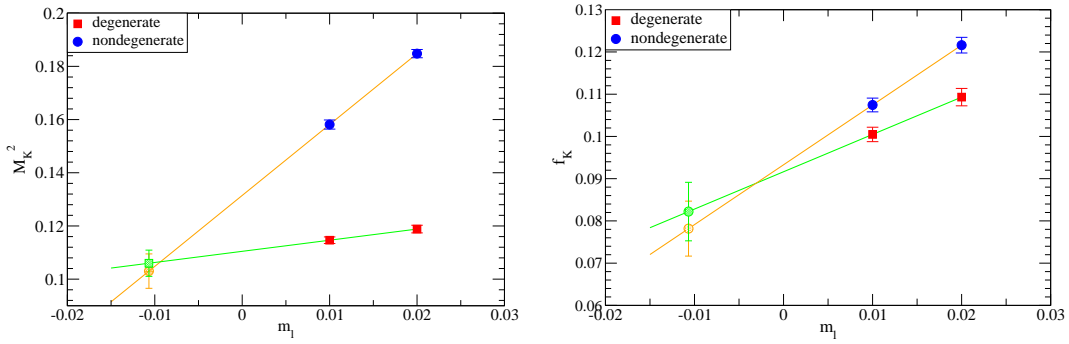


Figure 3: Estimate the effects of nondegeneracy.

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