Partially quenched chiral perturbation theory
and numerical simulations

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Abstract

The dependence of the pseudoscalar meson mass and decay constant is compared
to one-loop Partially Quenched Chiral Perturbation Theory (PQChPT) in a numerical
simulation with two light dynamical quarks. The characteristic behaviour with
chiral logarithms is observed. The values of the fitted PQChPT-parameters are in
a range close to the expectation in continuum in spite of the fact that the lattice
spacing is still large, namely $a \simeq 0.28 \text{fm}$.

1 Introduction

In numerical Monte Carlo simulations of QCD Chiral Perturbation Theory (ChPT)
\cite{1} is often used to guide the extrapolation to the physical values of the three light
quark masses ($m_u \simeq m_d$ and $m_s$). In this procedure not only the lattice gauge theory
results are established but also useful information is obtained about the values of
the Gasser-Leutwyler parameters of ChPT. In fact, recently several groups explored this possibility in quenched \[2\] and unquenched simulations with Wilson-type \[3\] and staggered \[4, 5\] quarks. (For a review see \[6\].)

In order to achieve small systematic errors the simulations themselves have to be performed in a range of quark masses where the applied one-loop (NLO) ChPT-formulas give a good approximation. In particular, the characteristic chiral logarithms have to appear in the quark mass dependence of different physical quantities. This applies both to original ChPT as well as to PQChPT \[7, 8\]. However, in most recent simulations – especially with Wilson-type quarks – this condition is not fulfilled because they are performed in the range \(m_{u,d} \geq \frac{1}{2} m_s\). Estimates based on present knowledge of the ChPT parameters indicate (see, for instance, \[9\]) that at least \(m_{u,d} \leq \frac{1}{4} m_s - \frac{1}{5} m_s\) has to be reached. (See also the summary of the panel discussion at the Boston Lattice Conference \[10\].) Another requirement is that the virtual effects of the \(s\)-quark also has to be taken into account by simulating with three light dynamical quarks.

Since the dynamical quarks in most unquenched simulations do not satisfy the above bound, it is not surprising that the chiral logarithms have not been observed \[11, 12, 13, 14, 15, 16\]. This was the main motivation of our collaboration to start exploring the possibility of simulating QCD with light quarks in the range \(m_{ud} \leq \frac{1}{2} m_s\) \[17, 18, 19, 20, 21\]. In these simulations we use the two-step multiboson (TSMB) algorithm for dynamical fermions \[22\] and consider for the moment \(N_s = 2\) dynamical “sea” quarks. The case of \(N_s = 3\) is also under study \[23\]. Our first simulations were oriented towards the investigation of simulation costs as a function of the quark mass and were performed on modest size lattices (typically \(8^3 \cdot 16\) with lattice spacings of the order \(a \simeq 0.27\) fm – a value where continuum behaviour is not necessarily expected. Therefore, it came to us as a surprise that plotting the pseudoscalar (“pion”) mass and decay constant as a function of the quark mass (in the form suggested by \[24, 25\]) the chiral logarithmic behaviour has been qualitatively displayed \[19, 20\].

Encouraged by this result we picked out a point with \(m_{ud} \simeq \frac{1}{4} m_s\) and performed a high statistics run on \(16^4\) lattice in order to study the dependence on the valence quark mass in a sufficiently large physical volume. This has the advantage that by taking ratios of the masses and decay constants the \(Z\)-factors of renormalization cancel. This removes an uncertainty in \[19, 20\] where the \(Z\)-factors have been neglected by setting them to \(Z \equiv 1\). In our analysis of simulation data we applied PQChPT for Wilson lattice fermions \[26\] which take into account leading lattice artefacts of \(O(a)\).

The plan of this paper is as follows: in the next section the one-loop PQChPT
formulas for Wilson lattice fermions will be recapitulated. In section 3 the numerical simulation data will be analyzed and discussed.

2 PQChPT formulas

Our analysis of the valence quark dependence of the pseudoscalar mass \( m_\pi \) and decay constant \( f_\pi \) is based on the one-loop PQChPT formulas for the Wilson lattice action as derived in [26]. Instead of the quantities with dimension mass-square \( \chi_A \) and \( \rho_A \) of ref. [26] we prefer to use the dimensionless ones

\[
\chi_A = \frac{2B_0m_q}{f_0^2}, \quad \rho_A = \frac{2W_0ac_{SW}}{f_0^2} .
\] (1)

Here \( m_q \) is the quark mass, \( a \) the lattice spacing, \( B_0 \) and \( W_0 \) are parameters of dimension mass and \( (\text{mass})^3 \), respectively, which appear in the leading order (LO) chiral effective Lagrangian, \( c_{SW} \) is the coefficient of the \( \mathcal{O}(a) \) chiral symmetry breaking term and \( f_0 \) is the value of the pion decay constant at zero quark mass. (Its normalization is such that the physical value is \( f_0 \approx 93 \text{ MeV} \).) In ref. [26] the case of three non-degenerate quark flavours is considered. Here we consider a general number \( N_s \) of equal mass sea quarks.

The next to leading order (NLO) PQChPT formula for the pion decay constant is in this case:

\[
\frac{f_{AB}}{f_0} = 1 - \frac{N_s}{128\pi^2} \left\{ (\chi_A + \chi_S + \rho_A + \rho_S) \log \left( \frac{1}{2}(\chi_A + \chi_S + \rho_A + \rho_S) \right) \\
+ (\chi_B + \chi_S + \rho_B + \rho_S) \log \left( \frac{1}{2}(\chi_B + \chi_S + \rho_B + \rho_S) \right) \right\} \\
+ \frac{1}{64N_s\pi^2} \left\{ \chi_A + \chi_B + \rho_A + \rho_B - 2\chi_S - 2\rho_S + (\chi_B - \chi_A + \rho_B - \rho_A)^{-1} \\
\cdot \left[ 2(\chi_A + \rho_A)(\chi_B + \rho_B) - (\chi_S + \rho_S)(\chi_A + \chi_B + \rho_A + \rho_B) \log \left( \frac{\chi_A + \rho_A}{\chi_B + \rho_B} \right) \right] \right\} \\
+ 2\tilde{L}_5(\chi_A + \chi_B) + 2\tilde{W}_5(\rho_A + \rho_B) + 4N_s\tilde{L}_4\chi_S + 4N_s\tilde{W}_4\rho_S .
\] (2)

Here A and B denote generic quark indices: S will be the label for the sea quarks V for valence quarks. For the pion mass squared we have:

\[
\frac{m^2_{AB}}{f_0^2} = \frac{1}{2}(\chi_A + \chi_B + \rho_A + \rho_B) + \frac{1}{32N_s\pi^2} \left( \frac{\chi_A + \chi_B + \rho_A + \rho_B}{\chi_B - \chi_A + \rho_B - \rho_A} \right) \\
\cdot \left\{ (\chi_A + \rho_A)(\chi_S - \chi_A + \rho_S - \rho_A) \log(\chi_A + \rho_A) \\
- (\chi_B + \rho_B)(\chi_S - \chi_B + \rho_S - \rho_B) \log(\chi_B + \rho_B) \right\}
\]
\[ +4N_s(2\bar{L}_6 - \bar{L}_4)\chi_S(\chi_A + \chi_B) + 2(2\bar{L}_8 - \bar{L}_5)(\chi_A + \chi_B)^2 \]

\[ +4N_s(\bar{W}_6 - \bar{L}_4)\chi_S(\rho_A + \rho_B) + 4N_s(\bar{W}_6 - \bar{W}_4)\rho_S(\chi_A + \chi_B) \]

\[ +2(2\bar{W}_8 - \bar{W}_5 - \bar{L}_5)(\chi_A + \chi_B)(\rho_A + \rho_B) \, . \]  

(3)

The NLO parameters \(\bar{L}_k\) and \(\bar{W}_k\) are related to \(L_k\) and \(W_k\) in ref. [9, 26] by

\[ \bar{L}_k \equiv L_k - c_k \log(f_0^2), \quad \bar{W}_k \equiv W_k - d_k \log(f_0^2), \]  

(4)

where the coefficients of the logarithms are given by

\[ c_4 = \frac{1}{256\pi^2}, \quad c_5 = \frac{N_s}{256\pi^2}, \quad c_6 = \frac{(N_s^2 + 2)}{512N_s^2\pi^2}, \quad c_8 = \frac{(N_s^2 - 4)}{512N_s\pi^2}, \]  

(5)

respectively,

\[ d_4 = \frac{1}{256\pi^2}, \quad d_5 = \frac{N_s}{256\pi^2}, \quad d_6 = \frac{(N_s^2 + 2)}{256N_s^2\pi^2}, \quad d_8 = \frac{(N_s^2 - 4)}{256N_s\pi^2}. \]  

(6)

The relations in (4) have the unpleasant feature that logarithms of a dimensionful quantity appear. One can avoid this by introducing

\[ L'_k \equiv L_k - c_k \log(\mu^2), \quad W'_k \equiv W_k - d_k \log(\mu^2), \]  

(7)

where \(\mu\) is the mass scale introduced by dimensional regularization. Since \(L_k\) and \(W_k\) depend on \(\mu\) the choice of it in the logarithm is natural. In terms of \(L'_k\) and \(W'_k\) we have

\[ \bar{L}_k = L'_k - c_k \log\left(\frac{f_0^2}{\mu^2}\right), \quad \bar{W}_k = W'_k - d_k \log\left(\frac{f_0^2}{\mu^2}\right). \]  

(8)

Note that the NLO parameters \(\alpha_k\) in ref. [7] are related to \(L'_k\) by

\[ \alpha_k = 128\pi^2L'_k. \]  

(9)

The universal low energy scales \(\Lambda_{3,4}\) in ref. [24, 25] can be expressed, in the case of \(N_s = 2\), by the following combinations of the coefficients \(\bar{L}_k\):

\[ -\frac{1}{256\pi^2} \log \frac{\Lambda_3^2}{f_0^2} = 2\bar{L}_8 - \bar{L}_5 + 4\bar{L}_6 - 2\bar{L}_4, \]

\[ \frac{1}{64\pi^2} \log \frac{\Lambda_4^2}{f_0^2} = 2\bar{L}_4 + \bar{L}_5. \]  

(10)

In this paper we are interested in the valence quark mass dependence of \(f_\pi\) and \(m_\pi^2\) for fixed sea quark mass parameter \(\chi_S\). Therefore it is natural to introduce the ratios of the other mass parameters to \(\chi_S\):

\[ \xi \equiv \frac{\chi_V}{\chi_S}, \quad \eta \equiv \frac{\rho_S}{\chi_S}, \quad \zeta \equiv \frac{\rho_V}{\rho_S} = \frac{\rho_V}{\eta \chi_S}. \]  

(11)
Once relations (11) are substituted in (2)-(3), the logarithmic dependence on $\chi_S$ can be absorbed in the NLO parameters if one introduces
\[
L_{Sk} \equiv \bar{L}_k - c_k \log(\chi_S) = L'_k - c_k \log \left( \frac{f_0^2}{\mu^2} \chi_S \right),
\]
\[
W_{Sk} \equiv \bar{W}_k - d_k \log(\chi_S) = W'_k - d_k \log \left( \frac{f_0^2}{\mu^2} \chi_S \right).
\]
Let us note that the argument of the last logarithms here can also be written as
\[
\frac{f_0^2}{\mu^2} \chi_S = \frac{2B_0 m_{qs}}{\mu^2}.
\]
In this paper we keep the sea quark mass ($\chi_S$) fixed and vary the valence quark mass ($\chi_V = \xi \chi_S$). Expanding the ratio of decay constants up to first order in the one-loop corrections one obtains
\[
R_{fVV} \equiv \frac{f_{VV}}{f_{SS}} = 1 + 4(\xi - 1)\chi_S L_{S5}
\]
\[
- \frac{N_s \chi_S}{64\pi^2} (1 + \xi + 2\eta) \log \frac{1 + \xi + 2\eta}{2} + \frac{N_s \chi_S}{32\pi^2} (1 + \eta) \log (1 + \eta),
\]
and similarly
\[
R_{fVS} \equiv \frac{f_{VS}}{f_{SS}} = 1 + 2(\xi - 1)\chi_S L_{S5} + \frac{\chi_S}{64N_s\pi^2} (\xi - 1) - \frac{\chi_S}{64N_s\pi^2} (1 + \eta) \log \frac{\xi + \eta}{1 + \eta}
\]
\[
- \frac{N_s \chi_S}{128\pi^2} (1 + \xi + 2\eta) \log \frac{1 + \xi + 2\eta}{2} + \frac{N_s \chi_S}{64\pi^2} (1 + \eta) \log (1 + \eta).
\]
In case of the ratios of $m_\pi^2$ we expand up to first order in the “correction” which now also includes the $O(a)$ terms of the tree-level expressions:
\[
R_{mVV} \equiv \frac{m_{VV}}{m_{SS}} = \xi + \eta - \eta \xi
\]
\[
+ 8\xi(\xi - 1)\chi_S (2L_{S8} - L_{S5}) + 8N_s(\xi - 1)\eta \chi_S (L_{S4} - W_{S6})
\]
\[
+ \frac{\chi_S}{16N_s\pi^2} (\xi - 1)(\xi + \eta) - \frac{\chi_S}{16N_s\pi^2} (1 + \eta) \log (1 + \eta)
\]
\[
+ \frac{\chi_S}{16N_s\pi^2} (2\xi^2 - \xi - \eta + 3\eta \xi) \log (\xi + \eta),
\]
and
\[
R_{mVS} \equiv \frac{m_{VS}}{m_{SS}} = \frac{1}{2}(1 + \xi + \eta - \eta \xi)
\]
\[
+ 2(\xi + 1)(\xi - 1)\chi_S (2L_{S8} - L_{S5}) + 4N_s(\xi - 1)\eta \chi_S (L_{S4} - W_{S6})
\]
\[
- \frac{\chi_S}{32N_s\pi^2} (\xi + 1)(1 + 2\eta) \log (1 + \eta)
\]
\[
+ \frac{\chi_S}{32N_s\pi^2} (\xi^2 + \xi + \eta + 3\eta \xi) \log (\xi + \eta).
\]
In these expressions it is assumed that the $O(a)$ mass terms $\rho$ are the same for valence quarks and the sea quark, namely $\rho_V = \rho_S$. This is the case if only the hopping parameter $\kappa$ is changed. Changing $\rho_V = \zeta \eta \chi_S$ can be investigated by changing the Wilson-parameter $r$ in the Wilson fermion action, too.

Up to now we considered the valence quark mass dependence for unchanged sea quark masses. Let us remark that the formulas for the sea quark mass dependence can also be written in a similar form as eqs. (14)-(17). In this case it is advantageous to fix a reference sea quark mass $\chi_R$ (see [2]) and introduce the variables

$$\sigma \equiv \frac{\chi_S}{\chi_R}, \quad \omega \equiv \frac{\rho_R}{\chi_R}, \quad \tau \equiv \frac{\rho_S}{\rho_R} = \frac{\rho_S}{\omega \chi_R}.$$  \hspace{1cm} (18)

Instead of the NLO parameters in (12) the appropriate ones are then obviously

$$L_{Rk} \equiv L_k - c_k \log \left( \frac{f_0}{\mu^2} \chi_R \right), \quad W_{Rk} \equiv W_k' - d_k \log \left( \frac{f_0}{\mu^2} \chi_R \right).$$  \hspace{1cm} (19)

3 Numerical results

We performed Monte Carlo simulations with $N_s = 2$ degenerate sea quarks on a $16^4$ lattice at $\beta = 4.68$, $\kappa = 0.195$ and investigated the valence quark mass dependence at $\kappa = 0.1955, 0.1945, 0.1940, 0.1930, 0.1920$. The statistics corresponds to 1180 gauge field configurations. The error analysis was based on the linearization method [27]. Since $r_0/a = 1.76(6)$ the lattice spacing is $a \simeq 0.28$ fm. This means that the physical lattice extension is rather large: $L \simeq 4.5$ fm. The value of the quark mass parameter is given by $a m_\pi = 0.519(1)$ as $M_r \equiv (r_0 m_\pi)^2 \simeq 0.83$. This is about $\frac{1}{4}$ of the value of $M_r$ for the strange quark $M_r^{\text{strange}} \simeq 3.1$.

The ratios in eqs. (14)-(17) as a function of the quark mass ratio ($\xi$) depend on five parameters, namely $\chi_S, \eta, L_{S5}, (2L_{S8} - L_{S5})$ and $(L_{S4} - W_{S6})$. With our choice of the valence hopping parameters and with our statistics most of the multi-parameter fits were unstable therefore our analysis is based one a sequence of single or double parameter fits. The stability of the multi-parameter fits can be improved by optimizing the choice of valence quark mass values, which we did not exploit this time.

A very useful quantity is the double ratio of decay constants [14] which does not depend on any of the NLO coefficients. In other words there one can see the chiral logarithms alone. The NLO formula is:

$$RRf \equiv \frac{f_{VS}^2}{f_{VV} f_{SS}} = 1 + \frac{\chi_S}{32 N_s \pi^2} (\xi - 1) - \frac{\chi_S}{32 N_s \pi^2} (1 + \eta) \log \frac{\xi + \eta}{1 + \eta}.$$  \hspace{1cm} (20)

Because of the $O(a)$ contributions this has two parameters: $\chi_S$ and $\eta = \rho_S/\chi_S$. For performing two-parameter fits some timeslice distance pairs were chosen and the fits
Figure 1: The valence quark mass dependence of the double ratio of pion decay constants \( RR_f \). Besides the "fit" the two other curves show the \( \mathcal{O}(a) \) contribution ("eta") and the physical contribution obtained at \( \eta = 0 \) ("chi").

of the pion- and quark mass were taken from them. Useful choices are, for instance, 4-5, 4-6 or 5-6. (The way physical quantities were obtained has been described in detail in [17]). The result of the two-parameter fit was (see figure 1):

\[
\chi_S = 9.2 \pm 2.5 , \quad \eta = 0.14 \pm 0.30 .
\]

(21)

The value of \( \chi_S \) has the right order of magnitude. Indeed, from the axial Ward identity we obtain \( r_0 m_q S = 0.06 Z_q^{-1} \). Using this and the phenomenological estimates \( r_0 f_0 = 0.23, r_0 B_0 = 7.0 \), where the value of \( B_0 \) refers to the \( \overline{\text{MS}} \) scheme at \( \mu = 2 \text{ GeV} \), we deduce \( \chi_S^{\text{estimate}} \simeq 16 Z_q^{-1} \). Here \( Z_q \) is an unknown \( Z \)-factor relating the bare lattice quark mass to the renormalized one at 2 GeV, which is typically of \( \mathcal{O}(1) \). Another estimate can be obtained by using the tree-level ChPT formula \( \chi_S^{\text{estimate}} \approx M_r/(r_0 f_0)^2 \approx 15.7 \).

After determining \( \chi_S \) and \( \eta = \rho_S/\chi_S \) from the double ratio \( RR_f \) one can fit the other ratios to obtain estimates of the NLO coefficients. A nice linear combination
of mass-squared ratios is:

\[ LRm \equiv 2Rm_{VS} - Rm_{VV} = 1 - 4(\xi - 1)^2\chi_S(2L_{S8} - L_{S5}) - \frac{\chi_S}{16N_s\pi^2}(\xi - 1)(\xi + \eta) \]

- \frac{\chi_S}{16N_s\pi^2}(1 + 2\eta)\log(1 + \eta) - \frac{\chi_S}{16N_s\pi^2}(\xi^2 - 2\xi - 2\eta)\log(\xi + \eta) \, . \quad (22)

This has only a single new parameter \( (2L_{S8} - L_{S5}) \) and the statistical errors are small, therefore one can also perform a two-parameter fit of \( \chi_S \) and \( (2L_{S8} - L_{S5}) \) with the result (\( \eta = 0.05 \) fixed, errors in last digits given in parentheses):

\[ 2L_{S8} - L_{S5} = -0.00203(5) \, , \quad 2\alpha_8 - \alpha_5 = 0.85(6) \, , \quad \chi_S = 5.2(1.1) \, . \quad (23) \]

\( \alpha_k \) denote the NLO parameters in \( (9) \) taken at the renormalization scale \( \mu = 4\pi f_0 \).

Fixing both \( \chi_S = 10.0 \) and \( \eta = 0.10 \) gives:

\[ 2L_{S8} - L_{S5} = -0.00177(3) \, , \quad 2\alpha_8 - \alpha_5 = 0.58(3) \, . \quad (24) \]

As figure 2 shows, with these parameters the last point is not perfectly fitted. A perfect fit is obtained with the parameters in \( (23) \).
Figure 3: The valence quark mass dependence of the ratio of pion decay constants $R_{fVV}$. Besides the “fit” the two other curves show the $O(a)$ contribution (“eta”) and the physical contribution obtained at $\eta = 0$ (“chi”).

The value of $L_{S5}$ can be determined from $R_{fVV}$. ($R_{fVS}$ gives very similar results.) In this case the statistical errors are larger, therefore only a single parameter fit is useful. The result for fixed $\chi_S = 10.0$ and $\eta = 0.10$ is (see figure 3):

$$ L_{S5} = 0.0034(1) , \quad \alpha_5 = 1.55(24) . $$

The errors given in (23)–(25) are the ones for the specified values of fixed parameters. The overall error is, of course, larger – as one can see, for instance, by comparing (23) and (24). The values of $(2\alpha_8 - \alpha_5)$ and $\alpha_5$ are somewhat larger than the results of UKQCD 3: $(2\alpha_8 - \alpha_5) = 0.36 \pm 0.10$ and $\alpha_5 = 1.22 \pm 0.11$ (only statistical errors quoted).

The double ratio of the pion mass squares 13

$$ RRm \equiv \frac{m_{V,S}^4}{m_{V,V}^2 m_{S,S}^2} = \frac{(\xi + 1)(\xi^2 + \xi - \eta + 2\eta\xi - \eta^2)}{4\xi^2} + \frac{\chi_S(\xi + 1)(\xi^2 + \xi + \eta + 3\eta\xi^2)\log(\xi + \eta)}{64N_\pi^2\xi^2} - \frac{\chi_S(\xi + 1)^2(2\eta + 1)\log(1 + \eta)}{64N_\pi^2\xi} $$
\[-\frac{\chi_S (\xi - 1)(\xi + 1)^2 (\xi + \eta)}{64 N_s \pi^2 \xi^2} + \frac{2 N_s \chi_S \eta (\xi + 1)(\xi - 1)^2}{\xi^2} (L_{S4} - W_{S6}) \]  

can be used to determine the fifth parameter \((L_{S4} - W_{S6})\). In this case a single parameter fit with fixed \(\chi_S = 10.0\) and \(\eta = 0.10\) gives \((L_{S4} - W_{S6}) = 0.00358(6)\).

The conclusion of this paper is that – once the quark masses are small enough – the qualitative behaviour of the low energy chiral effective theory with chiral logarithms is present even on coarse lattices. Since here ratios of pion masses and decay constants are considered the Z-factors of renormalization cancel, therefore the uncertainty about their \(\beta\)-dependence, which can influence the results of \([17, 19]\), is removed. The coefficients of the observed chiral logarithms and the fitted values of the Gasser-Leutwyler coefficients are close to expectation. This qualitative agreement of the results of a numerical simulation with (PQ)ChPT is quite satisfactory but for a quantitative determination of NLO ChPT parameters one has to perform extrapolations to \(a \to 0\) and \(m_q \to 0\). Since \(O(a)\) effects are taken into account in the analysis by the Rupak-Shoresh effective Lagrangian, the continuum limit will be reached asymptotically at the rate \(O(a^2)\).

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