Convergence issues in ChPT: a lattice perspective

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This review addresses the practical convergence of the ChPT series in the p-regime. In the SU(2) framework there is a number of new results, and improved estimates of $\bar{\ell}_3$ and $\bar{\ell}_4$ are available. In the SU(3) framework few new lattice computations have appeared and the improvement in the precision of the low-energy constants L_i is comparatively slow. I sketch some of the convergence issues genuine to extensions of ChPT which include additional sources of chiral symmetry breaking (finite lattice spacing) and/or violations of unitarity (different sea and valence quark masses). Finally, it is pointed out that the quark mass ratios m_u/m_d, m_s/m_d happen to be such that no reordering of the chiral series is needed to accommodate the experimental pion and kaon masses.
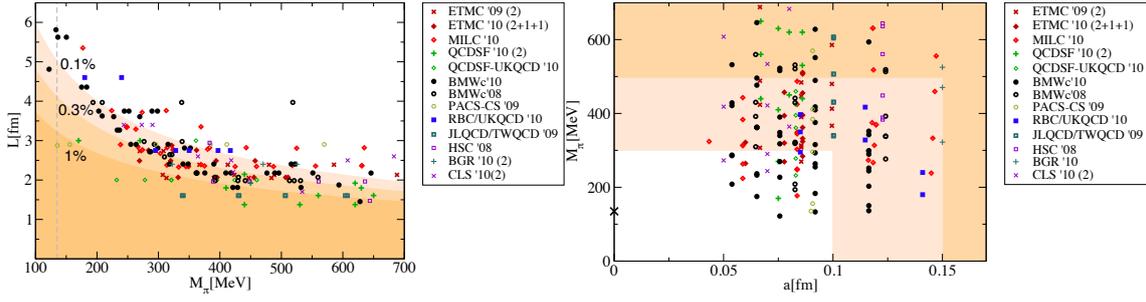
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Figure 1: Overview of the datasets accumulated in QCD ($N_f \geq 2$) by various collaborations as of 2011, plotted in the L versus M_π or the M_π versus a plane. The shaded backgrounds indicate the size of systematic effects due to the finite spatial volume or the chiral and continuum extrapolation. Figure taken from Ref. [2].

1. Introduction

Over the past few years computations in lattice QCD have greatly progressed. Today we aim for simulating $N_f = 2 + 1$ QCD (i.e. with a degenerate up and down quark mass m_{ud} and a separate strange quark mass in the determinant) right at the physical mass point $m_{ud} = (m_u^{\text{phys}} + m_d^{\text{phys}})/2$ and $m_s = m_s^{\text{phys}}$ where M_π^2 and $2M_K^2 - M_\pi^2$ take their physical values, in large boxes (up to 6 fm to control finite-size effects) and at several lattice spacings a (to allow for a continuum extrapolation $a \to 0$). This goal has been reached by the Wuppertal-Budapest collaboration (staggered fermions), the BMW collaboration (Wilson fermions), the PACS-CS collaboration (ditto), the MILC collaboration (staggered fermions) and the RBC/UKQCD collaboration (domain-wall fermions) – see the talk by Bob Mawhinney [1] for more details and Fig. 1 for an illustration (as of 2011).

These developments have a strong impact on the relation between Lattice QCD (LQCD) and Chiral Perturbation Theory (ChPT). In the past ChPT was used to guide the "chiral extrapolation" by which lattice physicists meant the extrapolation to $M_\pi \simeq 135$ MeV. In addition ChPT proved useful to correct data for the impact of the finite spatial box-size L, e.g. by providing the factor $M_X(\infty)/M_X(L)$ to be applied on the numerical data $M_X(L)$ for the mass of the state X. Now, the former application is less relevant, while the latter one is still extremely helpful (provided L is large enough so that ChPT can be applied). However, with todays lattices one can map out the quark mass dependence of various observables, and this provides a unique opportunity to determine the low-energy constants (LECs) of ChPT. The only "caveat" is that one must make sure that the data are in a regime where ChPT can be applied, i.e. converges (in a practical sense) well. The goal of this review is to provide examples of "good" and "bad" convergence and to discuss the status of lattice determinations of LECs in the SU(2) and SU(3) chiral frameworks.

2. Some Lattice and ChPT terminology

The purpose of this section is to recall some Lattice and ChPT terminology; the reader familiar with these is invited to move directly to Sec. 3.

ChPT is a rigorous framework to compute Green's functions of QCD, based on (*i*) symmetry, (*ii*) analyticity and (*iii*) [perturbative] unitarity. It is organized as an expansion in external momenta p^2 and quark masses m_q. At each order there is a number of new LECs which govern the momentum
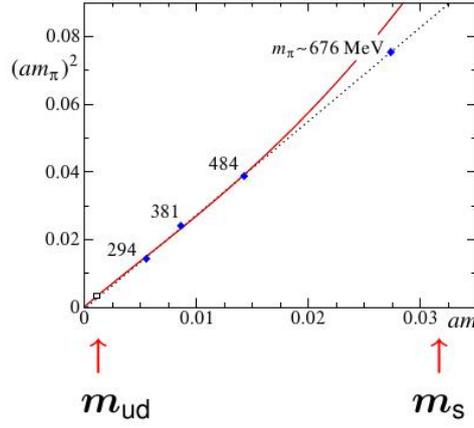
Figure 2: An early result for M_π^2 versus m_q in $N_f = 2$ QCD. The data are consistent with a linear behavior, yet ChPT predicts a curvature from which one is supposed to extract $\bar{\ell}_3$. Figure taken from Ref. [3].
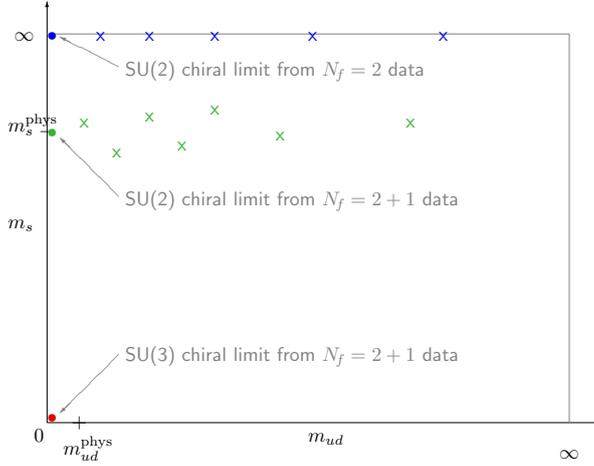

Figure 3: Cartoon of different data taking strategies in the (m_{ud}, m_s) plane. Simulations of QCD with $N_f = 2$ work effectively at $m_s = \infty$. Simulations with $N_f = 2 + 1$ tend to have m_s values in the vicinity of m_s^{phys}; for a controlled extrapolation to the SU(3) chiral limit additional data with $m_s \ll m_s^{\mathrm{phys}}$ are mandatory.

and quark-mass dependence of the Green's functions [at LO there are 2 parameters B, F in the SU(2) framework or B_0, F_0 in the SU(3) framework; at NLO there are 7 parameters $\bar{\ell}_i$ for SU(2) or 10 parameters $L_i^{\mathrm{ren}}(\mu)$ for SU(3)]. Those linear combinations of LECs which parameterize the p-dependence are usually best determined in experiment. By contrast, those linear combinations which determine the m_q-dependence are hard to get from experiment (in nature the quark masses can be varied in discrete steps only) and this creates an obvious opportunity for the lattice.

The standard counting rule is $p^2 \sim m$, but early on it was difficult to prove that the condensate parameter B or B_0 is large enough to warrant this counting (in phenomenology only the combination Bm_q or $B_0 m_q$ can be determined). Fig. 2 displays a historical plot by Lüscher [3] which shows that the lattice did step in to fill this gap: M_π^2 is in remarkably good approximation linear in m_q, and the slope is just $2B = 2\Sigma/F^2$. Moreover, the tiny deviation from linearity (which is not statistically significant in these data) bears the knowledge of $\bar{\ell}_3$. This illustrates that there is an enormous *hierarchy of difficulty* between determining the LECs at LO versus at NLO !
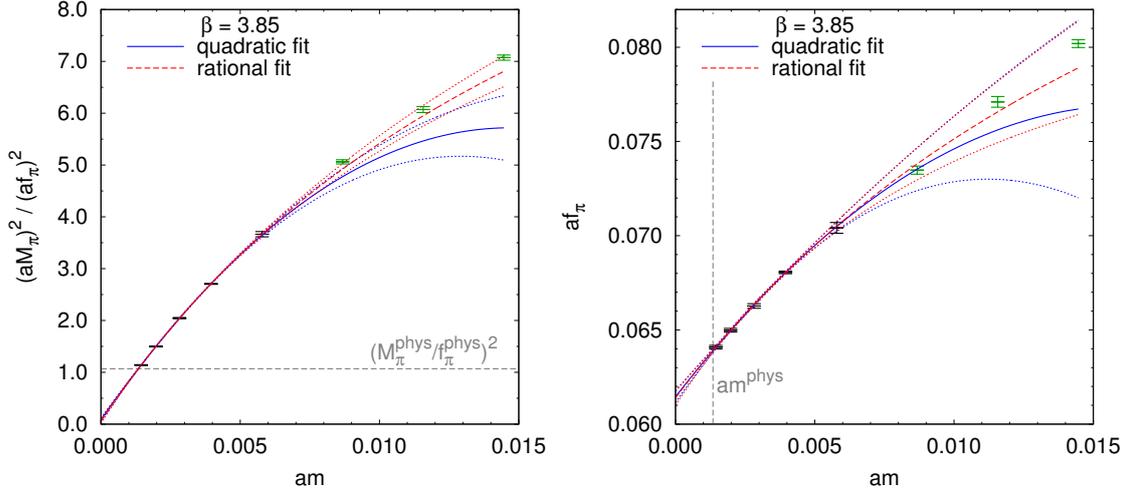
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Figure 4: Strategy of Ref. [5] for setting the scale and for adjusting m_{ud} to m_{ud}^{phys}. For each lattice spacing (bare coupling β) the data for $(aM_\pi)^2/(af_\pi)^2$ are interpolated/extrapolated to the point where this ratio assumes its physical value. The respective quark mass in lattice units is am_{ud}^{phys} (left), and by comparing the respective af_π to f_π^{phys} one finds a (right). See text for details. Figure taken from Ref. [5].

A few words on the relationship between $N_f = 2$ or $N_f = 2 + 1$ data and the SU(2) or SU(3) chiral frameworks are in order. Data with two degenerate dynamical flavors ($N_f = 2$) can only be analyzed with SU(2) formulas. The resulting LECs are logically different from those in nature, since the latter bear an implicit knowledge of m_s^{phys} (and heavier flavors). Also data with two degenerate light and a separate heavier flavor in the determinant ($N_f = 2+1$) may be analyzed in the SU(2) framework, cf. Fig. 3. If m_s was fixed at or near m_s^{phys} the resulting LECs may be identified with the phenomenological SU(2) LECs, since the implicit dependence of the latter on m_c^{phys} (and heavier flavors) is tiny. In addition, $N_f = 2 + 1$ data may be analyzed in the SU(3) framework, if the largest m_s used is small enough to warrant the chiral expansion. Hence, by increasing m_s^{max} the lattice may determine whether "catastrophic failure" occurs before or after reaching m_s^{phys}.

Sometimes lattice physicists analyze their data with *extended versions* of ChPT which are designed to parameterize the effects of *unitarity violation* (which come from $m_q^{\text{sea}} \neq m_q^{\text{val}}$ a.k.a. "partial quenching") and/or *finite lattice spacing* (specific to the lattice action used). It is important to keep in mind that these new capabilities bring in new convergence issues; it is well conceivable that there is a bound on the range of $|m_q^{\text{sea}} - m_q^{\text{val}}|$ that these theories may describe.

3. Success with the chiral SU(2) framework

An early (and I think particularly nice) paper in which the lattice demonstrated its ability to investigate convergence issues in the SU(2) framework and to pin down the corresponding LECs with good control over the chiral systematics is Ref. [4] by the JLQCD/TWQCD collaboration.

A more recent paper which I would like to discuss in some detail (perhaps because I'm an author) is [5]. It uses staggered $N_f = 2 + 1$ simulations with m_s tuned to m_s^{phys} and controls all sources of systematic error, including finite-size effects and cut-off effects (besides the chiral range). The scale is set by identifying the pion decay constant $f_\pi = \sqrt{2}F_\pi$ at the physical mass point with the
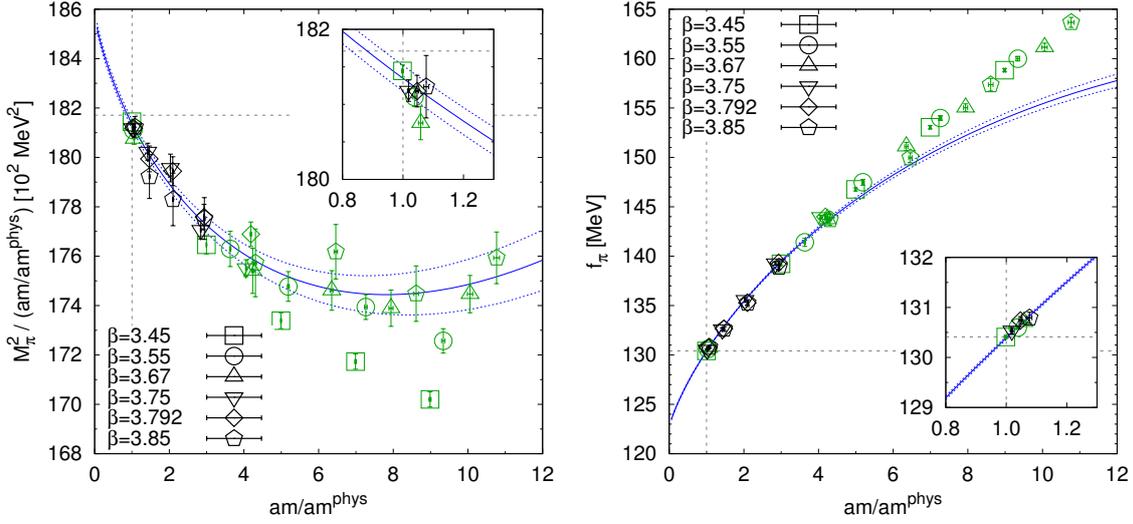
Figure 5: Plot of $M_\pi^2/(am_{ud}) \cdot (am_{ud}^{\mathrm{phys}})$ versus $(am_{ud})/(am_{ud}^{\mathrm{phys}})$ [left] and f_π [MeV] versus $(am_{ud})/(am_{ud}^{\mathrm{phys}})$ [right]. The latter quantity has no cut-off effects at the physical mass point, whereas the former one has cut-off effects at the few-permille level (see inserts). The LO+NLO fit includes data from the three finest lattices in the range $135\,\mathrm{MeV} \leq M_\pi \leq 240\,\mathrm{MeV}$ (black); other data (green) are disregarded. Figure taken from Ref. [5].
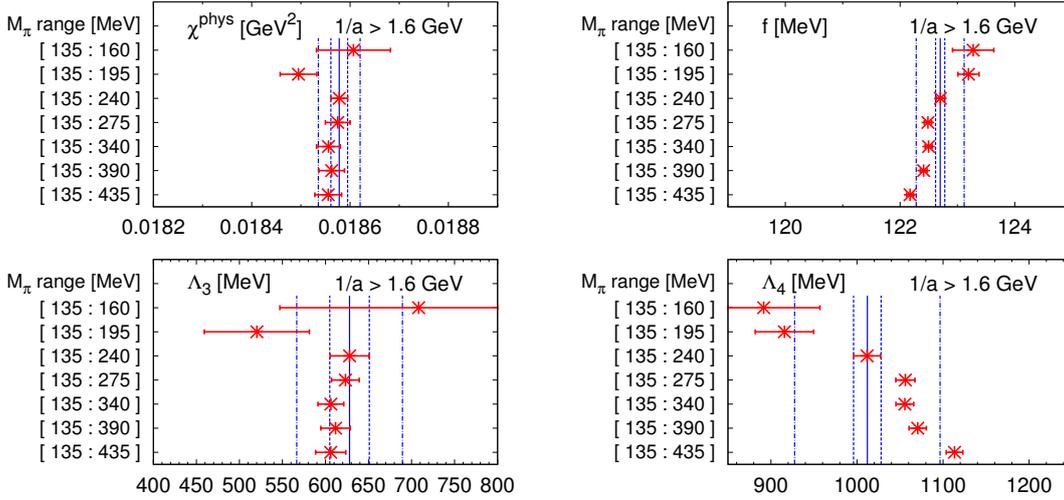

Figure 6: Behavior of the LECs at LO ($\chi = 2Bm$ and f [MeV], top) and at NLO (Λ_3 [MeV] and Λ_4 [MeV], bottom) as a function of the chiral range. Our preferred fit uses the range $135\,\mathrm{MeV} \leq M_\pi \leq 240\,\mathrm{MeV}$; the systematic error of the final result follows from the width of the distribution. Figure taken from Ref. [5].

PDG value, see Fig. 4 for details (there are some encouraging signs that the MILC collaboration might adopt this simple and compelling scale-setting strategy in future works, too).

The LECs are determined by a joint fit of the standard LO+NLO SU(2) formulas for M_π^2/m_{ud} and F_π as a function of m_{ud} (the abscissa value 1 in Fig. 5 indicates the physical pion mass). We get a decent description of the data if we restrict the fit to the three finest lattices (i.e. $a < 0.13\,\mathrm{fm}$) and the mass range $135\,\mathrm{MeV} \leq M_\pi \leq 240\,\mathrm{MeV}$. Alternative fit ranges affect $\chi^{\mathrm{phys}} = 2Bm_{ud}^{\mathrm{phys}}$ and Λ_3 (both extracted from M_π^2/m_{ud} versus m_{ud}) less severely than $f = \lim_{m_{ud}\to 0} f_\pi$ and Λ_4 (both extracted
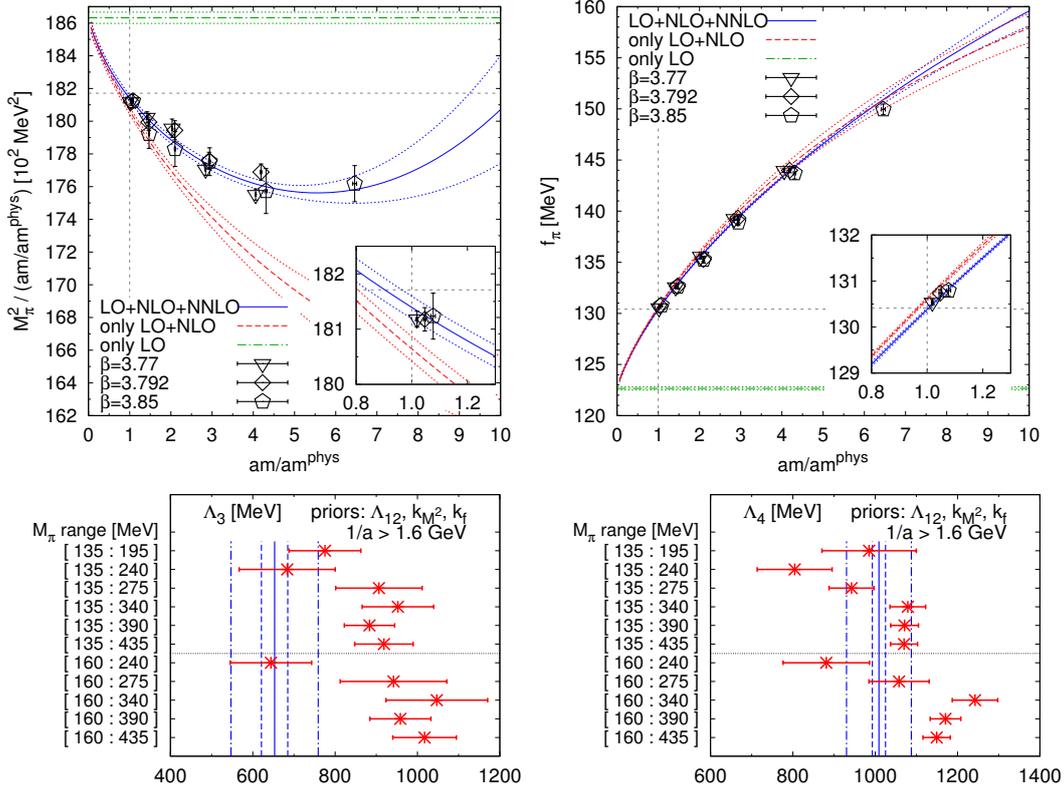
Figure 7: Data at the three finest lattice spacings together with a LO+NLO+NNLO fit (with priors for the NNLO parameters). The breakup into LO/NLO/NNLO contributions shows a convergence behavior, at the physical mass point, which is good for f_π (top right) and even excellent for M_π^2/m_{ud} (top left). For higher quark masses the situation may get reversed. The respective values of Λ_3 and Λ_4 are reasonably consistent with those from the pure LO+NLO fit (bottom, blue bands copied from Fig. 6). Figure taken from Ref. [5].

from f_π as a function of m_{ud}), see Fig. 6. The systematic uncertainty of the LECs is extracted from the variance over the 7 chiral fit ranges (all other uncertainties are massively subdominant).

With the restriction to the three finest lattice spacings ($a < 0.13$ fm) the data can even sustain a LO+NLO+NNLO joint chiral fit, provided we add (mild) priors to stabilize the NNLO coefficients (which we are not interested in anyway). A typical behavior is shown in Fig. 7. The point is that we can now perform a break-up into LO (green), LO+NLO (red) and LO+NLO+NNLO (blue) parts. At the physical mass point the numerical values of f_π [MeV] are 122.6, 130.7, 130.4, respectively, which I would term a "good" convergence behavior (the first shift is by 6.6%), and the numerical values of $M_\pi^2/m_{ud} \cdot m_{ud}^{\text{phys}}$ [10^2 MeV^2] are 186.3, 180.7, 181.4, respectively, which I would call an "excellent" convergence behavior (the first shift is by 3.0%). As the two lower panels of that figure indicate, this fit is not entirely immune against changes of the chiral fit range (in particular if the lower bound is increased), but the values of the NLO LECs Λ_3, Λ_4 stay reasonably consistent with what was obtained from the pure LO+NLO fit (blue bands for stat and $\sqrt{\text{stat}^2 + \text{syst}^2}$ errors).

We find $\bar{\ell}_3 = 3.16(10)_{\text{stat}}(29)_{\text{syst}}$ and $\bar{\ell}_4 = 4.03(03)_{\text{stat}}(16)_{\text{syst}}$ besides the LECs at LO [5]. A more extensive discussion of SU(2) LECs from the lattice along with some world-averages is found in [6]. It turns out that to date there is no significant difference for a given SU(2) LEC from $N_f = 2$ versus from $N_f = 2+1$ simulations. Hence unquenching effects from s-loops seem to be mild.
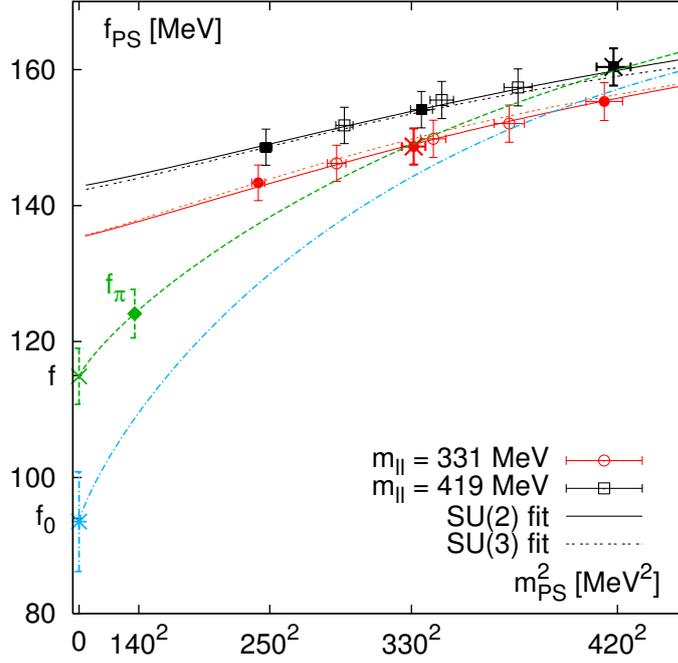
Figure 8: Partially quenched data by the RBC/UKQCD collaboration (as of 2008) for f_π (alias f_{PS}) versus m_{ud}^{val} (alias m_{PS}^2). They feature two unitary [m_{ll} instead of m_{PS}] data-points (bursts); the fits extract the decay constants f and f_0 in the SU(2) and SU(3) [unitary] chiral limits, respectively. Figure taken from Ref. [7].

4. Questions with the chiral SU(3) framework

It is known from phenomenology that $m_s^{phys} \simeq 95\,\text{MeV}$ (at $\mu = 2\,\text{GeV}$ in $\overline{\text{MS}}$ scheme) is at the edge of the regime where ChPT converges well. The good news is that the lattice can vary m_s around this value and explore the issue in more detail. The bad news is that many of the existing $N_f = 2 + 1$ studies are pounded with additional convergence issues that come from $m_q^{sea} \neq m_q^{val}$.

An older paper worth discussing is Ref. [7]; their famous plot is reproduced in Fig. 8. It shows their partially quenched data on two ensembles (red and black) versus m_{ud}^{val} and fitted with PQChPT. This fit yields the unitary f_π in two theories: (*i*) as a function of $m_{ud}^{sea} = m_{ud}^{val}$ at fixed $m_s^{sea} = m_s^{phys}$ [SU(2), green line] and (*ii*) as a function of $m_{ud}^{sea} = m_{ud}^{val} = m_s^{sea} = m_s^{val}$ [SU(3), blue line]. I think three points should be emphasized. First, the two unitary lines suggest $f/f_0 \equiv F/F_0 = 1.2(1)$ which is interesting because it specifies the amount of Zweig rule violation. Second, as pointed out by the authors, the extrapolated values f and f_0 lie significantly below the data. Finally, one should keep in mind that the not-so-great convergence apparent in this plot may – at least in part – be due to the fact that it is unnatural for PQChPT to accommodate nearly linear data (the curvature in the partially quenched logs must be counterbalanced by higher-order terms). In my opinion this calls for an investigation how the convergence pattern depends on the width of the partially quenched direction. For the progress achieved by RBC/UKQCD since publication of Ref. [7] see [1].

Another collaboration with an interesting $N_f = 2 + 1$ dataset is MILC. They have ensembles with $m_s \ll m_s^{phys}$, i.e. additional green crosses close to the *x*-axis in the cartoon of Fig. 3. In Ref. [8] they display a fit to their full (partially quenched) dataset along with the restriction of that fit to the unitary world where $m_q^{sea} = m_q^{val}$ for both $q = ud$ and $q = s$ (the red "full, cont, m_s" line in Fig. 9).
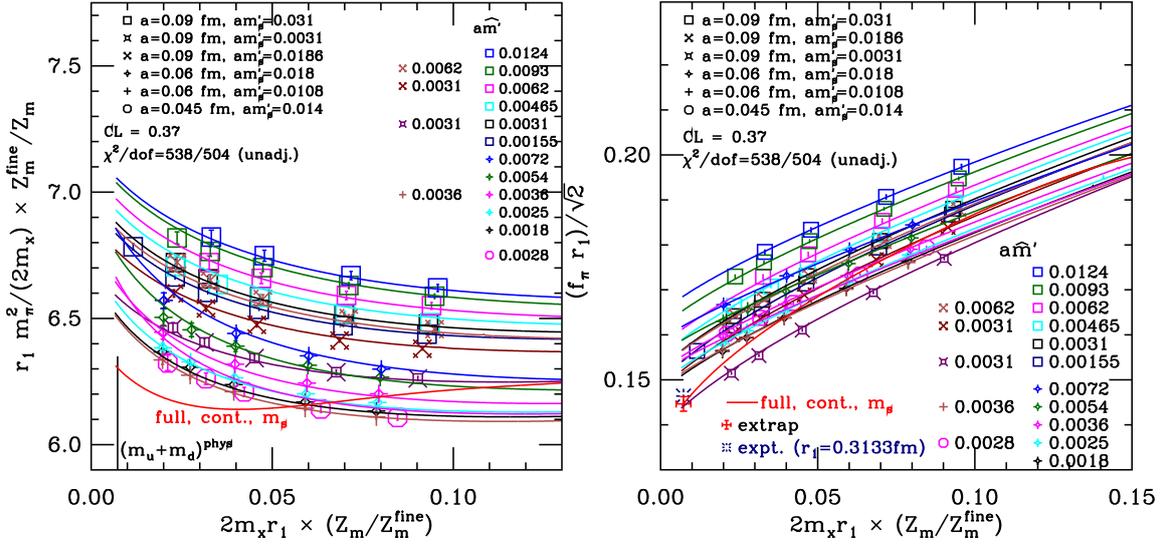
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Figure 9: Partially quenched data by the MILC collaboration (as of 2010) for M_π^2/m_{ud} (left) and f_π (right) versus m_{ud}^{val}. The unitary continuum behavior at $m_s = m_s^{\text{phys}}$ is shown in red. Figure taken from Ref. [8].
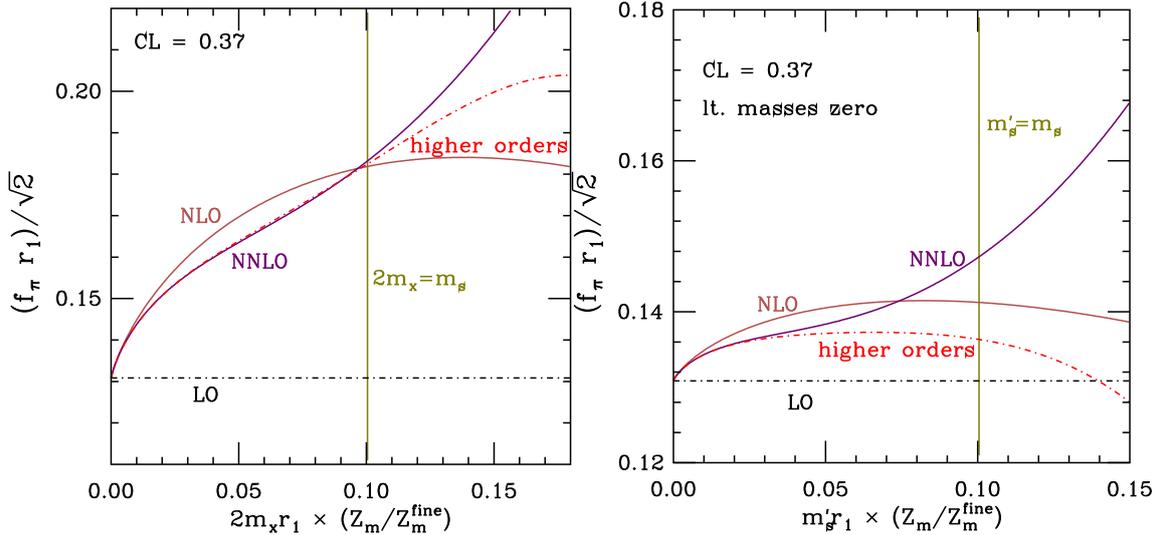

Figure 10: Breakup of the continuum extrapolated and unitary subset of the fit shown in the right panel of Fig. 9 into its LO/NLO/NNLO/higher-order-analytical contributions, both for the $m_{ud} = m_s$ diagonal line in Fig. 3 (left) and for the SU(2) chiral limit as a function of m_s (right). Figure taken from Ref. [8].

Fig. 10 shows the breakup of this unitary restriction into LO/NLO/NNLO/higher-order-analytical terms, both along the $m_{ud} = m_s$ diagonal line in the cartoon (left panel) and along the y-axis of the cartoon as a function of m_s (right panel). In the former case convergence seems to be good up to $2m_{ud} \simeq m_s^{\text{phys}}$ (marked by the green line). In the latter case the SU(2) convergence seems to depend on m_s; specifically near $m_s = m_s^{\text{phys}}$ (labeled $m_s' = m_s$) the convergence seems rather poor. This latter finding tends to be in conflict with the pattern observed in Fig. 7 from a direct SU(2) fit.

In short it seems fair to say that there are open issues regarding the convergence of (extended versions of) SU(3) ChPT on $N_f = 2+1$ ensembles. For numerical values of SU(3) LECs see [6].
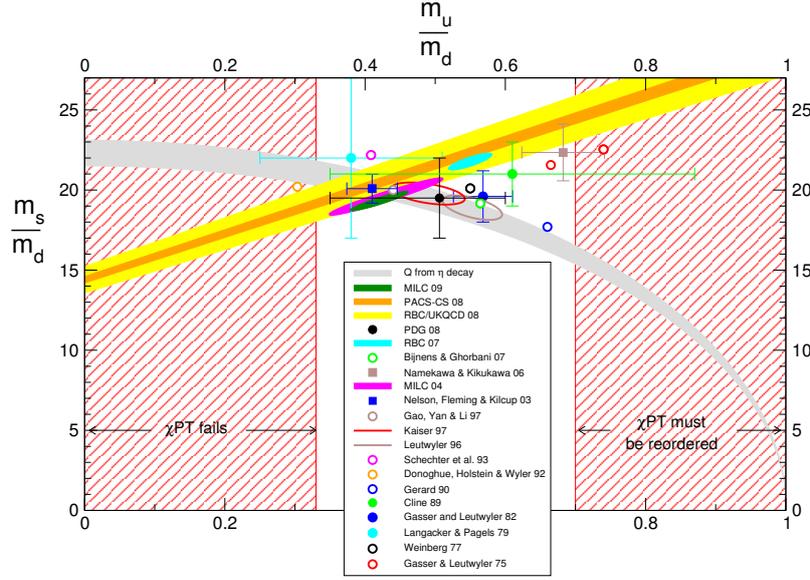
Figure 11: Some phenomenological and lattice determinations of $(m_u/m_d)^{\text{phys}}$ and $(m_s/m_d)^{\text{phys}}$ along with shaded areas for which ChPT augmented for electromagnetic effects would be in trouble if the experimental values of $M^2_{\pi^+} - M^2_{\pi^0}$ and $M^2_{K^+} - M^2_{K^0}$ are untouched. Figure taken from Ref. [9].

5. Brief comment on the viability of $m_u = 0$

It is well known that "$m_u = 0$" (in QCD) would provide a theoretically appealing solution to the strong CP problem. The question is just: Is it phenomenologically viable ?

Fig. 11 reproduces a plot from Ref. [9]. Leutwyler shows several results for $(m_s/m_d)^{\text{phys}}$ versus $(m_u/m_d)^{\text{phys}}$ along with red bands which indicate that ChPT augmented to account for electromagnetism fails to converge if the latter ratio would be below ~ 0.3 or above ~ 0.7 (which apparently is not the case). To avoid potential misunderstanding: There is no statement that ChPT+QED cannot describe a world with an up/down quark mass ratio of, say, 0.1 and $\alpha_{\text{QED}} \simeq 1/137$, if $M^2_{\pi^+} - M^2_{\pi^0}$ and $M^2_{K^+} - M^2_{K^0}$ change accordingly. The statement is that this extended chiral framework fails to converge if the meson mass splittings stay at their experimental values and nonetheless the internal m_u/m_d ratio is pinned to a value outside the white region. In short the physics question is: Does this indicate that "$m_u = 0$" is phenomenologically not viable or does it, to the contrary, just signal an inability of ChPT+QED to reconcile the beautiful solution with experimental facts ?

Over the years the lattice has made great progress at pinning down the quark mass ratio m_u/m_d (and also m_s/m_{ud}, both in QCD) independently, i.e. with steadily decreasing chiral input. An early study by MILC used ChPT+QED in the pion/kaon system and found $m_u/m_d = 0.43(1)(8)$ [10]. A calculation by BMW used more robust information about strong isospin breaking from $\eta \to 3\pi$ decays and found $m_u/m_d = 0.45(1)(3)$ [11]. There are several new results with quenched/full QED on full QCD backgrounds, e.g. Blum et al. [12], PACS-CS [13], RM123 [14] and BMW [15], which find significant but non-dramatic corrections to Dashen's theorem, indicating that m_u/m_d is away from zero by $O(10)$ standard deviations and well inside the white region in Fig. 11.

Of course, one may choose to wait for a fullQCD+fullQED study (without reweighting), but with hindsight one may say that nature solves the strong CP problem not by "$m_u = 0$".

6. Summary

Let me summarize the salient points in a few short statements:

1. The lattice community is at the point where physical quark masses can be simulated, i.e. ensembles with physical values of $(M_\pi^2, 2M_K^2 - M_\pi^2)$ in large enough boxes and at several lattice spacings can be generated. As a result chiral extrapolation formulas are now less important (while finite volume correction formulas are still in high demand), and the lattice is in a unique position to compute the chiral LECs from first principles.

2. The SU(2) framework is best served by current $N_f = 2$ and $N_f = 2 + 1$ simulations where (in the latter case) $m_s \simeq m_s^{\mathrm{phys}}$. For $m_{ud} \simeq m_{ud}^{\mathrm{phys}}$ the ChPT convergence seems to be rapid. The SU(2) LECs from $N_f = 2$ and $N_f = 2 + 1$ simulations are logically different, but currently no numerical difference is seen, i.e. unquenching effects due to s-loops seem to be mild.

3. The SU(3) framework requires data with $m_s \ll m_s^{\mathrm{phys}}$ to control ChPT systematics, as shown by MILC. There are issues regarding the convergence pattern as well as the size of unitarity violations and/or cut-off effects that can be parameterized by extended versions of ChPT.

4. Given the experimental values of the meson mass splittings $M_{\pi^+}^2 - M_{\pi^0}^2$ and $M_{K^+}^2 - M_{K^0}^2$, the chiral framework with electromagnetic effects included would be in trouble if m_u/m_d (in QCD) would be significantly different from a value ~ 0.5. Evidence is mounting that this is not a deficiency of ChPT – there is a number of lattice results which exclude the esthetically pleasing solution "$m_u = 0$" to the strong CP problem at the multi-sigma level.

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