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How far can you go ? Surprises and pitfalls in three-flavour chiral extrapolations

Sébastien Descotes-Genon[*†]
Laboratoire de Physique Théorique,
CNRS/Univ. Paris-Sud 11 (UMR 8627), 91405 Orsay Cedex, France
E-mail: `descotes@th.u-psud.fr`

The increasing accuracy of experimental data in flavour physics requires a corresponding improvement on the theoretical side, in particular concerning the non-perturbative dynamics of QCD. This has prompted the lattice community to aim at an unprecedented accuracy in form factors and matrix elements. However, in the light sector, the meson masses remain too heavy for an interpolation, which makes it necessary to rely on Chiral Perturbation Theory to perform extrapolations in the light quark masses. This makes it all the more necessary to assess precisely the range of validity of this theory. More precisely, the presence of strange quark pairs in the sea may have a significant impact of the pattern of chiral symmetry breaking : in particular large differences can occur between the chiral limits of two and three massless flavours (i.e., whether m_s is kept at its physical value or sent to zero). We recall some indications of such a scenario in QCD, in relation with the peculiar dynamics of the scalar sector. We explain how this could affect the convergence of three-flavour chiral series, commonly used to extrapolate the results of lattice simulations. Finally, we indicate how lattice simulations with three dynamical flavours could unveil such an effect through the quark-mass dependence of light meson masses and decay constants.

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1. Two chiral limits of interest

Because of the mass hierarchy among light quarks, the strange quark may play a special role in the low-energy dynamics of QCD. It is light enough to allow for a combined expansion of observables in powers of m_u, m_d, m_s around the $N_f = 3$ chiral limit (meaning 3 massless flavours): $m_u = m_d = m_s = 0$. But it is sufficiently heavy to induce significant changes in order parameters from the $N_f = 3$ chiral limit to the $N_f = 2$ chiral limit: $m_u = m_d = 0$ and m_s physical. Finally, it is too light to suppress efficiently loop effects of massive $\bar{s}s$ pairs (contrary to heavier quarks) [1].

Two different versions of Chiral Perturbation Theory have been developed around these two limits. In the $N_f = 2$ massless limit, only the pions play a particular role and thus are the only available degrees of freedom. The $N_f = 3$ chiral limit promotes pions, kaons and η as the degrees of freedom : this second version of χPT is richer, discusses more processes in a larger range of energy, but contains more unknown low-energy constants (LECs) and may have a slower convergence. In each limit, the LECs encode the pattern of chiral symmetry breaking, cannot be computed within χPT and must be determined from experiment. Obviously, LECs in both theories are related since the $N_f = 2$ theory can be obtained from $N_f = 3$ χPT by restricting it to the pion sector and integrating out kaons and eta, treated as massive particles. However, the details of the connection between the two theories remain under debate.

Indeed, due to $\bar{s}s$ sea-pairs, order parameters such as the quark condensate and the pseudoscalar decay constant, $\Sigma(N_f) = -\lim_{N_f}\langle\bar{u}u\rangle$ and $F^2(N_f) = \lim_{N_f} F_\pi^2$, can reach significantly different values in the two chiral limits ($\lim_{N_f}$ denoting the chiral limit with N_f massless flavours) [1]. An illustration is provided by the quark condensate in the two limits:

$$\Sigma(2) = \Sigma(2;m_s) = \Sigma(2;0) + m_s \frac{\partial\Sigma(2;m_s)}{\partial m_s} + O(m_s^2) \tag{1.1}$$

$$= \Sigma(3) + m_s \lim_{m_u,m_d\to 0} i\int d^4x\, \langle 0|\bar{u}u(x)\,\bar{s}s(0)|0\rangle + O(m_s^2) \tag{1.2}$$

Here, $\bar{s}s$-pairs are involved through the two-point correlator $\langle(\bar{u}u)(\bar{s}s)\rangle$, which violates the Zweig rule in the vacuum (scalar) channel [1]. This loop effect disappears in the large-N_c limit, which is known to fail in the 0^{++} channel due to the complicated structure of broad resonances, corresponding to poles of the scattering matrix located far away from the real axis (see for instance [2] for a discussion of the lightest scalar resonances).

Arguments based on the spectrum of the Dirac operator [1] indicate that this effect should suppress order parameters when $m_s \to 0$: $\Sigma(2) \geq \Sigma(3)$ and $F^2(2) \geq F^2(3)$. Since the quark condensate(s) and the pseudoscalar decay constant(s) are the building blocks of the two versions of χPT at leading order, a strong decrease from $N_f = 2$ to $N_f = 3$ should have a direct impact on the structure of the two theories. We discuss some available data on the pattern of chiral symmetry breaking in both chiral limits in turn.

[1] Like all the terms in the m_s-expansion of $\Sigma(2)$, this correlator is a $SU_L(2)\times SU_R(2)$ order parameter related to the spontaneous breakdown of $N_f = 2$ chiral symmetry, and this for any value of m_s. The (scheme-dependent) high-energy contributions to eq. (1.2) should be proportional to $m = m_u = m_d$ and thus drop from the relation once the $N_f = 2$ chiral limit has been taken (in contrast with the quark condensates arising in OPE at non-vanishing m_u, m_d, m_s, which exhibit such ultraviolet divergences).

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2. The situation in the $N_f = 2$ limit

A few years ago, the Brookhaven E865 collaboration provided new data on $K_{\ell 4}$ decays [3]. Building upon the dispersive analysis of $\pi\pi$ scattering [4], we extracted the two-flavour order parameters [5]:

$$X(2) = \frac{(m_u + m_d)\Sigma(2)}{F_\pi^2 M_\pi^2} = 0.81 \pm 0.07 \qquad Z(2) = \frac{F^2(2)}{F_\pi^2} = 0.89 \pm 0.03 \tag{2.1}$$

A different analysis, with an additional theoretical input from the scalar radius of the pion, led to a larger value for $X(2)$ [6].

The situation is somewhat modified by new data from the NA48 collaboration [7], which show some discrepancy with the E865 phase shifts in the higher end of the allowed phase space. The role of isospin breaking corrections is under discussion currently. The preliminary values of the phase shifts [7] tend to increase the value of the $I = J = 0$ $\pi\pi$ scattering length, and to decrease the value of the two-flavour quark condensate, possibly pushing $X(2)$ down to 0.7.

The Gell-Mann–Oakes–Renner relation and its siblings correspond to $X(2) = Z(2) = 1$ and such deviations from unity may seem fairly unimpressive. However one should remember these are $N_f = 2$ chiral expansions in powers of m_u and m_d *only*. Indeed, $X(2)$ and $Z(2)$ indicate the convergence of $N_f = 2$ chiral expansions of $F_\pi^2 M_\pi^2$ and F_π^2 respectively : they measure the relative size of the leading-order term in these expansions. One usually expects a far quicker convergence of $N_f = 2$ chiral series, with much smaller next-to-leading order corrections (below 10%) [5].

3. The situation in the $N_f = 3$ limit

To include K- and η-mesons dynamically, one must use three-flavour χPT, where the expansion in the three light quark masses starts around the $N_f = 3$ vacuum $m_u, m_d, m_s = 0$. Here, strange sea-quark loops may have a dramatic effect on $N_f = 3$ chiral expansions. The leading-order (LO) term, which depends on the $O(p^2)$ low-energy constants $F^2(3)$ and $\Sigma(3)$, would be damped, whereas next-to-leading-order (NLO) corrections could be enhanced, in particular those related to the violation of the Zweig rule in the scalar sector. For instance, the Gell-Mann–Oakes–Renner relation would not be saturated by its LO term and would receive sizeable numerical contributions from terms treated as NLO in the chiral counting scheme.

Indirect estimates [8, 9] suggest a very significant effect. At NLO the violation of the Zweig rule in the scalar sector is encoded in the two LECs L_4 and L_6. Dispersive estimates of the correlator $\langle(\bar{u}u)(\bar{s}s)\rangle$, related to L_6 [8], indicate that the quark condensate may drop by a half from $N_f = 2$ to $N_f = 3$, i.e. when m_s is sent from its physical value down to zero (such a decrease has been observed by the MILC collaboration [10]). On the other hand [9], the dispersive study of low-energy πK scattering through Roy-Steiner equations and the naive comparison with NLO $N_f = 3$ chiral expansions yields $L_4(M_\rho) = (0.53 \pm 0.39) \cdot 10^{-3}$.

Such a value may seem rather small, but one should not forget the m_s-enhancement of the contributions of L_4 and L_6 in chiral series. Take for instance

$$F_\pi^2 = F(3)^2 + 16(m_s + 2m)B_0\Delta L_4 + 16mB_0\Delta L_5 + O(m_q^2) \tag{3.1}$$

where $B_0 = -\lim_{m_u,m_d,m_s\to 0}\langle\bar{u}u\rangle/F_\pi^2$, and we have put together NLO low-energy constants and chiral logarithms : $\Delta L_5 = L_5(M_\rho) + 0.67\cdot 10^{-3}$ and $\Delta L_4 = L_4(M_\rho) + 0.51\cdot 10^{-3}$ (which is enhanced by a factor of m_s/m). If we assume that the LO contribution is numerically dominant (i.e., $F_\pi^2 = F(3)^2$ to a very good approximation), we can perform the following manipulations:

$$\frac{F(3)^2}{F_\pi^2} = \frac{F^2(3)}{F^2(3)+O(m_q^2)} = 1 - 8\frac{2M_K^2+M_\pi^2}{F_\pi^2}\Delta L_4 - 8\frac{M_\pi^2}{F_\pi^2}\Delta L_5 + O(m_q^2) = 1 - 0.51 - 0.04 + O(m_q^2) \tag{3.2}$$

where we have used $1/(1+x) = 1-x$ and eq. (3.1) at the second step, and the second and third terms of the last equality are obtained using $L_4(M_\rho) = 0.5\cdot 10^{-3}$ and $L_5(M_\rho) = 1.4\cdot 10^{-3}$ respectively (these values are used for illustrative purposes). Eq. (3.2) is clearly in contradiction with the original assumption $F_\pi^2 \simeq F(3)^2$. A similar game can be played with L_6 and $F_\pi^2 M_\pi^2$.

We can draw several conclusions from this simple exercise. A small positive value of $L_4(M_\rho)$ or of $L_6(M_\rho)$ is enough to invalidate the usual assumption of a rapid convergence of $N_f = 3$ chiral series (an issue to be remembered when one tries to extract the values of LECs in lattice simulations). In addition, we may encounter chiral series $A = A_{LO} + A_{NLO} + A\delta A$ with a good overall convergence, i.e., $\delta A \ll 1$ but the numerical balance between LO and NLO depends on the relevance of strange sea-quark loops. The numerical competition between formal LO and NLO makes approximations such as $1/(1+x) \simeq 1-x$ or $(m_s+m)B_0 \simeq M_K^2$ rather hazardous, leading to potential contradictions and/or slow convergence for some chiral expansions.

Actually, such difficulties in the convergence are encountered when NNLO computations are fitted to experimental data. A good example can be found among the reference fits in ref. [11]: for instance, the so-called Fit 10 yields : $(M_\pi^2)_{th} = (M_\pi^2)_{exp}[0.736 + 0.006 - 0.258]$, corresponding to the relative size of LO, NLO and NNLO respectively. If confirmed, such difficulties in the convergence of three-flavour chiral expansions should be considered as a very serious problem and a source of sizable systematics in lattice results relying on chiral extrapolations on a large range of quark masses.

4. Constraints from $\pi\pi$ and πK scatterings

We would like to cope with the potentially "large" values of L_4 and L_6, and the resulting numerical competition between formal LO and NLO contributions in chiral series. To do so, we have introduced a framework, called Resummed Chiral Perturbation Theory (ReχPT) [12], where we define the appropriate observables to consider and the treatment of their chiral expansion [12, 13, 14]:

1. Consider a subset of observables that are assumed to have a good overall convergence – we call them "good observables". They must form a linear space, which we choose to be that of connected QCD correlators (of vector/axial currents and their divergences) as functions of external momenta, away from any kinematic singularities. This rule selects in particular F_P^2 and $F_P^2 M_P^2$ ($P = \pi, K$).

2. Take each observable and write its NLO chiral expansion in terms of the chiral couplings : F_0, B_0, $L_i\ldots$

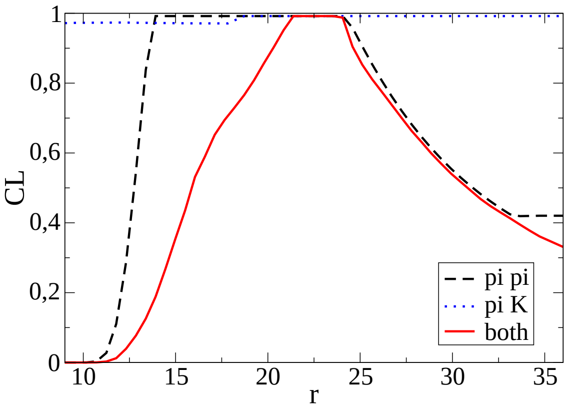

Figure 1: Profiles for the confidence levels of $r = m_s/m$ (left) and $X(3) = 2m\Sigma(3)/(F_\pi^2 M_\pi^2)$ (right). In each case, the results are obtained from $\pi\pi$ scattering only (dashed line), πK scattering only (dotted line), or both sources of information (solid line).

3. In theses formulae, reexpress the bare couplings in terms of physical quantities (masses, decay constants...) if justified by physics considerations (e.g., position of unitarity cuts) The result is called "bare expansion".

4. In these bare expansions, reexpress $O(p^2)$ and $O(p^4)$ LECs in terms of:

$$r = \frac{m_s}{m}, \qquad X(3) = \frac{2m\Sigma(3)}{F_\pi^2 M_\pi^2}, \qquad Z(3) = \frac{F^2(3)}{F_\pi^2}, \tag{4.1}$$

and NNLO remainders, using the bare expansions for the masses and decay constants of the pseudoscalar mesons π, K, η.

This simple recipe provides a resummation of the potentially large effect of the Zweig-rule violating couplings L_4 and L_6 [13, 12], hence the name of "Resummed Chiral Perturbation Theory" (ReχPT) given to this framework. Since we want to cope with the possibility of a numerical competition between (formal) LO and NLO terms in chiral series, some usual $O(p^4)$ results are not valid any longer : for instance $r = m_s/m$ is not fixed by M_K^2/M_π^2 and can vary from 8 to 40, L_5 is not fixed by the ratio of F_K/F_π.

In this framework, one can derive the NLO amplitudes corresponding to $\pi\pi$ and πK scatterings, which provide information on $N_f = 2$ and $N_f = 3$ patterns of chiral symmetry breaking. The smallest uncertainties on the chiral expansion are expected to occur in the unphysical region, far away from the non-analyticities due to unitarity. One can exploit dispersive relations, such as Roy equations [4] and Roy-Steiner equations [9], to reconstruct the amplitudes in this unphysical point from the phase shifts from threshold up to energies around 1 GeV. Matching the dispersive and chiral representations of the amplitude in a frequentist framework provides constraints (in terms of confidence Levels) on the main parameters of interest for three-flavour χPT [12]. As an illustration, fig. 1 shows the situation for $r = m_s/m$ and $X(3) = 2m\Sigma(3)/(F_\pi^2 M_\pi^2)$. A more detailed analysis provides the following constraints from the combination of $\pi\pi$ and πK scatterings:

$$r \geq 14.8\,, \quad X(3) \leq 0.83\,, \quad Y(3) \leq 1.1\,, \quad 0.18 \leq Z(3) \leq 1\,. \qquad [68\%\text{CL}] \tag{4.2}$$

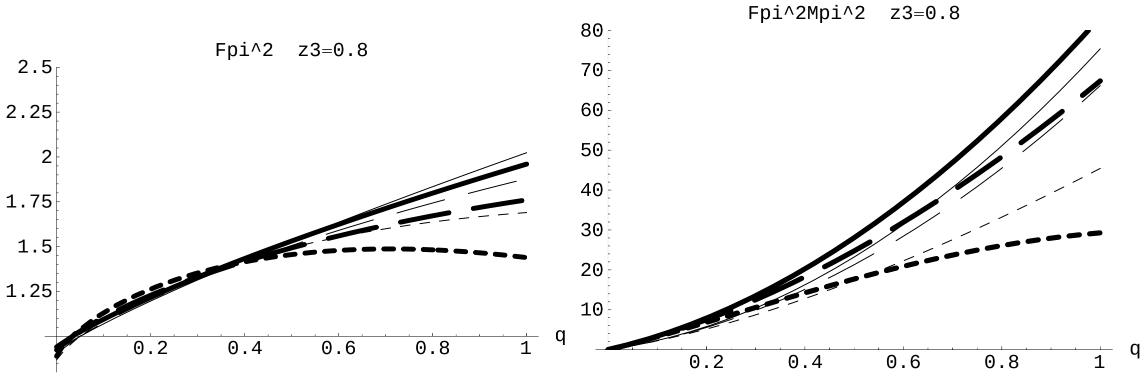

Figure 2: $\tilde{F}_\pi^2/F_\pi^2$ (left) and $\tilde{F}_\pi^2\tilde{M}_\pi^2/(F_\pi^2 M_\pi^2)$ (right) as functions of $q = \tilde{m}/m_s$. Solid, long-dashed and dashed curves correspond respectively to $X(3) = 0.8, 0.4, 0.2$. Thick (thin) lines are drawn for $r = 30$ (20). We set $Z(3) = 0.8$ and NNLO remainders are neglected.

Therefore, one can extract only mild constraints on the parameters of interest from experimental data : it is far from clear whether the usual description of chiral symmetry breaking, triggered by a large quark condensation and independent from strange sea-quark effects, holds or not.

5. Three-flavour χPT and lattice simulations

Lattice simulations may suffer from unexpected systematics in chiral extrapolations due to a strong m_s-dependence of chiral order parameters, and the resulting numerical competition between LO and NLO in three-flavour chiral series. But they may also shed some light on this problem, since they allow one to vary the quark masses, and thus enhance or suppress Zweig-rule violating contributions accordingly [14]. We consider a lattice simulation with (2+1) flavours : two flavours are set to a common mass $\tilde{m}$, whereas the third one is kept at the same mass as the physical strange quark m_s. Each quantity X observed in the physical situation (m, m, m_s) has a lattice counterpart $\tilde{X}$ for $(\tilde{m}, \tilde{m}, m_s)$. One can study the variation of $\tilde{F}_P^2$ and $\tilde{F}_P^2\tilde{M}_P^2$ according to

$$q = \frac{\tilde{m}}{m_s}, \qquad r = \frac{m_s}{m}, \qquad X(3) = \frac{2m\Sigma(3)}{F_\pi^2 M_\pi^2}, \qquad Z(3) = \frac{F^2(3)}{F_\pi^2} \tag{5.1}$$

Figure 2 illustrates how the dependence of hadronic observables on quark masses is related to Zweig-rule violating sea-quark effects: if the latter are large [$X(3) = 0.2 < X(2)$, dashed line], the curves bend more than in the case of negligible sea-quark loops [$X(3) = 0.8 \sim X(2)$, solid line].

Actually, lattice simulations are performed in a finite spatial box, whereas time is sent to infinity to single out the ground state. For sufficiently large boxes, the low-energy effective theory is identical to χPT, with the same values of the chiral couplings as in an infinite volume. The only difference arises in the propagators of the Goldstone modes, so that the chiral series for $\tilde{F}_P^2$ and $\tilde{F}_P^2\tilde{M}_P^2$ change only through tadpole logarithms. One can extend ReχPT to cope with such a problem by noting that only a part of finite-volume corrections computed at NLO in χPT has to involve the physical masses of the Goldstone bosons [14]. The relative finite-volume corrections for these observables are significant for $L = 1.5$ fm, but much smaller for $L = 2.5$ fm. In addition, the corrections are smaller for $\tilde{F}_\pi^2\tilde{M}_\pi^2$ than for the decay constant. By inspection, we see that $\tilde{F}_P^2\tilde{M}_P^2$

$(P = \pi, K)$ in large volumes is a quantity for which we manage a good control of finite-volume effects, whatever the impact of sea $s\bar{s}$ pairs on the pattern of $N_f = 3$ chiral symmetry breaking [14]. More specifically, the two ratios:

$$R_\pi = \frac{1}{q}\frac{\tilde{F}_\pi^2 \tilde{M}_\pi^2}{F_\pi^2 M_\pi^2}, \qquad R_K = \frac{2}{(q+1)}\frac{\tilde{F}_K^2 \tilde{M}_K^2}{F_K^2 M_K^2}, \tag{5.2}$$

are only mildly affected by finite-volume effects, and their q-dependence should provide valuable information on the importance of strange-quark loops. NNLO remainders blur slightly the picture, but they do not prevent the assessment of the effect.

6. Conclusion

The presence of massive $s\bar{s}$-pairs in the QCD vacuum may induce significant differences in the pattern of chiral symmetry breaking between the $N_f = 2$ and $N_f = 3$ chiral limits. This effect, related to the violation of the Zweig rule in the scalar sector, may destabilise three-flavour chiral expansions numerically and may yield large systematics for chiral extrapolations of lattice data down to very light quark masses. We have compared the situation in the two- and three-flavour chiral limits : the combination of $\pi\pi$ and πK data does not favour the usual picture of a large quark condensation independent of the number of massless flavours. We indicated how chiral extrapolations of lattice results with three dynamical quarks could be affected in the case of significant differences between the $N_f = 2$ and $N_f = 3$ chiral limits. In addition, we suggested a way to test this scenario on the lattice, through two dimensionless ratios which prove sensitive to this effect, with only a mild impact of finite-volume corrections.

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