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Resumming QCD vacuum fluctuations
in three-flavor Chiral Perturbation Theory

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Abstract. Due to its light mass, of order $\Lambda_{\rm QCD}$, the strange quark can play a special role in chiral symmetry breaking (χSB): differences in the pattern of χSB in the limits $N_f = 2$ ($m_u, m_d \to 0$, m_s physical) and $N_f = 3$ ($m_u, m_d, m_s \to 0$) may arise due to vacuum fluctuations of $s\bar{s}$ pairs, related to the violation of the Zweig rule in the scalar sector and encoded in particular in the $O(p^4)$ low-energy constants L_4 and L_6. In case of large fluctuations, we show that the customary treatment of $SU(3) \times SU(3)$ chiral expansions generates instabilities upsetting their convergence. We develop a systematic program to cure these instabilities by resumming non-perturbatively vacuum fluctuations of $s\bar{s}$ pairs, in order to extract information about χSB from experimental observations even in the presence of large fluctuations. We advocate a Bayesian framework for treating the uncertainties due to the higher orders. As an application, we present a three-flavor analysis of the low-energy $\pi\pi$ scattering and show that the recent experimental data imply a lower bound on the quark mass ratio $2m_s/(m_u + m_d) \geq 14$ at 95% confidence level. We outline how additional information may be incorporated to further constrain the pattern of χSB in the $N_f = 3$ chiral limit.

1 Introduction

Light quarks have their own hierarchy of masses. On one hand, m_u and m_d are much smaller than any intrinsic QCD scale, and their non-zero values induce only small corrections to the $SU(2) \times SU(2)$ chiral limit, in which $m_u = m_d = 0$. A systematic expansion in m_u and m_d, keeping all remaining quark masses at their physical values, defines the two-flavor chiral perturbation theory (χPT) [1]. On the other hand, the mass m_s of the strange quark is considerably higher (see, e.g., [2] and references therein for recent determinations); indeed, it is nearly of the order of $\Lambda_{\rm QCD}$, the characteristic scale describing the running of the QCD effective coupling. Nevertheless, a slowly convergent $SU(3) \times SU(3)$ chiral expansion is conceivable [3]. This is suggested from a comparison of the kaon mass M_K with the mass scale $\Lambda_H \sim 1\,{\rm GeV}$ of (strange) QCD bound states not protected by chiral symmetry: $M_K^2/\Lambda_H^2 \sim 0.25$–$0.30$. Due to the rather specific

value of m_s, the strange quark plays a special role among all six quarks.

(i) m_s is small enough to be used as an expansion parameter (at least in some restricted sense) and to relate properties of the QCD vacuum in the $SU(3) \times SU(3)$ chiral symmetry limit $m_u = m_d = m_s = 0$ to observable quantities.

(ii) Unlike m_u, m_d, the strange-quark mass is sufficiently large, $m_s \sim \Lambda_{\rm QCD}$, to influence the magnitude of order parameters characteristic of the $SU(2) \times SU(2)$ chiral limit $m_u, m_d = 0$ with m_s fixed at its physical value.

(iii) At the same time, m_s is not large enough to suppress loop effects of massive $\bar{s}s$ vacuum pairs. This is to be contrasted with heavy quarks $Q = c, b, t$ for which $m_Q \gg \Lambda_{\rm QCD}$ and the effect of $\bar{Q}Q$ pairs on the vacuum structure is expected to be tiny.

The above remarks single out the role of massive strange sea quarks, and suggest a possibly different behavior for $N_f = 2$ and $N_f = 3$ chiral dynamics. The origin of this difference clearly appears in connection with the possibility that in the vacuum channel ($J^{PC} = 0^{++}$) the Zweig rule and the $1/N_c$ expansion break down. This is strongly suggested by scalar meson spectroscopy [4], sum rule studies [5–8], as well as by instanton-inspired mod-

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els [9][1]. Furthermore, the enhancement of Zweig-rule violating effects of $\bar{s}s$ pairs on chiral order parameters has a natural theoretical interpretation as a consequence of fluctuations of the lowest eigenvalues of Euclidean QCD Dirac operator, in particular of their density [10]. These fluctuations would only affect quantities dominated by the infrared end of the Dirac spectrum [11]; however, this is precisely the case of chiral order parameters such as the quark condensate and the pion decay constant. (Most of the observables not protected by chiral symmetry are not especially sensitive to small Dirac eigenvalues, and they have no particular reason to break the Zweig rule or the $1/N_c$ expansion.) Fluctuations of small Dirac eigenvalues lead to a large long-range correlation between 0^+ massive $\bar{s}s$ and massless $\bar{u}u + \bar{d}d$ pairs. This correlation enhances the $SU(2) \times SU(2)$ order parameters,

$$\Sigma(2) = -\lim_{m_u, m_d \to 0} \langle \bar{u}u \rangle|_{m_s = \text{physical}} , \qquad (1)$$

$$F(2)^2 = \lim_{m_u, m_d \to 0} F_\pi^2|_{m_s = \text{physical}} , \qquad (2)$$

by a contribution which is induced from vacuum $\bar{s}s$ pairs. The "induced condensate" and "induced decay constant" [11,12] are proportional to m_s and vanish in the $SU(3) \times SU(3)$ chiral limit $m_u = m_d = m_s = 0$. As a result the $N_f = 3$ condensate $\Sigma(3)$ and the decay constant $F(3)^2$ can be substantially suppressed compared to the corresponding two-flavor order parameters,

$$\Sigma(2) > \Sigma(3) = \Sigma(2)|_{m_s=0} , \qquad (3)$$

$$F(2)^2 > F(3)^2 = F(2)^2|_{m_s=0} . \qquad (4)$$

The existence of this paramagnetic effect and its sign can be expected on general theoretical grounds [11], but its magnitude depends on the size of fluctuations of small Dirac eigenvalues, which is hard to infer from first principles. A general discussion of the interplay between chiral order and fluctuations in the QCD vacuum can be found in [13].

The main question to be asked is: how can the effect of vacuum fluctuations on chiral symmetry breaking be detected experimentally? Recall that two-flavor order parameters are most easily accessible via low-energy $\pi\pi$ scattering. Using accurate recent data [14], we have inferred values for the $N_f = 2$ condensate and decay constant; expressed in suitable physical units, we found [15]

$$X(2) = \frac{(m_u + m_d)\Sigma(2)}{F_\pi^2 M_\pi^2} = 0.81 \pm 0.07 , \qquad (5)$$

$$Z(2) = \frac{F(2)^2}{F_\pi^2} = 0.89 \pm 0.03 . \qquad (6)$$

The fact that both $X(2)$ and $Z(2)$ are rather close to 1 indicates that, as long as m_s is kept at its physical value, the effect of non-zero m_u, m_d is indeed small. This in turn suggests that the standard two-flavor χPT is a well-behaved expansion [1]; its leading order, described by the decay

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[1] It should also be visible in fully unquenched lattice simulations.

constant $F^2 \equiv F(2)^2$ and by the $N_f = 2$ quark condensate $\Sigma(2) \equiv F^2 B$, is dominant. On the other hand, the three-flavor order parameters $\Sigma(3)$ and $F(3)^2$ are more difficult to pin down, since they require an extrapolation to $m_s = 0$. The latter necessitates the use of three-flavor χPT, including more observables such as the masses and decay constants of the whole octet of Goldstone bosons, the K–π form factors, K–π scattering amplitude, etc. The $N_f = 3$ χPT involves more low-energy constants starting in order $O(p^4)$, and higher orders are likely to be more important than in the two-flavor case. Most existing analyses [3,16–18] are based on the explicit assumption that the effect of vacuum fluctuations of $\bar{s}s$ pairs on order parameters is small: it is usually assumed that the two parameters of the $O(p^2)$ Lagrangian $F_0 \equiv F(3)$ and $\Sigma(3) \equiv F_0^2 B_0$ are such that $F_0 \approx F_\pi$ and $(m_u + m_d)\Sigma(3) \approx F_\pi^2 M_\pi^2$, i.e., that the corrections due to non-vanishing m_s can be treated as a small perturbation.

A closely related assumption concerns the smallness of the two $O(p^4)$ low-energy constants (LECs) $L_6^r(\mu)$ and $L_4^r(\mu)$ which describe the large-N_c suppressed and Zweig-rule violating effects of fluctuations in the vacuum channel. Experimental information on the actual size of these two constants has been rather scarce; for a long time it was customary to posit $L_6^r(M_\rho) = (-0.2 \pm 0.3) \times 10^{-3}$ and $L_4^r(M_\rho) = (-0.3 \pm 0.5) \times 10^{-3}$ as an input to both one-loop [3,16] and two-loop calculations [17,18]. More recently, attempts of indirect estimates of L_4 and L_6 have appeared, all pointing towards small positive values compared to the old Zweig-rule based estimates mentioned above. Rapidly convergent sum rules for the correlator $\langle(\bar{u}u)(\bar{s}s)\rangle$ [5–8] yield the rough estimate $L_6^r(M_\rho) = (0.6 \pm 0.3) \times 10^{-3}$, while from the analysis of π–K sum rules [19] it has been concluded that $L_4^r(M_\rho) = (0.2 \pm 0.3) \times 10^{-3}$. The last conclusion has been confirmed in a recent two-loop fit to the scalar form factors [20]. The point is that the effect of such small shifts on order parameters is amplified by large coefficients: with the above estimates, $\Sigma(3)$ and $F(3)^2$ can be suppressed compared to $\Sigma(2)$ and $F(2)^2$ respectively by as much as a factor of 2. In this way, vacuum fluctuations of $\bar{s}s$ pairs could lead to a particular type of instability in three-flavor χPT.

The main purpose of the present work is to investigate instabilities in $N_f = 3$ χPT that would specifically arise from the (partial) suppression of order parameters $\Sigma(3)$ and F_0^2, and to propose a systematic non-perturbative modification (resummation) of the standard χPT recipe that could solve the problem. We assume that the whole expansion of relevant observables in powers of m_s is globally – though slowly and at most asymptotically – convergent. The problem may occur with the enhancement of particular terms of the type $m_s L_6$ or $m_s L_4$ that appear with large coefficients and can be identified as arising from fluctuation of vacuum $\bar{s}s$ pairs. These terms are responsible for the important "induced contributions" to $\Sigma(2)$ and $F(2)^2$, explaining why $\Sigma(2)$ and $F(2)^2$ at physical m_s could be substantially larger than their $m_s = 0$ limit $\Sigma(3)$ and $F(3)^2$ respectively. We show that in order to solve this particular problem it is not necessary to modify the

standard chiral counting rules as in generalized χPT [21]. The modification we propose is more modest: within the standard expansion scheme in powers of quark masses and external momenta, it appears to be sufficient to resum the fluctuation terms driven by $m_s L_4$ and $m_s L_6$ in the usual perturbative reexpression of the order parameters $m_s \Sigma(3)$ and F_0^2 in terms of observables such as $M_\pi, M_K, \ldots$ and physical decay constants. This resummation is of importance for the purpose of extracting the value of $N_f = 3$ order parameters from experiment.

The possible effects of vacuum fluctuations in three-flavor χPT and their resummation are discussed in Sects. 2 and 3. These two sections are focused on Goldstone boson masses and decay constants, which are the observables directly entering the reexpression of order parameters $m\Sigma(3)$ and F_0^2. In our approach, the influence of higher χPT orders ($O(p^6)$ and higher) is encoded into a few parameters referred to as "NNLO remainders", which are kept through the whole analysis whatever their values. The latter depend on the model one takes for the higher order counterterms and one hopes that they remain reasonably small independently of the model used. The result of this part of our article is an exact expression of L_4, L_5, L_6 and L_8 in terms of the three fundamental parameters

$$X(3) = \frac{(m_u + m_d)\Sigma(3)}{F_\pi^2 M_\pi^2} , \quad Z(3) = \frac{F_0^2}{F_\pi^2} , \quad r = \frac{2m_s}{m_u + m_d} , \tag{7}$$

and four NNLO remainders. Using these expressions inside the χPT formulae for various additional observables, one can hope to pin down the values of $X(3), Z(3)$ and r for a given set of assumptions on higher orders (NNLO remainders). The logical structure of the problem naturally calls for a Bayesian statistical type approach [22].

As a first application we consider the three-flavor analysis of $\pi\pi$ scattering, since today rather accurate data exist in this case and we know from past studies [11,13] that a strong correlation exists between the value of r and the characteristics of the two-flavor chiral limit as revealed in low-energy $\pi\pi$ scattering. In Sect. 4 a quantitative analysis of this correlation is presented for the first time. On the other hand, the $N_f = 3$ order parameters $X(3)$ and $Z(3)$ cannot be extracted from the $\pi\pi$ data alone. In Sect. 5 we survey some possibilities of learning about these fundamental order parameters from π–K scattering, $\eta \to 3\pi$ decays, OPE condensates and sum rules and, last but not least, from lattice simulations with three fully dynamical fermions: we present the corresponding extrapolation formulae using our resummed χPT formulation.

2 Convergence and instabilities of $N_f = 3$ chiral expansion

We first recall the general structure of three-flavor χPT [3], emphasizing where and how the instabilities due to vacuum fluctuations of $\bar{s}s$ pairs [11] could possibly show up. Unless stated otherwise, a typical quantity subject to

the expansion in powers of running quark masses m_u, m_d, m_s will be thought of as a connected QCD correlation function of quark currents (V, A, S, P) with external momenta fixed somewhere in a low-energy region away from the singularities generated by Goldstone bosons. We will take as a working hypothesis that the usual low-energy observables, e.g., Goldstone boson masses, decay constants, form factors and scattering amplitudes (at particular kinematical points), when linearly expressed through such QCD correlation functions, exhibit optimal convergence properties. While a similar assumption is implicitly made in the standard off-shell formulation of χPT [1,3], we will shortly argue that in the presence of important vacuum fluctuations this assumption should be understood as a restriction: observables that are not *linearly* expressible in terms of QCD correlators, e.g., *ratios* of Goldstone boson masses, need not admit a well convergent perturbative treatment and they should be treated with a particular care. This selects for instance $F_\pi^2 M_\pi^2$, F_π^2 and $F_\pi^2 F_K^2 A_{\pi K}$ (where $A_{\pi K}$ denotes the πK scattering amplitude), but rules out M_π^2.

2.1 The bare χPT series

The chiral expansion of symmetry-breaking observables in terms of the three lightest quark masses m_u, m_d, m_s is actually not a genuine power series expansion, due to the presence of chiral logarithms, which reflect infrared singularities characteristic of the chiral limit. One can nevertheless give an unambiguous scale-independent meaning to the renormalized coefficients of each power of individual quark masses. An observable A can be represented as a formal series

$$A = \sum_{j,k,l} m_u^j m_d^k m_s^l A_{jkl}, \tag{8}$$

where the coefficients $A_{jkl}[m_u, m_d, m_s; B_0, F_0; L_1^r(\mu) \ldots L_{10}^r(\mu); C_1^r(\mu) \ldots C_{90}^r(\mu); \ldots]$ are defined in terms of the constants contained in the effective Lagrangian.

(i) The basic order parameters B_0 and F_0 which are related to the three-flavor chiral limit of the quark condensate and of the pion decay constant respectively,

$$\Sigma(3) = - \lim_{m_u, m_d, m_s \to 0} \langle \bar{u}u \rangle ,$$
$$F_0 \equiv F(3) = \lim_{m_u, m_d, m_s \to 0} F_\pi , \tag{9}$$
$$B_0 = \frac{\Sigma(3)}{F(3)^2} ;$$

(ii) the 10 $O(p^4)$ LECs $L_i^r(\mu)$;
(iii) the 90 $O(p^6)$ LECs $C_i^r(\mu)$ [23], and eventually higher order counterterms. All LECs are renormalized at the scale μ. In addition, the A_{jkl} depend logarithmically on the quark masses through the Goldstone boson masses in the loops, and this dependence is such that for each jkl the coefficient A_{jkl} is independent of the scale μ. The representation (8) has been explicitly worked out for some observables to one [3] and two loops [17,18,20] and there is no

doubt that it extends to all orders of the chiral expansion. We shall refer to the expansion expressed in the form (8) as a *bare expansion*, to emphasize that it is entirely written in terms of the parameters of the effective Lagrangian – no reexpression of the latter in terms of observable quantities has been performed. It is crucial that even before one starts rewriting and reordering the series (8) in powers of Goldstone boson masses, the full renormalization of the bare expansion (8) can be performed order by order in the quark masses. Consequently, the coefficients A_{jkl} are finite as well as cut-off and renormalization-scale independent for all values of quark masses and of (renormalized) LECs in the effective Lagrangian.

In view of possible applications, we are concerned with practical questions related to the convergence properties of the bare χPT expansion (8) in QCD. The latter will depend on the values of running quark masses and on the values of the LECs at the typical hadronic scale $\Lambda_H \sim M_\rho$ set by the masses of non-Goldstone hadrons. In particular, one should question the convergence of the bare chiral expansion for the actual values of quark masses and not just in the infinitesimal vicinity of the chiral limit. In the real world, all three quarks, u, d, s, are sufficiently light,

$$m_u(\Lambda_H), m_d(\Lambda_H) \ll m_s(\Lambda_H) \ll \Lambda_H , \qquad (10)$$

to expect a priori some (at least asymptotic) convergence of the three-flavor bare χPT series. As pointed out in [7, 11], instabilities of the latter can nevertheless occur due to fluctuations of massive $\bar{s}s$ pairs in the vacuum. The importance of such pairs is measured by the strength of the effective QCD coupling; i.e., comparing m_s with Λ_{QCD}, rather than with the hadronic scale Λ_H. Furthermore, the impact of these fluctuations is proportional to m_s. Hence, instabilities due to fluctuations of vacuum quark–antiquark pairs turn out to be particularly relevant for strange quarks and could manifest themselves when two- and three-flavor chiral expansions are compared.

It has been argued [7,11] that fluctuations of $\bar{s}s$ pairs lead to a partial suppression of the three-flavor condensate $\Sigma(3)$, reducing the relative importance of the first term in the bare expansion of the Goldstone boson masses. We can consider for instance the Ward identity related to the mass of the pion (from now on we neglect isospin breaking and take $m_u = m_d = m$):

$$F_\pi^2 M_\pi^2 = 2m\Sigma(3) + 2mm_s Z^s$$
$$+ 4m^2 \left[A + Z^s + \frac{B_0^2}{32\pi^2} \left(3 \log \frac{M_K^2}{M_\pi^2} + \log \frac{M_\eta^2}{M_K^2} \right) \right]$$
$$+ F_\pi^2 M_\pi^2 d_\pi . \qquad (11)$$

The parameters Z^s and A are defined in terms of the LECs $L_6(\mu), L_8(\mu)$ and logarithms of Goldstone boson masses (their expression is recalled in Appendix A). Vacuum fluctuations of $\bar{s}s$ pairs show up in the term $m_s Z^s$. For the physical value of $m_s \sim \Lambda_{QCD}$, the corresponding $O(p^4)$ term $2mm_s Z^s$ can be as important [5,7,8] as the leading-order condensate term $2m\Sigma(3)$. Even then, the remainder d_π, which collects all $O(p^6)$ and higher contributions, can

still be small: $d_\pi \ll 1$. In other words, vacuum fluctuations need not affect the *overall* convergence of the bare chiral expansions such as (8) or (11) at least for some well-defined selected class of observables.

2.2 The role of NNLO remainders

Let us write a generic bare expansion (8) in a concise form:

$$A = A_{LO} + A_{NLO} + A\,\delta A. \qquad (12)$$

Equation (12) is an identity: A_{LO} collects leading powers in quark masses in the bare expansion (8) (e.g., the condensate term in (11)), A_{NLO} consists of all next-to-leading contributions (the second and third terms in (11)), whereas $A\,\delta A$ stands for the sum of all remaining terms starting with the next-to-next-to-leading order (NNLO). In (11), the latter is denoted $\delta(F_\pi^2 M_\pi^2) \equiv d_\pi$.

With this setting, A can be identified with the exact (experimental) value of the observable A. Usually, A_{LO} corresponds to the $O(p^2)$ contribution, A_{NLO} to $O(p^4)$ and $A\,\delta A$ collects all higher orders starting with $O(p^6)$[2]. δA will be referred to as "NNLO remainder". A precise definition of δA involves some convention in writing the argument in the chiral logarithms contained in the one-loop expression for A_{NLO}. To illustrate this point, consider the typical next-to-leading expression:

$$A_{NLO} = \sum_{qq'} m_q m_{q'} \left[a_{qq'}(\mu) + \sum_{PQ} a_{qq'}^{PQ} k_{PQ}(\mu) \right] , \quad (13)$$

or

$$A_{NLO} = \sum_{q} m_q \left[a_q(\mu) + \sum_{PQ} a_q^{PQ} k_{PQ}(\mu) \right] , \qquad (14)$$

corresponding respectively to a leading-order term $A_{LO} = O(m_{quark})$ and $A_{LO} = O(1)$. Here $q, q' = (u, d, s)$ and P, Q label Goldstone bosons. We have introduced the loop factor in the general case of unequal masses [3]:

$$k_{PQ}(\mu) = \frac{1}{32\pi^2} \frac{M_P^2 \log(M_P^2/\mu^2) - M_Q^2 \log(M_Q^2/\mu^2)}{M_P^2 - M_Q^2} , \qquad (15)$$

which in the limit of equal masses becomes

$$k_{PP}(\mu) = \frac{1}{32\pi^2} \left[\log \frac{M_P^2}{\mu^2} + 1 \right] . \qquad (16)$$

In (13) and (14), the constants $a_{qq'}(\mu)$ [$a_q(\mu)$] are expressed in terms of $O(p^4)$ LECs $L_i^r(\mu)$ multiplied by the appropriate powers of B_0 and F_0. These constants are defined in the chiral limit and are consequently independent of the quark masses, similarly to the known numerical coefficients $a_{qq'}^{PQ}$ [a_q^{PQ}].

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[2] The case of a quantity whose expansion only starts at $O(p^4)$ or higher requires particular care.

The only requirement from χPT is that A_{NLO} reproduces the $O(p^4)$ behavior in the limit of small quark masses $m_{\text{quark}} \to 0$; i.e., when the Goldstone boson masses M_P^2 in the loop factors (15) and (16) are replaced by their respective leading-order contributions. Once this mathematical condition is satisfied, different ways of writing the arguments of the chiral logarithms for *physical values* of quark masses merely correspond to different conventions in defining the NNLO remainders δA. For observables of the form of (13) and (14) at $O(p^4)$, we will use the convention which consists in writing in (15) the physical values of the Goldstone boson masses M_P^2; alternatively, we could have used the sum of LO and NLO contributions to M_P^2. This concerns, in particular, the expansion of the Goldstone boson masses and decay constants. In the latter case one has $P = Q$ and the convention simply amounts to writing the $O(p^4)$ tadpoles, in the notation of [3], as follows:

$$\mu_P = \frac{1}{32\pi^2} \frac{M_P^2\big|_{\text{LO}}}{F_0^2} \log \frac{M_P^2\big|_{\text{phys.}}}{\mu^2} \,. \qquad (17)$$

The same rule can be applied to the unitarity corrections arising in the bare expansion of subtraction constants that define form factors and low-energy $\pi\pi$ [24] and πK [19, 25, 26] amplitudes. Such a prescription (details are given in Sect. 4.1) will suffice for the quantities considered in this article.

Not much is known about the size of the NNLO remainders despite the fact that complete $SU(3) \times SU(3)$ two-loop calculations do exist for some observables [17, 18, 20] and the general structure of the generating functional is known to this order [23]. Following this line, the bare expansion can be pushed further and the NNLO remainder δA can be represented as

$$A \, \delta A = \Delta_{2L}^A(\mu) + \Delta_{1L}^A(\mu) + \Delta_{\text{tree}}^A(\mu) + \dots \,, \qquad (18)$$

where the ellipsis stands for $O(p^8)$ and higher contributions. The splitting of the $O(p^6)$ part [23] into the genuine two-loop contribution Δ_{2L} (containing only $O(p^2)$ vertices), the one-loop contribution Δ_{1L} (with the insertion of a single $O(p^4)$ vertex) and the tree $O(p^6)$ contribution Δ_{tree} depends on the renormalization scale and scheme.

Several ingredients are actually needed to estimate δA from the representation (18). The first two terms (loop contributions) depend respectively on $O(p^2)$ parameters mB_0, m_sB_0, F_0 and on $O(p^4)$ LECs $L_i^r(\mu)$. Furthermore, the tree-level counterterms $\Delta_{\text{tree}}^A(\mu)$ are built up from the 90 LECs $C_i^r(\mu)$ that define the $O(p^6)$ effective Lagrangian. Even if some of them can presumably be determined from the momentum dependence of form factors, decay distributions and scattering amplitudes (e.g., quadratic slopes), the remaining unknown $O(p^6)$ constants, which merely describe the higher order dependence on quark masses, are probably much more numerous than the observables that one can hope to measure experimentally. At this stage some models (resonance saturation, large N_c, NJL, ...) and/or lattice determinations are required [27], but the large number of terms contributing to a given Δ_{tree}^A makes

the resulting uncertainty in δA delicate to estimate. Finally, it is worth stressing that only the sum of the three components shown in (18) is meaningful. An estimate of the size of the NNLO remainders is therefore not possible without a precise knowledge of the $O(p^2)$ and $O(p^4)$ constants mB_0, F_0 and the L_i's.

In this paper, we do not address the problem of determining the NNLO remainders on the basis of (18). We are going to show that interesting non-perturbative conclusions can be reached, even if we do not decompose the NNLO remainders and investigate the behavior of the theory as a function of their size. We are primarily interested in the constraints imposed by experimental data on the fundamental QCD $SU(3) \times SU(3)$ chiral order parameters (and quark mass ratio)

$$X(3) = \frac{2m\Sigma(3)}{M_\pi^2 F_\pi^2}, \quad Z(3) = \frac{F^2(3)}{F_\pi^2}, \quad r = \frac{m_s}{m}, \quad (19)$$

$$Y(3) = \frac{2mB_0}{M_\pi^2} = \frac{X(3)}{Z(3)} \,, \qquad (20)$$

under various theoretical assumptions on the NNLO remainders (i.e., on higher χPT orders). A suitable approach to this problem is provided by Bayesian statistical inference [22]. (See Appendix B for a brief review adapted to the case of χPT.) The output of this analysis is presented as marginal probability distribution functions for the fundamental parameters (19) and it depends not only on the experimental input but also on the state of our knowledge of higher χPT orders. In this approach the latter dependence is clearly stated and can be put under control: the analysis can be gradually refined if new information on the relevant NNLO remainders becomes available either through (18) or in another way.

We start with a very simple theoretical assumption on higher orders: the bare chiral expansion of "good observables" as defined at the beginning of this section is *globally convergent*. By these words, we mean that the NNLO remainder δA in the identity (12) is small compared to 1:

$$\delta A \ll 1 \,, \qquad (21)$$

for the physical values of the quark masses and for the actual size of the $O(p^2)$ and $O(p^4)$ parameters. On general grounds, one expects $\delta A = O(m_{\text{quark}}^2)$. In the worst case, its size should be $\delta A = O(m_s^2) \sim (30\%)^2 = 0.1$, but in many situations δA turns out to be $O(m_s m)$ or even $O(m^2)$ and is therefore more suppressed[3]. These cases are usually identified as a consequence of $SU(2) \times SU(2)$ low-energy theorems. (Such suppressions are not claimed from arguments based on the Zweig rule, since we never assume the latter.) However the NNLO remainders will not be neglected or used as small expansion parameters in the following.

On the other hand, no particular hierarchy will be assumed between the leading $O(p^2)$ and next-to-leading

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[3] We take as order of magnitudes 10% for $O(m)$ contributions and 30% for $O(m_s)$ terms. This can be related to the typical sizes of violation for $SU(2) \times SU(2)$ and $SU(3) \times SU(3)$ flavor symmetries.

$O(p^4)$ components of (12). By definition, for infinitesimally small quark masses m_u, m_d, m_s, one should have

$$A_{\mathrm{NLO}} \ll A_{\mathrm{LO}}, \qquad X_A \equiv \frac{A_{\mathrm{LO}}}{A} \sim 1. \qquad (22)$$

However, due to vacuum fluctuations of $\bar{q}q$ pairs, the condition (22) can be easily invalidated for the physical value of $m_s \sim \Lambda_{\mathrm{QCD}}$: as discussed in [11], the three-flavor condensate $\Sigma(3)$ in (11) may be of a comparable size to – or even smaller than – the term $m_s Z^s$, reflecting the vacuum effects of massive $\bar{s}s$ pairs. At the same time, vacuum fluctuations need not affect the overall convergence of the bare chiral expansion (11), i.e., the condition (21) can still hold for "good observables" such as $F_\pi^2 M_\pi^2$. We will call *conditionally convergent* an observable for which $\delta A \ll 1$ but the hierarchy condition (22) does not hold.

2.3 Instabilities in chiral series

Standard χPT consists of two different steps.
(1) The first step coincides with what has been described above as the "bare expansion" in powers of quark masses and external momenta. The coefficients of this expansion are unambiguously defined in terms of parameters of the effective Lagrangian $B_0, F_0, L_i, \ldots$, independently of the convergence properties of the bare expansion.
(2) The second step consists in rewriting the bare expansion as an expansion in powers of Goldstone boson masses, by eliminating order by order the quark masses m and m_s and the three-flavor order parameters $\Sigma(3)$, $F(3)$ in favor of the physical values of Goldstone boson masses M_P^2 and decay constants F_P^2. For this aim one inverts the expansion of the Goldstone boson masses:

$$2mB_0 = M_\pi^2 \left(1 + \sum_P c_P^B M_P^2 + \ldots\right), \qquad (23)$$

where c_P^B contains the low-energy constants L_i and the chiral logarithms. A similar "inverted expansion" is worked out for F_0^2:

$$F_0^2 = F_\pi^2 \left(1 + \sum_P c_P^F M_P^2 + \ldots\right), \qquad (24)$$

and for the quark mass ratio

$$\frac{m_s + m}{2m} = \frac{M_K^2}{M_\pi^2} \left(1 + \sum_P c_P^r M_P^2 + \ldots\right). \qquad (25)$$

As a result of these two steps, observables other than M_π^2, M_K^2, F_π^2 (already used in (23), (24) and (25)) are expressed as expansions in powers of M_P^2 and $\log M_P^2$ with their coefficients depending on the constants L_i, C_i, etc.

We now argue that large vacuum fluctuations of $\bar{s}s$ pairs could represent a serious impediment to the second step, i.e., to the perturbative reexpression of order parameters. This may happen if the bare expansion (12)

of Goldstone boson masses and decay constants is only conditionally convergent: the leading and next-to-leading contributions are then of comparable size, $A_{\mathrm{LO}} \sim A_{\mathrm{NLO}}$, despite a good global convergence $\delta A \ll 1$. Let us concentrate on the three-flavor GOR ratio $X(3)$, defined in (19), which measures the condensate $\Sigma(3)$ in the physical units $F_\pi^2 M_\pi^2$. In the definition of $X(3)$ we can replace $F_\pi^2 M_\pi^2$ by its bare expansion (11) and investigate the behavior of $X(3)$ in limits of small quark masses. First of all, in the $SU(2) \times SU(2)$ chiral limit one obtains

$$\lim_{m \to 0} X(3) = \frac{\Sigma(3)}{\Sigma(2)} \qquad (m_s \text{ fixed}), \qquad (26)$$

from the definition of the two-flavor condensate $\Sigma(2) \equiv \lim_{m \to 0} F_\pi^2 M_\pi^2 / (2m)$. On the other hand, if both m and m_s tend to zero, we obtain by definition

$$\lim_{m, m_s \to 0} X(3) = 1. \qquad (27)$$

Consequently, as long as the three-flavor condensate $\Sigma(3)$ is suppressed with respect to the two-flavor condensate $\Sigma(2)$ ($\Sigma(3) \sim \Sigma(2)/2$ is suggested by the sum rule analysis in [5,6,8]), the physical value of $X(3)$ cannot be simultaneously close to its limiting values in both $SU(2) \times SU(2)$, (26), and $SU(3) \times SU(3)$, (27).

We expect the limit "$m \to 0$, m_s physical" to be a good approximation of the physical situation of very light u and d quarks, and thus the limiting value expressed by (26) to be quite close to the physical $X(3)$. On the other hand, the variation of $X(3)$ between $m_s = 0$ and m_s physical may be substantial, due to important fluctuations of the lowest modes of the (Euclidean) Dirac operator [10], which correspond to a significant Zweig-rule violating correlation between massless non-strange and massive strange vacuum pairs [11]. The latter contribute to the two-flavor condensate by the amount $m_s Z^s$. (We see from (11) that $\Sigma(2) = \Sigma(3) + m_s Z^s + \ldots$) As long as $\Sigma(3)$ is comparable to (or smaller than) the "induced condensate" $m_s Z^s$, the hierarchy condition between LO and NLO (22) will be violated for the bare expansion (11), in spite of a good global convergence $d_\pi \ll 1$. The inverted expansion of $X(3)$, in which $F_\pi^2 M_\pi^2$ is replaced by its expansion (11),

$$X(3) = \frac{1}{1 + \dfrac{m_s Z^s}{\Sigma(3)} + \ldots} = 1 + \sum_P c_P^X M_P^2 + \ldots, \qquad (28)$$

would then be invalidated by large coefficients, even for quite modest (and realistic) values of m_s at $1\,\mathrm{GeV}$ around $150\,\mathrm{MeV}$ [2]. In such a case, it is not a good idea to replace in higher orders of the bare expansion $X(3)$ by 1, $2mB_0$ by M_π^2, F_0^2 by F_π^2, etc.

A comment is in order before we describe in detail the non-perturbative alternative to eliminating order by order the condensate parameters and quark masses in bare χPT expansions. The previous example of $X(3)$ can be stated as a failure of the bare expansion of $1/F_\pi^2 M_\pi^2$. Let us remark that this is perfectly compatible with our assumption that the bare expansion of the QCD two-point function of axial-current divergences (i.e., $F_\pi^2 M_\pi^2$) converges

globally. Indeed, consider a generic observable A with its bare expansion (22). The latter unambiguously defines the coefficients of the bare expansion of $1/A$:

$$B = B_{\text{LO}} + B_{\text{NLO}} + B\,\delta B\,, \qquad B \equiv \frac{1}{A}\,, \qquad (29)$$

in terms of those of A:

$$B_{\text{LO}} = \frac{1}{A_{\text{LO}}}\,, \qquad B_{\text{NLO}} = -\frac{A_{\text{NLO}}}{A_{\text{LO}}^2}\,, \qquad (30)$$

$$\delta B = \frac{(1 - X_A)^2}{X_A^2} - \frac{\delta A}{X_A^2}\,, \qquad X_A \equiv \frac{A_{\text{LO}}}{A}\,. \qquad (31)$$

One observes that the global convergence of A does not necessarily imply the convergence of $B = 1/A$. If the expansion of A is only conditionally convergent, i.e., if the relative leading-order contribution X_A is not close to 1, then $\delta(1/A)$ need not be small – even in the extreme case $\delta A = 0$. This explains the origin of instabilities and large coefficients in the inverted expansion such as (23), (24) or (28). At the same time, it motivates the restriction to a *linear space* of "good observables" for which $\delta A \ll 1$. The latter is assumed to be represented by connected QCD correlators, and a priori excludes non-linear functions of them, such as ratios.

3 Constraints from Goldstone boson masses and decay constants

The conditional convergence of $F_P^2 M_P^2$ and/or of F_P^2 does not by itself bar experimental determination of the three-flavor order parameters $X(3)$ and $Z(3)$. It just may prevent the use of perturbation theory in relating them to observable quantities. In this section a systematic non-perturbative alternative is considered in detail.

The starting point is the standard bare expansion of $F_P^2 M_P^2$ and F_P^2 for $P = \pi, K, \eta$. (See (11) for the pion case.) As discussed above, these particular combinations of masses and decay constants are expected to converge well, since they are linearly related to two-point functions of axial/vector currents and of their divergences taken at vanishing momentum transfer. As long as $Z(3) = F_0^2/F_\pi^2 \sim 1$, the convergence of M_P^2 would be as good as for $F_P^2 M_P^2$. If however F_P^2 is only conditionally convergent (i.e., $Z(3)$ significantly smaller than 1), the expansion of M_P^2 could become unstable, in contrast to that of $F_P^2 M_P^2$; the perturbative expansion of $1/F_P^2$ would then exhibit very poor convergence. We have no prejudice in this respect: the size of $Z(3)$ as well as that of $X(3)$ remains an open problem until they are inferred from the data.

The expansion of $F_P^2 M_P^2$ and F_P^2 can be written in the generic form (12), denoting the corresponding NNLO remainders by d_P and e_P respectively. The LO of $F_P^2 M_P^2$ is given by the condensate $\Sigma(3)$ and the NLO contribution is fully determined by the standard $O(p^4)$ LECs $L_6(\mu), L_8(\mu)$ (and L_7 in the case of the η meson). Similarly, at LO F_P^2 coincides with the order parameter $F_0^2 = F^2(3)$ and the NLO contribution is given in terms of $L_5(\mu)$

and $L_4(\mu)$. All necessary formulae can be found in [13]. Here, we follow the notation of the above reference and for the reader's convenience the bare expansions of $F_P^2 M_P^2$ and F_P^2 are reproduced in Appendix A.

3.1 Pions and kaons

For $P = \pi, K$ the mass and decay constant identities (Ward identities) consist of four equations that involve $X(3), Z(3), r = m_s/m, L_6, L_8, L_4, L_5$ and the four NNLO remainders d_π, d_K, e_π, e_K. These identities – given in Appendix A – are *exact* as long as the remainders d_P, e_P are maintained in the formulae and no expansion is performed.

As explained in [11,13], we can combine the mass and decay constant identities (recalled in Appendix A) to obtain two relations between the order parameters X, Y, Z and the fluctuation parameters ρ and λ:

$$X(3) = 1 - \epsilon(r) - [Y(3)]^2 \rho/4 - d,$$
$$Z(3) = 1 - \eta(r) - Y(3)\lambda/4 - e, \qquad (32)$$

where the functions of the quark mass ratio are[4]

$$\epsilon(r) = 2\frac{r_2 - r}{r^2 - 1}, \quad r_2 = 2\left(\frac{F_K M_K}{F_\pi M_\pi}\right)^2 - 1 \sim 36\,,$$

$$\eta(r) = \frac{2}{r - 1}\left(\frac{F_K^2}{F_\pi^2} - 1\right)\,, \qquad (33)$$

and the following linear combinations of NNLO remainders arise:

$$d = \frac{r + 1}{r - 1}d_\pi - \left(\epsilon(r) + \frac{2}{r - 1}\right)d_K\,, \qquad (34)$$

$$e = \frac{r + 1}{r - 1}e_\pi - \left(\eta(r) + \frac{2}{r - 1}\right)e_K\,. \qquad (35)$$

The LECs L_6 and L_4 enter the discussion through the combinations

$$\lambda = 32\frac{M_\pi^2}{F_\pi^2}(r + 2)\Delta L_4\,, \qquad \rho = 64\frac{M_\pi^2}{F_\pi^2}(r + 2)\Delta L_6\,, \quad (36)$$

where the scale-independent differences $\Delta L_i = L_i^r(\mu) - L_i^{\text{crit}}(\mu)$ involve the critical values of the LECs defined by

$$L_4^{\text{crit}}(\mu) = \frac{1}{256\pi^2}\log\frac{M_K^2}{\mu^2} \qquad (37)$$
$$- \frac{1}{128\pi^2}\frac{r}{r^2 + r - 2}\left\{\log\frac{M_K^2}{M_\pi^2} + \left(1 + \frac{1}{2r}\right)\log\frac{M_\eta^2}{M_\pi^2}\right\}\,,$$

$$L_6^{\text{crit}}(\mu) = \frac{1}{512\pi^2}\left(\log\frac{M_K^2}{\mu^2} + \frac{2}{9}\log\frac{M_\eta^2}{\mu^2}\right)$$
$$- \frac{1}{512\pi^2}\frac{r}{r^2 + r - 2}\left(3\log\frac{M_K^2}{M_\pi^2} + \log\frac{M_\eta^2}{M_K^2}\right)\,. \qquad (38)$$

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[4] In this paper, we take the following values for the Goldstone boson masses and decay constants: $M_\pi = 139.6\,\text{MeV}$, $M_K = 493.7\,\text{MeV}$, $M_\eta = 547\,\text{MeV}$, $F_\pi = 92.4\,\text{MeV}$ and $F_K/F_\pi = 1.22$.

The critical values of L_4 and L_6 are only mildly dependent on r; for $r = 25$,

$$L_6^{\mathrm{crit}}(M_\rho) = -0.26 \cdot 10^{-3},$$

$$[r = 25] \qquad (39)$$

$$L_4^{\mathrm{crit}}(M_\rho) = -0.51 \cdot 10^{-3}.$$

The remaining two equations of the π–K system can be reexpressed as a relation between $\epsilon(r)$ and L_8 on one hand and between $\eta(r)$ and L_5 on the other hand:

$$\epsilon(r) = 16 \frac{M_\pi^2}{F_\pi^2} [Y(3)]^2 \Delta L_8 - d', \qquad (40)$$

$$\eta(r) = 8 \frac{M_\pi^2}{F_\pi^2} Y(3) \Delta L_5 - e'. \qquad (41)$$

These relations involve the combinations of the NNLO remainders $d' = d - d_\pi$ and $e' = e - e_\pi$. At large values of r (≥ 15), $\epsilon(r)$ and $\eta(r)$ are suppressed and $d' \ll d \sim d_\pi$, $e' \ll e \sim e_\pi$.

The LECs arise in (40) and (41) through the differences

$$\Delta L_8 = L_8^r(\mu) - \frac{1}{512\pi^2} \left[\log \frac{M_K^2}{\mu^2} + \frac{2}{3} \log \frac{M_\eta^2}{\mu^2} \right]$$

$$- \frac{1}{512\pi^2(r-1)} \left(3 \log \frac{M_K^2}{M_\pi^2} + \log \frac{M_\eta^2}{M_K^2} \right), \quad (42)$$

$$\Delta L_5 = L_5^r(\mu) - \frac{1}{256\pi^2} \left[\log \frac{M_K^2}{\mu^2} + 2 \log \frac{M_\eta^2}{\mu^2} \right] \qquad (43)$$

$$- \frac{1}{256\pi^2(r-1)} \left(3 \log \frac{M_\eta^2}{M_K^2} + 5 \log \frac{M_K^2}{M_\pi^2} \right).$$

These differences combine the (renormalized and quark mass independent) constants L_8, L_5 and chiral logarithms so that they are independent of the renormalization scale μ. For $r = 25$, we obtain

$$\Delta L_5 = L_5^r(M_\rho) + 0.67 \cdot 10^{-3},$$

$$[r = 25] \qquad (44)$$

$$\Delta L_8 = L_8^r(M_\rho) + 0.20 \cdot 10^{-3}.$$

3.2 Perturbative reexpression of order parameters

The four exact equations (32), and (40) and (41) can be used to illustrate explicitly the instabilities which may arise in the perturbative expression of $X(3)$ and $Z(3)$ in powers of M_P^2. In the perturbative treatment of three-flavor χPT [3], one uses the fact that $Y(3) = 1 + O(M_P^2)$ to set systematically $Y(3) = 1$ whenever it appears in the NLO term. One first uses (40) and (41) to eliminate F_K^2/F_π^2 and $r = m_s/m$ in terms of ΔL_5 and ΔL_8. The result reads

$$\frac{F_K^2}{F_\pi^2} = 1 + 8 \frac{M_K^2 - M_\pi^2}{F_\pi^2} \Delta L_5 + \dots, \qquad (45)$$

$$r + 1 = 2 \frac{M_K^2}{M_\pi^2} \left(1 + 8 \frac{M_K^2 - M_\pi^2}{F_\pi^2} [\Delta L_5 - 2\Delta L_8] + \dots \right). \qquad (46)$$

In these formulae the quark mass ratio r appearing in the expressions for ΔL_i has to be replaced by its leading-order value (obtained from (46)):

$$r_0 = 2 \frac{M_K^2}{M_\pi^2} - 1 \sim 24. \qquad (47)$$

Strictly speaking, (45) and (46) do not get any direct contribution from the vacuum fluctuation of $\bar{s}s$ pairs which violate the Zweig rule and are tracked by L_6 and L_4. The situation is quite different in the case of the identities (32) for $X(3)$ and $Z(3)$, where the terms describing fluctuations are potentially dangerous. Expressing them perturbatively one gets

$$X(3) = 1 - 16 \frac{M_\pi^2}{F_\pi^2} \Delta L_8 - 16 \frac{2M_K^2 + M_\pi^2}{F_\pi^2} \Delta L_6 + \dots,$$

$$(48)$$

$$Z(3) = 1 - 8 \frac{M_\pi^2}{F_\pi^2} \Delta L_5 - 8 \frac{2M_K^2 + M_\pi^2}{F_\pi^2} \Delta L_4 + \dots \quad (49)$$

The large coefficients characteristic of the perturbative treatment of $1/(F_\pi^2 M_\pi^2)$ – and to some extent also of $1/F_\pi^2$ – now become visible. Equations (48) and (49) lead numerically to

$$X(3) = 1 - 37\Delta L_8 - 950\Delta L_6 + \dots, \qquad (50)$$

$$Z(3) = 1 - 18\Delta L_5 - 475\Delta L_4 + \dots \qquad (51)$$

In (48) and (49), the main NLO contribution comes from the M_K^2-enhanced term proportional to the $O(p^4)$ Zweig-rule violating LECs L_6 and L_4. If the latter stay close to their critical values (corresponding to (39) for $r = 25$), the NLO contributions remain small. On the other hand, even though the values of L_4 and L_6 are unknown yet, dispersive relations have been used to constrain their values: $L_6^r(M_\rho) = (0.6 \pm 0.2) \cdot 10^{-3}$ based on sum rules for the correlator $\langle (\bar{u}u + \bar{d}d)\bar{s}s \rangle$ [5,6,8], and $L_4^r(M_\rho) = (0.2 \pm 0.3) \cdot 10^{-3}$ from πK scattering data [19]. Such estimates – rather different from the critical values – suggest a significant violation of the Zweig rule in the scalar sector, and an important role for the vacuum fluctuations of $s\bar{s}$ pairs in the patterns of chiral symmetry breaking.

As an exercise, for illustrative purposes, we will now use the central values of the above sum rule estimates to study the convergence of (48) and (49). We actually aim in this paper at providing a framework to determine more accurately the size of vacuum fluctuations directly from experimental observables. If we take $L_5^r(M_\rho) = 1.4 \cdot 10^{-3}$ and $L_8^r(M_\rho) = 0.9 \cdot 10^{-3}$ [3,16], the numerical evaluation of (48) and (49) leads to the decomposition

$$\mathrm{Qty} = \mathrm{LO} + [\mathrm{fluct} + \mathrm{other}] + \mathrm{NNLO},$$

$$X(3) \equiv \frac{2m\Sigma(3)}{F_\pi^2 M_\pi^2} = 1 - [0.82 + 0.04] + O(p^4),$$

$$Z(3) \equiv \frac{F(3)^2}{F_\pi^2} = 1 - [0.34 + 0.04] + O(p^4),$$

$$(r + 1) \frac{M_\pi^2}{2M_K^2} = 1 - [0.00 + 0.06] + O(p^4). \qquad (52)$$

For each quantity, the right-hand side is the sum of the leading term (1), the NLO term (the sum in brackets) and higher order terms. The NLO term is decomposed into its two contributions: the first one comes from the fluctuation term (proportional to ΔL_4 or ΔL_6) and the second one collects all other NLO contributions. Fluctuation parameters have a dramatic effect on the convergence – they are the only terms enhanced by a factor of M_K^2 in (48) and (49).

It should be stressed that the instability of the perturbative expansion of $X(3)$ and $Z(3)$ does not originate from higher order terms in the expansion (11) of $F_\pi^2 M_\pi^2$. The latter actually factorize and can be cleanly separated from the effect of vacuum fluctuations. This can most easily be established in the $SU(2) \times SU(2)$ limit (26). Using a bar to indicate that a quantity is evaluated for $m = 0$ and fixed $m_s \neq 0$, one has

$$\Sigma(2) = \lim_{m \to 0} \frac{F_\pi^2 M_\pi^2}{2m} = \Sigma(3) + 32 B_0^2 m_s \overline{\Delta L_6} + \Sigma(2) \bar{d}_\pi , \tag{53}$$

where

$$\overline{\Delta L_6} = L_6^r(\mu) - \frac{1}{512\pi^2} \left(\log \frac{\bar{M}_K^2}{\mu^2} + \frac{2}{9} \log \frac{\bar{M}_\eta^2}{\mu^2} \right) . \tag{54}$$

Consequently,

$$\bar{X}(3) = \frac{\Sigma(3)}{\Sigma(2)} = \frac{1}{1 + 32 \dfrac{m_s B_0}{F_0^2} \overline{\Delta L_6}} (1 - \bar{d}_\pi) . \tag{55}$$

We expect the effect of non-zero m to be tiny; in particular, $\overline{\Delta L_6} \simeq \Delta L_6, d_\pi \simeq \bar{d}_\pi = \bar{d} = O(m_s^2)$ and $\bar{X}(3) \simeq X(3)$. Similarly, using the expansion of decay constants displayed in Appendix A, one gets

$$\bar{Z}(3) = \frac{F(3)^2}{F(2)^2} = \frac{1}{1 + 16 \dfrac{m_s B_0}{F_0^2} \overline{\Delta L_4}} (1 - \bar{e}_\pi) , \tag{56}$$

where $\bar{e}_\pi = \bar{e} = O(m_s^2)$ and

$$\overline{\Delta L_4} = L_4^r(\mu) - \frac{1}{256\pi^2} \log \frac{\bar{M}_K^2}{\mu^2} . \tag{57}$$

Equations (55) and (56) are exact identities, in which the whole effect of higher orders is gathered into the $O(m_s^2)$ NNLO remainders $\bar{d}_\pi$ and $\bar{e}_\pi$. Even if the latter are small ($\sim 10\%$), the expansion of $\bar{X}(3)$ and $\bar{Z}(3)$ in powers of m_s may break down, provided the magnitudes of ΔL_6 and ΔL_4 are as mentioned above. The $SU(2) \times SU(2)$ limit of (48) and (49) just exhibits the first term of such an expansion. Let us stress that we chose the $SU(2) \times SU(2)$ limit for simplicity here, but that the factorization of higher order corrections is a general result (holding even for $m \neq 0$) [13].

One more remark is in order concerning the special case in which both $\overline{\Delta L_4}$ and $\overline{\Delta L_6}$ are large, but satisfy

$$\overline{\Delta L_4} = 2 \overline{\Delta L_6} . \tag{58}$$

With this particular relation between the low-energy constants, one has

$$\bar{Y}(3) = \frac{\bar{X}(3)}{\bar{Z}(3)} = \lim_{m \to 0} \frac{2m B_0}{M_\pi^2} = \frac{1 - \bar{d}_\pi}{1 - \bar{e}_\pi} \approx 1 . \tag{59}$$

This would describe a situation in which the (large) vacuum fluctuations suppress both the condensate $\Sigma(3)$ and the decay constant F_0^2, i.e., partially restore the chiral symmetry, and yet the ratio $\Sigma(3)/F_0^2 = B_0$ remains nonzero.

3.3 Non-perturbative elimination of $O(p^4)$ LECs

We have just seen that the perturbative treatment of the chiral series fails if vacuum fluctuations of $\bar{q}q$ pairs are large, resulting in instabilities in the chiral expansions. In this case, the non-linearities in (32), relating order and fluctuation parameters, are crucial, and we must not linearize these relations (hence the inadequacy of a perturbative treatment).

We should therefore treat (32) without performing any approximation. Following [13], we can exploit (32) to express the chiral order parameters $X(3)$ and $Z(3)$ as functions of the fluctuation parameters ρ and λ. The ratio of the order parameters $Y(3)$ is[5]

$$Y(3) = \tag{60}$$
$$\frac{2[1 - \epsilon - d]}{1 - \eta - e + \sqrt{[1 - \eta - e]^2 + [\rho - \lambda][1 - \epsilon - d]}} ,$$

where $\epsilon = \epsilon(r)$ and $\eta = \eta(r)$. The non-linear character of (32) results in the (non-perturbative) square root. We see that the behavior of $Y(3)$ is controlled by the fluctuation parameter $\rho - \lambda$, i.e., $2L_6 - L_4$, as can be seen from (36).

The perturbative treatment sketched in the previous section corresponds to linearizing (60), assuming that the fluctuation parameter $\rho - \lambda \ll 1$. This is invalid if large fluctuations occur: ρ and/or λ are then numerically of order 1, although they count as $O(p^2)$ in the chiral limit. Equation (60) leads to the suppression of $Y(3)$, which would contribute to a stabilization of (32) by reducing the contribution proportional to the fluctuation parameters ρ and λ. As discussed extensively in [13], different behaviors of the fluctuation parameters can result in a rather varied range of patterns of chiral symmetry breaking.

We would like to extract information about $N_f = 3$ chiral symmetry breaking from physical observables, even in the event that the perturbative expansion breaks down. We could proceed in the same way as in [13] and express as many quantities as possible in terms of L_4 and L_6, in order to stress the role played by vacuum fluctuations. In the present paper, we find it more convenient to take as independent quantities the (more fundamental) chiral order parameters $X(3)$ and $Z(3)$. We should emphasize that this

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[5] The quadratic equation for $Y(3)$ admits two solutions, but only one of them corresponds to the physical case (see [13] for more details).

corresponds to a different choice from that adopted in the perturbative treatment of chiral series: in standard χPT, $X(3)$, $Z(3)$, r, F_K/F_π are iteratively expressed in terms of L_4, L_5, L_6, L_8. In contrast, we start by the same four identities and express non-perturbatively L_4, L_5, L_6, L_8 in terms of $X(3)$, $Z(3)$, r, F_K/F_π; this is a sensible treatment provided that both LO and NLO terms are considered.

Keeping in mind that LO and NLO contributions can have a similar size, we treat as exact identities the expansions of good observables in powers of quark masses and exploit the mass and decay constant identities to re-express $O(p^2)$ and $O(p^4)$ LECs in terms of r, $X(3)$, $Z(3)$, observable quantities and NNLO remainders. This leads to

$$F_0^2 = F_\pi^2 Z(3), \tag{61}$$

$$2mB_0 = M_\pi^2 Y(3), \tag{62}$$

$$2m_s B_0 = r M_\pi^2 Y(3), \tag{63}$$

and to

$$[Y(3)]^2 L_6^r(\mu) = \frac{1}{16(r+2)} \frac{F_\pi^2}{M_\pi^2}[1 - X(3) - \epsilon(r) - d]$$
$$+ \frac{[Y(3)]^2}{512\pi^2}\left(\log\frac{M_K^2}{\mu^2} + \frac{2}{9}\log\frac{M_\eta^2}{\mu^2}\right) \tag{64}$$
$$- \frac{[Y(3)]^2 r}{(r-1)(r+2)}\frac{1}{512\pi^2}\left(3\log\frac{M_K^2}{M_\pi^2} + \log\frac{M_\eta^2}{M_K^2}\right),$$

$$[Y(3)]^2 L_8^r(\mu) = \frac{F_\pi^2}{16M_\pi^2}[\epsilon(r) + d']$$
$$+ \frac{[Y(3)]^2}{512\pi^2}\left(\log\frac{M_K^2}{\mu^2} + \frac{2}{3}\log\frac{M_\eta^2}{\mu^2}\right)$$
$$+ \frac{[Y(3)]^2}{512\pi^2(r-1)}\left(3\log\frac{M_K^2}{M_\pi^2} + \log\frac{M_\eta^2}{M_K^2}\right), \tag{65}$$

$$Y(3) L_4^r(\mu) = \frac{1}{8(r+2)}\frac{F_\pi^2}{M_\pi^2}[1 - Z(3) - \eta(r) - e]$$
$$+ \frac{Y(3)}{256\pi^2}\log\frac{M_K^2}{\mu^2} \tag{66}$$
$$- \frac{Y(3)}{128\pi^2(r+2)}\left(\frac{2r+1}{2r-2}\log\frac{M_\eta^2}{M_K^2} + 2\frac{4r+1}{4r-4}\log\frac{M_K^2}{M_\pi^2}\right),$$

$$Y(3) L_5^r(\mu) = \frac{F_\pi^2}{8M_\pi^2}[\eta(r) + e']$$
$$+ \frac{Y(3)}{256\pi^2}\left(\log\frac{M_K^2}{\mu^2} + 2\log\frac{M_\eta^2}{\mu^2}\right)$$
$$+ \frac{Y(3)}{256\pi^2(r-1)}\left(3\log\frac{M_\eta^2}{M_K^2} + 5\log\frac{M_K^2}{M_\pi^2}\right). \tag{67}$$

These equations are derived from (32), (43) and (42), and they have a much simpler expression in terms of ΔL_i, introduced in (37) and (38), and (42) and (43), rather

than L_i ($i = 4, 5, 6, 8$):

$$Y^2(3)\Delta L_6 = \frac{1}{16(r+2)}\frac{F_\pi^2}{M_\pi^2}[1 - \epsilon(r) - X(3) - d], \tag{68}$$

$$Y^2(3)\Delta L_8 = \frac{1}{16}\frac{F_\pi^2}{M_\pi^2}[\epsilon(r) + d'], \tag{69}$$

$$Y(3)\Delta L_4 = \frac{1}{8(r+2)}\frac{F_\pi^2}{M_\pi^2}[1 - \eta(r) - Z(3) - e], \tag{70}$$

$$Y(3)\Delta L_5 = \frac{1}{8}\frac{F_\pi^2}{M_\pi^2}[\eta(r) + e']. \tag{71}$$

The above identities are useful as long as the NNLO remainders are small. The presence of powers of $Y(3)$, i.e., B_0, follows from the normalization of the scalar and pseudoscalar sources in [3]: these powers arise only for $O(p^4)$ LECs related to chiral symmetry breaking (two powers for L_6, L_7, L_8, one for L_4 and L_5) and are absent for LECs associated with purely derivative terms.

Plugging these identities into the χPT expansions corresponds therefore to a resummation of vacuum fluctuations, as opposed to the usual (iterative and perturbative) treatment of the same chiral series. We can then reexpress the observables in terms of the three parameters of interest, $X(3)$, $Z(3)$, r, and the NNLO remainders. Before describing how to exploit experimental information to constrain these parameters, we should first comment on the case of the η meson.

3.4 The η-mass and the Gell-Mann–Okubo formula

It remains for us to discuss the mass and decay constant of η as constrained by Ward identities for two-point functions of the eighth component of the axial current and of its divergence. This results into two additional relations (given in Appendix A) that involve one new NLO constant L_7 and two extra NNLO remainders d_η and e_η. These two identities will be used to reexpress the LEC L_7 in terms of the order parameters and quark mass ratio, and to eliminate the decay constant F_η, which is not directly accessible experimentally. This new discussion is closely related to the old question [28] whether the remarkable accuracy of the Gell-Mann–Okubo (GO) formula for Goldstone bosons finds a natural explanation within χPT and what it says about the size of the three-flavor condensate.

The combination

$$D_{GO} = 3F_\eta^2 M_\eta^2 - 4F_K^2 M_K^2 + F_\pi^2 M_\pi^2 \tag{72}$$

does not receive any $O(p^2)$ contribution from the genuine condensate $\Sigma(3)$. The η-mass identity (152) leads to the following simple formula for D_{GO}, expressed in units $F_\pi^2 M_\pi^2$:

$$\Delta_{GO} \equiv \frac{D_{GO}}{F_\pi^2 M_\pi^2} = 16\frac{M_\pi^2}{F_\pi^2}(r-1)^2[Y(3)]^2(2L_7+\Delta L_8)+d_{GO}, \tag{73}$$

where ΔL_8 was defined in (42). Similarly, the identity for F_η (153) can be put into the form

$$\frac{F_\eta^2}{F_\pi^2} = 1 + \frac{4}{3}\left(\frac{F_K^2}{F_\pi^2} - 1\right) \tag{74}$$

$$+ \frac{1}{48\pi^2}\frac{M_\pi^2}{F_\pi^2}Y(3)\left[(2r+1)\log\frac{M_\eta^2}{M_K^2} - \log\frac{M_K^2}{M_\pi^2}\right] + e_{\mathrm{GO}}.$$

Equations (73) and (74) are exact as long as the NNLO remainders

$$d_{\mathrm{GO}} = 3\frac{F_\eta^2 M_\eta^2}{F_\pi^2 M_\pi^2}d_\eta - 4\frac{F_K^2 M_K^2}{F_\pi^2 M_\pi^2}d_K + d_\pi\,,$$

$$e_{\mathrm{GO}} = \frac{F_\eta^2}{F_\pi^2}e_\eta + \frac{4}{3}\frac{F_K^2}{F_\pi^2}e_K - \frac{e_\pi}{3} \tag{75}$$

are included. If one follows Sect. 3.2 and treats the exact formulae (73) and (74) perturbatively, one reproduces the $O(p^4)$ expressions given in [3], as expected.

Remarkably, the identities (73) and (74) are simpler and more transparent than their perturbative version, and we find them useful to make a few numerical estimates which may be relevant for a discussion of the GO formula. For this purpose we shall use the value $r = r_0 \sim 24$ of the quark mass ratio and neglect for a moment the NNLO remainders d_{GO} and e_{GO}, as well as the error bars related to the experimental inputs on masses and decay constants. For this exercise, we also disregard isospin breaking and electromagnetic corrections. First, the dependence of F_η on $Y(3) = 2mB_0/M_\pi^2$ is negligibly small:

$$\frac{F_\eta^2}{F_\pi^2} = 1.651 + 0.036 \cdot Y(3)\,. \tag{76}$$

In the estimate of $\Delta_{\mathrm{GO}} = D_{\mathrm{GO}}/F_\pi^2 M_\pi^2$, we use $F_\eta^2/F_\pi^2 = 1.687$ and find

$$\Delta_{\mathrm{GO}} = 77.70 - 74.46 + 1 = 4.24\,. \tag{77}$$

We have split the result into the three contributions corresponding respectively to η, K and π, in order to emphasize the accuracy of the formula. If we drop the decay constants in Δ_{GO}, we obtain

$$\bar{\Delta}_{\mathrm{GO}} = \frac{3M_\eta^2 - 4M_K^2 + M_\pi^2}{M_\pi^2} = 46.06 - 50.03 + 1 = -2.97\,. \tag{78}$$

Hence, apart from a change of sign, this more familiar definition of the GO discrepancy is of a comparable magnitude as Δ_{GO}. For the reasons already stressed, the interpretation in terms of QCD correlation functions is more straightforward when $F_P^2 M_P^2$ is used.

If the origin of the GO formula were to be naturally explained by the dominance of the $O(p^2)$ condensate term in the expansion of $F_P^2 M_P^2$, the order of magnitude of the estimate (77) should be reproduced by (73) for a typical order of magnitude of the $O(p^4)$ LECs L_8 and L_7 without

any fine tuning of their values. Using (40) and neglecting the NNLO remainder d', one gets

$$16\frac{M_\pi^2}{F_\pi^2}(r-1)^2[Y(3)]^2\Delta L_8 = 22.5 \qquad [r=r_0]. \tag{79}$$

Hence, the typical $O(p^4)$ contribution ΔL_8 to Δ_{GO} happens to be nearly one order of magnitude bigger than the estimate (77). The latter can only be reproduced by tuning very finely the LEC L_7:

$$[Y(3)]^2(\Delta L_8 + 2L_7) \simeq 1.3 \times 10^{-4}\,, \tag{80}$$

to be compared with the above estimate $[Y(3)]^2\Delta L_8 \simeq 1.2 \times 10^{-3}$. All this of course does not reveal any contradiction, but it invalidates the customary "explanation" of the GO formula and the standard argument against a possible suppression of the three-flavor condensate $\Sigma(3)$. Therefore, the fact that the GO formula is satisfied so well remains unexplained independently of the size of $\Sigma(3)$ and of the vacuum fluctuations. The last point can be explicitly verified: the genuine condensate contribution $\Sigma(3)$ as well as the induced condensate $m_s Z^s$, which represents an $O(p^4)$ contribution to $F_P^2 M_P^2$, both drop out of the GO combination (72).

We now return to our framework: we do not assume a particular hierarchy between LO and NLO contributions to chiral series, and we do not neglect any longer the NNLO remainders (in the case of the η meson, d_{GO} and e_{GO} might be sizeable and should be kept all the way through). It is possible to use the previous formulae to reexpress L_7 in a similar way to (64)–(67):

$$[Y(3)]^2 L_7 = \frac{1}{32(r-1)^2}\frac{F_\pi^2}{M_\pi^2} \tag{81}$$

$$\times\left[\frac{3F_\eta^2 M_\eta^2 - 4F_K^2 M_K^2 + F_\pi^2 M_\pi^2}{F_\pi^2 M_\pi^2} - (r-1)^2[\epsilon(r)+d']\right.$$

$$\left. - \frac{3F_\eta^2 M_\eta^2 d_\eta - 4F_K^2 M_K^2 d_K + F_\pi^2 M_\pi^2 d_\pi}{F_\pi^2 M_\pi^2}\right].$$

This expression should be used to reexpress nonperturbatively L_7 in terms of chiral order parameters (F_η^2 is given by (74)). We can already notice that in (81), the first contribution, which corresponds to Δ_{GO}, is 5 to 10 times suppressed with respect to the second term $(r-1)^2[\epsilon(r)+d']$.

4 Three-flavor analysis of $\pi\pi$ scattering

The quantities $B_0 m$, r, F_0, $L_4,...,L_8$ appear in the bare chiral series up to NLO. The procedure outlined above allows us to express these eight quantities in terms of the masses and decay constants of Goldstone bosons. Apart from the (presumably small) six NNLO remainders d_P and e_P, this leaves three unknown parameters. We choose these three parameters to be the order parameters $X(3)$

and $Z(3)$, and the quark mass ratio r. The remaining terms of the $O(p^4)$ chiral Lagrangian, involving the LECs L_1, L_2, L_3, L_9, and L_{10}, do not affect the symmetry-breaking sector of the underlying theory in which we are mainly interested here.

The counting of the degrees of freedom is completely analogous to the one described in [17], where a global two-loop fit has been performed to the masses, decay constants and K_{e4} form factors. In this reference, the LECs L_1, L_2 and L_3 were also included and constrained by the three experimental results corresponding to the two K_{e4} form factors at threshold and to their slope. The three parameters left undetermined in the fits of [17] are the ratio of quark masses r and the $O(p^4)$ LECs L_4 and L_6. The unknown $O(p^6)$ LECs, estimated in the above reference through a resonance saturation assumption, introduce some theoretical uncertainty. In our approach, this uncertainty is included in the NNLO remainders. We keep the latter throughout our calculation; however, at some point of the numerical analysis we will have to make an educated guess as to their sizes. The main differences between our approach and that of [17] lie in our use of a non-perturbative resummation of instabilities, compared to the canonical two-loop perturbative elimination of $O(p^4)$ LECs; in our choice of $X(3), Z(3), r$ as the three undetermined parameters, rather than L_4, L_6, r; and in our treatment of higher order remainders: in [17] they are computed up to $O(p^6)$, and the additional LECs arising at this order are estimated through resonance saturation.

In order to constrain our three independent parameters, more information is needed. In the present section we will examine the impact of our knowledge of $\pi\pi$ scattering observables. We have previously analyzed the $\pi\pi$ data of [14] in terms of two-flavor order parameters, allowing a rather precise determination of them [15]: $X(2) = 0.81 \pm 0.07$ and $Z(2) = 0.89 \pm 0.03$. However, the $\pi\pi$ scattering parameters are more sensitive to the two-flavor order parameters than to the three-flavor ones [7, 11,29]. Expanding $X(2)$ in $SU(3) \times SU(3)$ χPT one can obtain [11]

$$
X(2)(1 - \bar{d}_\pi) = \frac{r}{r+2} \left[1 - \epsilon(r) - d - Y(3)^2 f_1 \right]
$$
$$
+ \frac{2}{r+2} X(3) , \quad (82)
$$

where f_1 is a (small) combination of chiral logarithms, whose precise definition is recalled in (105) below; in [11] the estimate $f_1 \sim 0.05$ was obtained.

If $\epsilon(r)$ is not close to 1, i.e., if r larger than 15, the term in square brackets in (82) is dominant. Then $X(2)$ has only a very weak (r-suppressed) sensitivity to $X(3)$. On the other hand, its value is strongly correlated with r. We expect therefore $\pi\pi$ scattering to provide us with valuable information about the quark mass ratio r, but not about the $N_f = 3$ order parameters $X(3)$ and $Z(3)$. This section is devoted to designing a framework testing this expectation in a quantitative way.

4.1 Low-energy $\pi\pi$ amplitude

Considerable progress has been achieved recently in the understanding of $\pi\pi$ scattering. The solutions of the Roy equations [30] allow one to express the amplitude, in the whole energy domain below 800 MeV, in terms of only two parameters (e.g., the scalar scattering lengths, or the parameters $\alpha_{\pi\pi}$ and $\beta_{\pi\pi}$ defined below), with very small uncertainty. It is therefore possible to determine experimentally these two parameters in a model-independent way. Furthermore, at low energy the $\pi\pi$ amplitude is strongly constrained by chiral symmetry, crossing and unitarity. It can be expressed, up to and including terms of order $(p/\Lambda_H)^6$, as follows:

$$
A_{\pi\pi}(s|t,u) = P(s|t,u) + \bar{J}(s|t,u) + O[(p/\Lambda_H)^8], \quad (83)
$$

where $P(s|t,u)$ is a polynomial conveniently written (following the conventions and notation of [24]) in the form

$$
P(s|t,u) = \frac{\alpha_{\pi\pi}}{F_\pi^2} \frac{M_\pi^2}{3} + \frac{\beta_{\pi\pi}}{F_\pi^2} \left(s - \frac{4M_\pi^2}{3} \right) \quad (84)
$$
$$
+ \frac{\lambda_1}{F_\pi^4} \left(s - 2M_\pi^2 \right)^2 + \frac{\lambda_2}{F_\pi^4} \left[\left(t - 2M_\pi^2 \right)^2 + \left(u - 2M_\pi^2 \right)^2 \right]
$$
$$
+ \frac{\lambda_3}{F_\pi^6} \left(s - 2M_\pi^2 \right)^3 + \frac{\lambda_4}{F_\pi^6} \left[\left(t - 2M_\pi^2 \right)^3 + \left(u - 2M_\pi^2 \right)^3 \right] ,
$$

in terms of six subthreshold parameters $\alpha_{\pi\pi}, \beta_{\pi\pi}, \lambda_1 \ldots \lambda_4$. $\bar{J}(s|t,u)$ collects the unitarity cuts arising from elastic $\pi\pi$ intermediate states. At low energy, the contributions of $K\bar{K}$ and $\eta\eta$ intermediate states are not neglected but expanded and absorbed into the polynomial $P(s|t,u)$. The general form of $\bar{J}(s|t,u)$ is dictated by successive iterations of the unitarity condition, and it is entirely determined by the first four subthreshold parameters up to $O(p^6)$:

$$
\bar{J}(s|t,u) = U(s)\bar{J}_{\pi\pi}(s)
$$
$$
+ [(s-u)V(t) + W(t)]\bar{J}_{\pi\pi}(t) \quad (85)
$$
$$
+ [(s-t)V(u) + W(u)]\bar{J}_{\pi\pi}(u) + \ldots ,
$$

where

$$
\bar{J}_{\pi\pi}(s) = \frac{s}{16\pi^2} \int_{4M_\pi^2}^\infty \frac{\mathrm{d}x}{x(x-s)} \sqrt{\frac{x - 4M_\pi^2}{x}} , \quad (86)
$$

U, V, W are polynomials given in terms of the parameters $\alpha_{\pi\pi}, \beta_{\pi\pi}, \lambda_1, \lambda_2$ and the ellipsis stands for (known) $O(p^6)$ contributions. (For a more explicit form, see (3.18) and (3.47) of [24].)

As a first step, the general representation (83) of the low-energy $\pi\pi$ amplitude can be matched with experimental phase shifts [14] and with the solution of the Roy equations [30] in order to determine the subthreshold parameters $\alpha_{\pi\pi}, \beta_{\pi\pi}, \ldots$ This has been done in [15], independently of any χPT expansion or predictions, leading to the following values:

$$
\alpha_{\pi\pi} = 1.381 \pm 0.242 , \qquad \beta_{\pi\pi} = 1.081 \pm 0.023 , \quad (87)
$$

with the correlation coefficient between the two parameters $\rho_{\alpha\beta} = -0.14$.

At the second stage, χPT can be used to expand the subthreshold parameters $\alpha_{\pi\pi}, \beta_{\pi\pi}, \lambda_1, \ldots, \lambda_4$ in powers of quark masses $m_u = m_d = m$ and/or m_s, thereby constraining the possible values of the chiral order parameters. Notice that the expansion of the subthreshold parameters is expected to converge better than that of the scattering lengths, the latter being more sensitive to small variations of the pion mass. Similarly, as already discussed in Sects. 2 and 3, one should bear in mind the possibility of a strong dependence of F_π^2 on m_s: it seems therefore preferable to consider the expansion of $F_\pi^4 A_{\pi\pi}$, i.e., the on-shell four-point function of the axial-vector current (rather than the scattering amplitude itself) in powers of quark masses and external pion momenta. In [15] the corresponding expansion of subthreshold parameters $\alpha_{\pi\pi}$ and $\beta_{\pi\pi}$ in powers of m (with m_s fixed at its physical value) was converted into a determination of the two-flavor order parameters $X(2)$ and $Z(2)$. Now we consider the "bare expansion" of $F_\pi^2 M_\pi^2 \alpha_{\pi\pi}$ and of the slope parameter $F_\pi^2 \beta_{\pi\pi}$ in powers of m and m_s in order to investigate directly how tightly the available $\pi\pi$ experimental information constrains the three-flavor condensate $X(3)$ and decay constant F_0 (or $Z(3)$), and the quark mass ratio $r = m_s/m$.

In order to establish the "bare" $SU(3) \times SU(3)$ expansion of $F_\pi^2 M_\pi^2 \alpha_{\pi\pi}$ and of $F_\pi^2 \beta_{\pi\pi}$ we proceed as follows. We start by rewriting the LO and NLO χPT contributions in a form similar to (83):

$$F_\pi^4 A_{\pi\pi}(s|t,u) = F_\pi^4 P^r(s|t,u) + F_\pi^4 J^r(s|t,u) + \ldots \quad (88)$$

$P^r(s|t,u)$ collects all LO and NLO tree and tadpole contributions and is of the form (84) with the two cubic terms omitted. The second term collects the one-loop contribution of order $O(p^4)$. Both are renormalized and separately depend on the renormalization scale μ. The loop part reads

$$\begin{aligned}
F_\pi^4 J^r(s|t,u) = {} & s^2 \left[\frac{1}{2} J_{\pi\pi}^r(s) + \frac{1}{8} J_{KK}^r(s) \right] \\
& + M_\pi^4 \left[-\frac{1}{2} J_{\pi\pi}^r(s) + \frac{1}{18} J_{\eta\eta}^r(s) \right] \\
& + \frac{1}{4} \left[(t - 2M_\pi^2)^2 J_{\pi\pi}^r(t) + (u - 2M_\pi^2)^2 J_{\pi\pi}^r(u) \right] \\
& + (s-u)t \left[M_{\pi\pi}^r(t) + \frac{1}{2} M_{KK}^r(t) \right] \\
& + (s-t)u \left[M_{\pi\pi}^r(u) + \frac{1}{2} M_{KK}^r(u) \right].
\end{aligned} \quad (89)$$

Here J_{PP}^r and M_{PP}^r are the standard loop functions for the Goldstone boson P (see, e.g., [24]). They are related to the functions $\bar{J}_{PP}(s)$ through

$$J_{PP}^r(s) = \bar{J}_{PP}(s) - 2k_{PP}, \quad (90)$$

$$M_{PP}^r(s) = \frac{s - 4M_P^2}{12s} \bar{J}_{PP}(s) - \frac{1}{6} k_{PP} + \frac{1}{288\pi^2}. \quad (91)$$

At low energy and for $P = K, \eta$, the loop functions are replaced by their expansion at small s:

$$J_{PP}^r = -2k_{PP}, \quad M_{PP}^r = -\frac{1}{6} k_{PP}. \quad (92)$$

In these equations, we have $k_{PP} = [\log(M_P^2/\mu^2)+1]/32\pi^2$.

Multiplying (85) by F_π^4 and dropping all terms beyond $O(p^4)$, one should recover the formula (89). This fact can be used to work out the bare expansion of the subthreshold parameters contained in $F_\pi^4 P(s|t,u)$. Comparing (85) and (89) leads to

$$\begin{aligned}
F_\pi^4 P(s|t,u) = {} & F_\pi^4 P^r(s|t,u) - s^2 \left(k_{\pi\pi} + \frac{1}{4} k_{KK} \right) \\
& + M_\pi^4 \left(k_{\pi\pi} - \frac{1}{9} k_{\eta\eta} \right) \\
& - \frac{1}{2} [(t - 2M_\pi^2)^2 + (u - 2M_\pi^2)^2] k_{\pi\pi} \\
& - \frac{1}{6} [(s-u)t + (s-t)u] \left(k_{\pi\pi} + \frac{1}{2} k_{KK} - \frac{1}{48\pi^2} \right),
\end{aligned} \quad (93)$$

which holds for all powers of s, t, u provided that one retains just the LO and NLO powers in quark masses in the expression of corresponding coefficients. In agreement with the convention explained in Sect. 2.2, we keep the physical Goldstone boson masses in the arguments of chiral logarithms arising from both tadpoles and unitarity loops. The right-hand side of (93) is checked to be independent of the renormalization scale μ. The resulting "bare expansion" of the two subthreshold parameters which carry information on the symmetry-breaking sector reads

$$\begin{aligned}
F_\pi^2 M_\pi^2 \alpha_{\pi\pi} = {} & 2m\Sigma(3) + 16m^2 A + 2m(8m + m_s)Z^s \\
& - 8m^2 B_0(\xi + 2\tilde{\xi}) \\
& + \frac{1}{8\pi^2} m^2 B_0^2 \left(4\log\frac{M_K^2}{M_\pi^2} - \frac{7}{3} \right) + F_\pi^2 M_\pi^2 d_{\alpha,\pi\pi},
\end{aligned} \quad (94)$$

$$\begin{aligned}
F_\pi^2 \beta_{\pi\pi} = {} & F_0^2 + 4m\xi + 2(4m + m_s)\tilde{\xi} \\
& + \frac{1}{4\pi^2} mB_0 \left[\log\frac{M_\eta^2}{M_K^2} + 2\log\frac{M_K^2}{M_\pi^2} - \frac{5}{4} \right] + F_\pi^2 e_{\beta,\pi\pi}.
\end{aligned} \quad (95)$$

The subthreshold parameters are thus expressed in terms of $A, Z^s, \xi, \tilde{\xi}$, which are defined in Appendix A as scale-invariant combinations of the $O(p^4)$ LECs and chiral logarithms. In order to account for NNLO and higher chiral orders, we have added in (94)–(95) the direct NNLO remainders $d_{\alpha,\pi\pi}$ and $e_{\beta,\pi\pi}$. (Their exact role in our analysis will be discussed shortly.) We would like to stress that the only quantities we really subject to a chiral expansion are the subthreshold parameters multiplied by appropriate powers of F_π^2 and M_π^2. The scattering amplitude as a function of s, t, u is given by (83), which holds up to and including $O(p^6)$ accuracy with all singularities and threshold factors correctly described using the physical Goldstone boson masses.

We have just illustrated how the bare expansion of subthreshold parameters is obtained in practice. The last

step now consists in replacing in the bare expansion (94) and (95) the parameters of the Lagrangian mB_0, m_sB_0 $L_4(\mu), L_5(\mu), L_6(\mu), L_8(\mu)$ by the three basic QCD parameters $X(3), Z(3), r = m_s/m$ using the identities (61)–(67), which yields

$$
\begin{aligned}
\alpha_{\pi\pi} &= 1 + 3\frac{r\epsilon(r)}{r+2} + 2\frac{1-X(3)}{r+2} \\
&+ 4\frac{1-Y(3)}{r+2} - 2\frac{Y(3)r\eta(r)}{r+2} \\
&- \frac{M_\pi^2}{32\pi^2 F_\pi^2}Y(3)^2\left\{\frac{7}{3}\right. \\
&+ \frac{r}{r^2+r-2}\left[(r+2)\log\frac{M_\eta^2}{M_K^2} - (r-2)\log\frac{M_K^2}{M_\pi^2}\right]\bigg\} \\
&- \frac{6}{r+2}d + \frac{4Y(3)}{r+2}e - 2Y(3)e' + [(d_\alpha - d) + 4d'],
\end{aligned} \tag{96}
$$

$$
\begin{aligned}
\beta_{\pi\pi} &= 1 + \frac{r\eta(r)}{r+2} + 2\frac{1-Z(3)}{r+2} \\
&+ \frac{M_\pi^2}{32\pi^2 F_\pi^2}Y(3)\{-5 \\
&+ \frac{r}{r^2+r-2}\left[(2r+1)\log\frac{M_\eta^2}{M_K^2} + (4r+1)\log\frac{M_K^2}{M_\pi^2}\right]\bigg\} \\
&- \frac{2}{r+2}e + [(e_\beta - e) + 2e'].
\end{aligned} \tag{97}
$$

These equations relate the two observable quantities $\alpha_{\pi\pi}$ and $\beta_{\pi\pi}$ to the three independent parameters $X(3), Z(3), r$ (recall that $Y(3) = X(3)/Z(3)$), and contain the dependence on the *direct* remainders $d_{\alpha,\pi\pi}, e_{\beta,\pi\pi}$ as well as on the *indirect* ones, stemming from the mass and decay constant identities. The order of magnitude of such remainders can be estimated and will be discussed later.

4.2 The Bayesian approach

The determination of the three-flavor order parameters from the experimental knowledge of $\alpha_{\pi\pi}$ and $\beta_{\pi\pi}$ is a subtle issue, due to the non-linear character of (96) and (97) and to the fact that our three independent parameters are subject to constraints (e.g., they have to be positive). Moreover, the NNLO remainders are in fact unknown; we can only estimate their order of magnitude. One is led to consider them as sources of error, but the propagation of errors is not so straightforward, precisely because of the above-mentioned non-linearities. For these reasons the standard method of maximum likelihood is inadequate in this case. A convenient approach is provided by Bayesian analysis [22], as described in Appendix B.

We introduce the correlated probability density function $P_{\exp}(\alpha_{\pi\pi}, \beta_{\pi\pi})$,

$$
P_{\exp}(\alpha_{\pi\pi}, \beta_{\pi\pi}) = \frac{\sqrt{\det C}}{2\pi}\exp\left(-\frac{1}{2}V^{\mathrm{T}}CV\right),
$$

$$
V = \begin{pmatrix} \alpha_{\pi\pi} - \alpha_{\exp} \\ \beta_{\pi\pi} - \beta_{\exp} \end{pmatrix}, \quad C = \begin{pmatrix} c_{11} & c_{12} \\ c_{12} & c_{22} \end{pmatrix}, \quad (98)
$$

with $1/c_{11} = \delta_\alpha^2(1-\rho_{\alpha\beta}^2)$, $1/c_{22} = \delta_\beta^2(1-\rho_{\alpha\beta}^2)$, $1/c_{12} = -\delta_\alpha\delta_\beta(1-\rho_{\alpha\beta}^2)/\rho_{\alpha\beta}$, and where $\alpha_{\exp}, \beta_{\exp}, \delta_\alpha, \delta_\beta$ and $\rho_{\alpha\beta}$ are the experimental results, uncertainties and correlations given in (87). This distribution summarizes the experimental result: the two numbers, $\alpha_{\exp}$ and $\beta_{\exp}$, given with an accuracy specified by the matrix C. Suppose now that we know, independently, the true values of $(\alpha_{\pi\pi}, \beta_{\pi\pi})$; (98) can then be interpreted as the probability of obtaining, when performing an experiment, the values $(\alpha_{\exp}, \beta_{\exp})$, i.e., the actual observed values, given our independent knowledge of $(\alpha_{\pi\pi}, \beta_{\pi\pi})$. Equation (98) is completely symmetric under exchange of $(\alpha_{\pi\pi}, \beta_{\pi\pi})$ with $(\alpha_{\exp}, \beta_{\exp})$.

This last interpretation is suitable for our problem, in which theory relates the subthreshold parameters $\alpha_{\pi\pi}$ and $\beta_{\pi\pi}$ to the three parameters $X(3), Z(3), r$ and to the remainders:

$$
\alpha_{\pi\pi} = \mathcal{A}[r, Y(3), Z(3), \delta_1, \delta_2, \delta_3, \delta_4], \tag{99}
$$
$$
\beta_{\pi\pi} = \mathcal{B}[r, Y(3), Z(3), \delta_2, \delta_5]. \tag{100}
$$

The relevant remainders, denoted by δ_i, $i = 1, ..., 5$, are defined in Table 1; δ_6 and δ_7 are additional remainders discussed in the following section. Therefore we can say that the probability of obtaining the data effectively observed, for a given choice of $r, Y(3), Z(3), \delta_i$, is

$$
P(\mathrm{data}|r, Y, Z, \delta_i) = P_{\exp}[\mathcal{A}(r, Y, Z, \delta_i), \mathcal{B}(r, Y, Z, \delta_i)]. \tag{101}
$$

This quantity is the likelihood of the observed experimental data. Indeed, it is not what we are interested in: data have certainly been observed, whereas the theoretical parameters are unknown to us. Instead, the probability that we need is $P(r, Y, Z, \delta_i|\mathrm{data})$. This object can be calculated as a result of a statistical inference using Bayes' theorem, at the price of introducing some "subjective" a priori knowledge of the theoretical parameters, $\pi(r, Y, Z, \delta_i)$. The result of the experiment is viewed as an update of our previous knowledge of the theoretical parameters, represented by the "prior" $\pi(r, Y, Z, \delta_i)$,

$$
\begin{aligned}
&P(r, Y, Z, \delta_i|\mathrm{data}) \hspace{3cm} (102) \\
&= \frac{P(\mathrm{data}|r, Y, Z, \delta_i)\cdot\pi(r, Y, Z, \delta_i)}{\int \mathrm{d}r\,\mathrm{d}Y\,\mathrm{d}Z\,\mathrm{d}\delta_i\,P(\mathrm{data}|r, Y, Z, \delta_i)\cdot\pi(r, Y, Z, \delta_i)}.
\end{aligned}
$$

The stronger the significance of the data, the weaker will be the dependence of the final result on our choice of the prior.

4.3 Choice of the prior

The prior should reflect our beliefs about the theoretical parameters before our learning of experimental results. If we have no reason to prefer one value to any other, then a flat prior should be chosen. We certainly have to implement the requirement of positivity for $X(3)$ and $Z(3)$, so

Table 1. Definition of NNLO remainders. σ_i denotes the expected order of magnitude, and barred remainders are taken in the $N_f = 2$ chiral limit

Remainder	Definition	σ_i
δ_1	d	0.1
δ_2	e	0.1
δ_3	e'	0.01
δ_4	$(d_{\alpha,\pi\pi} - d) + 4d'$	0.03
δ_5	$(e_{\beta,\pi\pi} - e) + 2e'$	0.03
δ_6	$[(1 + 2/r)(\bar{d}_\pi - d) + 2d/r]/(1 - d)$	0.03
δ_7	$[(1 + 2/r)(\bar{e}_\pi - e) + 2e/r]/(1 - e)$	0.03

the support of the function π will have a lower boundary at $X(3) = 0$, $Z(3) = 0$. A similar requirement can be applied to the two-flavor order parameters $X(2)$ and $Z(2)$. Using their expansions in the $SU(3) \times SU(3) \chi$PT one can obtain [11]

$$X(2)(1 - \bar{d}_\pi) = X(3) \qquad (103)$$
$$+ \frac{r}{r+2}\left[1 - X(3) - \epsilon(r) - d - Y(3)^2 f_1\right],$$
$$Z(2)(1 - \bar{e}_\pi) = Z(3) \qquad (104)$$
$$+ \frac{r}{r+2}\left[1 - Z(3) - \eta(r) - e - Y(3)g_1\right],$$

where f_1 and g_1 are (small) combinations of chiral logarithms,

$$f_1 = \frac{M_\pi^2}{32\pi^2 F_\pi^2}\left[\frac{r}{r-1}\left(3\log\frac{M_K^2}{M_\pi^2} + \log\frac{M_\eta^2}{M_K^2}\right)\right.$$
$$\left. -(r+2)\left(\log\frac{M_K^2}{\bar{M}_K^2} + \frac{2}{9}\log\frac{M_\eta^2}{\bar{M}_\eta^2}\right)\right], \qquad (105)$$

$$g_1 = \frac{M_\pi^2}{32\pi^2 F_\pi^2}\left[\frac{4r+1}{r-1}\log\frac{M_K^2}{M_\pi^2} + \frac{2r+1}{r-1}\log\frac{M_\eta^2}{M_K^2}\right.$$
$$\left. -(r+2)\log\frac{M_K^2}{\bar{M}_K^2}\right], \qquad (106)$$

estimated in [11] as $f_1 \sim 0.05$ and $g_1 \sim 0.07$, and barred quantities refer to the $SU(2) \times SU(2)$ chiral limit. The positivity of $X(2)$ and $Z(2)$ implies then a lower bound for the indirect remainders δ_1 and δ_2,

$$X(2) \geq 0 \leftrightarrow \delta_1 \leq \delta_1^{\max} = 1 - \epsilon(r) - Y(3)^2 f_1,$$
$$(107)$$
$$Z(2) \geq 0 \leftrightarrow \delta_2 \leq \delta_2^{\max} = 1 - \eta(r) - Y(3)g_1.$$
$$(108)$$

Actually one can also establish some upper bounds for the order parameters $X(3)$ and $Z(3)$ using the so-called paramagnetic inequalities (3) and (4) stated in [11][6], which

---

[6] The statement is that chiral order parameters dominated by the infrared end of the spectrum of the Euclidean Dirac

translate into lower bounds for the remainders δ_6 and δ_7 defined in Table 1,

$$X(3) \leq X(2) \qquad (109)$$
$$\leftrightarrow \delta_6 \geq \delta_6^{\min} = 1 - \frac{1 - \delta_1 - \epsilon(r) - Y(3)^2 f_1}{X(3)(1 - \delta_1)},$$
$$Z(3) \leq Z(2) \qquad (110)$$
$$\leftrightarrow \delta_7 \geq \delta_7^{\min} = 1 - \frac{1 - \delta_2 - \eta(r) - Y(3)g_1}{Z(3)(1 - \delta_2)}.$$

The ratio of order parameters $Y(3)$ is also bounded from above, as can be seen from (60):

$$Y(3) \leq Y^{\max} = 2\frac{1 - \epsilon(r) - \delta_1}{1 - \eta(r) - \delta_2}. \qquad (111)$$

We do not assume any further knowledge about the three-flavor order parameters. The hypothesis of a strict convergence of the chiral series, in the sense that every order of the expansion should be smaller than the previous one, would lead to the choice of a prior concentrated around the values $X(3) \sim 1$ and $Z(3) \sim 1$. In our approach this is not required; we allow the data to indicate whether vacuum fluctuations destabilize the chiral series or not. Therefore, apart from the constraints listed above, we will choose a flat prior for the three-flavor order parameters. In fact, this statement is ambiguous, since we have introduced three different quantities, $X(3)$, $Y(3)$ and $Z(3)$, related by $X(3) = Y(3)Z(3)$. If we restrict the problem to a flat prior in two parameters among $[X(3), Y(3), Z(3)] \equiv (X, Y, Z)$, we can get three different prior p.d.f.'s in (Y, Z):

$$(X, Z): \pi(Y, Z)dYdZ = dXdZ = ZdYdZ$$
$$\hookrightarrow \pi(Y, Z) = Z,$$
$$(X, Y): \pi(Y, Z)dYdZ = dXdY = YdYdZ$$
$$\hookrightarrow \pi(Y, Z) = Y,$$
$$(Y, Z): \pi(Y, Z)dYdZ = dYdZ$$
$$\hookrightarrow \pi(Y, Z) = 1.$$
$$(112)$$

A physical argument helps us to select one of these possibilities. When $Z(3)$ vanishes, chiral symmetry restoration occurs and the marginal probabilities of the chiral order parameters must vanish. This can be obtained if the prior p.d.f. vanishes in the limit $Z(3) \to 0$, which is realized in the case of a flat prior in (X, Z). Henceforth, we will focus on this case and therefore take $\pi(Y, Z) = Z$ inside the range allowed by the positivity and paramagnetic constraints, and $\pi(Y, Z) = 0$ outside.

Inspired by (32), we restrict the range of variation of r such that $0 \leq \epsilon(r) \leq 1$, which yields the range

$$r_1 \leq r \leq r_2, \qquad (113)$$

with

$$r_1 = 2\frac{F_K M_K}{F_\pi M_\pi} - 1 \sim 8, \quad r_2 = 2\frac{F_K^2 M_K^2}{F_\pi^2 M_\pi^2} - 1 \sim 36. \quad (114)$$

---

operator should decrease as the number of massless flavors increases. The paramagnetic inequalities also apply to $X(N_f)$ and $Z(N_f)$, for $N_f = 2, 3$.

No other previous knowledge is supposed for the quark mass ratio r, so the prior is taken to be flat in r over this allowed domain.

Finally, we must discuss how to treat the remainders $\delta_1, \ldots, \delta_7$. We recall that they are defined as the NNLO contributions in the chiral expansions of a selected class of observables, for which a good overall convergence is expected. Therefore, the remainders should be small. This expectation can be implemented in the prior by considering the remainders as Gaussian distributions centered at zero, with widths corresponding to their expected order of magnitude. Since the size of the corrections in the chiral series is 30% for the three-flavor expansions and 10% for the two-flavor ones, we will use the following rule of thumb, already introduced in footnote 3: the typical size of the remainders is $(30\%)^2 = 0.1$ for genuine $O(m_s^2)$ remainders like d, e, $30\% \times 10\% = 0.03$ for an $O(m_s m)$ combination of remainders (such as $d_\alpha - d$, $e_\beta - e$; see below), and 0.01 for $e' = O(e/r)$ and $d' = O(d/r)$. These assumptions for the widths of the Gaussian distributions of the remainders are collected in the last column of Table 1.

As far as Table 1 is concerned, we still have to show that the two combinations $d_{\alpha,\pi\pi} - d_\pi$ and $e_{\beta,\pi\pi} - e_\pi$, contributing to the remainders δ_4 and δ_5, are of order $O(mm_s)$, instead of $O(m_s^2)$. This follows from a $SU(2) \times SU(2)$ low-energy theorem: consider the subthreshold parameters $\alpha_{\pi\pi}$ and $\beta_{\pi\pi}$ in the $N_f = 2$ chiral limit, $m_u, m_d \to 0$; from their $SU(2) \times SU(2)$ chiral expansion in powers of m – (32) and (33) of [15] – it is straightforward to conclude that

$$\lim_{m \to 0} \alpha_{\pi\pi} = 1, \quad \lim_{m \to 0} \beta_{\pi\pi} = 1. \tag{115}$$

Then we combine the $SU(3) \times SU(3)$ chiral expansions of the subthreshold parameters and the mass and decay constant identities for the pion, by subtracting (143) from (96) [and (148) from (97)], which yields the following equalities:

$$F_\pi^2 M_\pi^2 (\alpha_{\pi\pi} - 1) = 12m^2 A + 12m^2 Z^s$$
$$-M_\pi^2 Y(3)4m(\xi + 2\tilde\xi)$$
$$+\frac{M_\pi^4}{32\pi^2} Y(3)^2 \left(\log \frac{M_K^2}{M_\pi^2} - \log \frac{M_\eta^2}{M_K^2} - \frac{7}{3} \right)$$
$$+F_\pi^2 M_\pi^2 (d_{\alpha,\pi\pi} - d_\pi), \tag{116}$$
$$F_\pi^2 (\beta_{\pi\pi} - 1) = 2m\xi + 4m\tilde\xi$$
$$+\frac{M_\pi^2 Y(3)}{16\pi^2} \left(\log \frac{M_\eta^2}{M_K^2} + 2\log \frac{M_K^2}{M_\pi^2} - \frac{5}{2} \right)$$
$$+F_\pi^2 (e_{\beta,\pi\pi} - e_\pi). \tag{117}$$

On the right-hand side of (116) [(117)], all the terms involving $O(p^4)$ LECs and chiral logarithms are of $O(m^2)$ [$O(m)$]. If we divide (116) by $F_\pi^2 M_\pi^2$ [(117) by F_π^2] and take the $N_f = 2$ chiral limit $m \to 0$, all the terms vanish apart from the NNLO remainders. The latter must therefore fulfill the following condition:

$$\lim_{m \to 0} (d_{\alpha,\pi\pi} - d_\pi) = 0, \quad \lim_{m \to 0} (e_{\beta,\pi\pi} - e_\pi) = 0, \tag{118}$$

so that the difference between $d_{\alpha,\pi\pi}$ and d_π [$e_{\beta,\pi\pi}$ and e_π] is only of order $O(mm_s)$.

Having collected all the ingredients for our choice of the prior, we can now perform the integration over the NNLO remainders to obtain $P(r, Y, Z|\text{data})$. If we integrate the latter with respect to two parameters, we end up with the marginal (posterior) probabilities:

$$P(r|\text{data}) = \int dY\, dZ\, P(r, Y, Z|\text{data}), \tag{119}$$

$$P(Y|\text{data}) = \int dr\, dZ\, P(r, Y, Z|\text{data}), \tag{120}$$

$$P(Z|\text{data}) = \int dY\, dY\, P(r, Y, Z|\text{data}), \tag{121}$$

$$P(X|\text{data}) = \int dr\, dY\, dZ\, \delta(YZ - X)\, P(r, Y, Z|\text{data})$$
$$= \int dr\, dZ\, \frac{1}{Z} P(r, X/Z, Z|\text{data}). \tag{122}$$

The precise expression of P and the numerical evaluation of these integrals are detailed in Appendix C.

4.4 Discussion and results

Even if no information from $\pi\pi$ scattering data is included, the results of the integrations (119)–(122) are non-trivial, because of the interplay of the various constraints imposed. For instance, the prior for r, when integrated over all other variables, will no longer be uniform. The probability density profiles of Fig. 1 are obtained by replacing $P(r, Y, Z, \delta_i|\text{data})$ with $\pi(r, Y, Z, \delta_i)$ and integrating over all but one variable. They can be interpreted as a measure of the "phase space" for each parameter allowed by the theoretical constraints. The significance of the $\pi\pi$ data will be seen in the modification induced with respect to such "reference" density profiles.

In the present framework, we may make more quantitative the well-known mechanism by which a low value of r implies a suppression of the quark condensate [11]. In Fig. 2 we show the reference probability density profiles for X, when the quark mass ratio r is taken fixed at different values, $r = 25, 20, 15, 10$. (The ratio of the order parameters $Y(3)$ behaves similarly.)

Notice that for small values of r, for which $X(3)$ is very small, the two-flavor order parameter $X(2)$ should also be small. This is clear from inspection of (103) and (104), because $\epsilon(r) \sim 1$. Since we know from our $SU(2) \times SU(2)$ analysis [15] of the same $\pi\pi$ data that $X(2)$ is very close to 1, we can expect that such data will constrain r to stay away from such small values. This is what we observe in Fig. 3, in which we show the marginal probability density profile for r with the inclusion of the $\pi\pi$ experimental data.

These data induce a substantial change in the distribution as compared to the reference probability density profile (restricted phase space). However, such a broad distribution cannot be used for a real determination of r; at most a lower bound for r can be given in probabilistic
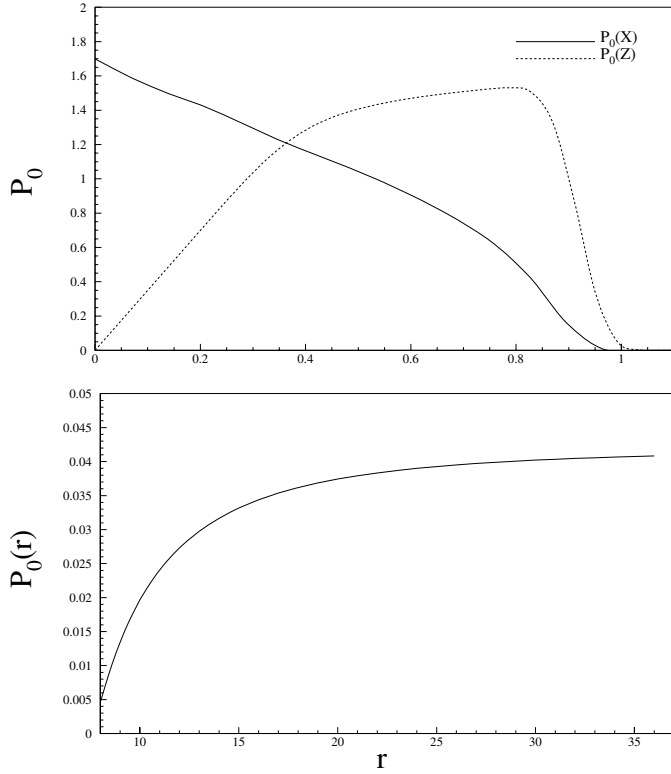
Fig. 1. The reference probability density profiles for the order parameters $X(3)$ (full) and $Z(3)$ (dashed) [top], and for the quark mass ratio r [bottom]
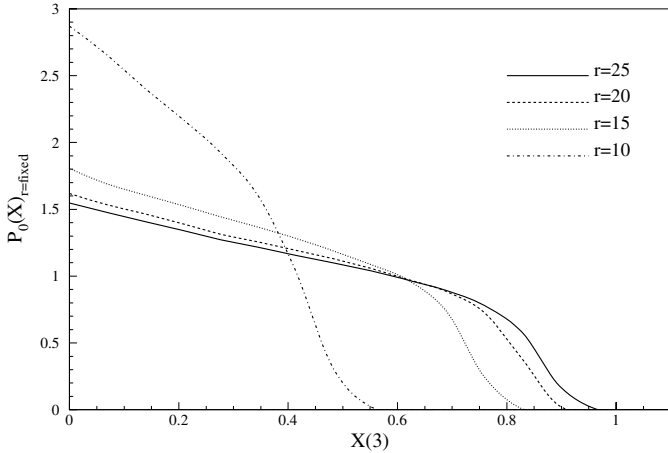

Fig. 2. The reference probability density profiles for the order parameter $X(3)$ when the quark mass ratio r is taken fixed at four different values
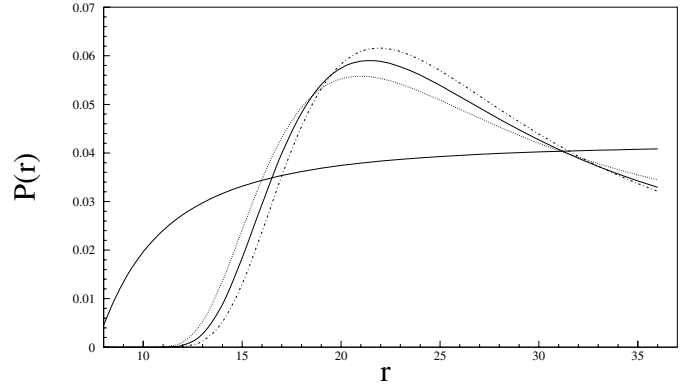

Fig. 3. The probability density profile for r inferred from the $\pi\pi$ data (thick lines) as compared to the reference one (thin dotted line). The different curves represent different choices for the prior. The full line corresponds to the choice of priors indicated in the previous section. The dashed-dotted line is obtained by reducing the widths for the prior distributions of the remainders by a factor of 2, the dotted line by increasing the widths by a factor of 2

tuations. It is therefore not surprising that similar values of r are obtained through the perturbative expansion (46) or the non-perturbative framework presented above. Such similarity is actually a welcome check of the approach advocated in this paper.

We also show in Fig. 3 the dependence of the inferred probability density profile on the initial choice of the prior: the full line refers to the choice of priors described in Sect. 4.3, while the dashed-dotted one (dotted one) corresponds to a distribution for the remainders with half widths (double widths), as compared to Table 1. As expected, broader Gaussians for the NNLO remainders lead to a flatter p.d.f. for r – the impact of experimental information is weakened when higher orders are allowed to be larger. If the most probable value of r depends to some extent on the choice of the prior, the same is not true for the 95% lower bound, which is almost the same for all distributions.

A comment on the so-called "Kaplan–Manohar ambiguity" is in order here. In [31], it was shown that the sum of the $O(p^2)$ and $O(p^4)$ chiral Lagrangian remained unchanged under a shift in the quark masses:

$$m \to m + \lambda m m_s \,, \qquad m_s \to m_s + \lambda m^2 \,, \qquad (123)$$

and a corresponding redefinition of the $O(p^4)$ LECs $L_{6,7,8}$. This seemingly prevents any determination of the quark mass ratio r. However, the Kaplan–Manohar ambiguity also induces a shift in the $O(p^6)$ terms included in the NNLO remainders (neglected in a perturbative treatment of $O(p^4)$ expansions). We have assumed a good overall convergence of the chiral series and therefore required small NNLO remainders, which corresponds to fixing the Kaplan–Manohar ambiguity. We point out that this hypothesis is not specific to our framework and is a fairly general assumption when dealing with chiral series.

On the other hand not much deviation is caused by $\pi\pi$ data with respect to the reference profiles for $X(3)$, $Z(3)$
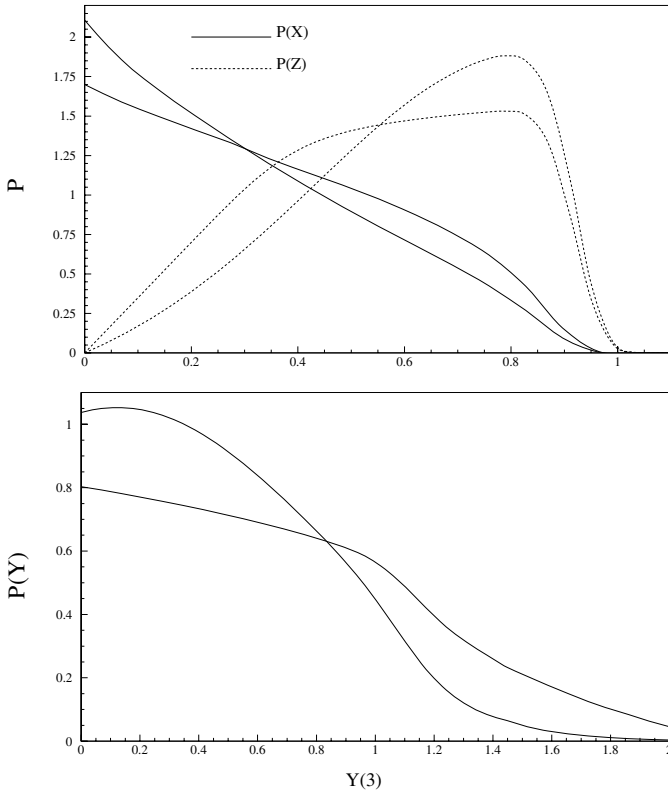
terms: $r \geq 14$ at 95% confidence level. The most probable value of r lies at $r = 21$–22, very close to standard expectations. Indeed, the motivation for the rearrangement of the chiral expansions, namely the possible importance of vacuum fluctuations and their potential to destabilize the chiral series, is not essential in the case of r: the fluctuation parameters L_4 and L_6 are absent from the perturbative reexpression of the chiral series of r, see (46), which may thus exhibit no instability even in the case of large fluc-

Fig. 4. The probability density profiles as inferred from the $\pi\pi$ data (thick lines) compared to the reference one, representing the phase space (thin lines). Full lines refer to $X(3)$, dashed lines to $Z(3)$ [top] and full lines to the ratio of order parameters $Y(3)$ [bottom]

and $Y(3)$, as is clear from Fig. 4. This is an indication of the fact that $\pi\pi$ data, as was expected, are not sensitive enough to $X(3)$ and $Z(3)$. Their determination would require the inclusion of other observables, which we discuss now.

5 Other sources of constraints on $X(3)$ and $Z(3)$

We now briefly mention some possible sources of independent experimental information on the three-flavor chiral order parameters $X(3)$ and $Z(3)$, or equivalently on the $O(p^4)$ fluctuation parameters $Y^2(3)L_6$ and $Y(3)L_4$. The combination of $O(p^4)$ LECs $(\Delta L_8 + 2\Delta L_6)$, invariant under the Kaplan–Manohar transformation, is of particular interest. It appears in many observables and has remained undetermined so far. $Y^2(3)L_8$ is essentially given by r through (40): $Y^2(3)\Delta L_8 = 0.99 \cdot 10^{-3}$ for $r = 25$ (where the NNLO remainders are neglected). From the positivity of $X(3)$ and its relation to the fluctuation parameter L_6 (32), one gets the following upper bound for L_6:

$$Y^2(3)\Delta L_6 \leq \frac{1}{16(r+2)}\frac{F_\pi^2}{M_\pi^2}[1 - \epsilon(r) - d], \qquad (124)$$

which implies that $Y^2(3)\Delta L_6 \leq 0.98 \cdot 10^{-3}$ for $r = 25$ (with an expected uncertainty of 10 % from NNLO remainders). Between the limit of no fluctuations and that of maximal fluctuations, the combination of LECs $Y^2(3) \times [\Delta L_8 + 2\Delta L_6]$ can thus vary in the range:

$$1.0 \cdot 10^{-3} \leq Y^2(3)[\Delta L_8 + 2\Delta L_6] \leq 3.0 \cdot 10^{-3}. \quad [r = 25] \tag{125}$$

This combination can be perturbatively related to the LEC $\bar{\ell}_3$ [1] of the $N_f = 2$ chiral Lagrangian; see (11.6) in [3]. In the limit of no fluctuations, $\bar{\ell}_3$ is a positive number of $O(1)$; the estimate $\bar{\ell}_3 = 2.9 \pm 2.4$ was obtained in [1] under the assumption of the validity of the Zweig rule. If larger vacuum fluctuations make $Y^2(3)[\Delta L_8 + 2\Delta L_6]$ increase, $\bar{\ell}_3$ decreases towards negative values with a larger magnitude. Thus, in principle, the size of vacuum fluctuations could be investigated through an accurate determination of $\bar{\ell}_3$ obtained from $\pi\pi$ scattering parameters. Unfortunately, experimental information at such an accuracy is not available due to a large uncertainty in the scattering length a_0^2, which is not tightly constrained by available K_{e4} decay experiments[7]. Therefore, we have to consider other sources of information in order to constrain the $N_f = 3$ order parameters.

5.1 Goldstone boson scattering and decays

In order to estimate the size of the vacuum fluctuations of $s\bar{s}$ pairs, processes directly involving strange mesons are required. Before sketching how our method could be extended to the relevant processes, we want to comment on a few estimates of the $O(p^4)$ LECs L_4 and L_6 that are available in the literature. These estimates show a common feature: they rely on the standard (perturbative) treatment of vacuum fluctuations, assuming that the latter are small, but they lead to L_4 and L_6 becoming significantly larger than their critical values. These estimates should therefore be considered at most as valuable hints of the internal inconsistency of the perturbative treatment.

Büttiker et al. [33] have analyzed the $\pi K \to \pi K$ and $\pi\pi \to K\bar{K}$ amplitudes, thereby obtaining the amplitudes at threshold and in the subthreshold region. Comparing these results with the $O(p^4)$ χPT expansion of Bernard et al. [25], they determine the LECs L_i $(i = 1, 4)$ and the combination $L_8 + 2L_6$:

$$10^3[L_8^r + 2L_6^r](M_\rho) = 3.66 \pm 1.52. \tag{126}$$

The large uncertainty quoted is reflected in the uncertainty in the scattering lengths combination $a_0^{1/2} + 2a_0^{3/2}$. This could improve considerably once experimental results from πK atoms become available. However, the analysis

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[7] The available $\pi\pi$ scattering data were analyzed in [15], yielding $\bar{\ell}_3 = -18.5 \pm 16.7$ and thus suggesting an important role played by vacuum fluctuations. If the experimental information on the $I = 2$ channel is replaced by a theoretical constraint concerning the scalar radius of the pion [32,15], $\bar{\ell}_3$ becomes a small positive number compatible with the absence of fluctuations.

is based on $O(p^4)$ χPT, in which the implicit assumption is made that $Y(3) = 1$. From our bounds (125), taking $Y(3) = 1$, we obtain

$$0.27 \leq 10^3 [L_8^r + 2L_6^r](M_\rho) \leq 2.3. \quad [r = 25, Y(3) = 1] \tag{127}$$

It is clear that the values for $L_8 + 2L_6$ given in [33] are barely compatible with the assumption of $Y(3) = 1$. Furthermore, the authors of [33] estimate $10^3 L_4^r(M_\rho) = 0.50 \pm 0.39$, which implies $10^3 \Delta L_4 = 1.0 \pm 0.39$ and suggests significant violation of the Zweig rule in the scalar sector [see (51)]. Both remarks call for a comparison of πK scattering amplitudes with a chiral expansion treating non-perturbatively (possibly large) vacuum fluctuations [26].

Recently, Bijnens and Dhonte [20] have calculated the π and K scalar form factors at two loops in $N_f = 3$ χPT; they then fit their results to the corresponding dispersive representation based on the solution of the multi-channel Omnès–Muskhelishvili equations [5,6]. In order to obtain "decent fits" for the form factors at zero momentum transfer, they found that the LECs L_4 and L_6 had to satisfy the constraint

$$L_6^r(M_\rho) \lesssim 0.6 \times L_4^r(M_\rho) + 0.4 \cdot 10^{-3}. \tag{128}$$

If we take this to imply that $[2L_6^r - L_4^r](M_\rho) \lesssim 0.8 \cdot 10^{-3}$, then we can rewrite the constraint in terms of the fluctuation parameters ρ, λ introduced in Sect. 3:

$$\rho - \lambda \lesssim 1.6. \qquad [r = 25] \tag{129}$$

Recalling (60), the convergence of the perturbative expansion of $Y(3) = 2mB_0/M_\pi^2$ requires $\rho - \lambda \ll 1$. Viewed in this light, the constraint of [20] is not surprising: it is simply the observation that the authors, within their perturbative analysis, cannot find a good fit to a perturbative χPT expansion in the presence of large vacuum fluctuations. In addition, they find that requiring that the values of the scalar form factors at zero not deviate too much from their lowest order values leads to the estimate $0.3 \leq 10^3 L_4^r(M_\rho) \leq 0.6$. Note that this result is roughly in agreement with that of [33] discussed above. According to Table 2 of [20], this value of L_4 leads to a suppression of $Z(3)$ down to half of $Z(2)$, as can be checked from (32). All these considerations suggest sizeable vacuum fluctuations in the scalar sector.

We outline now how additional observables coming from Goldstone boson scattering and decay could be incorporated naturally in the Bayesian machinery, in order to constrain the size of vacuum fluctuations, or equivalently $X(3)$ and $Z(3)$. The most obvious candidate is πK scattering. The first step consists in using analyticity, unitarity, crossing symmetry in conjunction with experimental data in order to constrain as much as possible the low-energy πK scattering amplitude [33]. The second stage corresponds to an analysis similar to that in the case of $\pi \pi$ scattering: establish a dispersive representation of the amplitude with subthreshold parameters (i.e., subtraction constants like $\alpha_{\pi\pi}$ and $\beta_{\pi\pi}$), determine

the value of these parameters from experiment, then include these parameters as additional observables for the Bayesian analysis. The expected outcome should be more stringent constraints on $X(3)$ and $Z(3)$ [26].

The decay $\eta \to 3\pi$ is a second process of interest [34]. The standard treatment of this decay starts with the ratio $A_{\eta \to 3\pi}/\Delta_K$, where $A_{\eta \to 3\pi}$ is the decay amplitude and $\Delta_K = (M_{K^+}^2 - M_{K^0}^2)_{\rm QCD}$. This ratio is then perturbatively reexpressed in terms of the Goldstone boson masses and a single $O(p^4)$ LEC L_3. As stressed previously, a bare chiral expansion of ratios of QCD correlation functions that are only conditionally convergent may exhibit instabilities. To cope with possibly large vacuum fluctuations, a better starting point could be the expansion of the quantity $F_\pi^3 F_\eta A_{\eta \to 3\pi}$, which is linearly related to a QCD correlation function. Such an expansion will involve more LECs and order parameters and allow the extraction of the latter from the data. Since the decay $\eta \to 3\pi$ is forbidden in the isospin limit $m_u = m_d$, we must start by extending the previous discussion of Goldstone boson masses and decay constants to include isospin breaking. A dispersive representation of the amplitude $A_{\eta \to 3\pi}$ must then be written to define convenient observables. The dispersion relations are here more involved than in the case of $\pi \pi$ and πK scattering: they require studying $\eta \pi \to \pi \pi$ and performing subsequently an analytical continuation to the (physical) decay channel. The observables thus defined, related to the behavior of the decay amplitude at the center of the Dalitz plot (via slope parameters), can be exploited in our Bayesian framework in order to constrain further the three-flavor chiral order parameters and to extract the quark mass ratios m_u/m_s and m_d/m_s.

5.2 Two-point functions and sum rules

In this paper, our aim was in particular to pin down $X(3)$, i.e., the $N_f = 3$ chiral condensate measured in physical units, which governs the behavior of QCD correlation functions in the limit $m_u = m_d = m_s = 0$. Related though different quantities arise when the high-energy limit of the same correlation functions is studied through the operator product expansion (OPE). Local condensates appear then, and those with the lowest dimension are

$$\Sigma_u = -\langle 0|\bar{u}u|0\rangle, \quad \Sigma_d = -\langle 0|\bar{d}d|0\rangle, \quad \Sigma_s = -\langle 0|\bar{s}s|0\rangle, \tag{130}$$

where the physical vacuum of the theory is denoted $|0\rangle$ with all the quarks carrying their physical masses: no chiral limit is taken.

These OPE quark condensates occur in various sum rules for two-point correlators and could thus be determined in this framework [35]. First, they arise (multiplied by a mass term) in the high-energy tail of the correlators as dimension-4 operators. (For example, see [36] for the case of pseudoscalar densities.) Next, in some sum rules, normal-ordered condensates of the type (130) appear through chiral Ward identities. For instance, in the case of the divergence of the strangeness-changing vector current [37,38], the strange-quark mass is determined via a

sum rule with no subtraction, but another sum rule can be written with the subtraction constant $(m_s - m_u)(\Sigma_s - \Sigma_u)$, providing in principle some information on the OPE quark condensates. Unfortunately, the high-energy tail of the (Borel transformed) two-point function involved in this case has a QCD expansion which behaves quite badly and prevents any accurate determination. Lastly, the OPE quark condensates arise when factorization is invoked to reexpress higher-dimensional four-quark operators as the square of $\bar{q}q$ vacuum expectation values.

We stress that the OPE quark condensates $\Sigma_u, \Sigma_d, \Sigma_s$ have a different definition (and thus value) from the chiral condensates that we have considered here and in [15]:

$$\Sigma(2) \equiv - \lim_{m_u, m_d \to 0} \langle 0|\bar{u}u|0\rangle$$
$$= \lim_{m_u, m_d \to 0} \Sigma_u = \lim_{m_u, m_d \to 0} \Sigma_d \,, \qquad (131)$$
$$\Sigma(3) \equiv - \lim_{m_u, m_d, m_s \to 0} \langle 0|\bar{u}u|0\rangle$$
$$= \lim_{m_u, m_d, m_s \to 0} \Sigma_u = \lim_{m_u, m_d, m_s \to 0} \Sigma_d$$
$$= \lim_{m_u, m_d, m_s \to 0} \Sigma_s \,. \qquad (132)$$

In particular, $\Sigma_u, \Sigma_d, \Sigma_s$ exhibit an ultraviolet divergence that must be renormalized; therefore, their definitions and their values depend on the convention applied. It is possible to relate them to $\Sigma(3)$ using $N_f = 3$ χPT. For instance, if we take (9.1) in [3] in the isospin limit, we get

$$X_{u,d} \equiv \frac{2m\Sigma_{u,d}}{F_\pi^2 M_\pi^2}$$
$$= X(3)$$
$$+ [Y(3)]^2 \frac{M_\pi^2}{F_\pi^2} \left[16(r+2)\Delta L_6 + 4(2\Delta L_8 + \Delta H_2) \right]$$
$$+ d_{\Sigma;u,d} \qquad (133)$$
$$= 1 - \frac{1}{2}\epsilon(r) + 4[Y(3)]^2 \frac{M_\pi^2}{F_\pi^2}\Delta H_2 - d + \frac{1}{2}d' + d_{\Sigma;u,d} \,,$$

$$X_s \equiv \frac{2m\Sigma_s}{F_\pi^2 M_\pi^2}$$
$$= X(3)$$
$$+ [Y(3)]^2 \frac{M_\pi^2}{F_\pi^2} \left[16(r+2)\Delta L_6 + 4r(2\Delta L_8 + \Delta H_2) \right]$$
$$+ d_{\Sigma;s}$$
$$= 1 + \frac{r-2}{2}\epsilon(r) + 4r[Y(3)]^2 \frac{M_\pi^2}{F_\pi^2}\Delta H_2$$
$$- d + \frac{r}{2}d' + d_{\Sigma;s} \,, \qquad (134)$$

where the NNLO remainders are denoted $d_{\Sigma;u,d}$ and $d_{\Sigma;s}$, and the $O(p^4)$ high-energy counterterm H_2^r arises in the combination

$$\Delta H_2 = H_2^r(\mu) - \frac{1}{128\pi^2}\left(\frac{1}{2}\log\frac{M_K^2}{\mu^2} + \frac{1}{3}\log\frac{M_\eta^2}{\mu^2} \right)$$
$$- \frac{1}{256\pi^2(r-1)}\left(3\log\frac{M_K^2}{M_\pi^2} + \log\frac{M_\eta^2}{M_K^2} \right) \,. \qquad (135)$$

The value of such high-energy counterterms cannot be fixed by low-energy data only, and their presence in the chiral expansions is merely a manifestation of the renormalization-scheme dependence of the OPE quark condensates.

An interesting relation, free from high-energy counterterms, exists between the OPE condensates:

$$\frac{rX_{u,d} - X_s}{r-1} = 1 - \epsilon(r) - d + \frac{r}{r-1}d_{\Sigma;u,d} - \frac{1}{r-1}d_{\Sigma;s} \,. \qquad (136)$$

Two conclusions can be drawn from this relation. First, for r larger than 15, (136) shows that $X_{u,d}$ is close to $[1 - \epsilon(r) - d]$, while we see from (82) that $X(2)(1 - \bar{d}_\pi)$ equals $[1 - \epsilon(r) - d]$ up to $1/r$-suppressed corrections. $\Sigma_{u,d}$ should thus be very close to $\Sigma(2)$, which was expected since the u, d quarks are very light and the physical world is near the $N_f = 2$ chiral limit.

The second conclusion is that $X_s - X_{u,d}$ can hardly be obtained from such a relation, since $X_{u,d}$ and $1 - \epsilon(r) - d$ largely cancel. Thus, very accurate knowledge of r and $X_{u,d}$ would be needed to determine X_s this way. More generally, the possibility of significant vacuum fluctuations of $s\bar{s}$ pairs makes it difficult to relate in a quantitative way $\Sigma(3)$ and the OPE quark condensates Σ_{ud}, Σ_s.

Such a relation between OPE and chiral quark condensates is naturally relevant for the description of K decays. In particular, some $K \to \pi\pi$ weak matrix elements are related to VEVs of four-quark operators in the $N_f = 3$ chiral limit, thanks to sum rules for vector–axial or scalar–pseudoscalar correlators [39]. These sum rules are evaluated by splitting the integral in two energy domains: the low-energy region is described by experimental data, while the high-energy behavior is obtained through the operator product expansion, which involves a priori OPE quark condensates. However, since the sum rules are evaluated in the chiral limit $m_u = m_d = m_s \to 0$, these condensates actually reduce to the $N_f = 3$ chiral condensate $\Sigma(3)$.

The dispersive estimates of $K \to \pi\pi$ matrix elements could thus be affected at three different stages by significant vacuum fluctuations of $s\bar{s}$ pairs leading to smaller values of $\Sigma(3)$. Firstly, extrapolating the weak matrix elements from the $N_f = 3$ chiral limit to the physical values of the u, d, s quarks could not be carried out on the basis of the usual treatment and values of LECs of $N_f = 3$ χPT, since the latter assume from the start a leading contribution from $\Sigma(3)$. Moreover, the very estimate of the sum rule could be modified because of the change in the high-energy behavior of the correlator in the chiral limit. The third question concerns dimension-6 four-quark condensates, which appear at higher orders of OPE and are often related to the square of a $\bar{q}q$ condensate through factorization, on the basis of large-N_c arguments. The presence of large $q\bar{q}$ fluctuations might render such an assumption invalid.

5.3 Implications for lattice simulations

In principle, the lattice should represent a particularly favorable domain to study how QCD at low energy de-

pends on the light-quark masses and how this dependence is connected to the vacuum fluctuations of $q\bar{q}$ pairs. Recent progress has been made in this field. Discretizations of the Dirac operator have been discovered with highly desirable qualities for the simulation of light quarks. In particular, Ginsparg–Wilson fermions [40] do not break chiral symmetry explicitly. A second (cheaper) option consists in twisted-mass lattice QCD [41], where a parametrized rotation of the mass matrix allows one to restore chiral symmetry partially in observables through an averaging procedure. Another avenue is provided by staggered fermions [42], which allows one to study an odd number of flavors, at the cost of introducing unwanted flavor degeneracies.

Vacuum fluctuations of $q\bar{q}$ pairs are typical sea-quark effects. The fermionic determinant plays here an essential role, since we are interested in chiral parameters dominated by the infrared end of the Dirac spectrum [10,11]. In order to study these effects on the lattice, it is therefore mandatory to generate data for three dynamical flavors. For this particular purpose, one cannot rely on quenched data (with no dynamical quark) or on data generated with only two dynamical quarks – even though they can be of interest for observables relatively insensitive to the fermion determinant, e.g., M_ρ.

We will now illustrate, by considering "bare" expansions of "good" observables such as $F_\pi^2 M_\pi^2$ and F_π^2, how lattice data could probe vacuum fluctuations of $q\bar{q}$ pairs and how chiral extrapolations should be dealt with if the latter turn out to be significant. We consider a slightly optimistic situation where lattice data with reasonable accuracy can be generated for three light dynamical flavors. For simplicity, we choose to work in the limit of degenerate strange and light-quark masses. The analysis could be done for independent variations of the quark masses, but the attendant complications do not add anything essential to our conclusions. Moreover, it is likely that realistic lattice calculations are more easily performed in this simplified situation. On the lattice, we denote by m_L the common mass of the three degenerate light flavors and by M_L^2 and F_L^2 the common mass and decay constant of the eight degenerate Goldstone bosons. We keep m and m_s for the physical values of the quarks and $F_\pi^2, M_\pi^2, \dots$ for the physical values of the Goldstone boson observables.

The observables F_L^2 and $F_L^2 M_L^2$ have thus the form

$$F_L^2 M_L^2 = 2m_L B_0 F_0^2$$
$$+ 64m_L^2 B_0^2 \left[3L_6(\mu) + L_8(\mu) - \frac{1}{96\pi^2} \log \frac{M_L^2}{\mu^2} \right]$$
$$+ F_L^2 M_L^2 d_L , \qquad (137)$$
$$F_L^2 = F_0^2$$
$$+ 16m_L B_0 \left[3L_4(\mu) + L_5(\mu) - \frac{3}{128\pi^2} \log \frac{M_L^2}{\mu^2} \right]$$
$$+ F_L^2 e_L , \qquad (138)$$

where the remainders d_L, e_L are of order m_L^2.

Since B_0, F_0 and the LECs L_i are all defined in the $N_f = 3$ chiral limit and are thus independent of the quark masses, we may use (61)–(67) to eliminate them in favor

of the real-world parameters $X(3), Y(3), Z(3), r$ and the physical values of the masses and couplings of the Goldstone bosons, leading to

$$F_L^2 M_L^2 = b\, F_\pi^2 M_\pi^2 X(3)$$
$$+ b^2 \frac{F_\pi^2 M_\pi^2}{r+2} \left\{ 3[1 - X(3) - d] + (r-1)[\epsilon(r) + d'] \right\}$$
$$+ 2b^2 M_\pi^4 Y(3)^2 \left\{ \frac{-1}{32\pi^2(r+2)} \left(3\log \frac{M_K^2}{M_\pi^2} + \log \frac{M_\eta^2}{M_K^2} \right) \right.$$
$$\left. + \frac{1}{16\pi^2} \left(\log \frac{M_K^2}{M_L^2} + \frac{1}{3} \log \frac{M_\eta^2}{M_L^2} \right) \right\} + F_L^2 M_L^2 d_L , \quad (139)$$
$$F_L^2 = F_\pi^2 Z(3)$$
$$+ b \frac{1}{r+2} F_\pi^2 \left\{ 3[1 - Z(3) - e] + (r-1)[\eta(r) + e'] \right\}$$
$$- b \frac{M_\pi^2 Y(3)}{32\pi^2} \left[\frac{1}{r+2} \left(3\log \frac{M_\eta^2}{M_K^2} + 7\log \frac{M_K^2}{M_\pi^2} \right) \right.$$
$$\left. - 2 \left(\log \frac{M_\eta^2}{M_L^2} + 2\log \frac{M_K^2}{M_L^2} \right) \right] + F_L^2 e_L , \qquad (140)$$

Taking the ratio of these equations gives M_L^2 implicitly as a function of $b = m_L/m$. The remainders d, e enter the resulting expressions multiplied by a factor of b/r; we will ignore them as well as the $1/r$-suppressed contributions from d', e'.

Since the chiral expansion requires small values of m_L, while present day lattice simulations prefer m_L on the order of m_s, it is important to ascertain if there is a range of variation for m_L in which our equations may be applied and still give valuable results. There are two different conditions to be met. First, as m_L increases, the degenerate mass M_L increases, eventually exceeding M_K, M_η; this in itself is of concern, since the chiral expansion becomes unreliable as M_L approaches values typical of relevant hadronic resonances. In addition, the terms logarithmic in M_L^2 become negative, and eventually the procedure described above is unstable. Therefore, we will restrict the range of variation of m_L so that these logarithmic terms do not contribute more than 25% of the total. This stability criterion constrains the allowed region in the space of parameters $X(3), Z(3), r, m_L$; however, this region includes values of interest. For example, in Fig. 5 we show the allowed region in $X(3), m_L/m$ for the illustrative choice $Z(3) = 0.6, r = 25$. For $m_L/m \leq 20$, all values of $X(3)$ are possible. As can be seen in Fig. 6, with such a constraint on m_L/m, we satisfy also the first requirement since M_L does not exceed $1.5 \cdot M_K$.

For values of $Z(3)$ between 0.4 and 0.8 and of r between 20 and 30, we find that the allowed region does not qualitatively change: so long as we keep m_L/m less than 20, then all values of $X(3)$ are permitted according to our stability criterion. Consider, then, the variation of F_L^2 and of $F_L^2 M_L^2$ as functions of m_L, for fixed $Z(3)$ and r, as shown in Figs. 7 and 8 in the illustrative case $Z(3) = 0.6, r = 25$. From (139) and (140), the general dependence on $X(3)$ is apparent: the $X(3)$-dependence must vanish for small
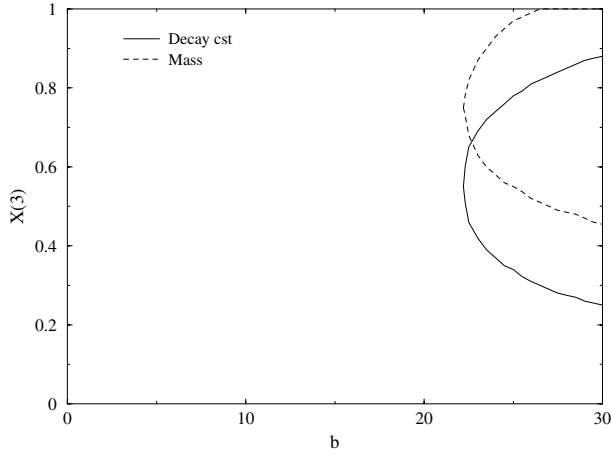
Fig. 5. Stability criterion for $Z(3) = 0.6, r = 25$. Inside the circle in full line [dashed line], the term logarithmic in M_L contributes more than 25% to F_L^2 [$F_L^2 M_L^2$]. All NNLO remainders are set to zero
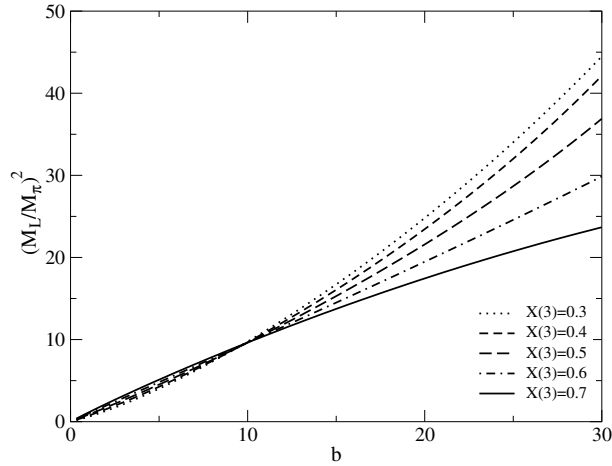

Fig. 7. $F_L^2 M_L^2/(F_\pi M_\pi)^2/b$ as a function of b. Each line corresponds to a different value of $X(3)$, whereas r is set to 25. All NNLO remainders are set to zero

Fig. 6. M_L^2/M_π^2 as a function of $b = m_L/m$ for $Z(3) = 0.6, r = 25$. All NNLO remainders are set to zero

Fig. 8. F_L^2/F_π^2 as a function of b. Each line corresponds to a different value of $X(3)$, whereas r is set to 25. All NNLO remainders are set to zero

$b = m_L/m$ as well as for $b = m_L/m \sim (r + 2)/3 \sim 10$ (apart from a residual dependence from the logarithms). Therefore, the region of interest is $10 \leq b \leq 20$. Fortunately, even in this restricted interval, there is considerable dependence on $X(3)$, especially for $F_L^2 M_L^2/b$. A good knowledge of the spectrum in this range would allow us to discriminate at least between the most extreme possibilities ($X(3)$ close to $X(2)$, $X(3)$ close to 0)[8]. We stress that

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[8] A first step in this direction was proposed by considering the dependence on m and m_s of the Goldstone boson masses to extract the values of some low-energy constants for partially quenched staggered fermions [43]. However, this was achieved by relying on the chiral expansion of M_P^2, with a perturbative reexpression of the fundamental parameters $r, X(3), Z(3)$ in terms of Goldstone boson masses. Moreover, the $O(p^4)$ LECs L_4 and L_6 related to the vacuum fluctuations were eliminated through a perturbative redefinition of the parameters involved in the chiral series. As discussed in Sects. 2 and 3, this proce-
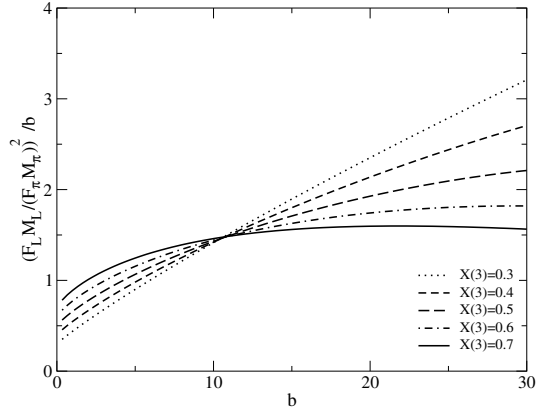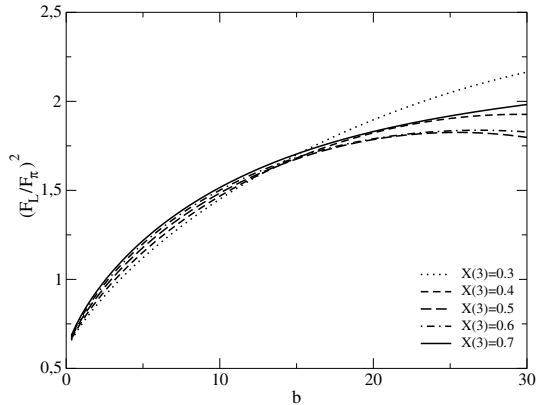
not all the observables are equivalent for this study: for instance, M_L^2 exhibits a much weaker sensitivity to vacuum fluctuations, as shown in Fig. 6. This cancellation between L_6 and L_4 in the case of the masses is quite usual [13] and does not mean that the effect is absent for all observables, as seen from Figs. 7 and 8.

We have not included the NNLO remainders d_L and e_L here, but it is a straightforward exercise to take them into account. We can check their size by writing them in the following form:

$$F_\pi^2 M_\pi^2 d_\pi = m_s^2 m D_1 + m_s m^2 D_2 + m^3 D_3 ,$$
$$F_\pi^2 e_\pi = m_s^2 E_1 + m_s m E_2 + m^2 E_3 , \qquad (141)$$

where D_i and E_i do contain $O(p^6)$ LECs and chiral logarithms. If we neglect the dependence of the chiral logarithms on the quark masses when they vary from m, m_s to m_L, the same quantities will appear in the analogous

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dure need not be correct in the case of large vacuum fluctuations.

expression for $F_L^2 M_L^2 d_L, F_L^2 e_L$:

$$\frac{d_L}{d_\pi} = \left[\frac{bF_\pi^2 M_\pi^2}{F_L^2 M_L^2}\right] \frac{b^2}{r^2} \left[\frac{D_1 + D_2 + D_3}{D_1 + D_2/r + D_3/r^2}\right],$$

$$\frac{e_L}{e_\pi} = \left[\frac{F_\pi^2}{F_L^2}\right] \frac{b^2}{r^2} \left[\frac{E_1 + E_2 + E_3}{E_1 + E_2/r + E_3/r^2}\right]. \qquad (142)$$

We can check easily that the first factor is of order one in each case (see for instance Figs. 7 and 8). Therefore, we conclude that the remainders d_L, e_L are expected to be of order m_L^2, i.e., of order $0.1 \cdot b^2/r^2$ (i.e., 10% or less). Once the remainders are included, an accurate determination of $Z(3)$ is quite difficult, because F_L^2 does not exhibit a strong sensitivity to the latter. But $X(3)$ is still accessible because of the strong variation in the curvature of $F_L^2 M_L^2$ as a function of b.

6 Summary and conclusion

The large-N_c suppressed low-energy constants $L_4^r(\mu)$ and $L_6^r(\mu)$ encode fluctuations of vacuum $\bar{s}s$ pairs. We have analyzed the influence of these fluctuations on the convergence of $N_f = 3$ χPT.

(i) For the physical value of m_s, we assume a global (though possibly slow) convergence of the $SU(3) \times SU(3)$ chiral expansion applied to low-energy connected QCD correlation functions and to observables that are linearly related to the latter: typical examples are F_P^2, $F_P^2 M_P^2$, $F_\pi^4 A_{\pi\pi \to \pi\pi}$, $F_\pi^2 F_K^2 A_{\pi K \to \pi K}$, etc. For such quantities, the bare expansion (as defined in Sect. 2) expressed in terms of the order parameters $\Sigma(3)$ and F_0 and in powers of quark masses m_u, m_d, m_s is likely characterized by relatively small higher order corrections starting at NNLO.

(ii) Vacuum fluctuations of $\bar{s}s$ pairs affect in particular the next-to-leading-order (NLO) contributions to $F_\pi^2 M_\pi^2$ and F_π^2 through terms $m_s L_6$ and $m_s L_4$, which appear in χPT with large coefficients. They reflect Zweig-rule violation and large $1/N_c$ corrections in the scalar channel. Unless L_6 and L_4 are very precisely tuned to their critical values $L_6^{\text{crit}}(M_\rho) = -0.26 \cdot 10^{-3}$, $L_4^{\text{crit}}(M_\rho) = -0.51 \cdot 10^{-3}$, the vacuum fluctuation NLO contribution to $F_\pi^2 M_\pi^2$ and/or to F_π^2 becomes of comparable size or even larger than the corresponding leading-order (LO) contributions given by the three-flavor condensate $\Sigma(3)$ and by the pion decay constant F_0^2. In this case, the expansions of $X(3) = 2m\Sigma(3)/F_\pi^2 M_\pi^2$ and $Z(3) = F_0^2/F_\pi^2$ in powers of m_s break down despite the convergence of $F_\pi^2 M_\pi^2$ and F_π^2. As a result, $X(3)$ and $Z(3)$, which measure $N_f = 3$ order parameters in physical units, could be suppressed well below one, implying an instability of $N_f = 3$ χPT.

(iii) The instability due to vacuum fluctuations upsets the standard perturbative reexpression of the lowest order parameters $\Sigma(3)$ and F_0^2 as well as quark masses in favor of an expansion in terms of physical Goldstone boson masses, F_π and F_K. Instead, using the four mass and decay constant Ward identities, we non-perturbatively eliminate the LECs $L_4, L_5, L_6, (L_7), L_8$ in terms of the order parameters $X(3)$ and $Z(3)$, the quark mass ratio $r = m_s/m$ and

the four NNLO remainders d_π, d_K, e_π, e_K, which collect all higher order contributions starting at $O(p^6)$. This procedure amounts to an exact resummation of the standard perturbative reexpression of $X(3)$, $Z(3)$ and r and it applies even if the vacuum fluctuations suppress $X(3)$ and/or $Z(3)$.

(iv) In this way, values of the basic order parameters $X(3)$, $Z(3)$ and the quark mass ratio r can be constrained by experimental data as long as NNLO remainders are under control. In order to gradually incorporate theoretical conjectures about the order parameters $X(3)$ and $Z(3)$ (e.g., their positivity, paramagnetic inequalities), and on higher chiral orders (i.e., NNLO remainders), we propose to use Bayesian statistical inference. In this approach, previous knowledge of the parameters is encoded into the prior probability distribution function. At this step, some degree of arbitrariness is introduced, but the dependence on the choice of the prior is guaranteed to be weak if the data are significant enough.

(v) We have applied this procedure to the three-flavor analysis of elastic $\pi\pi$ scattering, in order to test the ability of the recent high-precision low-energy data obtained by the E865 Collaboration [14] to constrain three-flavor chiral dynamics. We have shown that, for the present state of experimental precision, the data cannot determine the two fundamental $N_f = 3$ chiral order parameters $X(3)$ and $Z(3)$. However, the low-energy $\pi\pi$ data is sufficient for us to put a quantitative lower bound on the quark mass ratio $r = m_s/m \geq 14$ at the 95% confidence level, and to determine the corresponding probability distribution function.

(vi) The Bayesian machinery is suitable for incrementally including further experimental information on low-energy observables, and seems especially well adapted in this context, in view of an extension of our analysis to valence s-quark effects. In particular, πK scattering appears to be rather promising, due to recent progress obtained through the solution of the corresponding Roy–Steiner equations [33]. We plan to address this issue in future publications [26].

(vii) The possible instability of $N_f = 3$ chiral expansions, and the prescription examined in this paper to treat it, are also relevant in other respects. One example is the evaluation of $K \to \pi\pi$ weak matrix elements from sum rules based on OPE: in particular, the extrapolation of the OPE condensate from the chiral limit to the physical values of the quark masses would not be possible on the basis of the usual treatment of $N_f = 3$ χPT formulas. A similar remark applies to the study of the quark mass dependence of Goldstone boson masses on the lattice and to determinations of the LECs by these means. We have shown how such a program could be pursued even in the presence of large fluctuations, provided simulations with three dynamical flavors would be available with quark masses as small as the physical strange-quark mass. It remains to be seen whether such simulations, with proper control of the continuum and thermodynamic limits, will be feasible in the near future.

(viii) In order to detect possibly large $\bar{s}s$ fluctuations, another strategy is conceivable: one might calculate and analyze as many quantities as possible within the standard $SU(3) \times SU(3)$ χPT, up to and including two loops, using the standard perturbative reexpression of low-energy parameters [17,20]. The instability of such χPT expansions could appear as an internal inconsistency of the result of corresponding fits with the assumptions underlying the perturbative treatment of standard χPT.

A Mass and decay constant identities

We recall for convenience the chiral expansion of the Goldstone boson masses as discussed in [11,13]:

$$F_\pi^2 M_\pi^2 = 2m\Sigma(3) + 2m(m_s + 2m)Z^s + 4m^2 A$$
$$+ 4m^2 B_0^2 L + F_\pi^2 M_\pi^2 d_\pi, \quad (143)$$
$$F_K^2 M_K^2 = (m_s + m)\Sigma(3) + (m_s + m)(m_s + 2m)Z^s$$
$$+ (m_s + m)^2 A + m(m_s + m)B_0^2 L + F_K^2 M_K^2 d_K, \quad (144)$$

The case of the η meson is discussed in Sect. 3.4 and below. The connection with the standard LECs of the $N_f \geq 3$ effective Lagrangian is

$$Z^s = 32 B_0^2 \left\{ L_6(\mu) - \frac{1}{512\pi^2} \left[\log \frac{M_K^2}{\mu^2} + \frac{2}{9} \log \frac{M_\eta^2}{\mu^2} \right] \right\}, \quad (145)$$

$$A = 16 B_0^2 \left\{ L_8(\mu) - \frac{1}{512\pi^2} \left[\log \frac{M_K^2}{\mu^2} + \frac{2}{3} \log \frac{M_\eta^2}{\mu^2} \right] \right\}. \quad (146)$$

The remainders $F_P^2 M_P^2 d_P$ collect all higher order terms, starting at the next-to-next-to-leading order $O(m_q^3)$, in agreement with the definition in [13], but different from that in [8]. The combination of chiral logarithms L is [13]

$$L = \frac{1}{32\pi^2} \left[3\log \frac{M_K^2}{M_\pi^2} + \log \frac{M_\eta^2}{M_K^2} \right]. \quad (147)$$

Similar expressions are derived for the decay constants:

$$F_\pi^2 = F^2(3) + 2(m_s + 2m)\tilde{\xi} + 2m\xi \quad (148)$$
$$+ \frac{1}{16\pi^2} 2m B_0 \left\{ \log \frac{M_\eta^2}{M_K^2} + 2\log \frac{M_K^2}{M_\pi^2} \right\} + F_\pi^2 e_\pi,$$

$$F_K^2 = F^2(3) + 2(m_s + 2m)\tilde{\xi} + (m_s + m)\xi + m B_0 L$$
$$+ F_K^2 e_K. \quad (149)$$

The scale-invariant constants ξ and $\tilde{\xi}$ are related to the LECs L_4 and L_5 as follows:

$$\tilde{\xi} = 8 B_0 \left\{ L_4(\mu) - \frac{1}{256\pi^2} \log \frac{M_K^2}{\mu^2} \right\}, \quad (150)$$

$$\xi = 8 B_{0n} \left\{ L_5(\mu) - \frac{1}{256\pi^2} \left[\log \frac{M_K^2}{\mu^2} + 2\log \frac{M_\eta^2}{\mu^2} \right] \right\}. \quad (151)$$

The remainders $F_P^2 e_P$ collect the NNLO terms $O(m_q^2)$. Equations (32), (40) and (41) in Sect. 3.2 can be obtained by combining the previous identities to eliminate the $O(p^4)$ LECs $A, Z_S, \xi, \tilde{\xi}$.

The identities for the η can be recast in a form reminiscent of the Gell-Mann–Okubo formula:

$$3F_\eta^2 M_\eta^2 - 4F_K^2 M_K^2 + F_\pi^2 M_\pi^2$$
$$= 4(r-1)m^2 \left\{ (r-1)(2Z^p + A) - B_0^2 L \right\}$$
$$+ 3F_\eta^2 M_\eta^2 d_\eta - 4F_K^2 M_K^2 d_K + F_\pi^2 M_\pi^2 d_\pi, \quad (152)$$
$$3F_\eta^2 - 4F_K^2 + F_\pi^2$$
$$= \frac{2m B_0}{16\pi^2} \left[(1+2r)\log \frac{M_\eta^2}{M_K^2} - \log \frac{M_K^2}{M_\pi^2} \right]$$
$$+ 3F_\eta^2 e_\eta - 4F_K^2 e_K + F_\pi^2 e_\pi. \quad (153)$$

The η-mass identity involves the new LEC $Z^p = 16 B_0^2 L_7$. We have also introduced the NNLO remainders d_η and e_η of order $O(m_q^2)$.

B χPT and Bayesian statistical analysis

One of the main achievements of $SU(3) \times SU(3)$ chiral perturbation theory consists in providing a consistent framework that includes all the constraints of chiral symmetry when one analyzes processes involving the Goldstone bosons π, K, η. This allows one to express observables as expansions in powers of momenta and quark masses up to a given order. Each order involves new low-energy constants whose values cannot be determined from chiral constraints, but nevertheless provide very much needed insight into the mechanism of chiral symmetry breaking.

We would like therefore to pin down (or at least constrain) LECs arising at first order in $SU(3) \times SU(3)$ chiral expansions – for instance, the quark condensate and the pseudoscalar decay constant in the limit $m_u, m_d, m_s \to 0$ – by using available experimental information.

We must therefore combine several sources of information.

(1) Experimental measurements of observables α_i: $P_j^{\exp}(\alpha_i)$. Their values have (possibly correlated) uncertainties which are described by probability distributions. In the theoretical basis that underlies the determination of these observables no use of χPT should have been made. For instance, solutions of Roy equations were required in addition to experimental phase shifts to extract $\pi\pi$ scattering parameters. As explained in Sect. 2.3, a reasonable

choice of observables can be derived from QCD correlation functions of currents and densities, away from kinematic singularities; e.g., one may choose $\pi\pi$ subthreshold parameters.

(2) Relations between the observables and theoretical parameters T_n: $\alpha_i = \mathcal{A}_i(T_n)$. We have explained how mass and decay constant identities can be used to eliminate some $O(p^4)$ LECs in chiral expansions of observables. We have chosen the theoretical parameters to be $X(3)$, $Z(3)$, r, and remainders that comprise NNLO and higher order corrections.

(3) Theoretical constraints/assumptions about the values of T_n: $\mathcal{C}_k(T_n)$. Chiral order parameters are constrained: for instance, vacuum stability requires $X(3) \geq 0$, whereas $Z(3)$ is positive by definition. We have also theoretical prejudices about NNLO remainders if we require an overall convergence of chiral expansions: the relative contribution of NNLO remainders must remain small.

It is quite easy to construct from these elements the likelihood function

$$\mathcal{L}(T_n) = P(\text{data}|T_n, H) = \prod_j P_j^{\text{exp}}[\mathcal{A}_i(T_n)], \qquad (154)$$

which is the probability of obtaining the observed data once a particular set of theoretical parameters is given (within the theoretical framework H). However, what we want is not $\mathcal{L}$, but rather the reverse quantity $P(T_n|\text{data}, H)$, i.e., the probability of having a particular set of theoretical parameters, taking into account the data.

This problem of "statistical inference" has a long history. A possible solution is provided by Bayesian analysis [22], which relies on Bayes' theorem:

$$P(T_n|\text{data}, H) = \frac{\mathcal{L}(T_n) \cdot \pi(T_n|H)}{\int [\text{d}T] \, \mathcal{L}(T_n) \cdot \pi(T_n|H)}, \qquad (155)$$

where π is the "prior" distribution, i.e., the probability associated with the theoretical parameters before the experimental results have been taken in consideration:

$$\pi(T_n) = P(T_n|H) = \prod_k \mathcal{C}_k(T_n). \qquad (156)$$

The denominator on the right-hand side of (155) is just a normalization factor. The marginal probability associated with a given theoretical parameter is obtained by integrating the joint probability $P(T_n|\text{data}, H)$ over all other theoretical parameters.

Let us mention that there is some arbitrariness in each of these ingredients. We could have chosen other observables, such as combinations of scattering lengths in which one-loop chiral logarithms cancel [32]. We could have added all $O(p^4)$ LECs to the set of theoretical parameters, and kept "bare" chiral expansions as relations among the observables. Finally, we could have computed $O(p^6)$ contributions to NNLO remainders and used resonance saturation to estimate the size of the remainders, following the procedure in [17].

In the present paper we have advocated a particular choice of observables as constituting a sensible starting point for a Bayesian analysis of data from $\pi\pi$ and πK scattering. Other choices of prior p.d.f.'s for the theoretical parameters (especially for the NNLO remainders) can be considered, as long as they are well motivated. However, the posterior probabilities should not be strongly sensitive to the choice of priors when a sufficient amount of experimental data is included in the analysis.

C Integration procedure for the analysis of $\pi\pi$ scattering

In Sect. 4, we apply Bayesian methods to perform a three-flavor analysis of $\pi\pi$ scattering, constructing a joint probability $P(r, Y, Z, \delta|\text{data})$. This gives the probability of having a particular choice of quark mass ratio r, order parameters $Y(3)$ and $Z(3)$ and NNLO remainders $\delta_{i=1\ldots7}$, once $\pi\pi$ scattering data is taken into account. By integrating over NNLO remainders, we obtain the joint probability

$$P(r, Y, Z|\text{data}) = \int \prod_{i=1}^{7} \text{d}\delta_i \; P(r, Y, Z, \delta|\text{data}) \qquad (157)$$

$$\propto \pi(Y, Z) \, \theta(r - r_1) \, \theta(r_2 - r) \, \theta[Z(3)] \, \theta[Y(3)]$$

$$\times \int^{\delta_1^{\max}} \text{d}\delta_1 \int^{\delta_2^{\max}} \text{d}\delta_2 \int_{\delta_6^{\min}} \text{d}\delta_6 \int_{\delta_7^{\min}} \text{d}\delta_7 \int \text{d}\delta_3 \, \text{d}\delta_4 \, \text{d}\delta_5$$

$$\times \prod_{i=1}^{7} G(\delta_i, \sigma_i) \exp\left(-\frac{1}{2} \mathcal{V}^T C \mathcal{V}\right) \theta[Y^{\max} - Y(3)],$$

$$(158)$$

where $\propto$ means "equals, up to a (numerical) normalization coefficient", C is the error matrix for the experimental data, (98), $G(\delta_i, \sigma_i)$ is the Gaussian function of δ_i with width σ_i, and $\mathcal{V}$ is defined in terms of the chiral series for $\alpha_{\pi\pi}$ and $\beta_{\pi\pi}$, (96) and (97):

$$\mathcal{V}(r, Y, Z, \delta) = \begin{pmatrix} \mathcal{A}(r, Y, Z, \delta) - \alpha_{\exp} \\ \mathcal{B}(r, Y, Z, \delta) - \beta_{\exp} \end{pmatrix}. \qquad (159)$$

Before any numerical evaluation, we can analytically compute some of the integrals. δ_4 and δ_5 have the same width $\sigma_4 = \sigma_5$ and appear only in the experimental distribution obtained from $\pi\pi$ scattering. We can therefore diagonalize the latter:

$$R^{\text{T}} R = R R^{\text{T}} = I, \qquad R C R^{\text{T}} = \begin{bmatrix} C_1 & 0 \\ 0 & C_2 \end{bmatrix}, \qquad (160)$$

to perform the integration[9] over δ_4 and δ_5:

$$\int \delta_4 \, \delta_5 \, G(\delta_4, \sigma_4) G(\delta_5, \sigma_4) \exp\left(-\frac{1}{2} \mathcal{V}^{\text{T}} C \mathcal{V}\right)$$

---

[9] A similar procedure can be followed in the case of different widths for the Gaussian prior p.d.f.'s for δ_4 and δ_5.

$$\propto \exp\left[-\frac{1}{2}(D_1 \mathcal{W}_1 + D_2 \mathcal{W}_2)\right], \tag{161}$$

$$D_i = \frac{C_i}{1 + C_i \sigma_4^2}, \quad \mathcal{W} = R \cdot \mathcal{V}(r, Y, Z, \delta_{1,2,3}; \delta_4 = \delta_5 = 0). \tag{162}$$

The integrals over δ_6 and δ_7 are simply Gaussians integrated over semi-infinite ranges, and are thus given in terms of the error function Erf. We obtain finally

$$\begin{aligned}
P&(r, Y, Z | \text{data}) \\
&\propto \pi(Y, Z)\, \theta(r - r_1)\, \theta(r_2 - r)\theta[Z(3)]\, \theta[Y(3)] \\
&\times \int^{\delta_1^{\max}} \mathrm{d}\delta_1 \int^{\delta_2^{\max}} \mathrm{d}\delta_2 \int \mathrm{d}\delta_3 \prod_{i=1}^{3} G(\delta_i, \sigma_i) \\
&\times \exp\left[-\frac{1}{2}(D_1 \mathcal{W}_1 + D_2 \mathcal{W}_2)\right] \\
&\times \left[1 - \text{Erf}\left(\frac{\delta_6^{\min}}{\sqrt{2}\sigma_6}\right)\right]\left[1 - \text{Erf}\left(\frac{\delta_7^{\min}}{\sqrt{2}\sigma_7}\right)\right] \\
&\times \theta[Y^{\max} - Y(3)].
\end{aligned} \tag{163}$$

In order to obtain the marginal probability for either r, $X(3)$, $Y(3)$ or $Z(3)$, we must perform a numerical integration over three remainders to obtain the joint probability $P(r, Y, Z|\text{data})$, and then integrate the result over two of the remaining three parameters. We restrict the integration over the remainders $\delta_{1,2,3}$ to the range $[-5\sigma_i, 5\sigma_i]$ (the upper bound can be smaller for $i = 1, 2$ due to the positivity constraints (107) and (108)). The range of integration for the two parameters that remain to be integrated is given by the theoretical constraints discussed in Sect. 4.

In order to appreciate the impact of the data in the Bayesian framework, it is quite interesting to consider the marginal probabilities obtained when no experimental information is included. In our particular case, this amounts to replacing the experimental distribution $P_{\exp}(\alpha, \beta)$ by 1, or equivalently to setting the matrix C to 0. We obtain then the following p.d.f.:

$$\begin{aligned}
P_0&(r, Y, Z | \text{data}) \\
&\propto \pi(Y, Z)\, \theta(r - r_1)\, \theta(r_2 - r)\, \theta[Z(3)]\, \theta[Y(3)] \\
&\times \int^{\delta_1^{\max}} \mathrm{d}\delta_1 \int^{\delta_2^{\max}} \mathrm{d}\delta_2 \int \mathrm{d}\delta_3 \prod_{i=1}^{3} G(\delta_i, \sigma_i)\theta[Y^{\max} - Y(3)] \\
&\times \left[1 - \text{Erf}\left(\frac{\delta_6^{\min}}{\sqrt{2}\sigma_6}\right)\right]\left[1 - \text{Erf}\left(\frac{\delta_7^{\min}}{\sqrt{2}\sigma_7}\right)\right].
\end{aligned} \tag{164}$$

P_0 is just the normalized prior p.d.f. and corresponds to the "phase space" allowed by the theoretical constraints and assumptions on the various parameters. The resulting marginal probabilities can be found in Sect. 4, where they are compared with the ones that include experimental knowledge of $\pi\pi$ scattering.

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