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NNLO Positivity Bounds on χPT for a General Number of Flavours

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We present positivity bounds, derived from the principles of analyticity, unitarity and crossing symmetry, that constrain the low-energy constants of chiral perturbation theory. Bounds are produced for 2, 3 or more flavours with equal meson masses, up to and including next-to-next-to-leading order (NNLO), using the second and higher derivatives of the amplitude. We enhance the bounds by using the most general isospin combinations posible (or higher-flavour counterparts thereof) and by analytically integrating the low-energy range of the amplitude. In addition, we present a powerful and general mathematical framework for efficiently managing large numbers of positivity bounds.

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Chiral Perturbation Theory (χPT) is the most widespread effective field theory (EFT) for low-energy QCD. However, its predictive power is limited by the number of free parameters (low-energy constants, LECs) in its Lagrangian [1–4]: Even neglecting non-strong interactions, 102 LECs appear up to NNLO in the low-energy expansion, corresponding to two-loop amplitudes, with another 1233 entering at the next order. Not all of these feature in amplitudes of interest, but the fact remains that the number of LECs limits the usefulness of higher-order χPT corrections to observables. Only the LO LECs, corresponding to the pion mass and decay constant, are known to high precision; the NLO LECs are known at the percent level, only educated guesses are available at NNLO, and nothing at all at N^{3}LO [5].

A possible mitigation of this issue comes from the fact that, besides measurements in experiments and on the lattice, it is possible to constrain the values of the LECs also from the purely theoretical side. All quantum field theories must obey the principles of analyticity, unitarity and crossing symmetry, but it turns out that these are not necessarily compatible with the assumption of perturbativity for an EFT; thus, imposing all four principles can lead to non-trivial requirements on the Lagrangian. This concept was pioneered by Martin [6] before the development of χPT as such, with renewed interest in recent decades [7–10]. Our work, published in full as Ref. [11], is based on the methods of Manohar & Mateu [12, 13] with further inspiration from Refs. [14, 15]; other recent work in similar directions includes Refs. [16–18].

1. Positivity Bounds

Throughout, we shall work in the isospin limit (all mesons having the same mass, M) and use the normalized Mandelstam variables $s = (p_1+p_2)^2/M^2$, $t = (p_1+p_3)^2/M^2$ and $u = (p_1+p_4)^2/M^2$.

Following Manohar & Mateu, the process of obtaining bounds starts with the isospin decomposition of the $2 \to 2$ pseudoscalar meson scattering amplitude,

$$T(s,t) = a_J T^J(s,t)\,, \tag{1}$$

implicitly summed over the label J, which for two-flavour χPT runs over isospin channels 0, 1 and 2; with three flavours, this generalizes to the five representation labels I, A, S, AS and SS, with a sixth, AA, appearing in the unphysical case of four or more flavours. With this decomposition, $s \to u$ crossing symmetry is implemented as

$$T^I(u,t) = C_u^{IJ} T^J(s,t)\,, \tag{2}$$

with the matrix C_u^{IJ} determined entirely from the group structure.

Next, we invoke analyticity to write the k-times-subtracted fixed-t dispersion relation,

$$a_J \frac{\mathrm{d}^k}{\mathrm{d}s^k} T^J(s,t) = \frac{k!}{2\pi i} \oint \mathrm{d}z\, \frac{a_J T^J(z,t)}{(z-s)^{k+1}}\,, \tag{3}$$

which through contour manipulation can be brought into the form

$$a_J \frac{\mathrm{d}^k}{\mathrm{d}s^k} T^J(s,t) = \frac{k!}{\pi} \int_4^\infty \mathrm{d}z \left[\frac{a_J}{(z-s)^{k+1}} + \frac{(-1)^k a_I C_u^{IJ}}{(z-u)^{k+1}} \right] \operatorname{Im} T^J(z+\varepsilon i,t)\,. \tag{4}$$

The two terms in parentheses stem from routing the contour along the cuts corresponding to the s- and u-channel, respectively; with normalized Mandelstam variables, 4 corresponds to threshold.

Above threshold, and within a wide domain of convergence, we may partial-wave expand the amplitude as

$$T^J(s,t) = \sum_{\ell=0}^{\infty}(2\ell+1) f_\ell^J(s) P_\ell\left(1 + \frac{2t}{s-4}\right), \tag{5}$$

where P_ℓ are Legendre polynomials, and the optical theorem (invoking unitarity) imposes for the partial-wave amplitudes f_ℓ^J that

$$\operatorname{Im} f_\ell^J(s) = s\sigma_\ell^J(s)\sqrt{1 - 4/s}\,, \tag{6}$$

which is positive above threshold since the partial-wave cross-sections $\sigma_\ell^J(s)$ are. Thus, in the range where $P_\ell\left(1 + \frac{2t}{s-4}\right)$ is positive, $\operatorname{Im} T^J(s,t)$ must be positive as well. Putting all of this together, we find

$$a_J \frac{\mathrm{d}^k}{\mathrm{d}s^k} T^J(s,t) \geq 0 \tag{7a}$$

$$\text{if} \quad a_I \left\{ \delta^{IJ} \left[\frac{z-u}{z-s}\right]^{k+1} + (-1)^k C_u^{IJ} \right\} \geq 0 \quad \text{for all } z \geq 4 \text{ and all } J\,, \tag{7b}$$

valid in the range $t \in [0,4]$, $s \in [-t,4]$, a below-threshold region free of singularities. As follows from the Froissart bound [19], $k \geq 2$ is necessary and sufficient for convergence. It furthermore turns out that odd k are useless with three or more flavours, and forbidden with two. Likewise, it can be shown that it suffices to satisfy eq. (7b) at $z = 4$ (threshold) and in the limit $z \to \infty$.

Equation (7) provides the means for producing positivity bounds by evaluating $a_J \mathrm{d}^k T^J(s,t)/\mathrm{d}s^k$ at fixed s, t in the region of validity. Conventionally, this is done with a_J fixed to one of the mass eigenstates — $\begin{pmatrix}0 & 0 & 1\end{pmatrix}$ for two-flavour $\pi^+\pi^+$ scattering, $\begin{pmatrix}0 & \frac{1}{5} & 0 & \frac{1}{2} & \frac{3}{10}\end{pmatrix}$ for three-flavour $\pi\eta$ scattering, etc. — but in the isospin limit, this is not necessary. The region in a_J-space that satisfies eq. (7b) is rather broad and depends on s, u — there is no need to require validity for *all* s, u, just at a fixed point — and thus gives a wide range of bounds.

Inspired by the approach taken in [14], one may explicitly evaluate the lowest portion of the integral in eq. (4), from 4 up to some λ, and subtract it from the equation before applying the positivity arguments to the right-hand side. This subtracts a known, positive quantity from the left-hand side of eq. (7a), thus strengthening the bounds. Alternatively, a broader choice of s, u and a_J becomes available, which produces new, possibly stronger bounds despite the subtracted quantity now being possibly negative. We have analytically performed the pertinent integral applied to the NNLO $2 \to 2$ n-flavour scattering amplitude [20] by integrating a wider class of functions that includes those appearing in the 1- and 2-loop equal-mass integrals, thus making this subtraction easy to perform. Care has to be taken with the choice of λ: larger values strengthen the bounds, but since it is done at fixed order in the low-energy expansion, the validity decreases as λ approaches the Chivukula–Dugan–Golden bound [21], $\lambda \sim 70/n$, at which perturbative breakdown is expected.

2. Linear Constraints

Our generalization of a_J beyond the mass eigenstates allows for the production of a practically unlimited number of independent bounds on the LECs, and our use of NNLO n-flavour χPT greatly increases the dimension of the parameter space: The LECs appear in the bounds as up to 20 independent linear combinations, although this is reduced by using two- or three-flavour χPT, by using higher derivative counts k, or by fixing $t = 4$, which is the value at which most strong bounds are obtained. Nevertheless, our bound-producing methods necessitate improved bound-managing methods; dissatisfied with those available in the literature, we have derived a new mathematical framework for this purpose.

Up to NNLO, $\mathrm{d}^k T(s,t)/\mathrm{d}s^k$ is an inhomogeneous linear function of the LECs; thus, the general expression of interest is of the form

$$\alpha_1 b_1 + \alpha_2 b_2 + \ldots + \alpha_N b_N = \boldsymbol{\alpha} \cdot \boldsymbol{b} \geq c\,, \tag{8}$$

where b_i are the values being constrained (here, the LECs) and α_i and c are known [here, from eq. (7a)]. Thus, we introduce *(linear) constraints*, denoted $\langle \boldsymbol{\alpha}, c\rangle$, and express the relation $\boldsymbol{\alpha} \cdot \boldsymbol{b} \geq c$ as '$\langle \boldsymbol{\alpha}, c\rangle$ is satisfied by $\boldsymbol{b}$'. We express the simultaneous application of multiple constraints as summation; thus, with

$$\Omega = \sum_i \langle \boldsymbol{\alpha}_i, c_i\rangle\,, \tag{9}$$

Ω is satisfied by $\boldsymbol{b}$ if and only if $\boldsymbol{b}$ satisfies all of $\langle \boldsymbol{\alpha}_i, c_i\rangle$. We denote by $\mathcal{B}(\Omega)$ the set of all points that satisfy Ω. Even if two constraints Ω and Ω' may be written as different sums, we consider them equal when $\mathcal{B}(\Omega) = \mathcal{B}(\Omega')$.

There is a natural notion of one constraint (Ω) being stronger than another (Ω'), which we write as $\Omega \geq \Omega'$ and define by $\mathcal{B}(\Omega) \subseteq \mathcal{B}(\Omega')$: Every point that satisfies Ω also satisfies Ω', but Ω may bring additional restrictions. When generating many constraints, we wish to only retain the strongest among them and discard the rest. Apart from some obvious identities such as

$$\begin{gathered} \Omega \leq (\Omega + \Omega') \geq \Omega', \qquad \langle \boldsymbol{\alpha}, c\rangle = \langle \boldsymbol{\alpha}/|c|, \mathrm{sgn}(c)\rangle \quad \text{if } c \neq 0\,, \\ \langle \boldsymbol{\alpha}, -1\rangle \leq \langle (1+\lambda)\boldsymbol{\alpha}, -1\rangle \leq \langle \boldsymbol{\alpha}, 0\rangle = \langle \lambda\boldsymbol{\alpha}, 0\rangle \leq \langle (1+\lambda)\boldsymbol{\alpha}, 1\rangle \leq \langle \boldsymbol{\alpha}, 1\rangle \quad \text{if } \lambda \geq 0\,, \end{gathered} \tag{10}$$

this is a highly nontrivial task, and is the focus of most of our effort. The fundamental result, proven in Ref. [11], is the following:

Proposition 1. *A linear constraint $\langle \boldsymbol{\beta}, d\rangle$ is weaker than the combined constraint $\Omega = \sum_i \langle \boldsymbol{\alpha}_i, c_i\rangle$, i.e. $\langle \boldsymbol{\beta}, d\rangle \leq \Omega$, if and only if there exist $\lambda_i \geq 0$ such that*

$$\boldsymbol{\beta} = \sum_i \lambda_i \boldsymbol{\alpha}_i\,, \qquad \sum_i \lambda_i c_i \geq d\,. \tag{11}$$

This, however, is rather indirect, since no indication is given of how to find these λ_i. A more direct result is the following:

Proposition 2. *Given Ω as above, there exists $\mho_d = \sum_j \langle \boldsymbol{n}_j, r_j\rangle$ such that $\langle \boldsymbol{\beta}, d\rangle \leq \Omega$ if and only if $\boldsymbol{\beta} \in \mathcal{B}(\mho_d)$.*

The constraint $\mho_d$ can be thought of as a dual of Ω; in fact, applying proposition 2 to $\mho_d$ for $d \neq 0$ recovers Ω (Corollary B.5 in Ref. [11]). We provide a straightforward algorithm for finding $\langle \boldsymbol{n}_i, r_i \rangle$, which is stated in detail in appendix B.4.1 of Ref. [11]. In short, one forms a set consisting of certain linear combinations of the $\boldsymbol{\alpha}_i$, and takes its *convex hull* (the smallest convex set containing it), for which efficient algorithms exist [22]. As a side-effect, one obtains the normal vectors of the facets of the hull's surface, and after discarding certain facets based on some straightforward conditions, these normal vectors are essentially $\boldsymbol{n}_j$. Furthermore, there is a direct relation (Proposition B.4 in Ref. [11]) between the $\boldsymbol{n}_j$ and the location of the vertices and edges of $\mathcal{B}(\Omega)$, which helps with visualization.

Lastly, we have the following:

Proposition 3. *Of all sets $\mathcal{S}$ such that $\Omega = \sum_{\langle \alpha, c \rangle \in \mathcal{S}} \langle \alpha, c \rangle$, there exists a smallest such set, denoted $\mathcal{R}(\Omega)$. As long as Ω is non-degenerate, i.e. $\mathcal{B}(\Omega)$ is not contained in any hyperplane, this smallest set is unique.*

Appendix B.4.4 of Ref. [11] covers the algorithm for finding $\mathcal{R}(\Omega)$, which essentially consists of retaining only those $\boldsymbol{\alpha}_i$ that end up on the surface of the aforementioned convex hull. Thus, we may generate as many constraints as we want, and proposition 3 will pick out those that are actually relevant for placing bounds on the LECs. One shortcoming is that some constraints only carve out a negligible corner of parameter space, while still being retained by the algorithms; we unfortunately do not have a systematic way of filtering out such 'near-irrelevant' constraints.

3. New Bounds on χPT

In this section, we present a selection of our results; a larger selection can be found in Ref. [11]. The simplest case is two-flavour χPT at NLO, where there are only two LECs ($\bar{l}_1$ and $\bar{l}_2$) and constraints are available from Manohar & Mateu [12]. We reproduce their bounds in fig. 1, along with our own. The basic ($\lambda = 4$) version of our constraints provides only marginal improvements on the Manohar–Mateu bounds, and in order to reach close to the experimental reference value [5], very aggressive integration is needed, too close to the Chivukula–Dugan–Golden bound ($\lambda \sim 35$) to be taken seriously.

The bounds change significantly when the NNLO amplitude is used, even when just considering the LECs that also feature at NLO. Two more NLO LECs ($\bar{l}_3$ and $\bar{l}_4$) enter the NNLO amplitude, along with four linear combinations of the NNLO LECs (not shown here). Figure 2 shows the bounds on the $\bar{l}_i$; there, also $k \geq 2$ can yield nontrivial bounds, although only $k = 4$ yields useful ones. With only modest integration, the allowed region in the $\bar{l}_1$–$\bar{l}_2$ plane becomes finite, albeit still not close to the experimental uncertainty. Note that the bounds on $\bar{l}_3$ are extremely weak, since the coefficient of $\bar{l}_3$ in the amplitude is very small.

With three flavours, the LECs entering at NLO are L_1^r, L_2^r and L_3^r (the 'r' indicating a different renormalization convention than the bar on $\bar{l}_i$). Thus, we use a three-dimensional visualization of the bounds, shown in fig. 3, which is generated using proposition 2.

Qualitatively, the bounds in fig. 3 are similar to those in fig. 1, although here there is no earlier result to compare to; Mateu [13] uses realistic meson masses. The bounds depend strongly on the choice of M (only $M = M_\pi$ is shown here) and are significantly more sensitive to integration (not

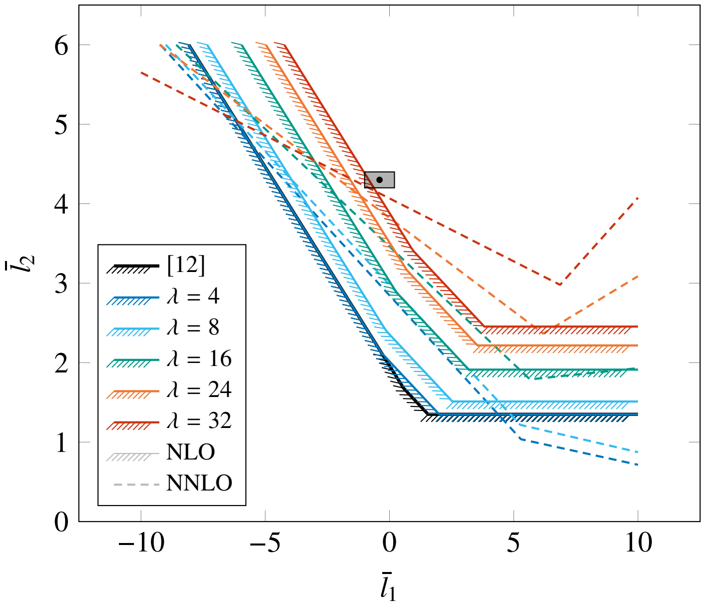

Figure 1: Two-flavour two-derivative NLO bounds on $\bar{l}_1, \bar{l}_2$ for various λ, as indicated in the legend, along with the Manohar–Mateu bound [12]. Each set of constraints is represented as a line with one side hatched; the hatched side is excluded by the constraints, and the other side corresponds to $\mathcal{B}(\Omega)$. The experimentally measured reference point $[\bar{l}_1 = -0.4(6),\ \bar{l}_2 = 4.3(1)]$ is drawn as a dot with an uncertainty region around it. For each bound, the direct NNLO counterpart (i.e. using the same λ, s, t and a_J) is drawn as a dashed outline.

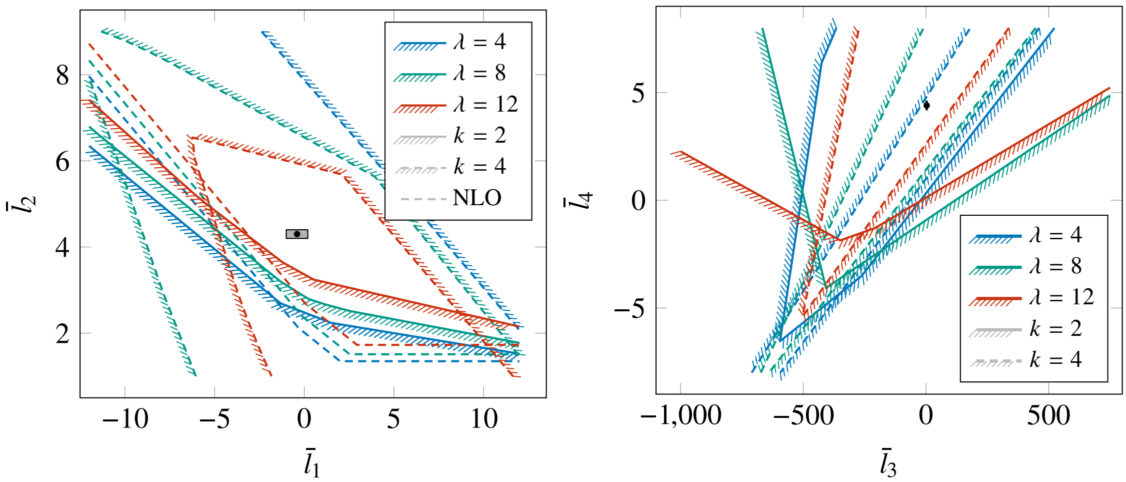

Figure 2: NNLO bounds on $\bar{l}_1, \bar{l}_2$ (left) and $\bar{l}_3, \bar{l}_4$ (right), displayed similarly to fig. 1. In each plot, the LECs not shown have been fixed to their reference values. For comparison, the corresponding NLO bounds shown in fig. 1 are drawn as a dashed outline.

shown) than their two-flavour counterparts. This sensitivity to the details of the isospin limit reduces the applicability of our $(n > 2)$-flavour bounds; unfortunately, the $2 \to 2$ scattering amplitude with realistic meson masses is not known at NNLO, just NLO [23].

At NNLO, in addition to $L^r_{1,2,3}$ whose NNLO bounds are shown in fig. 4, four more NLO LECs ($L^r_{4,5,6,8}$) and five linear combinations of NNLO LECs ($\Xi_{1,2,3}, \Gamma_3, \Delta_3$; these are defined in Ref. [11]) appear in the amplitude. The former (not shown) are bounded similarly to $\bar{l}_{3,4}$, and the reference point is excluded already at $\lambda = 4.5$. Several of the latter are constrained to finite ranges which exclude the reference point even without integration, as shown in fig. 5, although it must be kept in mind that the NNLO LECs are only roughly estimated in Ref. [5]. The bounds are quite sensitive to the values of the other LECs, which are fixed to their reference values to produce these figures,

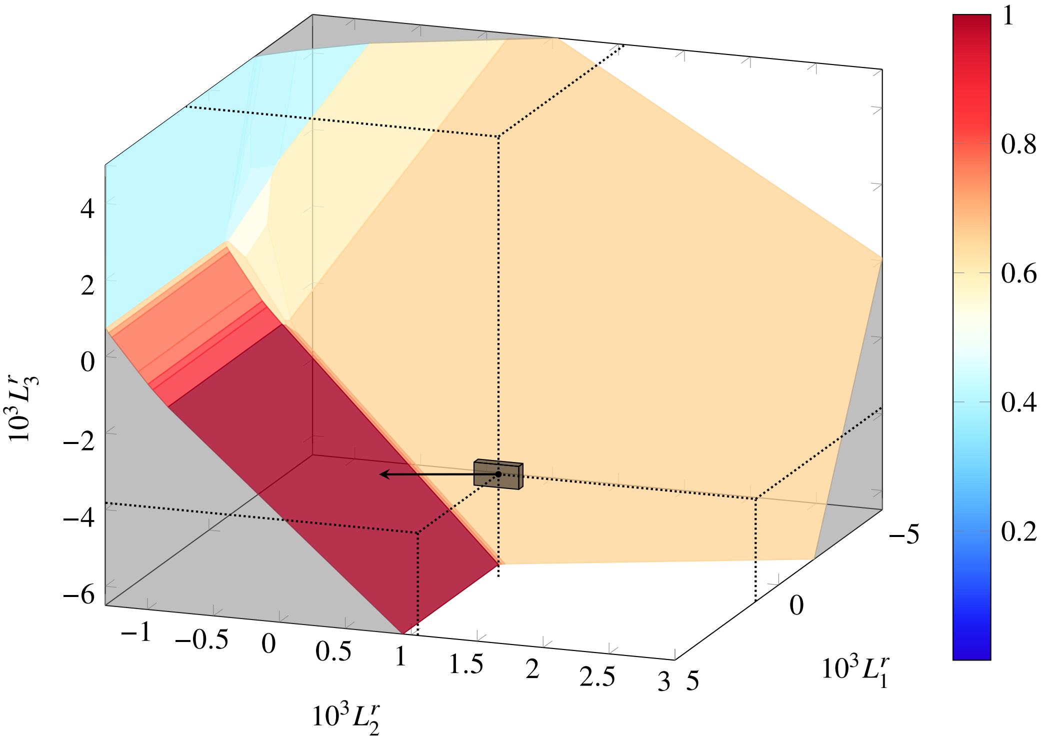

Figure 3: Three-flavour two-derivative NLO bounds on L_1^r, L_2^r and L_3^r. The space *outside* $\mathcal{B}(\Omega)$ is shown as a gray solid, with the empty space containing the reference point [$L_1^r = 0.00111(10)$, $L_2^r = 0.00105(17)$, $L_3^r = -0.00382(30)$] being a part of $\mathcal{B}(\Omega)$. The constraint surfaces are coloured according to the orthogonal distance to the reference point, denoted ρ, and the orthogonal line (which does not appear as such due to different axis scales) from the point to the surface is drawn whenever possible. Dotted lines are drawn parallel to the axes to clarify the reference point's position in space.

but no value of the NLO LECs within their experimental uncertainties allow the reference point to satisfy the bounds in fig. 5.

With four or more flavours, a few more LECs enter the amplitude, but their bounds (not shown) are qualitatively similar to those at three flavours. The bounds gradually grow weaker as the number of flavours increases, and asymptotically approach triviality (i.e. being satisfied by all points) as $n \to \infty$, as can be deduced from the amplitude. Many-flavour bounds are not readily interpreted due to the unphysicality of many-flavour χPT, and care must be taken about perturbativity, since the Chivukula–Dugan–Golden bound scales as $1/n$.

4. Summary and Outlook

We present the first general-flavour NNLO bounds, albeit in the isospin limit, and present some generalizations of the Manohar–Mateu method, in particular in the treatment of the isospin decomposition coefficient a_J. We also describe a new mathematical framework for managing large numbers of constraints in high-dimensional parameter spaces. In the cases where previously derived bounds exist, our results provide some improvement, but do not come close to the experimental uncertainty without the use of hard-to-motivate amounts of integration.

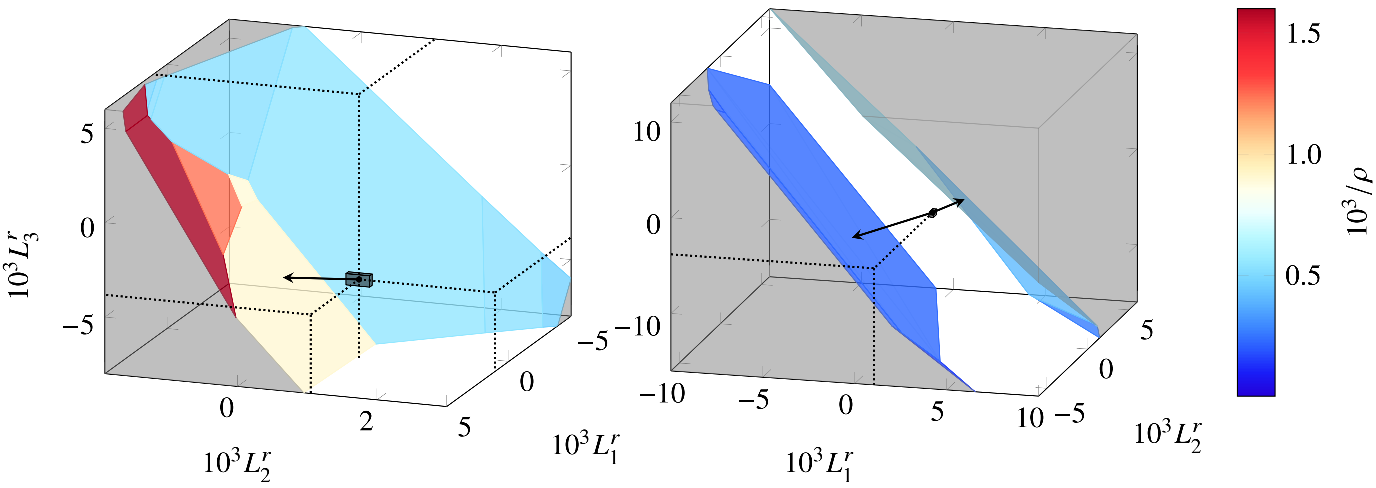

Figure 4: NNLO bounds on L_1^r, L_2^r and L_3^r, using two (left) and four (right) derivatives. Thus, the left figure is essentially the NNLO version of fig. 3. In the four-derivative case, $\mathcal{B}(\Omega)$ is actually finite: It is a lentil-shaped body whose largest dimension is about two orders of magnitude larger than the region shown in the figure. Note that the axes have been rotated relative to the left figure in order to make the inside of $\mathcal{B}(\Omega)$ reasonably visible.

Possible further development, besides refinement of our methods, would mostly require hitherto unknown amplitudes: NNLO beyond the isospin limit, or N^{3}LO, where an additional complication is that terms non-linear in the LECs appear, requiring generalization of the linear constraint framework. Alternatively, bounds on the recently calculated NLO $2 \to 4$ amplitudes [24, 25] could be explored, although this would require generalization of the derivation of bounds. Lastly, one can go beyond χPT; to a large extent, these methods could be applied as-is to other EFTs, such as those used in beyond-the-Standard-Model research.

Acknowledgments

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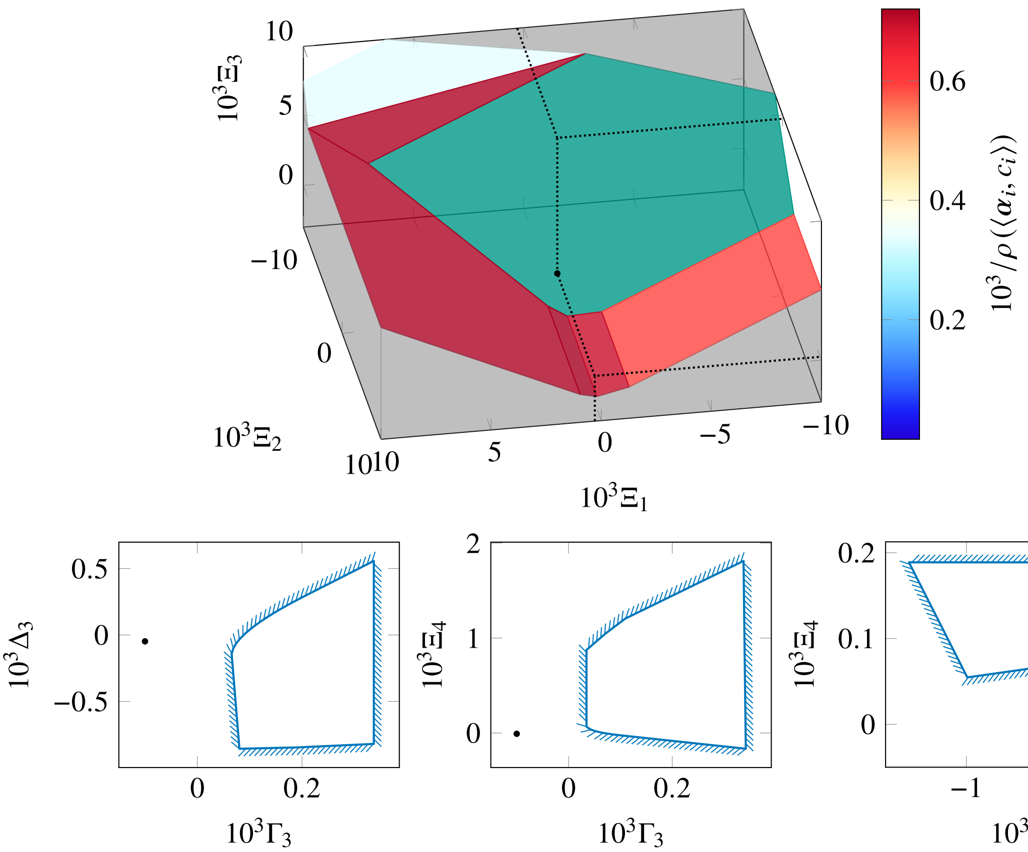

Figure 5: NNLO two-derivative bounds on $\Xi_{1,2,3}$ (top) and $\Gamma_3, \Delta_3, \Xi_3$ (bottom). Two-dimensional slices are used since the finite $\mathcal{B}(\Omega)$ makes three-dimensional representation difficult. The green constraint surface excludes the reference point $[\Xi_1 = 2.9 \cdot 10^{-4},\ \Xi_2 = 3.4 \cdot 10^{-4},\ \Xi_3 = 2.5 \cdot 10^{-4},\ \Xi_4 = -8 \cdot 10^{-6},\ \Gamma_3 = -1.0 \cdot 10^{-4},\ \Delta_3 = -4.8 \cdot 10^{-5}]$, albeit by a very small amount not visible at the scale of the figure. No uncertainties are available on the estimates of the NNLO LECs [5].

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