Chiral extrapolation and determination of low-energy constants from lattice data

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Abstract

We propose analytic approximations of chiral $SU(3)$ amplitudes for the extrapolation of lattice data to the physical meson masses. The method allows the determination of NNLO low-energy constants in a controllable fashion. We test the approach with recent lattice data for the ratio $F_K/F_\pi$ of meson decay constants.

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1. Introduction

In recent years, lattice QCD has made enormous progress in the light quark sector (see, e.g., Ref. [1]). State-of-the-art lattice studies employ quark masses corresponding to pion masses as low as 200 MeV, with kaon masses close to the physical value.

Extrapolation to the physical meson masses is performed in different ways. On one side of the theory spectrum, there are various smooth extrapolation formulas with more or less theoretical motivation. On the other side, the most sophisticated extrapolations are based on chiral perturbation theory (CHPT), the effective field theory of the standard model at low energies [2,3]. As the meson masses continue to approach the physical values in future high-statistics simulations [4], even simple-minded polynomial approximations will allow predicting physical quantities with ever better precision. However, a lot of information about QCD is lost in this way. On the other hand, CHPT provides the correct analytic structure of amplitudes in terms of several a priori undetermined constants, the so-called low-energy constants (LECs), which are independent of the light quark masses by definition.

Many of the higher-order LECs are difficult if not impossible to extract from actual experimental data. Lattice calculations offer a new environment for determining LECs because, unlike nature, the lattice physicist can tune the quark masses. For the chiral practitioner, it is then an advantage rather than a drawback that present lattice studies work with different meson masses larger than the physical values.

Many lattice groups use next-to-leading-order (NLO) CHPT results for the chiral extrapolations. As by-products, several LECs at this order, $O(p^4)$, have actually been determined this way (see, e.g., Ref. [5]). On the other hand, state-of-the-art NNLO CHPT results have only very recently been used for the interpretation of lattice data [6–8]. There are good reasons why lattice physicists have generally ignored available NNLO calculations so far: the results are quite involved and, what is even worse, they are mostly available in numerical form only, at least for chiral SU(3) (for a review of NNLO results, see Ref. [9]).

We propose in this note analytic approximations for NNLO CHPT amplitudes for chiral SU(3) that are more sophisticated than the double-log approximation [10], yet much simpler than the full numerical expressions. We first recapitulate CHPT to $O(p^6)$ for the generating functional of Green functions [11]. In the following, we recapitulate and reformulate the general treatment of

$$Z = Z_2 + Z_4 + Z_6 + \ldots$$

(1)

The NNLO functional $Z_6$ of $O(p^6)$ is itself a sum of different contributions shown pictorially in Fig. [1]. In the following, we recapitulate and reformulate the general treatment of

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1 A very recent simulation [4] already uses physical quark masses.
renormalization at $O(p^6)$ \cite{11}. In addition to tree diagrams of $O(p^6)$ (diagram g), there are two classes of contributions requiring separate treatments: irreducible (diagrams a,b,d) and reducible (diagrams c,e,f) contributions.

With dimensional regularization, the irreducible diagrams have both double- and single-pole divergences. Moreover, the single-pole divergences of each irreducible diagram are in general non-local. Renormalization theory guarantees, however, that the sum of the three diagrams has only local divergences \cite{11,13}, i.e., polynomials in momenta and masses in momentum space. Chiral symmetry guarantees that these divergences can be absorbed by the LECs of $O(p^6)$ via diagram g. In this process an arbitrary renormalization scale $\mu$ is generated. The sum of diagrams a,b,d,g is then finite and can be written in the form (details of the derivation will be given elsewhere \cite{14})

\[
Z_{a+b+d+g}^6 = \int d^4x \left\{ C_{a}(\mu) + \frac{1}{4F_0^2} \left( 4 \Gamma_{a}^{(1)} L - \Gamma_{a}^{(2)} L^2 + 2 \Gamma_{a}^{(L)}(\mu)L \right) \right\} O_a(x) + \frac{1}{(4\pi)^2} \left[ L_{i}(\mu) - \frac{\Gamma_{i}}{2} L \right] H_i(x;M) + \frac{1}{(4\pi)^2} K(x;M) \right\} .
\]

The structure (2) holds for chiral $SU(n)$ in general but we have already used the notation for $n = 3$. The monomials $O_a(x)$ $(a = 1, \ldots , 94)$ define the chiral Lagrangian of $O(p^6)$ \cite{15} with associated renormalized LECs $C_{a}^{\ast}(\mu)$, the $L_{i}(\mu)$ $(i = 1, \ldots , 10)$ are renormalized LECs of $O(p^4)$ with associated beta functions $\Gamma_i$ \cite{3} and the coefficients $\Gamma_{a}^{(1)}$, $\Gamma_{a}^{(2)}$ and $\Gamma_{a}^{(L)}$ are listed in Ref. \cite{11}. Repeated indices are to be summed over. $F_0$ is the meson decay constant in the chiral $SU(3)$ limit. The chiral log

\[
L = \frac{1}{(4\pi)^2} \ln M^2/\mu^2
\]

involves an additional (arbitrary) scale $M$ but $Z_{6}^{a+b+d+g}$ as well as the total generating functional are independent of both $\mu$ and $M$. $H_i(x;M)$ are one-loop functionals associated
with diagram d whereas the two-loop contributions (except for the chiral logs) are contained in the functional \( K(x; M) \). Unlike \( O_a(x) \), the functionals \( H_i(x; M), K(x; M) \) are non-local. The scale independence of the functional (2) can be derived with the help of renormalization group equations for the LECs \( C_a^\mu(\mu) \) [11] and \( L_i^\mu(\mu) \) [3], using also relations between the coefficients \( \Gamma_a^{(2)} \) and \( \Gamma_a^{(L)} [11] \).

As shown in Ref. [11], the sum of reducible diagrams c, e, f gives rise to a finite and scale independent functional with the conventional choice of chiral Lagrangians. It can be written in the form

\[
Z_6^{c+e+f} = \int d^4x \, d^4y \left[ \left( L_i^\mu(\mu) - \frac{\Gamma_i}{2} L \right) P_{i,\alpha}(x) + F_{\alpha}(x; M) \right] G_{\alpha,\beta}(x, y) - \left[ \left( L_j^\mu(\mu) - \frac{\Gamma_j}{2} L \right) P_{j,\beta}(y) + F_{\beta}(y; M) \right].
\]

Indices \( \alpha, \beta \) run from 1, \ldots, 8 (octet of pseudoscalar mesons), the \( P_{i,\alpha}(x) \) are local functionals, the one-loop contributions of diagrams c, e are contained in the non-local functionals \( F_{\alpha}(x; M) \) and the \( G_{\alpha,\beta}(x, y) \) are (functional) propagators.

The complete generating functional of \( O(p^6) \) is then given by the sum

\[
Z_6 = Z_6^{a+b+d+g} + Z_6^{c+e+f}.
\]

Once again, it is independent of both scales \( \mu \) and \( M \).

3. Analytic approximation for chiral \( SU(3) \)

As emphasized in the introduction, the genuine two-loop contributions contained in the functional \( K(x; M) \) are usually only available in numerical form for chiral \( SU(3) \). On the other hand, the one-loop contributions can be given in analytic form and the dependence on meson masses is manifest. For the chiral extrapolation of lattice results, we therefore suggest the following approximate form for the functional of \( O(p^6) \):

\[
Z_6^{\text{app}} = \int d^4x \left\{ \left[ C_a^\mu(\mu) + \frac{1}{4F_5^2} \left( 4 \Gamma_a^{(1)} L - \Gamma_a^{(2)} L^2 + 2 \Gamma_a^{(L)}(\mu) L \right) \right] O_a(x) + \frac{1}{(4\pi)^2} \left[ L_i^\mu(\mu) - \frac{\Gamma_i}{2} L \right] H_i(x; M) \right\} + \int d^4x \, d^4y \left\{ \left( L_i^\mu(\mu) - \frac{\Gamma_i}{2} L \right) P_{i,\alpha}(x) G_{\alpha,\beta}(x, y) \left( L_j^\mu(\mu) - \frac{\Gamma_j}{2} L \right) P_{j,\beta}(y) + 2 \left( L_i^\mu(\mu) - \frac{\Gamma_i}{2} L \right) P_{i,\alpha}(x) G_{\alpha,\beta}(x, y) F_{\beta}(y; M) \right\}.
\]

In contrast to the generalized double-log approximation [10], which can be recovered by setting the coefficients \( \Gamma_a^{(1)} \) and the functionals \( H_i(x; M), F_{\alpha}(x; M) \) to zero, the analytic approximation (5) is scale independent. This is an important asset for a reliable determination of renormalized LECs.

In addition to tabulated quantities [11], the finite and scale independent one-loop functionals \( H_i(x; M) \) \( (i = 1, \ldots, 10) \), \( F_{\alpha}(x; M) \) \( (\alpha = 1, \ldots, 8) \) must be determined from diagrams
d and e. If available, the corresponding amplitudes can be read off from existing calculations by collecting all amplitudes linear in the LECs $L_i^r(\mu)$.

Another attractive feature of (6) is its large-$N_c$ behaviour. It comprises all leading (generically: $C_a$, $L_i L_j$) and next-to-leading contributions ($L_i \times 1$-loop). Of the NNLO terms, it contains at least all chiral logs.

The amplitude for a given observable corresponding to the scale invariant functional (6) can now be determined in four steps.

1. Calculate all tree- and one-loop diagrams, i.e., the contributions from diagrams d,e,f,g in Fig. 1. In many cases of interest, these amplitudes are already available in the literature [9].

2. In the tree-level amplitude of $O(p^6)$ (diagram g), replace the LECs $C_a^r(\mu)$ by

$$C_a^r(\mu) \rightarrow C_a^r(\mu) + \frac{1}{4F_0^2} \left( 4 \Gamma_a^{(1)} L - \Gamma_a^{(2)} L^2 + 2 \Gamma_a^{(L)}(\mu)L \right). \quad (7)$$

We recall that the combination on the right-hand side of (7) is scale invariant.

3. Collect all contributions linear and bilinear in the LECs $L_i^r(\mu)$ in the remaining amplitude (diagrams d,e,f) and extract the chiral logs. The products $L_i^r(\mu)L$ from the irreducible parts must match the terms $$\Gamma_a^{(L)}(\mu)L$$ in (7). After performing this check, set all chiral logs $L = 0$ in this subset of terms (diagrams d,e,f), which amounts to replacing $\mu$ by $M$ in the one-loop functions.

4. Replace the bilinears $L_i^r(\mu)L_j^r(\mu)$ (due to reducible contributions: diagram f) by the scale invariant expressions

$$L_i^r(\mu)L_j^r(\mu) \rightarrow \left( L_i^r(\mu) - \frac{\Gamma_i}{2} L \right) \left( L_j^r(\mu) - \frac{\Gamma_j}{2} L \right). \quad (8)$$

Finally, in the remaining terms linear in the $L_i^r(\mu)$ (originating from diagrams d,e) replace

$$L_i^r(\mu) \rightarrow L_i^r(\mu) - \frac{\Gamma_i}{2} L. \quad (9)$$

The resulting scale invariant amplitude corresponds to the functional (6). The approximation consists in dropping $K(x;M)$ and the terms bilinear in $F_a(x;M)$ in the exact functionals (2) and (4), introducing a dependence on the scale $M$. This scale parametrizes the two-loop contributions not contained in (6). Transforming the one-loop functionals $H_i(x;M), F_a(x;M)$ back to $H_i(x;\mu), F_a(x;\mu)$, the only $M$-dependence resides in the chiral logs. The remaining (single and double) chiral logs can then only be due to the two-loop contributions because all other contributions are correctly included in the approximate functional (6) and are therefore independent of $M$. Experience with the double-log approximation [10] suggests that $M$ is naturally of the order of the kaon mass in $SU(3)$ calculations.

While the above approximation is motivated by large $N_c$, some of the terms not included in the approximate functional (6) have a relatively simple analytic form (products of one-loop amplitudes from diagrams a,c in Fig. 1). In practice, inclusion of those terms may improve the accuracy of the approximation for certain observables. We will come back to this issue in Ref. [14].
4. Application to lattice data for $F_K/F_{\pi}$

We apply the analytic approximation (4) to the ratio $F_K/F_{\pi}$ of meson decay constants. $F_K/F_{\pi}$ is well suited for an exploratory study for at least two reasons.

- At the scale $\mu = 0.77$ GeV, the genuine two-loop contribution amounts to $-0.005$ for physical masses, i.e., half a percent only \[6,16\].

- The detailed results of the BMW collaboration \[12\] provide an ideal laboratory for testing our approximation.

The approximate form of $F_K/F_{\pi}$ is given in the Appendix where all masses are lowest-order masses of $O(p^3)$ \[16,17\]. Since we work to $O(p^6)$ the masses in $R_4$ must be expressed in terms of the lattice masses to $O(p^4)$ \[3\]. The chiral limit value $F_0$ is deduced from the experimental value $F_\pi = 92.2$ MeV and physical meson masses, using again the relation to $O(p^4)$ \[3\].

Here we are mainly interested in getting information on the LECs of $O(p^6)$. Only two combinations of LECs appear: $C_{14} + C_{15}$ and $C_{15} + 2C_{17}$. Most of the $L_i$ also contribute to $F_K/F_{\pi}$. Several determinations of the $L_i^r$ are available in the literature \[18,19\]. All fits of the $L_i^r$ to $O(p^6)$ need to make some assumptions about the $C_i^r$, in particular for extracting $L_5^r$ from $F_K/F_{\pi}$. $L_5$ is the only LEC contributing to $F_K/F_{\pi}$ at $O(p^4)$. Moreover, $L_5^r$ appears at $O(p^6)$ to leading order in $1/N_c$. This suggests to fit the lattice data with the three parameters $L_5^r$, $C_{14}^r + C_{15}^r$ and $C_{15}^r + 2C_{17}^r$. For the remaining LECs of $O(p^4)$ we adopt the values of fit 10 of Ref. \[18\]. Since our approximation is scale independent we may choose the conventional scale $\mu = 0.77$ GeV.

Restricting the data sample of the BMW collaboration \[12\] to simulation points with $M_\pi < 450$ MeV, we are left with 13 data points. For this exploratory study, we take only the statistical errors of $F_K/F_{\pi}$ into account. After all, our main purpose is to investigate the capacity of lattice data for the determination of LECs but not to compete with the detailed analysis of Ref. \[12\].

Fitting the 13 data points with Eq. (13), we obtain for the LECs at $\mu = 0.77$ GeV

$$L_5^r = (0.76 \pm 0.09) \cdot 10^{-3}$$

$$C_{14}^r + C_{15}^r = (0.37 \pm 0.08) \cdot 10^{-3} \text{ GeV}^{-2}$$

$$C_{15}^r + 2C_{17}^r = (1.29 \pm 0.16) \cdot 10^{-3} \text{ GeV}^{-2}.$$  

(10)

The three parameters are strongly correlated, with correlation coefficients indicated below.

| $L_5^r$ | $C_{14}^r + C_{15}^r$ |
|---------|-----------------------|
| 0.69    | -0.87                 |
| $C_{15}^r + 2C_{17}^r$ | $L_5^r$ |
| -0.95   |                       |

(11)

Taking these correlations into account, $F_K/F_{\pi}$ for physical meson masses is found to be

$$F_K/F_{\pi} = 1.198 \pm 0.005,$$  

(12)

comparing well with the result $F_K/F_{\pi} = 1.192(7)_\text{stat}(6)_\text{syst}$ of Ref. \[12\]. We stress once more that our errors take only the statistical errors of the lattice values for $F_K/F_{\pi}$ into account. The same word of caution applies to $\chi^2/\text{dof} = 1.3$ for the quality of fit.
Although the functional [6] and therefore $F_K/F_\pi$ in [13] are independent of the renormalization scale $\mu$ there is a residual dependence on the scale $M$ of the chiral logs. As announced before, we adopt the natural choice $M = M_K$ (lattice value). Varying this scale by $\pm 20\%$, both $F_K/F_\pi$ and $L_5^r$ remain practically unchanged while the LECs of $O(p^6)$ vary within two standard deviations. Note that this range for $M$ includes $M_\eta$, which is given by the Gell-Mann-Okubo mass formula in the contribution of $O(p^6)$ and is therefore always less than 1.2 $M_K$ for the meson masses under consideration. Taking $M$ too low would enhance the chiral logs too much for an $SU(3)$ observable. The sensitivity to the scale $M$ could be substantially reduced if lattice simulations would use strange quark masses lighter than the physical value. In such a scenario the convergence properties of chiral $SU(3)$ could be improved altogether.

For the case at hand, $F_K/F_\pi$ and $L_5^r$ are insensitive to the approximation made, with uncertainties determined by lattice errors. The situation is opposite for the LECs of $O(p^4)$. Here the approximation errors definitely exceed the lattice errors. The dependence on the other LECs of $O(p^4)$ must be taken into account in addition.

Since $C_{15}$ is subleading in $1/N_c$ our fit determines essentially $C_{14}$ and $C_{17}$ [6]. Although the values depend of course on the input for the $L_5^r$ we have found generically that both $C_{14}$ and $C_{17}$ are positive and smaller than $10^{-3}$ GeV$^{-2}$, always taken at the usual scale $\mu = 0.77$ GeV. Comparing with resonance exchange predictions [20], our results indicate that multiscalar exchange is important for these LECs. With single resonance exchange only, we would have $C_{14}^R = C_{17}^R < 0$ instead [20]. Our result for $L_5^r$ lies in the range covered by other NNLO fits [18, 19].

We cannot compare directly with the results of Bernard and Pasemann [6] for $C_{14}^r + C_{15}^r$ and $C_{17}^r + 2C_{17}^r$. First of all, the results of the BMW collaboration were not yet available for their analysis and, what is probably more important, the value of $L_5^r$ was taken as input in Ref. [6]. For the reasons given earlier and because of the strong (anti-)correlations found we consider it more appropriate to fit $L_5$ together with the LECs of $O(p^6)$. Generically, we find somewhat bigger values for $C_{14}^r + C_{15}^r$ and $C_{17}^r + 2C_{17}^r$ than in Ref. [6].

5. Conclusions

Starting from the structure of the generating functional of Green functions to $O(p^6)$, we have proposed analytic approximations for chiral $SU(3)$ amplitudes that require the calculation of tree-level and one-loop diagrams only. The result serves two purposes:

- It provides flexible and user-friendly extrapolation formulas for lattice data.
- It allows for the determination of higher-order LECs that are otherwise difficult to extract from experimental data.

The approximate amplitudes are independent of the renormalization scale, a prerequisite for a reliable determination of LECs. In addition to including all chiral logs, the amplitudes contain all leading and next-to-leading terms in the $1/N_c$ expansion.

The approach will therefore be especially useful in cases where the genuine two-loop contributions are small, compatible with the large-$N_c$ counting. The ratio $F_K/F_\pi$ is an interesting observable with this property. Fitting the approximate expression for $F_K/F_\pi$ to recent lattice data, we obtain a value for $F_K/F_\pi$ in agreement with the detailed analysis of Ref. [12]. Both $F_K/F_\pi$ and $L_5^r$ are insensitive to the approximation made. The LECs of
\(O(p^6), C_{14}^r + C_{15}^r + C_{15}^r + 2 C_{17}^r,\) are consistent with expectations but subject to uncertainties exceeding the lattice errors.

Although the present study is mainly of exploratory nature we consider the results significant enough to warrant further investigations along these lines [14].

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Appendix: Approximate result for $F_K/F_\pi$ to $O(p^6)$

In the approximation defined by the functional (10), $F_K/F_\pi$ assumes the following form:

$$
F_K/F_\pi = 1 + R_4 + R_6
$$

(13)

$$
F_0^2 R_4 = 4 (M_K^2 - M_\pi^2) L_5 - 5 \overline{A}(M_\pi, \mu)/8 + \overline{A}(M_K, \mu)/4 + 3 \overline{A}(M_\eta, \mu)/8
$$

$$
F_0^4 R_6 = 8 F_0^2 (M_K^2 - M_\pi^2) (2 M_K^2 (C_{14} + C_{15}) + M_\eta^2 (C_{15} + 2 C_{17}))
$$

$$+ (M_K^2 - M_\pi^2) (-32 (M_\pi^2 + 2 M_K^2) L_4 L_5 - 8 (3 M_\pi^2 + M_K^2) L_5^3
$$

$$+ (25 M_\pi^2 + 17 M_K^2) L^2/32)
$$

+ $$(M_K^2 - M_\pi^2)/(4\pi)^2 (-2 (M_\pi^2 + M_K^2) L_1 - (M_\pi^2 + M_K^2) L_2 - (5 M_\pi^2 + M_K^2) L_3/18
$$

$$+ 6 (M_\pi^2 + 2 M_K^2) L_4 + (14 M_\pi^2 + 22 M_K^2) L_5/3 - 12 (M_\pi^2 + 2 M_K^2) L_6
$$

$$+ 16 (M_\pi^2 - M_K^2) L_7 - 4 (M_\pi^2 + 5 M_K^2) L_8 + (313 M_\pi^2 + 271 M_K^2) L/288)
$$

+ $5 \overline{A}(M_\pi, \mu)^2/8 - \overline{A}(M_K, \mu)^2/8 + \overline{A}(M_\pi, \mu) \overline{A}(M_K, \mu)/16
$$

$$- 3 \overline{A}(M_\pi, \mu) \overline{A}(M_\eta, \mu)/8 - 3 \overline{A}(M_K, \mu) \overline{A}(M_\eta, \mu)/16
$$

$$+ \overline{A}(M_\pi, \mu) (4 M_\pi^2 L_1 + 10 M_\pi^2 L_2 + 13 M_\pi^2 L_3/2 + 10 (M_\pi^2 + 2 M_K^2) L_4
$$

$$+ (19 M_\pi^2 - 5 M_K^2) L_5/2 - 10 (M_\pi^2 + 2 M_K^2) L_6 - 10 M_\pi^2 L_8
$$

$$- (361 M_\pi^2 + 131 M_K^2) L/288)
$$

$$+ \overline{A}(M_K, \mu) (-4 M_K^2 L_1 - 10 M_K^2 L_2 - 5 M_K^2 L_3 - 4 (M_\pi^2 + 2 M_K^2) L_4
$$

$$- (M_\pi^2 + M_K^2) L_5 + 4 (M_\pi^2 + 2 M_K^2) L_6 + 4 M_K^2 L_8 + (59 M_\pi^2 + 115 M_K^2) L/144)
$$

$$+ \overline{A}(M_\eta, \mu) (M_K^2 - M_\pi^2)/M_\pi^2 (9 M_\pi^2 L_7 - 3 M_\pi^2 L_8 + 5 M_\pi^2 L/32)
$$

$$+ \overline{A}(M_\eta, \mu) ((M_\pi^2/2 - 2 M_K^2) L_3 - 6 (M_\pi^2 + 2 M_K^2) L_4 - (7 M_\pi^2 + 23 M_K^2) L_5/6
$$

$$+ 6 (M_\pi^2 + 2 M_K^2) L_6 + 3 (3 M_\pi^2 M_K^2/M_\eta^2 - 7 M_\pi^2 + 4 M_K^2) L_7
$$

$$+ 3 (M_\pi^2 M_K^2/M_\eta^2 - 3 M_\pi^2 + 4 M_K^2) L_8
$$

$$- (15 M_\pi^2 M_\pi^2/M_\eta^2 - 44 M_\pi^2 - 19 M_K^2) L/96)
$$

The abbreviations $L_i = L_i^r(\mu)$, $C_\alpha = C_\alpha^r(\mu)$ have been used for a compact representation. The masses are the lowest-order meson masses of $O(p^2)$. $F_0$ is the meson decay constant in the chiral $SU(3)$ limit and the chiral log $L$ is defined in (11). The loop function $\overline{A}(M_\alpha, \mu)$ is defined as

$$
\overline{A}(M_\alpha, \mu) = \frac{M_\alpha^2}{(4\pi)^2} \log \frac{\mu^2}{M_\alpha^2}
$$

(14)
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