Two-Loop Analysis of the Pion Mass Dependence of the $\rho$ Meson

Malwin Niehus,1,*, Martin Hoferichter2,3,† Bastian Kubis,1,‡ and Jacobo Ruiz de Elvira2,§

1Helmholtz-Institut für Strahlen- und Kernphysik (Theorie) and Bethe Center for Theoretical Physics, Universität Bonn, 53115 Bonn, Germany
2Albert Einstein Center for Fundamental Physics, Institute for Theoretical Physics, University of Bern, Sidlerstrasse 5, 3012 Bern, Switzerland
3Institute for Nuclear Theory, University of Washington, Seattle, Washington 98195-1550, USA

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Analyzing the pion mass dependence of $\pi\pi$ scattering phase shifts beyond the low-energy region requires the unitarization of the amplitudes from chiral perturbation theory. In the two-flavor theory, unitarization via the inverse-amplitude method (IAM) can be justified from dispersion relations, which is therefore expected to provide reliable predictions for the pion mass dependence of results from lattice QCD calculations. In this work, we provide compact analytic expression for the two-loop partial-wave amplitudes for $J = 0, 1, 2$ required for the IAM at subleading order. To analyze the pion mass dependence of recent lattice QCD results for the $P$ wave, we develop a fit strategy that for the first time allows us to perform stable two-loop IAM fits and assess the chiral convergence of the IAM approach. While the comparison of subsequent orders suggests a breakdown scale not much below the $\rho$ mass, a detailed understanding of the systematic uncertainties of lattice QCD data is critical to obtain acceptable fits, especially at larger pion masses.

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Introduction.—While recent years have shown significant progress in understanding the QCD resonance spectrum from first principles in lattice QCD [1], most calculations are still performed at unphysically large pion masses, requiring an extrapolation to the physical point to make connection with experiment. Such extrapolations can be controlled using effective field theories, i.e., chiral perturbation theory (ChPT) [2–4] for observables that allow for a perturbative expansion. By definition, this precludes a direct application to resonances such as the $\rho$ meson in the $P$ wave of $\pi\pi$ scattering. In fact, spectroscopy results from lattice QCD are arguably most advanced for the $\rho$ meson [5–20], with even calculations at the physical point now available [20], which makes this channel the ideal example to study the details of the pion mass dependence. In addition, the $\pi\pi$ $P$ wave features prominently in a host of phenomenological applications, among them hadronic vacuum polarization [21–26], nucleon form factors [27–30], and the radiative process $\gamma\pi \rightarrow \pi\pi$ [31,32]. For the latter, a thorough understanding of the $\pi\pi$ $P$ wave is prerequisite for an analysis of the pion mass dependence of recent lattice results [33–35], see Ref. [36], and similarly for decays into three-pion final states [37].

On the technical level, the failure to produce resonant states is related to the fact that unitarity is only restored perturbatively in ChPT, so that any description of resonances requires a unitarization procedure. A widely used approach known as the inverse-amplitude method (IAM) achieves this unitarization by studying the unitarity relation for the inverse amplitude [38–46]. In particular, in the case of SU(2) ChPT the IAM procedure can be derived starting from a dispersion relation in which the discontinuity of the left-hand cut is approximated by its chiral expansion [41,42]. While Adler zeros induce a modification for the $S$ waves [47], the naive derivation of the IAM survives for the $P$-wave amplitude: writing the partial wave for $\pi\pi$ scattering $t(s)$ as

$$t(s) = t_2(s) + t_4(s) + t_6(s), \quad (1)$$

with the subscripts indicating the chiral order, the unitarized amplitude at next-to-leading order (NLO) becomes [39–41]

$$t_{\text{NLO}}(s) = \frac{|t_2(s)|^2}{t_2(s) - t_4(s)}, \quad (2)$$

while at next-to-next-to-leading order (NNLO) [42,45]...
the resonance parameters of the 
sions are provided for all partial waves up to 
stable two-loop fits to current lattice data. While expres-
straightforward to implement and devise a strategy for 
analytic expressions for the two-loop amplitudes that are 
sufficient quality to allow for meaningful two-loop fits. In 
considerably. Second, as shown in Refs. [51,52], the 
loop amplitudes, thus complicating their implementation 
one-loop amplitudes can be given in analytic form, sim-
the pion mass.
However, apart from Refs. [51,52] such studies have been 
restricted to one-loop order, so that it was not possible to 
scrutinize the convergence properties of the expansion in 
the pion mass.
The reason for this situation was twofold. First, while the 
one-loop amplitudes can be given in analytic form, sim-
larily compact expressions were not available for the two-
loop amplitudes, thus complicating their implementation 
considerably. Second, as shown in Refs. [51,52], the 
increased number of low-energy constants (LECs) renders 
the fits more volatile, so that lattice data need to reach a 
sufficient quality to allow for meaningful two-loop fits. In 
this Letter we address both points: we present compact 
analytic expressions for the two-loop amplitudes that are 
straightforward to implement and devise a strategy for 
stable two-loop fits to current lattice data. While expres-
sions are provided for all partial waves up to \( J = 2 \), we 
concentrate on the application to the \( \pi \pi \) \( P \) wave, including 
the resonance parameters of the \( \rho \) meson and its pole 
residue.
Partial waves in ChPT.—We express the partial waves 
\( t_I^J(s) \), where \( I \) and \( J \) stand for the isospin and angular 
momentum, respectively, in terms of the pion decay 
constant in the chiral limit \( F \) as well as the pion mass 
\( M_\pi \) (including quark mass corrections from the LEC \( t_0^J \)), 
to render the dependence on the physical pion mass 
explicit and exclude a spurious mass dependence arising 
from the transition \( F \to F_\pi \) [58]. We will follow the 
conventions of Refs. [3,61] for the one-loop LECs \( t_0^J \) 
and the two-loop LECs \( r_0^J \). First, the leading-order (LO) 
results are [62]

\[
t_0^J(s) = \frac{2s - M_\pi^2}{32\pi F^2}, \quad t_0^J(s) = \frac{s - 2M_\pi^2}{32\pi F^2},
\]

\[
t_1^J(s) = \frac{s - 4M_\pi^2}{96\pi F^2}, \quad t_2^J(s) = 0.
\]

At NLO, the partial-wave amplitudes can be written in the 
form [58]

\[
\text{Re } t_I^J(s) = \sum_{i=0}^2 b_i^J(s)|L(s)|^i + \sum_{i=1}^3 b_i^J(s)t_i^J, \tag{5}
\]

in terms of

\[
L(s) = \log \frac{1 + \sigma(s)}{1 - \sigma(s)}, \quad \sigma(s) = \sqrt{1 - \frac{4M_\pi^2}{s}}, \tag{6}
\]

and coefficient functions \( b_i^J(s), b_i^J(s) \), which apart from 
phase-space and angular-momentum factors are poly-

calculations involve \( N_f = 2 + 1 \) flavor simulations, but in 
either case the changes compared to the physical kaon 
mass, which determine the corrections to the LECs in two-


\[
\text{Im } t_4(s) = \sigma(s)|t_2(s)|^2, \quad \text{Im } t_0(s) = 2\sigma(s)t_2(s)\text{Re } t_4(s).
\]

Fits to lattice data.—From here on, we focus on the \( P \) 
wave of \( \pi \pi \) scattering, with both isospin \( I \) and angular 
momentum \( J \) equal to one. Its phase \( \delta(s) = \arg[t_1^J(s)] \) 
can be computed using lattice QCD via Lüscher’s quantization 
condition [1,63], which allows one to determine the phase 
shift given \( \pi \pi \) energy levels and vice versa. To illustrate the 
fitting strategy as well as the conclusions regarding the pion 
mass dependence of \( \delta \) and the \( \rho \) parameters, we analyze 
such energy levels as computed on the lattice by two 
different groups. First, the one from Ref. [17], based on 
gauge configurations generated by the CLS collaboration, 
accompanied by a determination of the pion decay constant 
[64]. There are six datasets (ensembles) at five different 
pion masses in the range 200 to 284 MeV. Second, we 
consider the energy levels from the Hadron Spectrum 
Collaboration [12,65], using one of their ensembles with 
\( M_\pi \approx 236 \) MeV and two with \( M_\pi \approx 391 \) MeV. Both lattice 
calculations involve \( N_f = 2 + 1 \) flavor simulations, but in 
either case the changes compared to the physical kaon 
mass, which determine the corrections to the LECs in two-
flavor ChPT [66,67], are negligibly small compared to 
other sources of uncertainty. In the following, we concen-
trate mainly on the fit to the CLS data; details of the fitting 
procedure and the fits to the Hadron Spectrum data are 
given in Ref. [58]. To reduce the impact of scale-setting 
uncertainties, i.e., the error that arises when determining the 
lattice spacing in physical units, we work in lattice units 
wherever possible.
The fit proceeds as follows. At NLO, Eq. (2) is used to 
compute the phase \( \delta \), which is subsequently inserted into
TABLE I. NLO LECs obtained from a fit to the CLS ensembles (evaluated at $\mu = 0.77$ GeV). The first error is the statistical one, while the second arises due to the error of the lattice spacing. For comparison, in the second column the values expected from ChPT analyses are given, while the third column contains the values extracted from $N_f = 2 + 1$ lattice QCD computations [72–77].

|         | Fit        | Ref. [71] | Ref. [72] |
|---------|------------|-----------|-----------|
| $(l_2^s - 2l_1^s) \times 10^3$ | 12.62(25)(0) | 9.9(1.3) | 19(17) |
| $l_1^s \times 10^3$ | $-2.6(1.1)(0.2)$ | 6.2(1.3) | 3.8(2.8) |

Lüscher’s quantization condition to determine the energy levels. Their distance to the energies as computed on the lattice is then minimized. Simultaneously, the pion decay constant is fit, using the ChPT expression truncated at NLO. In an NNLO fit, the same procedure is applied, with Eq. (3) instead of Eq. (2), and the pion decay constant truncated at NNLO. This means that at NLO only the LECs $l_1^s - 2l_1^r$ and $l_2^r$ appear, while the NNLO expressions depend on $l_1^r$, $l_2^r$, and $l_3^r$ as well as the parameters $a_{r_a,b,c}$ and $r_F$.

The minimization of the $\chi^2$ with respect to the fit parameters—most importantly the LECs—requires a sufficiently powerful algorithm. To find the global minimum, we first employ the differential evolution algorithm [68], whose results are subsequently refined via a modification of Powell’s method [69]. The former algorithm allows one to tackle the multidimensional, nonlinear optimization problem at hand in both a robust and efficient manner, if its parameters are adjusted carefully. Together with the improved lattice data the choice and tuning of this algorithm are crucial to obtain sound fits that are stable even when ensembles at only a few different pion masses are available, e.g., the two masses used by the Hadron Spectrum Collaboration.

There are three sources of error that need to be considered for a reliable uncertainty estimate: first, the statistical error of the lattice data; second, the error of the lattice spacing, which enters the ChPT expressions indirectly via the renormalization scale $\mu$ [58]; third, the error that arises as a result of the truncation of the chiral expansion (1), which we are able to study in detail by a comparison of the IAM at one- and two-loop order. The chiral expansion proceeds in $1/m^2$ as well as $a = M_\pi^2/M_\rho^2$, with the breakdown scale expected to be set by the $\rho$ mass since it is the lowest-lying resonance in the partial wave of interest. The energy dependence is resummed by the unitarization via the IAM, leaving the expansion in the pion mass as the most critical variable. Following Ref. [70], we estimate the truncation error of an observable $X$ as

$$\Delta X_{\text{NLO}} = aX_{\text{NLO}},$$

$$\Delta X_{\text{NNLO}} = \max \{a^2 X_{\text{NLO}}, a|X_{\text{NLO}} - X_{\text{NNLO}}|\}. \quad (9)$$

Results.—To fix the LECs it is necessary to control both the $s$ dependence and the mass dependence. Hence, we fit all

CLS ensembles from Ref. [17] simultaneously, once working to NLO and once working to NNLO, excluding only the ensemble N401 from the fit, since its pion decay constant has not been determined in Ref. [64]. To render the NNLO fit stable, it is necessary to put a constraint on the LEC $l_1^r$.

The parameter governs the relation between the pion mass $M_\pi$ and its value $M$ at LO in ChPT, information on which is not included in our fit. Thus we add a penalty term to the $\chi^2$ that favors values of $l_1^r$ around its reference value $0.8(3.8) \times 10^{-3}$ [71]. The LECs obtained at NLO are given in Table I, and the NNLO ones in Table II.

Since the amplitudes as given in Eqs. (2) and (3) have the appropriate analytic structure, they can be continued analytically to the second Riemann sheet, where the pole associated with the $\rho$ resonance is located. Extracting the mass $M_\rho$ and width $\Gamma_\rho$ from the pole position $s_p$ via $s_p = (M_\rho - i\Gamma_\rho/2)^2$ and the coupling $g$ of $\rho$ to $\pi\pi$ from the residue $r$ via $g_0^2 = 4\pi r/(4M_\rho^2 - s_p)$ yields the values shown in Table III. Also shown are the goodness of the fit as well as the obtained value of $F$, the pion decay constant in the chiral limit. The corresponding phase is depicted in Fig. 1. Here and in the following, the physical

| $l_1^s \times 10^3$ | $-6.1(1.8)(0.1)$ | $-4.03(63)$ |
| $l_2^s \times 10^3$ | $2.58(90)(7)$ | $1.87(21)$ |
| $l_4^s \times 10^3$ | $0.776(65)(4)$ | $0.8(3.8)$ |
| $l_2^r \times 10^3$ | $-33(13)(0)$ | $6.2(1.3)$ |
| $r_a \times 10^6$ | $28(12)(1)$ | $13$ |
| $r_b \times 10^6$ | $-4.8(2.6)(0.2)$ | $-9.0$ |
| $r_c \times 10^6$ | $2.1(1.3)(0.1)$ | $1.1$ |
| $r_F \times 10^3$ | $2.7(1.2)(0)$ | $0$ |

TABLE II. The same as Table I, but at NNLO. For the NNLO LECs we show the estimates from resonance saturation for comparison [78, 79], although the uncertainties especially in $r_{a,b}$ are substantial and difficult to quantify.

|         | Fit | Ref. [71] | Refs. [78, 79] |
|---------|-----|-----------|--------------|
| $\chi^2$/d.o.f. | 216/(122 – 9) = 1.91 | 165/(123 – 15) = 1.53 |
| BIC | 259 | 237 |
| $M_\rho$/MeV | 761.4(5.1)(0.3)(24.7) | 750(12)(1)(1) |
| $\Gamma_\rho$/MeV | 150.9(4.4)(0.1)(4.9) | 129(12)(1)(1) |
| Re$g$ | 5.994(54)(0)(194) | 5.71(23)(2)(1) |
| Im$g$ | 0.731(21)(0)(24) | 0.46(14)(2)(1) |
| $F$/MeV | 88.27(20.3)(0.04)(2.86) | 93.7(2.3)(0.1)(0.2) |

TABLE III. Results of NLO and NNLO fits to the CLS data, including the goodness of the fit, the properties of the $\rho$ resonance at the physical point, as well as the decay constant in the chiral limit. The first error is the statistical one, the second stems from the lattice spacing, the third is the truncation error estimated via Eq. (9). The Bayesian information criterion (BIC) is defined in terms of the number of fit parameters $|F|$ and the number of data points $N$ as $\text{BIC} = \chi^2 + |F| \log N$. 

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|---------|-----|------|
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point is simply defined by the Particle Data Group (PDG)
value of the charged pion mass, $M_\pi = 139.57\text{MeV}$ [80],
and $F$ is computed using the PDG value of $F_\pi$ as input.

Because of the unitarization via the IAM, the LECs are
expected to deviate to some extent from the ChPT reference
values [41–44]. Accordingly, all LECs agree well with
expectations, apart from a large discrepancy in $l_4'$ both at
NLO and NNLO. To understand its origin, we performed
an NLO fit to the pion decay constant alone (at NNLO
the fit becomes underconstrained), leading to $l_4' =
1.3(1.0) \times 10^{-3}$, in agreement with the Flavour Lattice
Averaging Group, but already in tension with phenomenol-
ogy. The remainder of the pull displayed in Table I originates
from the $\pi\pi$ data. This pull becomes exacerbated at NNLO,
but as indicated by the large uncertainties the sensitivity to
$l_4'$ is limited. Indeed, we observe only a moderate increase of
the $\chi^2$ if literature values of $l_4'$ are enforced, as well as a large
change to $l_4' = -16 \times 10^{-3}$ when employing a different
strategy for the scale setting [17]. We conclude that there is

FIG. 1. The phase at physical pion mass as extrapolated from
global fits to the CLS data; see Fig. 2 for color scheme. For
comparison, in black the result of the dispersive analysis [22].
The extrapolation is performed at fixed $E = \sqrt{s}$, but a trajectory
defined by fixed momentum instead would yield identical results.

FIG. 2. The pion mass dependence of the decay constant, the coupling, as well as the real and imaginary part of the $\rho$ pole as determined
via fits to the CLS data, with error bands corresponding to (in order of decreasing color saturation) the data error (statistical plus spacing),
the truncation error, and the total one. The dashed lines mark the physical pion mass. The decay constant is given in units of $F$ to reduce the
impact of the scale setting. Since the NLO and NNLO fits yield different values of $F$, their physical points in these units differ. Also shown
as black ranges are reference values, the $\rho$ characteristics taken from Ref. [82], and the decay constant from Refs. [72–77,80].
a tension between the pion decay constant in the chiral limit and \( \rho \) parameters, which at least in part may be related to scale-setting uncertainties [88].

In general, we note that the \( \chi^2 / \text{d.o.f.} \) improves significantly when going from NLO to NNLO, although a statistically fully acceptable fit would require a more detailed understanding of lattice artifacts. Moreover, in the terms defined in Ref. [81], \( \Delta \text{BIC} = 22 \) provides very strong evidence for the NNLO over the NLO IAM. Comparing the obtained \( \rho \) characteristics with the ones from Roy-like equations [82]—namely, \( M_\rho = 763.7^{+1.6}_{-1.3} \) MeV, \( \Gamma_\rho = 146.4^{+2.0}_{-2.2} \) MeV, and \( g = 5.98^{+0.04}_{-0.07} + i(-0.56)^{+0.10}_{-0.07} \)—shows that both the NLO and NNLO results are compatible with these already within statistical errors, with a 1.4\( \sigma \) discrepancy in the width at NNLO and a 2.2\( \sigma \) tension in \( \text{Im} \, g \) at NLO. However, only the NLO value of \( F \) is compatible with the literature value \( F = 86.89(58) \) MeV, which is obtained by combining the PDG value of \( F_\pi \) [80] with the Flavour Lattice Averaging Group \( N_f = 2 + 1 \) average of \( F_\pi / F \) [72–77].

Our main results are shown in Figs. 1 and 2, for the pion mass dependence of the phase shift, the decay constant, and the \( \rho \) resonance parameters. Most notably, the two-loop analysis allows us to improve the precision considerably when going beyond the physical point, once the truncation becomes the dominant source of error. Second, with error bands produced assuming a breakdown scale of \( M_\rho \), the NLO and NNLO bands mostly overlap, which indicates that the true breakdown scale of the theory may lie below the \( \rho \) mass, but not much.

Overall, the coupling shows a very mild mass dependence [49,51], as does the \( \rho \) mass. Toward the end of the fit range, the central value of the two-loop curve seems to decrease, in disagreement with the phenomenological expectation from both the Kawaiabayashi-Suzuki-Fayyazuddin-Riazuddin relation [83,84] and the expected ordinary \( q \bar{q} \) nature of the \( \rho \) meson [85]. This may again, in addition to the \( \chi^2 \) and the tension in \( \Gamma_\rho \), point to the impact of lattice artifacts, which the two-loop IAM becomes flexible enough to mimic.

Similar conclusions can be drawn from the fits to the data by the Hadron Spectrum Collaboration [58]. They also show a significant improvement of the \( \chi^2 \) when going from NLO to NNLO and a pion mass dependence that mimics the one depicted in Fig. 2, with the difference that \( M_\rho \) does not decrease at high pion masses, providing further evidence that this decrease may arise due to lattice artifacts. Notably, for the Hadron Spectrum data the \( \rho \) properties at the physical point are closer to the literature values at NLO than at NNLO.

Conclusions.—In this work we have presented compact analytic expressions for the two-loop partial-wave amplitudes for \( \pi \pi \) scattering up to \( D \) waves, with a first application to an analysis of lattice data for the \( P \)-wave amplitude and the \( \rho \) parameters. We have shown that two-loop fits do improve the fit quality and, by comparing NLO and NNLO results, found that the breakdown scale of the chiral expansion should not lie much below the expected scale set by the \( \rho \) mass. However, we also concluded that the current datasets cannot be described in a statistically satisfactory way, with a more detailed understanding of the lattice data required.

In the future, anticipated improvements in the precision of lattice QCD calculations will increase the need to match that precision in the analysis. In this work, we have demonstrated how to achieve two-loop precision in practice, using the example of the \( P \) wave, but once lattice calculations mature a similar analysis can be performed for other partial waves including the pion mass dependence of the \( f_0(500) \). Even once datasets at the physical point become available, the IAM will thus provide a tool for a high-precision analysis of lattice data.

Finite-volume energy levels taken from Refs. [12,65] were provided by the Hadron Spectrum Collaboration—no endorsement on their part of the analysis presented in the current paper should be assumed. In addition, we would like to thank John Bulava as well as ETMC for sharing lattice data with us. We thank Carsten Urbach for many useful discussions, and Raúl Briceño, Mattia Bruno, Christopher Thomas, Martin Ueding, Markus Werner, and David Wilson for valuable input. Financial support by the Bonn–Cologne Graduate School of Physics and Astronomy (BCGS), the DFG (CRC 110, “Symmetries and the Emergence of Structure in QCD”), the Swiss National Science Foundation, under Projects No. PCEFP2_181117 (M. H.) and No. PZ00P2_174228 (J. R. d. E.), and the DOE (Grant No. DE-FG02-00ER41132) is gratefully acknowledged.

\[ \text{niehus@hiskp.uni-bonn.de} \]
\[ \text{hoferichter@itp.unibe.ch} \]
\[ \text{akubis@hiskp.uni-bonn.de} \]
\[ \text{elvira@itp.unibe.ch} \]

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