Connecting physical resonant amplitudes and lattice QCD

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Abstract

We present a determination of the isovector, $P$-wave $\pi\pi$ scattering phase shift obtained by extrapolating recent lattice QCD results from the Hadron Spectrum Collaboration using $m_\pi = 236$ MeV. The finite volume spectra are described using extensions of Lüscher’s method to determine the infinite volume Unitarized Chiral Perturbation Theory scattering amplitude. We exploit the pion mass dependence of this effective theory to obtain the scattering amplitude at $m_\pi = 140$ MeV. The scattering phase shift is found to agree with experiment up to center of mass energies of 1.2 GeV. The analytic continuation of the scattering amplitude to the complex plane yields a $\rho$-resonance pole at $E_\rho = [755(2)(1)_{129}^{+129}(3)(1)_{236}^{+129} - 129(3)(1)_{129}^{+129}(3)(1)_{236}^{+129}]$ MeV. The techniques presented illustrate a possible pathway towards connecting lattice QCD observables of few-body, strongly interacting systems to experimentally accessible quantities.

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The spectrum of hadronic resonances has long served as a window into the non-perturbative nature of Quantum Chromodynamics (QCD), the fundamental theory of the strong force. Hadronic resonances are color-singlet combinations of the fundamental degrees of freedom of QCD (quarks, anti-quarks, and gluons). They are observed as unstable resonant enhancements in the scattering of QCD stable hadrons, such as the pion. A simple example of a hadronic resonance is the $\rho$ that occurs in $\pi\pi$ scattering. The non-perturbative nature of QCD makes direct determination of the properties of hadronic resonances a challenging task.

Presently, the only means to study properties of low-energy hadronic states in a systematically improvable way is to perform a non-perturbative numerical evaluation of the QCD path-integral, by statistically sampling the gauge fields in a discretized finite volume to obtain correlation functions. This program is known as lattice QCD. The last decade has witnessed a tremendous advance in the ability of the lattice QCD community to connect experimental phenomena directly to the standard model of particle physics. It is not unreasonable to expect that in the upcoming decade most “simple” observables, such as masses, decay constants and elastic form factors of low-lying QCD stable particles, will be computed using physical values of the quark masses and QCD+QED gauge configurations (see Refs. [1, 2, 3] for recent progress in this direction).

For hadronic resonances, and in general systems involving two or more stable hadrons, the challenges are far greater and further technological and formal developments are needed (see Refs. [4, 5, 6, 7] for recent reviews on the topic). In order to kinematically suppress multiparticle channels, many excited state calculations are performed using unphysically massive light quarks. Thus, it is desirable to devise a scheme for performing a controlled extrapolation to the physical mass.

As a step towards developing such a program, we present the first extrapolation of a resonant scattering amplitude obtained from lattice QCD. Specifically, we analyze isovector, $P$-wave $\pi\pi$ spectra in the elastic scattering region that have been determined by the Hadron Spectrum Collaboration using dynamical quark masses corresponding to $m_\pi = 236$ MeV [8].

Lattice QCD uses a discrete and finite spacetime. Discretization provides a natural high energy regulator for QCD and if a fine enough spacing is used this introduces negligibly small effects in the spectrum. Working in a finite, periodic volume transforms the continuum of infinite volume scattering states into a discrete spectrum of states. The non-perturbative mapping between finite and infinite volume observables was first derived in Refs. [9, 10] and is commonly referred to as the “Lüscher method”.

The mappings between finite and infinite volume amplitudes cannot be one-to-one due to two important facts. First, the reduction of rotational symmetry from a continuous group to a discrete group (e.g., cubic) assures mixing between different partial waves. Second, having lost the notion of asymptotic states, finite volume states will necessarily be an admixture of different hadronic states with the same quantum numbers (e.g., $\pi\pi$ and $K\bar{K}$ in the $I = 1$ channel). Many theoretical advances have guided the field. For example, several references have discussed the feasibility of studying coupled-channel scattering in...
a finite volume [11, 12, 13, 14] (see Refs. [15, 16] for the first application of this formalism to the study of πK, ηK) as well as three-body systems [17, 18, 19, 20]. These methods become increasingly cumbersome when applied to highly energetic few-body systems, such as exotic or hybrid resonances [21, 22, 23], as well as the phenomenologically interesting charmed and bottom decays (e.g., $D \rightarrow \pi \pi / K\bar{K}$ [13, 24]), where multiple few-body channels are open.

In this work, we investigate one of the most studied low-lying resonances, the $\rho$ [8, 25, 26, 27, 28, 29, 30, 31]. The $\rho$ is an isotriplet with $J^{PC} = 1^{-}$, and it decays strongly to $\pi \pi$ nearly 100% of the time [32]. Its mass, $\sim 770$ MeV, lies above the $\pi \pi$ and $4\pi$ thresholds, and is less than half a width ($\Gamma_{\rho} \sim 145$ MeV) away from the $6\pi$ threshold. The coupling to these channels are experimentally observed to be negligible, which would suggest that the finite volume effects associated with these thresholds are suppressed. Further work is needed to confirm and quantify this suppression.

To circumvent these subtleties, we perform an extrapolation to the physical point of the $\pi \pi$ scattering phase shift computed at $m_{\pi} = 236$ MeV [8]. At these quark masses, the $4\pi$, $6\pi$ and $K\bar{K}$ thresholds lie well above the $\rho$ resonance and can be safely ignored. To perform the extrapolation we use Unitarized Chiral Perturbation Theory (UχPT) [33, 34, 35, 36, 37], which we summarize below. The parameters of UχPT at $m_{\pi} = 236$ MeV are chosen in order to reproduce the lattice QCD spectrum, and once this is done the pion mass is set to its experimental value and a postdiction for the scattering phase shift is obtained. Although superficially the need to extrapulate may seem undesirable, the avoidance of thresholds makes this conjunction of a phenomenological effective field theory with the Lüscher method a fruitful alternative to a determination of the phase shift at the physical point.

UχPT was previously advocated in the literature as a tool to determine physical resonances from lattice QCD [38, 39, 40, 41, 42, 43, 44, 45, 46], and it has been used in the study of the quark-mass dependence of the $\rho$ mass [47] \(^1\). Instead of focusing on the pole of the resonant amplitude, which has been the main focus of previous chiral extrapolations, we fit the full resonant amplitude. Given the correlation between the energy- and quark-mass dependence of these amplitudes, we find that this is sufficient to obtain the quark-mass dependence of the amplitude and consequently its pole.

In ref. [8], a total of 22 $\pi \pi$ energy levels are obtained below the $4\pi / K\bar{K}$ thresholds. Also determined are energy levels above these thresholds, and from them the $K\bar{K}$ phase shift and $\pi \pi$, $K\bar{K}$ inelasticity are obtained using the formalism first presented in [12, 13]. In this work, we analyze only the states in the elastic region. To relate these to an infinite volume scattering amplitude, $M(P)$, we use the generalization of Lüscher’s formalism for two degenerate scalar particles in moving frames [9, 10, 49, 50, 51]

$$\det[F^{-1}(P, L) + M(P)] = 0, \quad (1)$$

where $F(P, L)$ is a function that depends on the total four-momentum $P$ and the spatial extent of the cubic volume $L$, and the determinant acts on the space of spherical harmonics (for an exact definition of these quantities see Ref. [50]). This expression is exact up to exponentially suppressed corrections that scale as $e^{-m_{\pi}q}$, which we can safely ignore given that $m_{\pi}L \gtrsim 4.4$ for the lattice used [8] \(^2\). Because the two particles are degenerate, odd and even partial waves do not couple, even when the system is in flight. Furthermore, in Ref. [8] it was shown that in the elastic region the $\ell \geq 3$ phase shifts are consistent with zero. Therefore, Eq. 1 effectively gives a one-to-one relation between the spectrum and the elastic $(\ell, I) = (1, 1) \pi \pi$ scattering amplitude. For real values of the relative momentum, $q$, the inverse of the scattering amplitude is related to the scattering phase shift $\delta$ in the standard way [50]

$$q \cot \delta_{I} = 16\pi E_{\pi \pi}^{*} \text{Re} \left[ \left( M_{I} \right)^{-1} \right], \quad (2)$$

where $E_{\pi \pi}^{*} = 2\sqrt{q^{2} + m_{\pi}^{2}}$ is the total energy in the center of mass (c.m.) frame.

We use SU(2) UχPT to obtain the $\pi \pi$ amplitude. Just like standard $\chi$PT [53, 54, 55, 56, 57, 58], UχPT allows one to evaluate observables analytically in a perturbative expansion defined by $(m_{\pi}/4\pi f_{\pi})^{\alpha}$, where $f_{\pi} = 92.2$ MeV [32] is the decay constant of the $\pi$. At each order in the expansion, one can write the scattering amplitude as a function of a finite number of LECs. At leading-order (LO) in the expansion only two LECs appear ($m_{0}$ and $f_{0}$). At next-to-leading order (NLO) four other LECs emerge ($\ell_{a1-4}$). See Appendix A for the Lagrangian as well as perturbative expressions for the pion mass, decay constant, and the pion-pion scattering amplitude. When performing the fit to the lattice spectrum, we fix $m_{0}$ such that $m_{\pi} = 236$ MeV. Given that the decay constant has not been determined, $f_{0}$ is fixed to reproduce the experimental value of $f_{\pi}$.

The $\ell'_{a}$ cannot be directly obtained from the physical values of the mass and decay constant, but can be accessed from the scattering amplitude. For the $\ell = 1$ partial wave, only two linear combinations of these are needed to describe the scattering phase shift ($\alpha_{1} \equiv -2\ell'_{1} + \ell'_{2}$ and $\alpha_{2} \equiv \ell'_{2}$). As discussed below, we fix these parameters by performing a fit to the lattice spectrum. Although the $\ell'_{a}$ are quark-mass independent in principle, by ignoring higher-order corrections the LECs will absorb a mild quark-mass dependence. See Ref. [60] for a recent review and discussion in the context of standard $\chi$PT.

The distinguishing feature of UχPT is its use of a procedure commonly referred to in the literature as the Inverse Amplitude Method [33, 35, 36] to ensure that the scattering amplitude satisfies unitarity. Effectively, in UχPT $s$-channel diagrams are summed in a geometric series using perturbation theory to all

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\(^1\)It has also been used to determine the low-energy coefficients (LECs) for heavy-light systems by studying the quark-mass dependence of the scattering phase shifts of weakly repulsive channels [48].

\(^2\)A subset of these exponential corrections has been determined for the $\pi \pi$ states with $\ell = 0$ [52] and $\ell = 1$ [38] partial waves.

\(^3\)For progress towards determining the decay constant of the ground state and excited states of the $\pi$ using these lattices, we point the reader to Ref. [59].

\(^4\)In Ref. [47] it is argued that these effects might be large for UχPT and higher order corrections might be needed. In this work we ignored higher order corrections, and these will be incorporated in future studies.
orders, while t- and u-channel diagrams are treated perturbatively to a finite order in the expansion described above. This procedure empirically extends the range of applicability of standard \( \chi PT \) to c.m. energies on the order of 1.2 GeV. Furthermore, unlike standard \( \chi PT \), \( \Upsilon PT \) has been shown to accurately describe low-lying resonances with a finite number of LECs [33, 35, 36], making it a desirable tool for the study of resonances from lattice QCD. By truncating the chiral expansion to NLO, one can write the unitarized scattering amplitude (see Appendix B for the derivation),

\[
M_{\Upsilon PT} = M_{\chi LO} - \frac{1}{M_{\chi LO} - M_{\chi NLO}} M_{\chi NLO},
\]

(3)

where \( M_{\chi LO} \) and \( M_{\chi NLO} \) are the LO and NLO \( \chi PT \) amplitudes detailed in Appendix A.

To perform a chiral extrapolation we must determine the lattice spacing. We use two definitions of the lattice spacing. First, we use the \( \Omega \) baryon mass, which has been determined to be \( a m_{\Omega}^{\text{lat}} = 0.2789(16) \) at these quark masses [8]. By setting this equal to \( a m_{\Omega}^{\text{phys}} \), where \( m_{\Omega}^{\text{phys}} = 1672.45(29) \) MeV is the mass of physical \( \Omega \) baryon, we obtain the lattice spacing \( a_{1}^{[1]} = 0.1668(10) \) GeV\(^{-1}\). Second, as shown in Fig. 1, we perform an extrapolation to the physical point of the lattice \( \Omega \) baryon mass using

\[
m_{\Omega}(m_{\pi}) = m_{\Omega}^{\text{lat}} + \alpha \frac{m_{\pi}^{2}}{m_{\Omega}^{2}} + \beta \frac{m_{\pi}^{4}}{m_{\Omega}^{2}},
\]

(4)
determined for four different values of \( \frac{m_{\pi}}{am_{\Omega}} \in [0.14 - 0.33] \) [65, 8]. We find \( a_{1}^{[2]} = 0.1630(14) \) GeV\(^{-1}\) with a \( \chi^2 / \text{d.o.f.} \) = 0.52. Assuming that \( a_{1}^{[1]} \) should coincide with \( a_{1}^{[2]} \), we perform all fits using both of these lattice spacings and any deviation of the result is incorporated into the systematic error. All central values below are obtained using the mean value of \( a_{1}^{[1]} \). As shown below, this 2\% error is the largest source of uncertainty in our final

result. It is important to recognize that this systematic error is improvable.

We determine the two unknown LECs by fitting the 22 energy levels obtained at a single quark mass and spatial volume. In practice, we input the \( \Upsilon PT \) amplitude into Eq. 1 and compute the spectra for a given set of LECs, \( E_{\chi PT}([\alpha]) \). By varying these LECs we minimize the \( \chi^2 ([\alpha]) \), defined as

\[
\chi^2 ([\alpha]) = \sum_{j,k} \delta E_{j}([\alpha]) C_{jk}^{-1} \delta E_{k}([\alpha])
\]

(5)

where \( \delta E_{j}([\alpha]) = [E_{j}^{\chi PT} - E_{j}^{\Upsilon PT}([\alpha])] \), and \([j,k]\) run over all 22 energy levels. As with the energy levels themselves, the elements of the covariance \( \Sigma \) matrix were provided by the Hadron Spectrum Collaboration [8]. The fit results in \( \chi^2 / N_{\text{d.o.f.}} = 1.26 \) for SU(2) \( \Upsilon PT \) and is shown in Fig. 2 compared to the lattice determined phase shifts. The LECs and correlations are found to be

\[
a_{1}(770 \text{ MeV}) = 14.7(4)(2)(1) \times 10^{-3}
\]

\[
a_{2}(770 \text{ MeV}) = -28(6)(3)(1) \times 10^{-3} \quad \begin{bmatrix} 1 & -0.98 \end{bmatrix}
\]

(6)

The first uncertainty is statistical, the second is the systematic due to the determination of the \( \pi \) mass and the anisotropy of the lattice \(^6\), and the third is an estimate of the systematic due to the determination of the lattice spacing. The symmetric matrix on the right of the coefficients denotes the statistical correlation between the two. By analytically continuing the scattering amplitude to complex values of \( s = (E_{\pi^{\ast}})^2 \) we obtain a resonance pole on the unphysical sheet, corresponding to taking the negative root when computing the c.m. momentum \( q^{\ast} \). At these quark masses, we find a \( \rho \) pole at \( E_{\rho} = 782(2) - \frac{1}{2} 85(2) \) MeV with a width, \( \Gamma_{\rho} \equiv -2 \text{Im}(E_{\rho}) = 85(2) \) MeV. We observe good agreement with the result from the Hadron Spectrum Collaboration where the poles were determined using other parameterizations of the scattering amplitude. This emphasizes the fact

\(^6\)The \( \pi \) mass was determined in lattice units to be \( a m_{\pi} = 0.03928(18) \). The anisotropy of that lattice is defined as \( \xi = a_{1}/a_{0} \) where \( a_{1} \) and \( a_{0} \) are the lattice spacings in the spatial and temporal extents. The anisotropy has been determined to be \( \xi = 3.4534(61) \).
that the lattice QCD spectrum properly constrains the scattering phase shift independently of the parameterization chosen.

The power of the $U_3$PT amplitude is that it allows one to extrapolate these quantities as a function of pion mass. In Fig. 3 we show the result of this exercise using the mean values of the coefficients in Eq. 6 and propagating both statistical and systematic uncertainties. We show the postdiction for $m_\pi = 140$ MeV and $m_\pi = 391$ MeV, where earlier calculation also extracted the $\pi\pi$ scattering amplitude containing the $\rho$ resonance [26]. We emphasize that in Ref. [47] it is clearly explained that $U_3$PT is not expected to reliably describe lattice QCD results above $m_\pi \sim 300 - 350$ MeV. Despite this formal constraint and the slight deviation at $m_\pi = 391$ MeV from the lattice results, $U_3$PT produces phase shifts that resemble both experimental and lattice determinations as a function of $m_\pi$.

In Fig. 4 we show a comparison of the results of the extrapolation using SU(2) and SU(3) versions of $U_3$PT. Given that SU(3)-breaking effects are large, SU(3) $\chi$PT has a poorer convergence than that the SU(2) counterpart. Therefore, we expect the SU(3) extrapolation to have a significantly larger systematic uncertainty. Assessing such systematic lies outside of the scope of the present work.

In Fig. 5 we present our final result for the chiral extrapolation of the $\pi\pi$ phase shift using SU(2) $U_3$PT. The result includes a propagation of statistical and systematic uncertainties. The largest uncertainty is due to the determination of the lattice spacing, where we aim to be conservative. Overall, we find good agreement with the experimental phase shift [66, 67] up to center of mass energies of 1.2 GeV, well above the $4\pi, 6\pi, K\bar{K}$ and $8\pi$ thresholds. By analytically continuing the amplitude into the complex plane, we find a postdiction of the $\rho$ pole at the physical point $E_\rho = \left[755(2)(1)^{(0)}_{02} - \frac{1}{2} 129(3)(1)^{(2)}_{12}\right]$ MeV.

In order to compare with experimental determinations of the mass and width of the $\rho$, we must restrict our attention to those determinations which have used the model-independent definitions $m_\rho = \text{Re}(E_\rho)$ and $\Gamma_\rho = -2\text{Im}(E_\rho)$. We contrast this with the standard procedure of quoting the mass and width parameters appearing in the Breit-Wigner parametrization of the scattering amplitude (as is done in the Particle Data Group book [32]). Only in the very narrow width limit do these two definitions coincide.

In Fig. 6 we show our determination of the $\rho$ pole. For comparison we show those obtained in Refs. [68, 62, 54, 69, 70, 71] by solving the Roy equation [72] and using experimental data as input. Since these results cover a large area, we highlight a dark point which encompasses all pole positions. Identifying this as an estimate of the overall systematic and statistical uncertainty, we find good agreement with our determination. We also show the pole position obtained in previous lattice QCD calculations [65, 26, 8], including those where the $\rho$ is stable. This plot serves as a nice illustration of the trajectory being taken by the $\rho$ pole as a function of $m_\pi$. For heavy quark masses, the $\rho$ is stable and its pole lies on the real axis. As the quark mass decreases, the $\rho$ becomes unstable and acquires a non-zero width, sending the pole off the real axis.

We compare the LECs determined here with those determined in Refs. [46, 47, 37]: $\alpha_1(770$ MeV) $\times 10^3 \in [9, 13]$ and $\alpha_2(770$ MeV) $\times 10^3 \in [1, 12]$. We observe a qualitative discrepancy between our determination of $\alpha_2$ and those determined in these references. This can be explained by two facts. First, as discussed in Ref. [34], the $\langle l, I \rangle = (1, 1)$ amplitude primarily depends on $\alpha_1$. Second, as mentioned above, the definition and value of these parameters depend on higher order corrections in the chiral expansion [47]. We suspect that by performing simultaneous fits of various channels while including higher order corrections one will see a convergence of these results. Implementing these techniques for channels including scalar resonances like the f0(500) would require using the modified Inverse Amplitude Method to have the correct analytic structure below threshold [61, 47]. The implementation of this awaits the lattice QCD calculation of these channels using $m_\pi = 236$ MeV.

Final remarks: We present the first extrapolation of a resonance amplitude from lattice QCD. To perform the extrapolation we used $U_3$PT, an effective field theory that at low-energies coincides with $\chi$PT and at high-energies generates resonances dynamically. In this framework, resonances are manifested nat-
$$m_{\pi} = 140 \text{ MeV} \quad m_{\rho} = 755(2)(1)(20) \text{ MeV} \quad \Gamma_{\rho} = 129(3)(1)(7) \text{ MeV}$$

\[ \Gamma = 2 \cdot \text{Im} \left( \frac{E}{\text{MeV}} \right) \]

- Which appear to play a negligible role.

- accommodating all open multiparticle channels will be available.

- not yet clear when a finite volume formalism rigorously accommodates phase shift up to energies above the $8\pi$.

- masses where the $\rho$ is stable [65] as well as unstable [26, 8].

- pole determinations from these references up to one standard deviation.

- these we highlight a black diamond whose uncertainty is defined to include all

- constrained from experimental data [gray diamonds] [68, 62, 54, 69, 70, 71].

- with pole determinations obtained from solutions to the Roy equation [72] constrained from experimental data [blue circles] performed using unphysically heavy quark

- from lattice QCD, in both the light and heavy quark sectors [26, 73, 74, 15, 16, 28, 75, 76].

It is desirable to study more complex systems such as highly energetic exotic hadrons (e.g., the $\pi (1400)$ resonance) or heavy meson weak decays (e.g., $D \rightarrow \pi \pi/K\bar{K}$ [13, 24]), however it is not yet clear when a finite volume formalism rigorously accommodating all open multiparticle channels will be available. We demonstrate that by properly constraining the scattering amplitude at a value of the pion mass where fewer channels are kinematically open, one can perform an extrapolation to the physical point.

These methods may be applied to obtain a wide range of hadron scattering amplitudes that are presently being extracted from lattice QCD, in both the light and heavy quark sectors [26, 73, 74, 15, 16, 28, 75, 76]. It is hoped that these concepts could be extended and applied to scattering processes containing highly excited and exotic resonances to gain deeper understanding of QCD and the excited spectrum of hadrons.

### Appendix A. Chiral Lagrangian and Scattering Amplitude

Here we present the key results of SU(2) $\chi$PT as derived in Ref. [38]. The relevant terms of the leading order (LO) and next-to-leading order (NLO) terms of the chiral Lagrangian (in the isospin limit $m_u = m_d$),

\[ \mathcal{L}_{\text{LO}} = \frac{f_0^2}{4} \text{Tr} \left( \partial_\mu U \partial^\mu U^\dagger \right) + \frac{m_0^2 f_0^2}{4} \text{Tr} \left( U^\dagger + U \right) \]

\[ \mathcal{L}_{\text{NLO}} = \frac{f_1}{4} \text{Tr} \left( \partial_\mu U \partial^\nu U^\dagger \right) + \frac{f_1^2}{4} \text{Tr} \left( \partial_\mu U \partial^\nu U^\dagger \right) \left[ \text{Tr} \left( U^\dagger U \partial^\nu U^\dagger \right) \right] \]

\[ + \frac{m_0^2 f_1^2}{16} \text{Tr} \left( U^\dagger + U \right) + \frac{m_0^2 f_0}{4} \text{Tr} \left( \partial^2 U^\dagger - \partial^2 U \right) + \ldots \]

(A.1)

are written in terms of the parameters $f_0$ (related to the pion decay constant) and $m_0$ (related to the pion mass), and the matrix of pion fields,

\[ U = \exp \left\{ \frac{i}{f_0} \begin{pmatrix} \pi^0 & \sqrt{2} \pi^- \\ \sqrt{2} \pi^+ & -\pi^0 \end{pmatrix} \right\}. \]

(A.2)
Divergences associated with loops with LO vertices are removed by renormalizing the $\ell_i$ LECs from the NLO Lagrangian and physical quantities depend on the renormalized LECs $\ell'_i(\mu)$. We use $\mu = 770$ MeV in this work. At this order in the chiral expansion, it is convenient to introduce $\mu$-independent expressions for the LECs, $\ell_i(m_0)$, that depend on the value of $m_0$,

$$\ell'_i = \frac{\gamma_i}{32\pi^2} \left[ \ell_i + \ln \left( \frac{m_0^2}{\mu^2} \right) \right],$$

(A.3)

where $\gamma_1 = \frac{1}{3}$, $\gamma_2 = \frac{2}{3}$, $\gamma_3 = -\frac{1}{3}$, and $\gamma_4 = 2$.

We use the standard NLO expressions [56, 57, 58] for the physical pion mass and decay constant,

$$m^2 = m^2_0 \left[ 1 - \frac{1}{32\pi^2} \frac{m^2_0}{f^2_0} \ell_3(m_0) + \ldots \right],$$

(A.4)

$$f_\pi = f_0 \left[ 1 + \frac{m^2_0}{16\pi^2} \frac{m^2_0}{f^2_0} \ell_2(m_0) + \ldots \right],$$

(A.5)

to solve for $m_0$ and $f_0$ perturbatively. To fix $m_0$ we use the value of $m_0$ that has been determined on the lattice, $m^\text{latt}_0$. Since $f_\pi$ has not been determined for these lattices, we resort to fixing $f_\pi$ using the experimental value, $f^\text{exp}_\pi$. This approximation forces us to use two different values of $m_\pi$ in our fits. More explicitly, for $m_0$ we use,

$$m^2 \approx m^\text{latt}_0 \left[ 1 + \frac{1}{32\pi^2} \frac{(m^\text{latt}_0)^2}{f^2_0} \ell_3(m^\text{latt}_0) + \ldots \right]$$

(A.6)

$$m_0^2 \approx \left( m^\text{latt}_0 \right)^2 \left[ 1 + \frac{1}{32\pi^2} \frac{(m^\text{latt}_0)^2}{f^2_0} \ell_3(m^\text{latt}_0) + \ldots \right],$$

(A.7)

were the ellipses denote corrections that appear at higher orders in the chiral expansion. Similarly, for $f_0$,

$$f_0 \approx f^\text{exp}_\pi \left[ 1 - \frac{1}{16\pi^2} \frac{(m^\text{exp}_\pi)^2}{f^2_\pi} \ell_2(m^\text{exp}_\pi) + \ldots \right].$$

(A.8)

The amplitudes depend on $1/f^2_0$, which we write here perturbatively

$$\frac{1}{f^2_0} \approx \frac{1}{f^\text{exp}_\pi f_\pi^2} \left[ 1 + \frac{2}{16\pi^2} \frac{(m^\text{exp}_\pi)^2}{f^2_\pi} \ell_2(m^\text{exp}_\pi) + \ldots \right].$$

(A.9)

The scattering amplitude prior to partial-wave projection, $A(s, t, u)$, can be written as

$$A_{\text{LO}}(s, t, u) = \frac{s - m^2}{f^2_\pi}$$

$$A_{\text{NLO}}(s, t, u) = \frac{s - m^2}{f^2_\pi} \frac{(m^\text{exp}_\pi)^2}{8\pi^2 f^4_\pi} \ell_4(m^\text{exp}_\pi) - \frac{m^2}{32\pi^2 f^2_\pi} \ell_3(m_\pi) + \frac{1}{6f^2_\pi} \left[ 3(s^2 - m^2_\pi) f(s) + [t(t - u) - 2m^2_\pi] f(t) \right] + \frac{1}{96\pi^2 f^2_\pi} \left[ 2 \ell_2(m_\pi) - 5/6 \right] \left[ s^2 + (t - u)^2 \right] - 12m^2_\pi s + 15m^4_\pi \right],$$

(A.10)

where

$$J(s) = \frac{1}{16\pi^2} \left[ \sqrt{1 - 4m^2_\pi/s} \ln \frac{\sqrt{1 - 4m^2_\pi/s - 1} + 2}{\sqrt{1 - 4m^2_\pi/s + 1}} \right].$$

(A.11)

Note that in Eq. A.10 we have implemented the perturbative expressions for $m_0^2$ and $f^2_0$ described above. In Eq. A.10 and Eq. A.11 we use the notation $m_\pi = m^\text{latt}_\pi$ and $f_\pi = f^\text{exp}_\pi$. The amplitude $A(s, t, u)$ can then be projected into a partial wave $\ell$ using,

$$M_\ell = \frac{1}{2} \int_0^{\pi/2} dz P_\ell(z) A(s, t(s, z), u(s, z))$$

(A.12)

where $z = \cos \theta$ and $\theta$ is the $s$-channel c.m. frame scattering angle. In this work, we also project onto the $l = 1$ channel,

$$M_1^\ell(s, t, u) = M(t, s, u) - M(u, t, s).$$

(A.13)

One can show that the only linear combinations of LECs contributing to the isotriplet scattering amplitude are $\alpha_1 = -2\ell'_1 + \ell'_2$ and $\alpha_2 \equiv \ell'_4$, which are the ones determined in this work.

### Appendix B. The Inverse Amplitude Method

Although U3PT has been extensively discussed in the literature, here we sketch the derivation of Eq. 3 presented in Ref. [36] in an effort to make this article more self-contained. The basic idea, as already mentioned above, is to assure that unitarity is satisfied exactly at each order in the chiral expansion. We begin by giving the standard relation between the $S$-matrix and the partial-wave projected scattering amplitude, $M$,

$$S = 1 + 2i\sigma M,$$

(B.1)

where $\sigma = g/16\pi f^2_\pi$. Unitarity enforces

$$\text{Im}(M) = |\sigma| |M|^2,$$

(B.2)

which is the familiar Optical Theorem. This condition can be rewritten as

$$\text{Im}(M^{-1}) = -\sigma,$$

(B.3)

which leads us to

$$M = (\text{Re}(M^{-1}) - i\sigma)^{-1}.$$  

(B.4)

If $M$ is evaluated perturbatively as detailed in Appendix A, $M = M_{\text{LO}} + M_{\text{NLO}} + \ldots$, we can expand its inverse to find,

$$M^{-1} = M_{\text{LO}}^{-1} \frac{1}{1 + M_{\text{LO}}^{-1} M_{\text{NLO}} + \ldots} = M_{\text{LO}}^{-1} \left( 1 - M_{\text{LO}}^{-1} M_{\text{NLO}} + \ldots \right).$$

(B.5)

Since $M_{\text{LO}}$ is real,

$$\text{Re}(M^{-1}) = M_{\text{LO}}^{-1} \left( 1 - \text{Re}(M_{\text{NLO}}) + \ldots \right),$$

(B.6)
which we insert into Eq. B.4 to find,
\[ M = \frac{1}{M_{LO}^{-1}} \left( 1 - M_{LO}^{-1} \text{Re}(M_{NLO}) + \ldots \right) - i \sigma \]
\[ \approx M_{LO}^{-1} \left( 1 - i \sigma \text{Re}(M_{NLO}) - i \sigma M_{NLO}^2 \right). \]  
(B.7)

Finally, let us return to Eq. B.2 and enumerate the unitarity constraints order by order,
\[ \text{LO} : \quad \text{Im}(M_{LO}) = 0 \]
\[ \text{NLO} : \quad \text{Im}(M_{NLO}) = \sigma M_{LO}^2. \]  
(B.8)

Thus, putting Eq. B.8 into Eq. B.7, we reproduce Eq. 3.

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References

[1] S. Borsanyi et al., Science 347, 1452 (2015), 1406.4088.
[2] S. Borsanyi et al. (Budapest-Marseille-Wuppertal), Phys.Rev.Lett. 111, 252001 (2013), 1306.2287.
[3] S. Aoki et al., Phys. Rev. D86, 034507 (2012), 1205.2961.
[4] R. A. Briceño, Z. Dавови и Т. Ц. Луу, J. Phys. G42, 023101 (2015), 1406.5673.
[5] R. A. Briceño, PoS LATTICE2014, 008 (2015), 1411.6944.
[6] T. Yamazaki, PoS LATTICE2014, 009 (2015), 1503.08671.
[7] S. Pervlovs, PoS LATTICE2014, 015 (2014), 1411.0405.
[8] D. J. Wilson, R. A. Briceño, J. J. Dudek, R. G. Edwards, and C. E. Thomas, Phys. Rev. D92, 094502 (2015), 1507.02599.
[9] M. Lüscher, Commun. Math. Phys. 105, 153 (1986).
[10] M. Lüscher, Nucl. Phys. B354, 531 (1991).
[11] S. He, X. Feng, and C. Liu, JHEP 07, 011 (2005), hep-lat/0504019.
[12] R. A. Briceño and Z. Dавови, Phys. Rev. D88, 094507 (2013), 1204.1110.
[13] M. T. Hansen and S. R. Sharpe, Phys. Rev. D86, 016007 (2012), 1204.0826.
[14] R. A. Briceño, Phys. Rev. D89, 074507 (2014), 1401.3312.
[15] J. J. Dudek, R. G. Edwards, C. E. Thomas, and D. J. Wilson (Hadron Spectrum), Phys. Rev. Lett. 113, 182001 (2014), 1406.4158.
[16] D. J. Wilson, J. J. Dudek, R. G. Edwards, and C. E. Thomas, Phys. Rev. D91, 054008 (2015), 1411.2004.
[17] M. T. Hansen and S. R. Sharpe, Phys. Rev. D90, 116003 (2014), 1408.5933.
[18] M. T. Hansen and S. R. Sharpe, Phys. Rev. D92, 114509 (2015), 1504.0428.
[19] R. A. Briceño and Z. Dădu, Phys.Rev. D87, 094507 (2013), 1212.3398.
[20] K. Polkrajča and A. Rusetsky, Eur. Phys. J. A48, 67 (2012), 1203.1241.
[21] J. J. Dudek, R. G. Edwards, M. J. Peardon, D. G. Richards, and C. E. Thomas, Phys. Rev. Lett. 103, 262001 (2009), 0909.0200.
Rept. 353, 207 (2001), hep-ph/0005297.

[63] R. García-Martin, R. Kaminski, J. R. Pelaez, J. Ruiz de Elvira, and F. J. Yndurain, Phys. Rev. D83, 074004 (2011), 1102.2183.

[64] I. V. Danilkin, L. I. R. Gil, and M. F. M. Lutz, Phys. Lett. B703, 504 (2011), 1106.2230.

[65] H.-W. Lin et al. (Hadron Spectrum), Phys. Rev. D79, 034502 (2009), 0810.3588.

[66] S. D. Protopopescu, M. Alston-Garnjost, A. Barbaro-Galtieri, S. M. Flattle, J. H. Friedman, T. A. Lasinski, G. R. Lynch, M. S. Rabin, and F. T. Solmitz, Phys. Rev. D7, 1279 (1973).

[67] P. Estabrooks and A. D. Martin, Nucl. Phys. B79, 301 (1974).

[68] P. Masjuan, J. Ruiz de Elvira, and J. J. Sanz-Cillero, Phys. Rev. D90, 097901 (2014), 1410.2397.

[69] Z. Y. Zhou, G. Y. Qin, P. Zhang, Z. Xiao, H. Q. Zheng, and N. Wu, JHEP 02, 043 (2005), hep-ph/0406271.

[70] R. García-Martin, R. Kaminski, J. R. Pelaez, and J. Ruiz de Elvira, Phys. Rev. Lett. 107, 072001 (2011), 1107.1635.

[71] P. Masjuan and J. J. Sanz-Cillero, Eur. Phys. J. C73, 2594 (2013), 1306.6306.

[72] S. M. Roy, Phys. Lett. B36, 353 (1971).

[73] J. J. Dudek, R. G. Edwards, M. J. Peardon, D. G. Richards, and C. E. Thomas, Phys. Rev. D83, 071504 (2011), 1011.6352.

[74] J. J. Dudek, R. G. Edwards, and C. E. Thomas, Phys. Rev. D86, 034031 (2012), 1203.6041.

[75] A. Martínez Torres, E. Oset, S. Prelovsek, and A. Ramos, JHEP 05, 153 (2015), 1412.1706.

[76] R. A. Briceño, J. J. Dudek, R. G. Edwards, C. J. Shultz, C. E. Thomas, and D. J. Wilson, Phys. Rev. Lett. 115, 242001 (2015), 1507.06622.