θ-dependence of the lightest meson resonances in QCD

Neramballi Ripunjay Acharya\textsuperscript{1,∗}, Feng-Kun Guo\textsuperscript{1,†}, Maxim Mai\textsuperscript{1,‡}, Ulf-G. Meißner\textsuperscript{1,2,§}

\textsuperscript{1}Helmholtz-Institut für Strahlen- und Kernphysik and Bethe Center for Theoretical Physics, Universität Bonn, D-53115 Bonn, Germany
\textsuperscript{2}Institute for Advanced Simulation, Institut für Kernphysik, Jülich Center for Hadron Physics, and JARA-FAME, Forschungszentrum Jülich, D-52425 Jülich, Germany

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Abstract

We derive the pion mass and the elastic pion-pion scattering amplitude in the QCD θ-vacuum up to next-to-leading order in chiral perturbation theory. Using the modified inverse amplitude method, we study the θ-dependence of the mass and width of the light scalar meson σ(500) and the vector meson ρ(770).

1 Introduction

Light flavor quantum chromodynamics (QCD) with up, down and strange quarks is a fascinating theory, that features only a few parameters. Variations of these parameters have been explored in great detail in the last decade. We mention in particular varying the quark masses to make contact with lattice simulations, but also variants of the theory with more light quark flavors or different numbers of colors have been studied. These studies mostly focused on the fate and exploration of the dynamical and explicit symmetry breaking that light flavor QCD exhibits. A much less explored territory relates to the θ-term of QCD, where

\begin{equation}
\mathcal{L}_θ = -\frac{θ}{64\pi^2} \epsilon^{\mu\nu\rho\sigma} G_{\mu\nu}^a G_{\rho\sigma}^a,
\end{equation}

where \(a = 1, \ldots, 8\) are color indices and \(G_{\mu\nu}^a\) is the gluon field strength tensor. While the upper limit on the neutron electric dipole moment poses a stringent limit on the value on \(θ\), where the latest determination gives \(|θ| < 7.6 \cdot 10^{-11}\) [1], it has been argued that based on the string theory landscape, \(θ\) might take natural values and that it is difficult to achieve a tiny value for it, see e.g. Ref. [2]. Independently of that, it is interesting to explore QCD at larger values of \(θ\). QCD at \(θ \sim π\) was already investigated in Refs. [3, 4]. Also, the pion and the nucleon mass were calculated at fixed topology in Ref. [5] to explore the connection between lattice QCD and physical observables. Further, Ubaldi [6] studied the effects that a non-zero strong-CP-violating parameter would have on the deuteron and di-proton binding energies and on the triple-alpha process using a somewhat simplified nuclear modeling. Even so the relevant energy scales in these systems exhibit some fine-tuning, no dramatic effect of varying \(θ\) was found. We also note a recent study on the relation between confinement and the θ-vacuum, see Ref. [7].

The θ-dependence of the pion mass has been given at leading order (LO) in chiral perturbation theory (ChPT) [5]. Here, we want to derive the pion mass in the θ-vacuum up to next-to-leading
order (NLO) as well as the corresponding pion-pion ($\pi\pi$) elastic scattering amplitude. Furthermore, we will calculate the $\theta$-dependence of the lightest resonances in QCD, the scalar meson $\sigma(500)$ and the vector meson $\rho(770)$. These are not only interesting by themselves, but also are important components in precision modelings of the nuclear forces, as used e.g. in the work on extracting limits on variations of the Higgs vacuum expectation value from the element abundances in Big Bang nucleosynthesis [8] (for related works using different frameworks, see Refs. [9, 10]). In the following, we assume that the $\sigma$ and the $\rho$ are generated from a resummation of pion-pion interactions evaluated at NLO in ChPT in the $\theta$-vacuum. Having calculated the $\theta$-dependent pion-pion scattering amplitude, it is straightforward to implement it into a unitarization (resummation) scheme that can generate the light resonances and thus gives their $\theta$-dependent properties. To be specific, we make use of the so-called (modified) inverse amplitude method, which is one, but not the only available, unitarization scheme that allows to perform this task.

Our work is organized as follows. In Sec. 2 we discuss the chiral effective Lagrangian in the $\theta$-vacuum, with particular emphasis on the two-flavor formulation and also including strong isospin breaking. Next, the $\theta$-dependent $\pi\pi$ scattering amplitude is constructed at NLO in Sec. 3. Armed with that, we then come to the central section 4, where the mass and the width of the $\sigma$ and the $\rho$ are calculated as a function of $\theta$. We end with a short summary and outlook in Sec. 5. The appendix contains some discussion of the vacuum alignment at NLO.

2 Chiral effective Lagrangian in the $\theta$-vacuum

At the lowest order, $\mathcal{O}(p^2)$, the SU($N$) chiral Lagrangian in the $\theta$ vacuum is [11, 12]

$$
\mathcal{L}_2 = \frac{F^2}{4} \langle D_{\mu} U^\dagger D^\mu U \rangle + \frac{F^2}{4} \langle \chi U^\dagger + \chi^\dagger U \rangle ,
$$

(2)

where $F$ is the pion decay constant in the chiral limit and $\chi = 2BM \exp(i\theta/N)$. Here, $M$ is the real and diagonal quark mass matrix, and the low-energy constant (LEC) $B = \Sigma/F^2$, with $\Sigma$ the absolute value of the flavor-averaged quark condensate in the chiral limit. The field $U \in \text{SU}(N)$ collects the Goldstone bosons of the theory. However, only for $\theta = 0$ the vacuum expectation value of it, which is the solution of the equations of motion for the zero-momentum mode, is trivial, i.e. $U_0 = 1$. In the general case, the vacuum is shifted from the unit matrix, and the vacuum alignment can be determined by minimizing the potential energy. Therefore, it is useful to separate the ground state $U_0$ from the quantum fluctuation $\tilde{U}$ containing the Goldstone boson fields as $U(x) = U_0 \tilde{U}(x)$. Thus, the ground state of the theory is given by minimizing the potential energy

$$
V_2 = -\frac{\Sigma}{2} \left\langle \left( U_0 e^{i\theta/N} + U_0 e^{-i\theta/N} \right) M \right\rangle .
$$

(3)

Because $M$ is diagonal, $U_0$ can be taken as diagonal as well without loss of generality. The special unitary matrix $U_0$ can be parametrized as

$$
U_0 = \text{diag}\{ e^{i\varphi_1}, e^{i\varphi_2}, \ldots, e^{i\varphi_N} \} , \quad \sum_f \varphi_f = 2n\pi \ (n \in \mathbb{Z}) .
$$

(4)

This leads to

$$
V_2 = -\Sigma \text{Re} \left\langle e^{-i\theta/N} U_0 M \right\rangle = -\Sigma \sum_f \cos \left( \varphi_f - \frac{\theta}{N} \right) m_f ,
$$

(5)

with $m_f$ the quark mass of flavor $f$.

For $\theta = \pi$, because the theory is periodic in $\theta$ with a period $2\pi$, the Lagrangian is invariant under CP and P transformations as they change $\theta$ to $-\theta$. However, it is well-known that at $\theta = \pi$, there is a spontaneous CP breaking, called Dashen’s phenomenon, because the CP conserving stationary point of the action is in fact a maximum and there are two degenerate CP violating vacua which are obtained by minimizing the potential energy [13].
2.1 Two-flavor case without isospin symmetry

In the rest of the paper, we will consider the two-flavor case and use the following parametrization

$$U_0 = \text{diag}(e^{i\varphi}, e^{-i\varphi}), \quad \hat{U} = e^{i\sqrt{2}\Phi}, \quad \Phi = \frac{1}{\sqrt{2}} \begin{pmatrix} \pi^0 & \sqrt{2}\pi^+ \\ \sqrt{2}\pi^- & -\pi^0 \end{pmatrix}. \quad (6)$$

We see that the angle $\varphi$ and the neutral pion field always appear in a linear combination $\varphi + \pi^0 / F$. Therefore, finding the stationary solution for $U_0$ by minimizing the potential energy with respect to $\varphi$ is equivalent to removing the tree-level tadpole for the neutral pion [13]. The minimization of $V_2$ gives [5]

$$(m_u + m_d)\sin \varphi \cos \frac{\theta}{2} - (m_u - m_d)\cos \varphi \sin \frac{\theta}{2} = 0$$

$$\Leftrightarrow \tan \varphi = -\epsilon \tan \frac{\theta}{2}, \quad (7)$$

where the average light quark mass $\bar{m} = (m_u + m_d) / 2$ and the parameter $\epsilon = (m_d - m_u) / (2\bar{m})$, that quantifies strong isospin breaking, are introduced. Actually, at $\theta = \pi$ and $\epsilon = 0$ the Eqs. (7) do not depend on $\varphi$ at all. This leads to a paradoxical situation of continuous vacuum degeneracy discussed in [3, 4] and resolved in [14] taking into account terms of the NLO chiral Lagrangian.

In the present work we also consider the NLO chiral Lagrangian [11]. In the SU(2)$\times$SU(2) notation of e.g. Ref. [15] it reads

$$\mathcal{L}_4 = \frac{l_1}{4} \left\langle D_\mu U^\dagger D^\mu U \right\rangle^2 + \frac{l_2}{4} \left\langle D_\mu U^\dagger D_\nu U \right\rangle \left\langle D^\mu U^\dagger D^\nu U \right\rangle + \frac{l_3}{16} \left\langle \chi^\dagger U + U^\dagger \right\rangle^2$$

$$+ \frac{l_4}{4} \left\langle D_\mu \chi^\dagger D^\mu U + D_\mu \chi D^\mu U^\dagger \right\rangle + \frac{l_5}{4} \left\langle U^\dagger F_{\mu\nu}^R U F^{L,\mu\nu} \right\rangle$$

$$+ \frac{l_6}{2} \left\langle F_{\mu\nu}^R D^\mu U D^\nu U^\dagger \right\rangle + \left\langle F_{\mu\nu}^L D^\mu U^\dagger D^\nu U \right\rangle - \frac{l_7}{16} \left\langle \chi^\dagger U - U^\dagger \right\rangle^2$$

$$+ \frac{h_1 + h_3}{4} \left\langle \chi^\dagger \chi \right\rangle + \frac{h_1 - h_3}{2} \text{Re} (\text{det} \chi) - h_2 \left\langle F_{\mu\nu}^L F^{L,\mu\nu} + F_{\mu\nu}^R F^{R,\mu\nu} \right\rangle, \quad (8)$$

where

$$D_\mu \mathcal{O} = \partial_\mu \mathcal{O} - i r_\mu \mathcal{O} + i \mathcal{O} l_\mu \quad \text{for} \quad \mathcal{O} = U, \chi$$

$$F_{\mu\nu}^R = \partial^\mu \chi^\nu - \partial^\nu \chi^\mu - i [r^\mu, r^\nu], \quad F_{\mu\nu}^L = \partial^\mu \chi^\nu - \partial^\nu \chi^\mu - i [l^\mu, l^\nu] \quad (9)$$

with $r^\mu$ and $l^\nu$ the right-handed and left-handed external fields, respectively.

In principle, with the introduction of the NLO Lagrangian as well as the one-loop contribution, the vacuum energy has changed, and the vacuum alignment needs to be re-determined. In particular, the $l_7$ term in the NLO Lagrangian is not minimized by the LO solution given in Eq. (7). This means that the $l_7$ term induces a shift to the LO vacuum alignment. However, as shown in Appendix A, this shift does not affect the calculation of the pion masses and the $\pi\pi$ scattering amplitudes up to NLO. Therefore, it is sufficient to consider the LO vacuum alignment in Eq. (7) for our purpose.\footnote{We will not discuss the complications at $\theta = \pi$. In that case, one needs to include the $l_7$ term as it determines the whole dynamics [3].}

2.2 $\theta$-dependence of the pion mass

Substituting $U_0$ with $\varphi$ given by Eq. (7) into the LO Lagrangian, we get the LO pion mass squared in the $\theta$-vacuum [5]

$$\tilde{M}^2(\theta) = 2B\bar{m} \cos \frac{\theta}{2} \sqrt{1 + \epsilon^2 \tan^2 \frac{\theta}{2}}, \quad (10)$$

which is the same for the neutral and charged pions.
At NLO, the pion masses receive contributions from both one-loop diagrams and the $l_3$ and $l_7$ terms. The divergence in the one-loop diagrams cancel exactly with that from $l_3$. We obtain

$$M_{\pi^+}^2(\theta) = \tilde{M}^2(\theta) + \frac{\tilde{M}^4(\theta)}{F^2} \left( \frac{1}{32\pi^2} \ln \frac{\tilde{M}^2(\theta)}{\mu^2} + 2l_3 + 2l_7 \left( \frac{1 - \epsilon^2}{1 + \epsilon^2 \tan^2(\theta/2)} \right)^2 \right),$$

$$M_{\pi^0}^2(\theta) = M_{\pi^+}^2(\theta) - 2l_7 \frac{\tilde{M}^4(\theta)}{F^2} \frac{\epsilon^2}{\cos^4(\theta/2) \left( 1 + \epsilon^2 \tan^2(\theta/2) \right)^2},$$ (11)

where $l_7^\ast$ is the scale-dependent finite part of $l_3$. At $\theta = 0$, these expressions reduce to the standard SU(2) relations derived in Ref. [11]. Using the positivity bound for $l_7$ obtained in Ref. [3], we find that the charged pion is always heavier than the neutral one.

For easy reference, we give the corresponding formulae for the much simpler isospin symmetric case with $m_u = m_d = \bar{m}$. In this case, the stationary solution of the vacuum energy has $\varphi = 0$. The pion mass up to NLO in the $\theta$-vacuum has one additional term compared with that in the $\theta = 0$ case, and is given by

$$M_{\pi}^2(\theta) = M^2(\theta) + \frac{M^4(\theta)}{F^2} \left( \frac{1}{32\pi^2} \ln \frac{M^2(\theta)}{\mu^2} + 2l_3^\ast + 2l_7 \tan^2 \frac{\theta}{2} \right)$$ (12)

with isospin symmetric LO pion mass

$$M_{\pi}^2(0) = 2B\bar{m} \cos \frac{\theta}{2}. \quad (13)$$

One sees that even in the isospin symmetric case, the NLO pion mass depends on $l_7$, and this additional term vanishes at $\theta = 0$.

### 3 ππ scattering amplitudes in a $\theta$-vacuum

The $\pi\pi$ scattering amplitude at NLO is the building block to generate the light mesons $\sigma(500)$ and $\rho(770)$ via unitarization. To be specific, we calculate the amplitude $A(s, t, u) = A_{\pi^+\pi^-\rightarrow\pi^0\pi^0}(s, t, u)$ which is used to get the following combinations with definite isospin ($I = 0, 1, 2$)

$$T^0(s, t) = 3A(s, t, u) + A(t, u, s) + A(u, s, t),$$

$$T^1(s, t) = A(t, u, s) - A(u, s, t),$$

$$T^2(s, t) = A(t, u, s) + A(u, s, t).$$ (14)

Later, we will also need the partial-wave projection for given isospin $I$ and angular momentum $L$

$$T^I_L(s) = \frac{1}{32\pi^2} \frac{1}{2} \int_{-1}^{+1} dz T^I(s, t) P_L(z)$$ (15)

with $P_L(z)$ the pertinent Legendre polynomials.

Up to the order $O(p^4)$, there are several contributions to the $\pi\pi$ scattering amplitude, as shown in Fig. 1. Diagram (a) gives

$$A_{(a)}(s, t, u) = \frac{1}{3F^2} \left\{ 3s + \tilde{M}_\theta^2 - 2 \left[ M_{\pi^0}^2(\theta) + M_{\pi^+}^2(\theta) \right] \right\},$$ (16)

in terms of $\tilde{M}_\theta^2 \equiv \tilde{M}^2(\theta)$, $M_{\pi^+}^2(\theta)$ and $M_{\pi^0}^2(\theta)$ given in Eqs. (10) and (11), respectively. Diagram (b) gives

$$A_{(b)}(s, t, u) = \frac{2l_3}{F^4} \left( s - 2\tilde{M}_\theta^2 \right)^2 + \frac{l_7}{F^4} \left[ 4\tilde{M}_\theta^2 \left( s - 2\tilde{M}_\theta^2 \right) + t^2 + u^2 \right] + \frac{8l_7}{3F^4} \tilde{M}_\theta^4 + \frac{32l_7B^4\bar{m}^4}{3F^4} \left[ (1 - \epsilon^2)^2 \sin^2 \theta - 2\epsilon^2 \right].$$ (17)
Figure 1: Feynman diagrams for the $\pi\pi$ scattering amplitude up to $O(p^4)$. Here the filled circles and square denote the vertices from the LO and NLO Lagrangian, respectively. The $t$ and $u$ channel two-point loops are not shown.

Diagram (c) includes the tadpole vertex correction from both the neutral and charged pions, and its contribution is

$$A_{(c)}(s, t, u) = \frac{1}{18 F^4} \left(31\hat{M}_\theta^2 - 20s\right) A_0 \left(\hat{M}_\theta^2\right),$$

(18)

$A_0(m^2)$ is the one-point loop integral (the tadpole) in $d$ space-time dimensions

$$A_0(m^2) := i\mu^{4-d}\int \frac{d^dl}{(2\pi)^d} \frac{1}{l^2 - m^2},$$

(19)

with $\mu$ the scale of dimensional regularization.

The two-point loops, diagram (d) and the corresponding $t$- and $u$-channel crossed diagrams, give

$$A_{(d)}(s, t, u) = \frac{1}{18 F^4} \left\{9 \left(\hat{M}_\theta^2 - s^2\right) B_0 \left(s, \hat{M}_\theta^2, \hat{M}_\theta^2\right) + 10s A_0 \left(\hat{M}_\theta^2\right)\right\} + \frac{1}{6 F^4} \left\{2\hat{M}_\theta^2 + 2\hat{M}_\theta^2(t - 2u) + t(u - t)\right\} B_0 \left(t, \hat{M}_\theta^2, \hat{M}_\theta^2\right) + \frac{2}{3}(t - 3u)A_0 \left(\hat{M}_\theta^2\right)$$

$$+ \frac{1}{48\pi^2} \left(\hat{M}_\theta^2 - s\right) \left(-6\hat{M}_\theta^2\right) + \frac{1}{6 F^4} \left\{2\hat{M}_\theta^2 + 2\hat{M}_\theta^2(u - 2t) + u(t - u)\right\} B_0 \left(u, \hat{M}_\theta^2, \hat{M}_\theta^2\right) + \frac{2}{3}(u - 3t)A_0 \left(\hat{M}_\theta^2\right)$$

$$+ \frac{1}{48\pi^2} \left(\hat{M}_\theta^2 - s\right) \left(u - 6\hat{M}_\theta^2\right),$$

(20)

where the first line corresponds to the $s$-channel charged and neutral pion loops, the second and third lines correspond to the $t$-channel loop, and the last two lines are for the $u$-channel loop. Here $B_0$ is the scalar two-point loop integral

$$B_0(q^2, m_1^2, m_2^2) := i\mu^{4-d}\int \frac{d^dl}{(2\pi)^d} \frac{1}{(l^2 - m_1^2)(l^2 + q^2 - m_2^2)}.$$

(21)

We also need to take into account the wave function renormalization for all external lines which is represented by diagram (e). This amounts to

$$A_{(e)}(s, t, u) = \frac{1}{2} \left(2\delta Z_{\pi} + 2\delta Z_{\pi^0}\right) \frac{1}{F^2} \left(s - \hat{M}_\theta^2\right) = \frac{4}{3F^2} A_0 \left(\hat{M}_\theta^2\right) \left(s - \hat{M}_\theta^2\right),$$

(22)

where $\delta Z_{\pi} = Z_{\pi} - 1$, with the wave function renormalization constant for both the neutral and charged pions given by

$$Z_{\pi} = 1 + \frac{2}{3F^2} A_0 \left(\hat{M}_\theta^2\right).$$

(23)

Using dimensional regularization for the loop integrals and summing up all contributions, we obtain a UV divergence-free and scale-independent amplitude. The $l_3$ and $l_7$ terms in Eq. (17)
cancel with the same terms in Eq. (16) that enter through the NLO mass expressions for the neutral and charged pions. The full amplitude reads

\[ A(s, t, u) = \frac{s - M_\rho^2}{F^2} + B(s, t, u) + C(s, t, u), \tag{24} \]

\[ B(s, t, u) = \frac{1}{6F^4} \left\{ 3(s^2 - M_\rho^2) \bar{J}(s) + \left[ t(t - u) - 2M_\rho^2 t + 4M_\rho^2 u - 2M_\rho^4 \right] \bar{J}(t) + \left[ u(u - t) - 2M_\rho^2 u + 4M_\rho^2 t - 2M_\rho^4 \right] \bar{J}(u) \right\}, \]

\[ C(s, t, u) = \frac{1}{96\pi^2 F^4} \left\{ 2 \left( \bar{l}_\theta - \frac{4}{3} \right) \left( s - 2M_\rho^2 \right)^2 + \left( \bar{l}_\theta - \frac{5}{6} \right) \left[ s^2 + (t - u)^2 \right] - 12M_\rho^2 s + 15M_\rho^4 \right\}. \]

Here, the \( \bar{l}_\theta \) are the scale-independent but quark mass-dependent, and thus \( \theta \)-dependent, LECs which are related to the renormalized ones as

\[ l'^r_i = \frac{\gamma_1}{32\pi^2} \left( \bar{l}_\theta + \ln \frac{M_\rho^2}{\mu^2} \right), \quad \gamma_1 = \frac{1}{3}, \quad \gamma_2 = \frac{2}{3}. \tag{25} \]

The finite loop function \( \bar{J} \) is given by

\[ \bar{J}(s) = \frac{1}{16\pi^2} \left( \sigma(s) \ln \frac{\sigma(s) - 1}{\sigma(s) + 1} + 2 \right), \quad \sigma(s) = \sqrt{1 - \frac{4M_\rho^2}{q^2}}. \tag{26} \]

We find that the \( \pi\pi \) scattering amplitude up to NLO in a \( \theta \)-vacuum, Eq. (24), takes exactly the same form as the well-known one in the vacuum with \( \theta = 0 \) [11], and the only change is to replace everywhere \( M^2(0) = 2B\bar{m} \) by \( M_\rho^2 \) given by Eq. (10). The reason is that vertices from terms of the form \( \langle \chi U + U^\dagger \chi \rangle \) can always be written in terms of \( M_\rho^2 \), while the \( l_7 \) term from diagram (b) gets cancelled with the one from diagram (a). Such a property does not hold at higher orders. For instance, considering the \( \pi\pi \) scattering at \( \mathcal{O}(\rho^6) \), there can be a one-pion exchange diagram with two CP-violating three-pion vertices (see Appendix A), which does not have any correspondence at \( \theta = 0 \). This behaviour of the \( \pi\pi \) scattering amplitude is reminiscent of the Kaplan-Manohar transformation [16], which is an accidental symmetry of the chiral Lagrangian at NLO.

### 4 \( \theta \)-dependence of the \( \sigma \) and \( \rho \) in the isospin limit

The \( \sigma(500) \) and the \( \rho(770) \) are the lightest two-flavor non-Goldstone mesons. They can be obtained from the chiral perturbation theory amplitudes by unitarization. There are various such unitarization schemes on the market, like the inverse amplitude method (IAM) to be used here [17]. In most cases, such a unitarization procedure amounts to a resummation of a certain class of diagrams to ensure exact two-body unitarity, which is only perturbative in ChPT, but such resummations are usually at odds with crossing symmetry. We do not want to enter a more detailed discussion on these issues here (see e.g. the early work in Ref. [18]), but rather employ the IAM as a tool to generate the light mesons from the \( \theta \)-dependent pion-pion interaction, which automatically leads to \( \theta \)-dependent properties of the \( \sigma \) and the \( \rho \).

The scattering amplitude for a given channel (with fixed isospin and angular momentum) up to NLO in the IAM is given by

\[ T(s) = \frac{(T_{(2)}(s))^2}{T_{(2)}(s) - T_{(4)}(s)}, \tag{27} \]

where \( T_{(2)}(s) \) and \( T_{(4)}(s) \) are the \( \pi\pi \) scattering amplitudes of leading and next-to-leading chiral order. This form is valid in the channel with \( I = J = 1 \) pertinent to the \( \rho \)-meson. As pointed out e.g. in Ref. [19], it requires modification in the \( I = J = 0 \) channel due to the presence of Adler zeros in the \( S \)-wave. The associated unphysical poles can be cancelled in rather natural
way as derived in Ref. [20] which is called the modified inverse amplitude method (mIAM). The corresponding scattering amplitude reads

\[
T(s) = \frac{(T_2(s))^2}{T_2(s) - T_4(s) + A_{\text{mIAM}}(s)},
\]

where \( s_A \) denotes the Adler zero of the full partial wave defined by the condition \( T(s_A) = 0 \), and \( ' \) denotes differentiation with respect to \( s \). The approximative Adler zeros at LO and NLO correspond to the energies \( s_2 \) and \( s_2 + s_4 \), determined by \( T_2(s_2) = 0 \) and \( T_2(s_2 + s_4) + T_4(s_2 + s_4) = 0 \), respectively. This mIAM has been used e.g. in Ref. [21] to study the quark mass dependence of the sigma and the rho. In particular, we will use the LECs \( l_1^r \) and \( l_2^r \) as determined in that paper at the scale \( \mu = 770 \text{ MeV} \),

\[
l_1^r = (-3.7 \pm 0.2) \times 10^{-3}, \quad l_2^r = (5.0 \pm 0.4) \times 10^{-3}.
\]

As mentioned in Ref. [21], the results of the IAM is insensitive to the values of \( l_3^r \) and \( l_4^r \) as long as they are within the uncertainties: \( l_3^r = (0.8 \pm 3.8) \times 10^{-3} \) and \( l_4^r = (6.2 \pm 5.7) \times 10^{-3} \). Taking the central values and the measured values of the pion mass and decay constant \( M_\pi = 138.04 \text{ MeV} \) (isospin averaged) and \( F_\pi = 92.21 \text{ MeV} \), the standard ChPT one-loop expressions yield \( M = 139.46 \text{ MeV} \) and \( F = 86.43 \text{ MeV} \).

The masses and widths of the \( \rho \) and \( \sigma \) resonances can be obtained by searching for the poles in the complex \( s \)-plane of the unitarized amplitudes. When the resonances are above the \( \pi\pi \) threshold, which is the case for the physical pion mass, we need to search for poles in the second Riemann sheet. The corresponding pole positions read

\[
\sqrt{s_\sigma} = (443.1 - i 217.4) \text{ MeV}, \quad \sqrt{s_\rho} = (751.9 - i 75.4) \text{ MeV}.
\]

We note that the mass of the \( \rho \) comes out somewhat below the physical value as it is common in such unitarization procedures. For a more detailed discussion on this issue, see e.g. Refs. [22, 23].

When isospin breaking is neglected, \( m_u = m_d \), the vacuum is not shifted, and we can use the usual ChPT Lagrangian and amplitudes directly. All the \( \theta \)-dependence of physical observables enters through Eq. (13) which finally leads to the mass and width of the \( \sigma \) and the \( \rho \) as a function of \( \theta \), shown in Fig. 2. The \( \theta \)-dependence of the \( \sigma \) mass is stronger than the one of the \( \rho \) mass since the former is in a \( S \)-wave while the latter is in a \( P \)-wave. Also, both widths show a somewhat stronger dependence on \( \theta \) which is due to the enlarged phase space as the pion mass decreases from its physical value when \( |\theta| \) increases from 0.
5 Summary and outlook

In this paper, we have studied the $\theta$-dependence of the lightest resonances in QCD. For that, we have derived the charged and neutral pion masses and the pion-pion scattering amplitude at NLO in the $\theta$-vacuum. We found that the NLO contributions proportional to $l_3$ and $l_7$ and entering via the pion mass formula and $\pi\pi$-contact terms cancel each other exactly. The $\sigma$ and the $\rho$ have been obtained from a unitarization of this amplitude using the so-called (modified) inverse amplitude method. This automatically generates $\theta$-dependent masses and widths of these resonances. Although the pion mass vanishes at $\theta = \pi$ at LO, no dramatic effects on the masses and widths of the $\sigma$ and the $\rho$ were found. However, it still remains to be seen how such modifications change the properties of nuclei, as the nuclear binding is fine tuned, and thus more sensitive to such parameter variations.

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A Vacuum alignment at NLO

In this appendix, we will discuss the vacuum alignment at NLO induced by the presence of the counterterms ($l_i$-terms) and the one-loop contribution. We will calculate the vacuum alignment perturbatively.

Because the shift of the LO vacuum alignment given in Eq. (7) is caused by the NLO terms in the chiral expansion, we assume that the angle $\varphi$ in $U_0 = \text{diag}\{e^{i\varphi}, e^{-i\varphi}\}$ can be split into

\[ \varphi = \varphi_0 + \alpha \varphi_1 \]  \hspace{1cm} (A.1)

with $\varphi_0$ determined by aligning the vacuum at LO, and $\alpha \varphi_1$ is the shift coming from the $\mathcal{O}(p^4)$ contribution to the vacuum energy. Here, $\alpha$ is a chiral scaling factor to make explicit that $\alpha \varphi_1$ is one order higher than $\varphi_0$ in the chiral expansion.\(^2\) The vacuum energy density up to NLO is given by

\[ e_{\text{vac}} = -\frac{F^2}{4} \left\langle \chi^\dagger U_0 + \chi U_0^\dagger \right\rangle - \frac{l_3}{16} \left\langle \chi^\dagger U_0 + \chi U_0^\dagger \right\rangle^2 + \frac{l_7}{16} \left\langle \chi^\dagger U_0 - \chi U_0^\dagger \right\rangle^2 
- \frac{h_1 + h_3}{4} \langle \chi^\dagger \chi \rangle - \frac{h_1 - h_3}{2} \text{Re} (\text{det} \chi) + e_{\text{vac}}^{(1\text{-loop})}, \]  \hspace{1cm} (A.2)

where we have neglected those $h_i$-terms which are independent of $U_0$, and $e_{\text{vac}}^{(1\text{-loop})}$ is the 1-loop effective potential whose explicit expression is \[24\] (see also Ref. \[25\] expanded up to $\theta^4$)

\[ e_{\text{vac}}^{(1\text{-loop})} = 3 M^4(\theta) \left[ \frac{\lambda}{2} + \frac{1}{128 \pi^2} \left( 1 - 2 \ln \frac{\Lambda^2}{\mu^2} \right) \right]. \]  \hspace{1cm} (A.3)

We may decompose the vacuum energy density into the LO and NLO contributions with the NLO one including all terms proportional to $\alpha$

\[ e_{\text{vac}} = e_{\text{vac}}^{(2)} + \alpha e_{\text{vac}}^{(4)}. \]  \hspace{1cm} (A.4)

\(^2\)The introduction of the scaling factor is only for convenience. It will be set to $\alpha = 1$ after $\varphi_1$ is calculated.
Substituting $U_0 = \text{diag}\{e^{i\varphi}, e^{-i\varphi}\}$ and Eq. (A.1) into Eq. (A.2), we get

$$e^{(2)}_{\text{vac}} = -F^2 M^2_\varphi, \quad M^2_\varphi = 2 B \tilde{m} \left( \cos \frac{\theta}{2} \cos \varphi_0 - \epsilon \sin \frac{\theta}{2} \sin \varphi_0 \right),$$

$$e^{(4)}_{\text{vac}} = \varphi_1 \frac{\partial e^{(2)}_{\text{vac}}}{\partial \varphi_0} + e^{(1\text{-loop})}_{\text{vac}} - \frac{l_3}{F^4} \left( e^{(2)}_{\text{vac}} \right)^2 - 4l_7 B^2 \tilde{m}^2 \left( \sin \frac{\theta}{2} \cos \varphi_0 + \epsilon \cos \frac{\theta}{2} \sin \varphi_0 \right)^2,$$

(A.5)

where we have neglected the terms independent of $\varphi$. The LO vacuum alignment is obtained by minimizing $e^{(2)}_{\text{vac}}$,

$$\frac{\partial e^{(2)}_{\text{vac}}}{\partial \varphi_0} = 0,$$

(A.6)

whose solution is given by $\varphi_0 = \bar{\varphi}_0$ with

$$\bar{\varphi}_0 = \arctan \left( -\epsilon \tan \frac{\theta}{2} \right).$$

(A.7)

With this value of $\varphi_0$, the LO vacuum energy density, normalized to 0 at $\theta = 0$, is [5]

$$e^{(2)}_{\text{vac}} = F^2 \left[ M^2(0) - \tilde{M}^2(\theta) \right],$$

(A.8)

where $M^2(0) = 2 B \tilde{m}$, and $\tilde{M}^2(\theta)$ is given in Eq. (10). The NLO vacuum energy density is

$$e^{(4)}_{\text{vac}} = e^{(1\text{-loop})}_{\text{vac}} - \tilde{M}^4(\theta) \left\{ l_3 + l_7 \left[ \frac{(1 - \epsilon^2) \tan(\theta/2)}{1 + \epsilon^2 \tan^2(\theta/2)} \right]^2 \right\}.$$  

(A.9)

The perturbation $\varphi_1$ due to the NLO terms is then determined by

$$\left. \frac{\partial e^{(4)}_{\text{vac}}}{\partial \varphi_0} \right|_{\varphi_0 = \bar{\varphi}_0} = 0.$$  

(A.10)

From Eq. (A.6), it is easy to see that the $l_3$ term does not have any effect. The vacuum alignment is equivalent to removing the tadpole of the neutral pion which causes vacuum instability [13] (see also, e.g., Refs. [26, 27, 28, 29]). In fact, with $\varphi_0 = \bar{\varphi}_0$, the SU(2) LO chiral Lagrangian does not have any term with odd number of pions because such a term is always proportional to

$$\cos \frac{\theta}{2} \sin \varphi_0 + \epsilon \sin \frac{\theta}{2} \cos \varphi_0 \propto \frac{\partial e^{(2)}_{\text{vac}}}{\partial \varphi_0}.$$  

(A.11)

This implies that the one-loop diagrams for producing a $\pi^0$ from the vacuum as shown in Fig. 3 have a vanishing amplitude. Thus, we have $\left( \partial e^{(1\text{-loop})}_{\text{vac}} / \partial \varphi_0 \right)_{\varphi_0 = \bar{\varphi}_0} = 0$. This can be checked explicitly with Eq. (A.3) noticing that $\tilde{M}^2(\theta) = M^2_\varphi|_{\varphi_0 = \bar{\varphi}_0}$. Therefore, Eq. (A.10) leads to a solution $\varphi_1 = \bar{\varphi}_1$ with

$$\bar{\varphi}_1 = \frac{4l_7 B \tilde{m}}{F^2} \left( 1 - \epsilon^2 \right) \frac{\tan(\theta/2) \sec(\theta/2)}{\left[ 1 + \epsilon^2 \tan^2(\theta/2) \right]^{3/2}}.$$  

(A.12)
This is the NLO perturbation to the LO vacuum alignment. Expanding it around $\theta = 0$, we reproduce the result derived in Ref. [29]

$$\bar{\varphi}_1 = \frac{2l_1 B \bar{m}}{F^2} \epsilon (1 - \epsilon^2) \theta + \mathcal{O} (\theta^2) . \tag{A.13}$$

This perturbation produces a CP violating three-pion vertex [28, 29] by substituting $U_0$ with $\varphi = \bar{\varphi}_0 + \bar{\varphi}_1$ into the LO Lagrangian, which turns out to be of $\mathcal{O} (p^4)$. Such a vertex contributes to the $\pi\pi$ scattering from $\mathcal{O} (p^6)$ and to the pion mass only starting at $\mathcal{O} (p^8)$. Furthermore, terms with even number of pions are CP conserving and receive contributions with an even power of $\bar{\varphi}_1$, so that the $\bar{\varphi}_1$-induced terms in the Lagrangian also start from $\mathcal{O} (p^6)$. Therefore, it is safe to make the vacuum alignment at LO for our calculation. It is for the same reason that the topological susceptibility up to NLO in the chiral expansion calculated in Ref. [25] agrees with that in Ref. [30], where the vacuum was aligned by minimizing the vacuum energy at LO and NLO, respectively.

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