

# Pion Scattering in Chiral Perturbation Theory on the Lattice

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# Introduction

Quantum chromodynamics (QCD), the theory of strong interaction, gives rise to a rich hadronic spectrum with pions as its lightest representatives. Due to the large coupling at low energies, however, this sector cannot be treated perturbatively and, so far, numerous of more or less efficient alternative techniques have been developed to handle the underlying phenomenology.

Especially the light mesons are very well described by chiral perturbation theory (ChPT), an effective field theory which captures the pions as the Nambu-Goldstone bosons of broken chiral symmetry and basically represents an expansion in terms of the quark masses and momenta [1, 2]. Pion scattering is one important application in ChPT, in which the experimental data for the scattering lengths agree to high accuracy with the theoretically determined values [3]. Yet, the aesthetic obstacle is that ChPT can be derived only based on pure considerations of symmetry. So far, there is no way to determine the coefficients of the involved operators, the so-called low energy constants, directly from QCD [4].

Quite the contrary is the case in lattice QCD, a non-perturbative method in which the discrete lattice represents a distinct regularization scheme in order to solve the functional integral of QCD. The big impact of lattice QCD is that its structure is perfectly fit to perform numerical simulations and, hence, to investigate the hadronic spectrum and important observables of QCD such as scattering lengths from first principles. Algorithmic progress and increasing computational power nowadays even allow dynamical, unquenched simulations. In this way, the S-wave pion scattering length  $a_0^2$  belonging to the isospin channels  $I = 2$  has been computed by the CP-PACS collaboration [5]. Unfortunately, the costs of such computations scale with powers of the inverse quark mass. Thus, the simulation of light quarks is extremely expensive [6]. For this reason, simulations are still performed with heavier quark masses than in nature. The results are then extrapolated to the physical point. The validity of this approach, however, strongly depends on the underlying fitting formulae. The general idea is to employ the results from ChPT as fitting formulae as long as the quark masses in the simulation

are sufficiently small. The quark masses are then considered as variables and the low energy constants as fitting parameters. As a byproduct, one obtains numerical estimates for the involved low energy constants which can then be compared with the phenomenologically determined values.

Since computations in lattice QCD strongly rely on the chosen lattice action, the framework of ChPT must be properly adapted to the underlying lattice theory in order to ensure the validity of the fitting process for a distinct observable. For the Wilson action, this has been done by developing a *Wilson chiral perturbation theory* (WChPT) [7–9]. This extended effective continuum theory takes explicitly into account the effects of a non-vanishing lattice spacing.

In this diploma thesis, pion scattering in WChPT is studied. The aim of the present work is to derive analytic expressions which can be used to fit numerical data obtained from pion scattering on the lattice. We compute the on-shell pion scattering amplitude to one loop assuming isospin symmetry for  $N_f = 2$ . From the amplitude, we derive with the effective range formalism analytic expressions for the scattering lengths  $a_l^I$  for the lowest non-vanishing partial waves  $l$  in all isospin channels  $I = 0, 1, 2$ . These are the scattering lengths  $a_0^0$ ,  $a_0^2$  and  $a_1^1$ . They can be used to extrapolate lattice data from pion scattering to the physical point.

In lattice QCD, the lattice spacing is, like the quark mass, a source of explicit chiral symmetry breaking. Therefore, we concentrate our calculations on two different regimes depending on the order of magnitude of the quark mass compared with the discretization effects of the lattice spacing: 1) The quark mass is of the same order of magnitude as the linear lattice spacing effects. 2) Higher order lattice artifacts are not negligible any more, such that the quark mass is of the same order of magnitude as the quadratic lattice spacing effects. For the first scenario, the  $a_0^2$  scattering length has already been computed [10]. In this thesis, we will compute the scattering lengths in the second scenario for all isospin channels. From this achievement, we will derive the corresponding expressions for the first regime and discuss the qualitative differences of the appropriate fitting formulae. Especially the differences to ChPT in the continuum will be discussed in detail.

The present work is structured as follows: In chapter 1, we extensively explain the machinery of ChPT and extend it to WChPT. In chapter 2, we apply the framework developed so far on the two quark mass scenarios mentioned above and construct the full necessary lagrangian. Then, the scattering amplitude is computed in chapter 3 and, finally, the scattering lengths and the corresponding fitting formulae are extracted in chapter 4.

# Chapter 1

## Chiral perturbation theory

In the first chapter, the concepts of ChPT are presented. We start with a very brief summary of QCD and its most important symmetries. Chiral symmetry and chiral symmetry breaking will lead us directly to the ideas of ChPT. The whole machinery will be explained in detail in the continuum such that the inclusion of the lattice spacing through WChPT can be developed in the last section.

### 1.1 Quantum chromodynamics

QCD is formulated as an  $SU(3)$  non-abelian gauge theory of color charge. It is constructed by claiming invariance of the action with respect to a distinct local continuous group transformation, in QCD, this is  $SU(3)$ . Let  $\hat{g}(x)$  be a representation of this group. If one considers, for example, a pure fermionic lagrangian  $\mathcal{L}_{\text{fer}} = \bar{\psi}(i\hat{\not{D}} - m)\psi$  and performs the group transformation  $\psi' = \hat{g}\psi$ , one finds that  $\mathcal{L}_{\text{fer}}$  is not invariant due to the derivative acting on the product  $\hat{g}\psi$ . However, the occurrence of additional terms which break the invariance can be compensated by introducing additional fields, gauge fields, whose transformation properties are constructed in such a way that the whole theory remains invariant. Finally, one can construct other  $SU(3)$  invariants out of the new gauge fields itself. The requirement of renormalizability, gauge invariance and Lorentz invariance then dictates the QCD lagrangian [11]. We will not outline this procedure in more detail but simply write down the gauge invariant QCD lagrangian and then subsequently explain the most

important features. Here it is:<sup>1</sup>

$$\mathcal{L}_{\text{QCD}} = -\frac{1}{4}F_a^{\mu\nu}F_{\mu\nu}^a + \sum_{\alpha} \bar{\psi}_j^{(\alpha)}(i\not{D}_{jk} - m^{(\alpha)}\delta_{jk})\psi_k^{(\alpha)} \quad (1.1)$$

The fermions which carry color charge are the quarks. We express this color by an additional index  $j = 1, 2, 3$  on the Dirac spinor  $\psi_j$ . This is not to be confused with the Dirac index which we suppress in order to keep the notation as simply as possible. The quarks appear in six different flavors  $\alpha = u, d, s, c, b, t$  whoses masses vary over many orders of magnitude. The lightest quarks, for instance, the up quark  $u$  and the down quark  $d$ , have masses around  $m_u = 1.5$  to  $3.3$  MeV and  $m_d = 3.5$  to  $6.0$  MeV, while the heaviest quark, the top quark  $t$  is around  $171$  GeV [13]. For the low energy effective theory, we will later restrict our calculations to the lightest quarks, the  $u$  and  $d$  quarks, and take the effects of heavy virtual quarks into consideration by properly adapting the effective low energy constants of the theory.  $D_{jk}^{\mu}$  in (1.1) is the covariant derivative. It is given by

$$\not{D}_{jk}\psi_k = \gamma^{\mu}(\delta_{jk}\partial_{\mu} + igA_{\mu}^a\frac{\lambda_{jk}^a}{2})\psi_k \quad (1.2)$$

where we have summed over repeated indices. The  $\lambda^a$  are the eight group generators for the  $d = 3$  fundamental representation of  $\text{SU}(3)$ . The  $A_{\mu}^a$  with color-index  $a = 1, \dots, 8$  are the  $\text{SU}(3)$  gauge fields, the gluons, which are the mediators of the strong interaction. The gauge fields themselves transform in the adjoint representation of  $\text{SU}(3)$ , unlike the quarks where each flavor transforms as the fundamental triplet representation.  $g$  is the strong interaction coupling constant. The first term in (1.1) is the non-abelian Maxwell term whose gauge field strength tensor  $F_{\mu\nu}^a$  is defined by

$$F_{\mu\nu}^a = \partial_{\mu}A_{\nu}^a - \partial_{\nu}A_{\mu}^a - gf^{abc}A_{\mu}^bA_{\nu}^c. \quad (1.3)$$

The gauge fields carry color charge (in contrast to quantum electrodynamics where the photons, the mediators of the electromagnetic interaction, do not carry any electric charge). The consequence thereof is that the gluons themselves interact, and this fact makes the theory very complicate.

Long before the discovery of QCD other symmetries of the strong interaction were known. These are the discrete symmetries of parity and charge conjugation as well as flavor symmetries. One can indeed check that (1.1) is CP invariant. Since the gluons are flavor independent, (1.1) further exhibits all the properties of the free quark model. This allows to discuss flavor symmetry independently of the complicated chromodynamic interaction.

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<sup>1</sup>So far, there is no experimental evidence that the strong interaction breaks the discrete symmetries of parity and charge conjugation. Therefore, we have neglected the CP breaking but renormalizable  $\theta$ -term. A detailed discussion can be found in [12].

## 1.2 Chiral symmetry

We consider the lagrangian for the free quark model

$$\mathcal{L}_{\text{quarks}} = \sum_{\alpha} \bar{\psi}^{(\alpha)} (i\gamma^{\mu} \partial_{\mu} - m^{(\alpha)}) \psi^{(\alpha)} = \bar{\psi} i\gamma^{\mu} \partial_{\mu} \psi - \bar{\psi} \hat{M} \psi \quad (1.4)$$

where we collected the quarks in a multiplet  $\psi$  of  $N_f$  flavors

$$\psi = \begin{pmatrix} \psi^{(u)} \\ \psi^{(d)} \\ \vdots \\ \psi^{(N_f)} \end{pmatrix} \quad (1.5)$$

and defined an appropriate diagonal mass matrix  $\hat{M}$ . In the chiral limit where  $\hat{M} = 0$ , (1.4) is invariant with respect to the following global symmetry transformations:<sup>2</sup>

$$\mathcal{V} : \quad \psi \longrightarrow \psi' = e^{i\alpha^a T^a} \psi, \quad (1.6)$$

$$\mathcal{A} : \quad \psi \longrightarrow \psi' = e^{i\beta^a T^a \gamma_5} \psi. \quad (1.7)$$

$\mathcal{V}$  is called vector transformation while  $\mathcal{A}$  defines the axial transformation involving  $\gamma_5$ . The  $T^a$  are the  $N_f^2 - 1$  generators of the  $SU(N_f)$  flavor group in the fundamental representation,  $\alpha^a$  and  $\beta^a$  are real continuous parameters. Further, we sum over repeated indices. With these definitions, we can determine the corresponding symmetry currents leading to the vector current  $V_{\mu}^a$  and to the axial vector current  $A_{\mu}^a$ :

$$V_{\mu}^a = \bar{\psi} T^a \gamma_{\mu} \psi, \quad (1.8)$$

$$A_{\mu}^a = \bar{\psi} T^a \gamma_{\mu} \gamma_5 \psi. \quad (1.9)$$

Taking the four-divergences and imposing the classical equations of motion we get

$$\begin{aligned} \partial^{\mu} V_{\mu}^a &= \bar{\psi} (\hat{M} T^a - T^a \hat{M}) \psi, \\ \partial^{\mu} A_{\mu}^a &= \bar{\psi} (\hat{M} T^a + T^a \hat{M}) \gamma_5 \psi. \end{aligned} \quad (1.10)$$

One immediately sees that for  $\hat{M} = 0$  both the vector and the axial vector current are conserved:  $\partial^{\mu} V_{\mu}^a = \partial^{\mu} A_{\mu}^a = 0$ . For  $\hat{M} \neq 0$ , however, the axial symmetry is explicitly broken. In the special case of degenerate quark masses, the mass matrix  $\hat{M}$  commutes with all generators  $T^a$  and we can conclude

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<sup>2</sup>We do not discuss here the additional  $U(1)_V \times U(1)_A$  symmetry which leads to baryon number conservation and to the famous Wess-Zumino-Witten anomaly.



from (1.10) that  $\partial^\mu V_\mu^a = 0$ . This means that for degenerate quark masses the  $SU(N_f)$  vector symmetry remains unbroken. According to Noether's theorem this generates a conserved symmetry charge, the vector charge

$$Q^a(t) = \int V_0^a(x) d^3x \quad \text{with} \quad \frac{dQ^a}{dt} = 0. \quad (1.11)$$

It satisfies an  $SU(N_f)$  charge algebra

$$[Q^a(t), Q^b(t)] = if^{abc} Q^c(t) \quad (1.12)$$

that allows us to organize the hadronic spectrum according to irreducible representations of  $SU(N_f)$ .

As mentioned in the previous section, the assumption of mass degeneracy is definitely not fulfilled. As an approximate symmetry, though, it makes sense for the light quarks. Compared with the QCD energy scale  $\Lambda_{\text{QCD}} \sim 1 \text{ GeV}$ , the masses of the up and down quarks are very small. Their mass difference, therefore, can be neglected in many calculations. As a consequence, the masses of particles in a distinct multiplet involving only  $u$  and  $d$  quarks like for example the pions or the nucleons are nearly degenerate. In the present work, we perform the calculations for  $N_f = 2$  in the limit where indeed  $m_u = m_d$  holds, i.e. we assume *isospin symmetry*.

Let us now come back to the massless case where  $\partial^\mu V_\mu^a = \partial^\mu A_\mu^a = 0$ . While the corresponding vector charges  $Q^a$  itself form a closed algebra, this is not the case for the axial charges  $Q^{5a}(t) = \int A_0^a(x) d^3x$  whose commutation relations are not independent from the vector charges:

$$[Q^a(t), Q^{5b}(t)] = if^{abc} Q^{5c}(t), \quad (1.13)$$

$$[Q^{5a}(t), Q^{5b}(t)] = if^{abc} Q^c(t). \quad (1.14)$$

Defining a left-handed and a right-handed charge

$$Q_L^a = \frac{1}{2}(Q^a + Q^{5a}) \quad \text{and} \quad Q_R^a = \frac{1}{2}(Q^a - Q^{5a}) \quad (1.15)$$

allows us to rewrite the commutation relations (1.12), (1.13) and (1.14) such that  $Q_L^a$  and  $Q_R^a$  separately fulfill the closure condition:

$$[Q_L^a(t), Q_L^b(t)] = if^{abc} Q_L^c(t), \quad (1.16)$$

$$[Q_R^a(t), Q_R^b(t)] = if^{abc} Q_R^c(t), \quad (1.17)$$

$$[Q_L^a(t), Q_R^b(t)] = 0. \quad (1.18)$$

These commutation relations are called *chiral algebra* and its symmetry charges generate the *chiral symmetry*  $SU(N_f)_L \times SU(N_f)_R$  in which both

$SU(N_f)_L$  and  $SU(N_f)_R$  are independent from each other. On the level of the symmetry currents, one defines correspondingly a left-handed current  $\mathcal{J}_{\mu L}^a$  and a right-handed current  $\mathcal{J}_{\mu R}^a$  as linear independent combinations of the vector and axial currents:

$$\mathcal{J}_{\mu L}^a = \frac{1}{2}(V_\mu^a + A_\mu^a) = \bar{\psi}\gamma_\mu \frac{1 + \gamma_5}{2} T^a \psi \quad (1.19)$$

$$\mathcal{J}_{\mu R}^a = \frac{1}{2}(V_\mu^a - A_\mu^a) = \bar{\psi}\gamma_\mu \frac{1 - \gamma_5}{2} T^a \psi \quad (1.20)$$

Taking the four-divergence of the left- and right-handed current and imposing (1.10) we see again, as expected, that for  $\hat{M} = 0$  both currents are conserved, i.e.  $\partial^\mu \mathcal{J}_{\mu L}^a = \partial^\mu \mathcal{J}_{\mu R}^a = 0$ . Equations (1.19) and (1.20) are a good starting point to get a deeper understanding of chirality. The operators

$$P_L = \frac{1 + \gamma_5}{2} \quad \text{and} \quad P_R = \frac{1 - \gamma_5}{2} \quad (1.21)$$

hold the property of being projection operators with  $P_L + P_R = 1$  and  $P_L P_L = P_L$  resp.  $P_R P_R = P_R$ . With some simple algebra, therefore, we can write the left-handed and the right-handed current (1.19) and (1.20) as

$$\mathcal{J}_{\mu L}^a = \bar{\psi}_L \gamma_\mu T^a \psi_L, \quad (1.22)$$

$$\mathcal{J}_{\mu R}^a = \bar{\psi}_R \gamma_\mu T^a \psi_R. \quad (1.23)$$

Each current consists at any time only of independent left-handed or right-handed spinors. This justifies the name chiral  $SU(N_f)_L \times SU(N_f)_R$  symmetry.<sup>3</sup>

If chiral symmetry was realized in nature as an exact symmetry, we would expect a chiral partner of degenerate mass and opposite parity for each observed particle. To every pseudoscalar meson like a pion, for instance, one would expect to find also a scalar counterpart. Since chiral symmetry is, though, explicitly broken by the mass term, we expect the spectrum of the two multiplets to differ only due to the strength of the explicit symmetry breaking term. In nature, however, we do not observe the appropriate scalar mesons. The same statement holds in the barionic sector where the multiplets of positive parity do not have a corresponding counterpart of negative parity.

One can explain this fact if one assumes that the global chiral symmetry is spontaneously broken down to a  $SU(N_f)$  vector symmetry. According to

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<sup>3</sup>The word ‘‘chiral’’ stems from ancient Greek  $\eta \chi\epsilon\iota\rho = \text{hand}$ . The left hand and the right hand cannot be translated or rotated into each other. Analogously, the chiral  $SU(N)_L \times SU(N)_R$  transformation means independent symmetry properties between left-handed and right-handed spinors.

the Nambu-Goldstone theorem every broken symmetry generator produces one massless spin zero particle, a Goldstone boson. As chiral symmetry is also explicitly broken, the Goldstone bosons are not exactly massless, but acquire a small mass.

This scenario fits perfectly into the phenomenological picture: The pions are very much lighter than the  $1^-$  vector mesons, the rho mesons. The same holds for the two  $SU(3)$  octets of pseudoscalar mesons and vector mesons, though, to a lesser extent due to the comparatively big mass of the strange quark. This suggests that we can interpret the pseudoscalar mesons as the Nambu Goldstone Bosons of the spontaneously broken chiral symmetry.

The pions as the lightest dynamical degrees of freedom in QCD form the starting point for chiral perturbation theory. The idea is to incorporate all the relevant symmetries of QCD as well as its symmetry breaking pattern in an effective field theory. Then, the pions no longer appear as composite particles but enter the theory as a multiplet of elementary pseudoscalar fields. At low energies, only the pions propagate mediating the dynamics of QCD. All heavy degrees of freedom are integrated out and enter the theory through effective low energy constants. In the pioneering work on chiral perturbation theory from Gasser and Leutwyler [1, 2] the effective theory is constructed in such a way that it leads to the same Ward identities which one encounters in QCD. Hence, the considerations of global symmetry are reproduced correctly at quantum level. However, there is no way of deriving the effective lagrangian from the underlying theory. There are only pure symmetry arguments which dictate the structure of the involved operators. Yet, the low energy constants multiplying these operators must be determined by experiment. Once they are fixed, however, the theory provides us with a useful tool to study low energy QCD. This is the main intention of chiral perturbation theory.

### 1.3 Chiral perturbation theory in the continuum

To explain the main features of chiral perturbation theory we first parameterize the relevant degrees of freedom, i.e. the pions as the Goldstone bosons. Then we explicitly construct the chiral effective lagrangian and finally we investigate the range of applicability of chiral perturbation theory.

We will develop the theory in terms of charge eigenstates  $\pi_i$  as linear combinations of the physical pion fields  $\pi^+$ ,  $\pi^-$  and  $\pi^0$ . With an appropriate

phase convention they are related as

$$\pi_1 = \frac{1}{\sqrt{2}}(\pi^+ + \pi^-), \quad \pi_2 = \frac{i}{\sqrt{2}}(\pi^+ - \pi^-), \quad \pi_3 = \pi^0. \quad (1.24)$$

These fields are collected in a vector  $\vec{\pi} = (\pi_1, \pi_2, \pi_3)$ . In a next step we incorporate the pattern of chiral symmetry breaking. Spontaneous symmetry breaking occurs if the groundstate of a theory is not invariant under a global symmetry which is present in the lagrangian. Let  $G$  be the full symmetry group of the lagrangian and  $H$  be a subgroup of  $G$  which leaves the ground state invariant. The bottom line is that there exists an isomorphic mapping  $\varphi$  between the coset space  $G/H$  and the Goldstone boson fields

$$\vec{\pi} \xrightarrow{g} \varphi(g, \vec{\pi}) \quad (1.25)$$

where  $g \in G$  is a representative of the chiral symmetry [4]. Such a mapping can be written in terms of an SU(2) matrix field

$$\Sigma = \exp(i\vec{\sigma}\vec{\pi}/f) \quad (1.26)$$

where  $\vec{\sigma}$  are the Pauli matrices. Furthermore, we introduced the pion decay constant for dimensional reasons. With this parametrization,  $\Sigma$  transforms bilinearly with respect to chiral transformations  $g$

$$\Sigma \xrightarrow{g} L\Sigma R^\dagger \quad (1.27)$$

where  $L$  and  $R$  are two independent SU(2) matrices [4]. We refer to (1.26) as the exponential parametrization of the pion fields. Note, however, that it does not define a vector space because  $\Sigma(\lambda\vec{\pi}) \neq \lambda\Sigma(\vec{\pi})$ , i.e. in this parametrization, the pion fields transform with a nonlinear representation of the symmetry group  $G$ .

We now embark upon the construction of the effective lagrangian. We will follow mainly the derivation in [12] and, therefore, adapt our notation to the case  $N_f = 3$ .<sup>4</sup> In order to correctly treat the classical symmetries at the quantum level we switch for a moment to the path integral framework to define a generating functional  $W$  of the theory. For this purpose, we slightly modify the QCD lagrangian (1.1). We take the chiral lagrangian with  $\hat{M} = 0$  and add local external sources coupling to distinct currents and densities. The currents in question are the left-handed and the right-handed currents (1.19) and (1.20) as well as the corresponding singlet currents where  $T^a = 1$ . The

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<sup>4</sup>One simply replaces  $\vec{\sigma}\vec{\pi}$  by the SU(3) analogon  $\vec{\lambda}\vec{\pi}$  with the eight Gell-Mann matrices in (1.26)

densities are the scalar densities  $\bar{\psi}\psi$  and  $\bar{\psi}T^a\psi$  as well as the pseudoscalar densities  $\bar{\psi}\gamma_5\psi$  and  $\bar{\psi}\gamma_5T^a\psi$ . Including the sources  $l_\mu(x)$ ,  $r_\mu(x)$ ,  $s(x)$  and  $p(x)$  the lagrangian reads

$$\begin{aligned} \mathcal{L}(l_\mu, r_\mu, s, p) = & -\frac{1}{4}F_a^{\mu\nu}F_{\mu\nu}^a + \bar{\psi}i\not{D}\psi - \bar{\psi}\gamma_\mu\frac{1+\gamma_5}{2}l^\mu\psi - \bar{\psi}\gamma_\mu\frac{1-\gamma_5}{2}r^\mu\psi \\ & -\bar{\psi}_L(s+ip)\psi_R - \bar{\psi}_R(s-ip)\psi_L. \end{aligned} \quad (1.28)$$

The source functions are space-time dependent  $3 \times 3$  matrices given by

$$l_\mu = l_\mu^0 + l_\mu^a T^a, \quad r_\mu = r_\mu^0 + r_\mu^a T^a, \quad s = s^0 + s^a T^a, \quad p = p^0 + p^a T^a \quad (1.29)$$

where  $a = 1, \dots, 8$  and the  $T^a$  are the generators of an SU(3) group in the fundamental representation. Further, we have written the scalar density and the pseudoscalar density as

$$\bar{\psi}\psi = \bar{\psi}_R\psi_L + \bar{\psi}_L\psi_R \quad \text{and} \quad \bar{\psi}\gamma_5\psi = \bar{\psi}_R\psi_L - \bar{\psi}_L\psi_R \quad (1.30)$$

using the projection operators  $P_L$  and  $P_R$  from the previous section. One gets the QCD lagrangian (1.1) by setting  $l_\mu = r_\mu = p = 0$  and  $s = \hat{M}$ . Setting all external sources equal to zero we obtain by construction the QCD lagrangian in the chiral limit. The left handed current (1.19), for instance, is computed by

$$\mathcal{J}_{\mu L}^a = -\frac{\partial \mathcal{L}}{\partial l_\mu^a(x)} = \bar{\psi}(x)\gamma_\mu\frac{1+\gamma_5}{2}T^a\psi(x). \quad (1.31)$$

The external sources, now, allow us to define a generating functional via the path integral as

$$W_{\text{QCD}} = \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D}A_\mu^a e^{i \int d^4x \mathcal{L}_{\text{QCD}}(\psi, \bar{\psi}, A_\mu^a, l_\mu, r_\mu, s, p)}. \quad (1.32)$$

If one knows the generating functional  $W$  of a theory, one can compute any desired matrix element of currents by taking functional derivatives with respect to the corresponding external sources. For example, the vacuum expectation value of the scalar density is computed by

$$\langle 0 | \bar{\psi}(x)\psi(x) | 0 \rangle = i \frac{\delta \ln W}{\delta s^0(x)} \Bigg|_{\substack{s=\hat{M} \\ l_\mu=r_\mu=p_\mu=0}}. \quad (1.33)$$

At a first glance, this approach looks like an increase in complexity. The point, however, is that it allows us to connect QCD with the low energy effective theory by simultaneously considering the effect of the sources in

QCD and in the effective theory. The aim of the low energy expansion is to maintain only the relevant degrees of freedom at the energy of interest, i.e., the Goldstone bosons. Hence, we write down a generating functional  $W_{\text{eff}}$  depending solely on the Goldstone fields and the sources:

$$W_{\text{eff}} = \int \mathcal{D}\Sigma e^{i \int d^4x \mathcal{L}_{\text{eff}}(\Sigma, l_\mu, r_\mu, s, p)}, \quad (1.34)$$

where  $\Sigma$  is the parameterization defined in (1.26). This means that we have to construct  $\mathcal{L}_{\text{eff}}$  in such a way that it reproduces the generating functional of the underlying theory in the low energy limit:

$$\lim_{E \rightarrow 0} W_{\text{QCD}}[l_\mu, r_\mu, s, p] \equiv W_{\text{eff}}[l_\mu, r_\mu, s, p]. \quad (1.35)$$

We only need to make sure that all the symmetries are mapped correctly from  $\mathcal{L}_{\text{QCD}}$  to  $\mathcal{L}_{\text{eff}}$  and that we have precise control over the range of the low energy expansion. The latter is done later by introducing a power counting scheme. The former will be investigated now.

The modified QCD lagrangian (1.28) exhibits an exact *local, chiral*  $SU(3)_L \times SU(3)_R$  invariance if we claim the external fields to transform as gauge fields. (This is the reason for the slightly artificial choice of matrices in (1.29).)

$$\begin{aligned} \psi_L &\rightarrow L(x)\psi_L, & \psi_R &\rightarrow R(x)\psi_R, \\ l_\mu &\rightarrow L(x)l_\mu L^\dagger(x) + i\partial_\mu L(x)L^\dagger(x), \\ r_\mu &\rightarrow R(x)l_\mu R^\dagger(x) + i\partial_\mu R(x)R^\dagger(x), \\ (s + ip) &\rightarrow L(x)(s + ip)R^\dagger(x). \end{aligned} \quad (1.36)$$

$L(x)$  represents the local  $SU(3)_L$  transformations and  $R(x)$  the local  $SU(3)_R$  transformations. In order to preserve these symmetries in the generating functional we construct  $\mathcal{L}_{\text{eff}}$  explicitly with these symmetries. In principle, this means that we extend the mapping (1.25) to a local symmetry  $\vec{\pi} \rightarrow \varphi(g(x), \vec{\pi})$ . In [1], it is shown that a sufficient condition for the Greens functions obtained from an effective lagrangian to obey the Ward identities of QCD is to incorporate the local  $SU(3)_L \times SU(3)_R$  symmetry of the external fields in the effective theory. This is the reason why the correct mapping of the symmetries of the QCD lagrangian to the effective theory also holds at quantum level and, hence, that (1.35) makes sense at all.

We now proceed in complete analogy to the  $SU(3)$  gauge theory of color charge in section 1.1. Since both  $l_\mu$  and  $r_\mu$  enter the theory as gauge fields, we construct a covariant derivative

$$D_\mu \Sigma = \partial_\mu \Sigma + il_\mu \Sigma - i\Sigma r_\mu \quad (1.37)$$

and field strength tensors

$$\begin{aligned} L_{\mu\nu} &= \partial_\mu l_\nu - \partial_\nu l_\mu + i[l_\mu, l_\nu], \\ R_{\mu\nu} &= \partial_\mu r_\nu - \partial_\nu r_\mu + i[r_\mu, r_\nu]. \end{aligned} \quad (1.38)$$

If we transform

$$\Sigma \rightarrow L(x)\Sigma R^\dagger(x), \quad (1.39)$$

then

$$D_\mu \Sigma \rightarrow L(x)D_\mu \Sigma R^\dagger(x), \quad (1.40)$$

and analogously we get for the field strength tensor

$$L_{\mu\nu} \rightarrow L(x)L_{\mu\nu}L^\dagger(x), \quad R_{\mu\nu} \rightarrow R(x)R_{\mu\nu}R^\dagger(x) \quad (1.41)$$

Defining  $\chi = 2B_0(s + ip)$  which transforms according to (1.36) like

$$\chi \rightarrow L(x)\chi R^\dagger(x) \quad (1.42)$$

and  $B_0$  being an appropriate constant of proportionality we have operators with definite transformation properties at hand to construct an effective chirally invariant lagrangian. Simply take  $\Sigma, \Sigma^\dagger, D_\mu \Sigma, D_\mu \Sigma^\dagger, \chi, \chi^\dagger$  and the field strength tensors and construct chirally invariant scalar functions that respect Lorentz invariance as well as parity and charge conjugation. This can neatly be done using traces in flavor space which we will denote with angled brackets. Take for example

$$\langle D_\mu \Sigma D^\mu \Sigma^\dagger \rangle \rightarrow \langle LD_\mu \Sigma R^\dagger R D^\mu \Sigma^\dagger L^\dagger \rangle = \langle D_\mu \Sigma D^\mu \Sigma^\dagger \rangle \quad (1.43)$$

$$\langle \chi \Sigma^\dagger + \Sigma \chi^\dagger \rangle \rightarrow \langle L \chi R^\dagger R \Sigma^\dagger L^\dagger + L \Sigma R^\dagger R \chi^\dagger L^\dagger \rangle = \langle \chi \Sigma^\dagger + \Sigma \chi^\dagger \rangle \quad (1.44)$$

We simply used the unitarity of both  $L$  and  $R$  as well as the cyclic property of traces. In the same way we can construct infinitely many chiral invariant operator functions.

We now investigate the anticipated power counting scheme in order to restrict our considerations to a limited number of operators. Lorentz invariance dictates that operators involving derivatives in Fourier space must always be  $\sim p^2, p^4, p^6, \dots$ . In the expansion every power of momentum counts as one power in energy. As will be justified later,  $\chi \sim E^2$  and, hence, contributes on the same level as  $p^2$ . All operators on this level will be collected in the leading order (LO) lagrangian  $\mathcal{L}_2$ . Correspondingly, we collect terms of order  $E^4$  in the next to leading order (NLO) lagrangian  $\mathcal{L}_4$  and so on. This allows us to write down the structure of the low energy expansion as

$$\mathcal{L}_{\text{eff}} = \mathcal{L}_2 + \mathcal{L}_4 + \mathcal{L}_6 + \dots \quad (1.45)$$

For low energies we consider only a limited number of operators. Let us, therefore, at first, construct the simplest term, the  $\mathcal{L}_2$  term. It reads

$$\mathcal{L}_2 = \frac{f^2}{4} \langle D_\mu \Sigma D^\mu \Sigma^\dagger \rangle + \frac{f^2}{4} \langle \chi \Sigma^\dagger + \Sigma \chi^\dagger \rangle. \quad (1.46)$$

These are all the operators on the  $E^2$  level. Hence, it is the most general  $\mathcal{L}_2$ . Remember that in the exponential representation of the Goldstone fields  $\Sigma$  is always dimensionless and does not contribute with its own power in energy, while  $D_\mu \Sigma \sim E$ . The pion decay constant of the chiral limit  $f$  is introduced such that the dimension of the lagrangian is four. The factor of four in the denominator is conventional.

(1.46) is still chirally invariant. Now, low energy QCD in the absence of sources is recovered setting  $l_\mu = r_\mu = p = 0$  and  $s = \hat{M}$ .

$$\mathcal{L}_2 = \frac{f^2}{4} \langle \partial_\mu \Sigma \partial^\mu \Sigma^\dagger \rangle + \frac{f^2}{4} \langle 2B_0 \hat{M} (\Sigma^\dagger + \Sigma) \rangle \quad (1.47)$$

We now see that we have correctly incorporated the symmetries into our theory: the second term is not chirally invariant any more, as in (1.4) the mass term is responsible for the explicit symmetry breaking. Essentially, what we have done is a so called spurion analysis. One simply promotes the explicitly symmetry breaking term to a spurion which respects the symmetry properties, in our case this is  $\chi$ . Then, one constructs the chiral symmetric lagrangian and finally sets the spurion to its actual physical value which destroys chiral invariance.

The lagrangian (1.47) is now expanded in terms of the pion fields and we can compute any desired correlation function using Feynman diagrams.<sup>5</sup> We will, nevertheless, encounter a serious problem. If we use the  $\mathcal{L}_2$  lagrangian (1.47) to compute a one loop diagram, the result will not be of order  $E^2$  any more but of order  $E^4$ . How loops afflict power counting in general, can be determined with Weinberg's power counting scheme [14]. It states that a diagram containing  $N_L$  loops contributes at a power  $E^{2N_L}$  higher than the tree level diagrams. Hence, using  $\mathcal{L}_2$  to one loop increases the power counting by a factor of  $E^2$  to  $E^4$ .

In the present work, we consider chiral perturbation theory to one loop. This is equivalent to an expansion in energy to order  $E^4$  if we use  $\mathcal{L}_2$  at tree level and to one loop as well as  $\mathcal{L}_4$  at tree level only. Using  $\mathcal{L}_4$  to one loop would correspond to  $E^6$  and it would make sense only if we included  $\mathcal{L}_2$  to two

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<sup>5</sup>Contrary to QCD whose interaction strength increases for low momenta, the interaction between the pions in the effective theory decreases for low energies and vanishes in the chiral limit for zero momentum. This justifies the name chiral perturbation theory.



loops, what would correspond to a two loop calculation. In the continuum such computations have been done [15, 16], however, they are very technical and complicated. For our final purpose to compute lattice corrections, such an enormous effort is not worthwhile.

For a complete one loop computation, we now need  $\mathcal{L}_4$ . Using the same arguments as for the derivation of  $\mathcal{L}_2$  one arrives at the following result [12]:

$$\begin{aligned}
\mathcal{L}_4 = & L_1 \langle D_\mu \Sigma D^\mu \Sigma^\dagger \rangle^2 + L_2 \langle D_\mu \Sigma D_\nu \Sigma^\dagger \rangle \langle D^\mu \Sigma D^\nu \Sigma^\dagger \rangle \\
& + L_3 \langle D_\mu \Sigma D^\mu \Sigma^\dagger D_\nu \Sigma D^\nu \Sigma^\dagger \rangle \\
& + L_4 \langle D_\mu \Sigma D^\mu \Sigma^\dagger \rangle \langle \chi \Sigma^\dagger + \Sigma \chi^\dagger \rangle + L_5 \langle D_\mu \Sigma D^\mu \Sigma^\dagger (\chi \Sigma^\dagger + \Sigma \chi^\dagger) \rangle \\
& + L_6 \langle \chi \Sigma^\dagger + \Sigma \chi^\dagger \rangle^2 + L_7 \langle \chi \Sigma^\dagger - \Sigma \chi^\dagger \rangle^2 + L_8 \langle \chi \Sigma \chi \Sigma + \Sigma \chi^\dagger \Sigma \chi^\dagger \rangle \\
& + iL_9 \langle L_{\mu\nu} D^\mu \Sigma D^\nu \Sigma^\dagger + R_{\mu\nu} D^\mu \Sigma^\dagger D^\nu \Sigma \rangle + L_{10} \langle L_{\mu\nu} \Sigma R^{\mu\nu} \Sigma^\dagger \rangle. \quad (1.48)
\end{aligned}$$

This is the most general lagrangian of order  $E^4$ .<sup>6</sup> In the following, we will set  $L_7 = 0$  since the corresponding operators mutually cancel unless isospin symmetry is explicitly broken (c.f. (A.11) in appendix A). Setting again the sources  $l_\mu = r_\mu = 0$  and  $\chi = \hat{M}$  we arrive at a lagrangian which can be used to compute tree level diagrams.

One problem of our low energy effective theory is that it is not renormalizable. In renormalized perturbation theory divergences can always be cancelled at any order by appropriate counterterms. In a non-renormalizable theory, this is not possible and one needs different counterterms at every higher order one considers. When we constructed  $\mathcal{L}_{\text{eff}}$ , we realized independently of renormalizability that the full low energy expansion contains infinitely many free parameters. We can, however, try to use the free parameters to renormalize the theory up to the order of expansion. The basic idea from Gasser and Leutwyler [1, 2], therefore, was to renormalize the low energy constants  $L_i$  from the NLO lagrangian  $\mathcal{L}_4$  in order to get finite results from one-loop computations with the LO lagrangian  $\mathcal{L}_2$ . What is actually done is that one performs the functional integral (1.32) with  $\mathcal{L}_2$  as lagrangian and an appropriate regularization, extracts the divergences and absorbs them in the Gasser-Leutwyler (GL) constants  $L_i$ .

The method outlined in [12] is based on the background field method whose main idea is to expand the field configuration  $\Sigma$  around the matrix  $\Sigma^*$  which solves the classical equations of motion. One then writes

$$\Sigma = \Sigma^* + \delta\Sigma = \Sigma^* e^{i\Delta} = \Sigma^* + i\Sigma^* \Delta - \frac{1}{2} \Sigma^* \Delta^2 + \dots \quad (1.49)$$

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<sup>6</sup>We do not consider any terms which consist only of pure sources like, for example,  $\langle \chi \chi^\dagger \rangle$  or  $\langle L_{\mu\nu} L^{\mu\nu} \rangle$ .

$\delta\Sigma$  represents the quantum fluctuations which one parametrizes, for instance, with an  $SU(3)$  matrix as  $\exp(\lambda^a \Delta^a)$ . The LO lagrangian is now expanded up to  $\mathcal{O}(\Delta^2)$ . Since  $\Sigma^*$  satisfies the equations of motion, there is no term linear in  $\Delta$  and one is left with an effective quadratic form in  $\Delta$ . In [12] it is further shown that performing the functional integral over  $\Delta$  results in an effective action in  $\Sigma^*$  which, if applied to the computation of matrix elements at tree level, corresponds to a one loop computation of the original action in  $\Sigma$ . Using dimensional regularization we can extract the operators in  $\Sigma^*$  that are multiplied by divergences. The clue is that these operators exhibit precisely the structure of the operators of the NLO lagrangian  $\mathcal{L}_4(\Sigma^*)$  which is used at tree level only, and, therefore, all divergences can be absorbed into the GL coefficients. This means that one renormalizes the whole generating functional to one loop.

If one carries out the rather technical renormalization process, the GL coefficients  $L_i$  are written as

$$L_i = L_i^r - \mu^{-\epsilon} \frac{\gamma_i}{32\pi^2} \left( \frac{2}{d-4} - \gamma + \ln(4\pi) + 1 \right). \quad (1.50)$$

$L_i^r$  denote the renormalized GL coefficients,  $\mu$  is the renormalization scale and  $\gamma = -\Gamma'(1) = 0.577\dots$  is the Euler-Mascheroni constant. One immediately sees that the expression diverges for  $d = 4$ . The  $\gamma_i$  are the renormalization constants and are listed in table 1.1. Note that they are given for the  $SU(2)$  case where we will perform our computation.

With the renormalized GL constants, we need not worry about renormalization any more, as long as we do not leave the one loop level with the lagrangian given above. The application of the method now always works equally:

1. Expand  $\mathcal{L}_2$  in terms of the pion fields to any desired order and compute all tree level and one loop matrix elements of the process
2. Calculate the appropriate tree level matrix elements with  $\mathcal{L}_4$
3. Replace the bare low energy constants with its renormalized counterparts in the sum of all diagrams. The result is finite by construction.

$i$	1	2	3	4	5	6	7	8	9	10
$SU(2) \quad \gamma_i$	$\frac{1}{12}$	$\frac{1}{6}$	0	$\frac{1}{8}$	$\frac{1}{4}$	$\frac{3}{32}$	0	0	$\frac{1}{6}$	$-\frac{1}{6}$

**Table 1.1:** Renormalization coefficients

The last task still undone is to justify that in our power counting scheme  $\chi \sim E^2$  holds indeed. Dimensional analysis in (1.47) dictates the mass dimension of the quantity  $2B_0 \hat{M}$  to be two. To get a physical interpretation of this quantity we expand (1.47) in terms of the pion fields. Since we assume isospin symmetry with  $m_u = m_d = m$ ,  $\chi$  further simplifies to

$$\chi = 2B_0 m \mathbf{1} = M_0^2 \mathbf{1} \quad (1.51)$$

where  $\mathbf{1}$  is the  $2 \times 2$  unit matrix and where we have defined

$$2B_0 m = M_0^2, \quad (1.52)$$

for simplicity of notation. The expansion is now straightforward and reads up to  $\mathcal{O}(\pi^4)$

$$\begin{aligned} \mathcal{L}_2 = & \frac{1}{2} \partial_\mu \vec{\pi} \cdot \partial^\mu \vec{\pi} - \frac{1}{2} M_0^2 \vec{\pi}^2 \\ & + \frac{1}{6f^2} \left( (\vec{\pi} \cdot \partial_\mu \vec{\pi})(\vec{\pi} \cdot \partial^\mu \vec{\pi}) - (\partial_\mu \vec{\pi} \cdot \partial^\mu \vec{\pi}) \vec{\pi}^2 \right) + \frac{1}{4!} \frac{M_0^2}{f^2} \vec{\pi}^4. \end{aligned} \quad (1.53)$$

This looks like a canonically normalized bosonic lagrangian with an interaction part consisting of derivative couplings and pure polynomial couplings. Since pions are bosons, we can indeed interpret the factor  $M_0^2$  in front of the quadratic portion of the fields as the squared tree level mass of the pion. Hence, we can conclude that the linear expansion in the mass of the quarks corresponds to a quadratic expansion in the pion mass, which justifies the assertion that  $\chi \sim E^2$ .

## 1.4 Effective theory with lattice corrections

As already mentioned in the previous section, one needs a distinct regularization to perform the functional integral of the theory in question. Essentially, a regulator introduces a cutoff which makes the ill-defined divergent path integral finite, yet, cutoff dependent. The physical observables, however, cannot depend on the regularization scheme and, therefore, the cutoff finally must be removed. Such a physical input forms the starting point for the Callan-Symanzik equation, one special realization of the renormalization group equations. With these equations, one can determine so-called beta function which describes the dependence of the coupling constant on the renormalization scale. We will not discuss the theory of renormalization here, however, we will use the associated result, that QCD is an asymptotically free theory which means that the coupling constant decreases at higher momenta and finally vanishes for infinite momenta.

In lattice regularization, Euclidean space-time is discretized by a hypercubic lattice with lattice spacing  $a$ . Now, the lattice spacing is the regulator and the cutoff can be interpreted as the momentum proportional to  $\frac{1}{a}$ . Since QCD is an asymptotically free theory, its beta function has a zero fixed point of the coupling constant for infinite momenta. This means that, at least theoretically, the theory has a well defined continuum limit for vanishing lattice spacing. The continuum limit in lattice QCD, however, is still a highly non trivial task. One usually fits the numerical data obtained at different finite lattice spacings and then extrapolates its values to the continuum.

Unfortunately, the number of floating point operations (flops) in today's simulations scales besides the volume and the lattice spacing dependence roughly speaking with the third power of the inverse quark mass [6]. This is the reason why the simulation of light quarks is extremely expensive. Although there lies big hope on new algorithms like the domain wall decomposition hybrid monte carlo algorithm whose quark mass dependence is supposed to scale only linearly with the inverse quark mass [17], simulations are not yet performed at the physical point but with quarks much heavier than in nature. One hopes to get faithful results by a subsequent extrapolation of the data to the physical point.

In a concrete computation one may proceed as follows: one simulates an observable like the scattering length on the lattice for various quark masses and determines the corresponding lattice spacing. Simultaneously, one determines the “physical” value of another reference observable corresponding to this artificial choice of quark masses.<sup>7</sup> One usually chooses an observable which strongly depends on the quark mass, for example the pion mass. In our example, one gets scattering lengths for different pion masses. Then, one can fit the observables (e.g. the scattering length) of different pion masses to an underlying fitting formula and extrapolate them to the physical point of the real world, i.e.  $M_\pi \simeq 135$  MeV.

The validity of such an approach strongly relies on the underlying fitting formulae. This is the point where ChPT enters the game, because, as an expansion in the quark masses, the formulae can be well suited as fitting formulae with the pion masses as variables. For this reason, we will finally express the observable, in our case the scattering lengths, in terms of the physical pion mass. ChPT that we have discussed so far, yet, only holds for the continuum. In order to take into account the lattice artifacts we extend the framework of ChPT to the lattice. First, though, we discuss the main

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<sup>7</sup>The bare quark mass on a lattice is simply a number without direct physical meaning and primarily serves as a free parameter. Each choice, however, corresponds to a distinct realization of observables, for example a pion which is three times larger than in the real world.

ideas of lattice QCD.

In the standard formulation of lattice QCD by Wilson [18] the quark fields  $\psi(x)$  reside on the sites  $x$  of the lattice and carry color, flavor and Dirac indices as in the continuum theory. The gauge fields are associated to the links of the lattice, represented through a field of SU(3) matrices  $U(x, \mu)$  where  $\mu$  indicates the space-time direction of the lattice links. In analogy to the continuum one can now construct a lattice gauge transformation

$$\psi(x) \rightarrow \Omega(x)\psi(x), \quad U(x, \mu) \rightarrow \Omega(x)U(x, \mu)\Omega(x + a\hat{\mu})^{-1} \quad (1.54)$$

where  $\hat{\mu}$  denotes the unit vector in direction  $\mu$ . With this definition the forward difference operator

$$\nabla_{\mu}\psi(x) = \frac{1}{a}[U(x, \mu)\psi(x + a\hat{\mu}) - \psi(x)] \quad (1.55)$$

is gauge covariant. With the appropriate backward difference operator  $\nabla_{\mu}^*$  the lattice Dirac operator is defined as<sup>8</sup>

$$D = \frac{1}{2}\{\gamma_{\mu}(\nabla_{\mu}^* + \nabla_{\mu}) - a\nabla_{\mu}^*\nabla_{\mu}\}. \quad (1.56)$$

The last term in (1.56), referred to as Wilson term, has no analogue to the continuum Dirac operator. It is introduced to remove the fermion doublers adding a  $1/a$  correction to their masses and, thus, making them infinitely heavy in the continuum limit. We can now write down the gauge invariant QCD action on the lattice by

$$S_{\text{lat}} = \frac{1}{g_0^2} \sum_p \text{tr}\{1 - U(p)\} + a^4 \sum_x \bar{\psi}(x)(D + m_0)\psi(x). \quad (1.57)$$

The sum over  $p$  denotes the sum over all oriented plaquettes  $p$  while  $U(p)$  is the product of gauge field variables around  $p$ .  $m_0$  is the bare lattice quark mass. Besides the color gauge symmetry, the Wilson action (1.57) exhibits the discrete symmetries of charge conjugation, parity and time reversal. The O(4) rotational invariance of Euclidean space-time, however, is reduced to the discrete hypercubic group. Analogously, the continuous translational invariance breaks down to the discrete translational symmetry in the lattice spacing. Note that even for  $m_0 = 0$  the theory is not chirally invariant any more due to the Wilson term which explicitly breaks chiral symmetry. We have regard to that by an additive mass renormalization proportional to  $1/a$ :

$$m = Z_m(m_0 - \frac{c}{a}). \quad (1.58)$$

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<sup>8</sup>For simplicity, we have set the Wilson parameter  $r$  equal to one.

$\frac{c}{a} = m_c$  is termed to as the critical mass. It can be defined, for instance, as the value where the pion becomes massless. For the distinct observable “pion mass”, chirality is “restored” in that sense that the pion becomes massless in the chiral limit, just like in the continuum. Note, however, that this procedure does not at all restore chirality in the theory.

In the previous section we discussed ChPT as the low energy effective theory of QCD which is valid only up to a certain energy scale. We now extend the discussion of effective theory to lattice theory. One can consider the momentum cutoff induced by the lattice spacing in a purely mathematical sense as a scale of new physics. Lattice QCD, then, is described as a continuous effective theory where the continuous QCD lagrangian (1.1) simply receives additive corrections through operators of higher dimension. The resulting Symanzik effective action [19] can be considered as an expansion in the lattice spacing

$$S_{\text{eff}} = \int d^4x \{ \mathcal{L}_0 + a\mathcal{L}_1 + a^2\mathcal{L}_2 + \dots \}. \quad (1.59)$$

$\mathcal{L}_0$  is the continuous QCD lagrangian,  $\mathcal{L}_1$  consists of operators of dimension 5 like, for example,  $\bar{\psi}D_\mu D_\mu\psi$ , correspondingly,  $\mathcal{L}_2$  is of mass dimension 6 and so on.<sup>9</sup> The constraint on the  $\mathcal{L}_k$  is simply to respect the symmetries of the lattice action, i.e. one claims gauge invariance and hypercubic symmetry as well as C, P and T invariance.

The effective action (1.59) is well suited to be incorporated into the framework of ChPT. We expect that for small masses and lattice spacings the dominant contribution in  $S_{\text{eff}}$  stems from  $\mathcal{L}_0$ , wherefore the theory will exhibit the same chiral symmetry breaking pattern as in the continuum with pions as Nambu-Goldstone bosons. The idea is to embed the lattice spacing  $a$  in the power counting scheme which so far consisted only of the quark mass  $m$  and the momentum  $p^2$ . Further, the operators of each  $\mathcal{L}_k$  in question must be investigated with respect to their chiral transformation properties. They can then be included via spurion analysis into a *chiral perturbation theory for Wilson fermions* (WChPT). The difference compared to the method outlined in section 1.3 is that besides the mass term, now also the lattice spacing is promoted to a spurion matrix field which guarantees the construction of chirally invariant terms with the appropriate pion fields. After setting the spurion to its original constant value the chiral theory explicitly breaks chiral symmetry like the corresponding Symanzik theory.

In [20] it is shown that up to  $\mathcal{O}(a)$  the effective lagrangian can be written

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<sup>9</sup>The notation must not be confused with the previous section where the leading order lagrangian of ChPT was also called  $\mathcal{L}_2$ .

as

$$\mathcal{L}_{\text{eff}} = \mathcal{L}_{\text{QCD}} + C a \bar{\psi} \sigma_{\mu\nu} F_{\mu\nu} \psi + \mathcal{O}(a^2) \quad (1.60)$$

where  $C$  is a complicated function of the gauge coupling of order unity. Hence, we have QCD with a Pauli term. The chiral symmetry breaking for this term is the same as for the mass term in continuum QCD and we can simply incorporate it into the chiral lagrangian by promoting  $a$  to a spurion  $\hat{\rho}$  and proceed in analogy to the quark mass. The additional term at leading order, for instance, is

$$\mathcal{L}_{\text{LO}}(\hat{\rho}) \sim \langle \hat{\rho} \Sigma^\dagger + \Sigma \hat{\rho}^\dagger \rangle. \quad (1.61)$$

after setting the spurion to its constant value we get

$$\mathcal{L}_{\text{LO}}(\rho) = -\frac{f^2}{4} \rho \langle \Sigma^\dagger + \Sigma \rangle \quad (1.62)$$

where we defined

$$\hat{\rho} = 2W_0 a \mathbf{1} = \rho \mathbf{1}. \quad (1.63)$$

$W_0$  is a constant of proportionality with mass dimension 3 such that the power counting scheme for the lattice spacing is of order  $E^2$  like for  $\chi$  and  $p^2$ . The minus sign in (1.62) is due to Euclidean space-time since from now on, we will perform all our computations in Euclidean space-time. The NLO  $\mathcal{O}(a)$  terms are constructed in [8] and the corresponding  $\mathcal{O}(a^2)$  terms in [9]. With these ingredients we can write down the full chiral effective lagrangian in Euclidean space-time with lattice corrections up to  $\mathcal{O}(a^2)$ . As usual, we divide it into a LO and a NLO contribution. The NLO part is further divided into the portion from continuous ChPT and an additional lattice part such that  $\mathcal{L}_{\text{NLO}} = \mathcal{L}_4 + \mathcal{L}'_4$ . In the notation of [9] these read:

$$\mathcal{L}_2 = \frac{f^2}{4} \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle - \frac{f^2}{4} M_0^2 \langle \Sigma + \Sigma^\dagger \rangle - \frac{f^2}{4} \rho \langle \Sigma + \Sigma^\dagger \rangle \quad (1.64)$$

and at NLO for the continuum

$$\begin{aligned} \mathcal{L}_4 = & -L_1 \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle^2 \\ & -L_2 \langle \partial_\mu \Sigma \partial_\nu \Sigma^\dagger \rangle \langle \partial_\mu \Sigma \partial_\nu \Sigma^\dagger \rangle \\ & -L_3 \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \partial_\nu \Sigma \partial_\nu \Sigma^\dagger \rangle \\ & +L_4 M_0^2 \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle \langle \Sigma + \Sigma^\dagger \rangle \\ & +L_5 M_0^2 \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger (\Sigma + \Sigma^\dagger) \rangle \\ & -L_6 M_0^4 \langle \Sigma + \Sigma^\dagger \rangle^2 \\ & -L_8 M_0^4 \langle \Sigma \Sigma + \Sigma^\dagger \Sigma^\dagger \rangle \end{aligned} \quad (1.65)$$

as well as the lattice part

$$\begin{aligned}
\mathcal{L}'_4 = & W_4 \rho \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle \langle \Sigma + \Sigma^\dagger \rangle \\
& + W_5 \rho \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger (\Sigma + \Sigma^\dagger) \rangle \\
& - W_6 \rho M_0^2 \langle \Sigma + \Sigma^\dagger \rangle^2 \\
& - W_8 \rho M_0^2 \langle \Sigma \Sigma + \Sigma^\dagger \Sigma^\dagger \rangle \\
& - W'_6 \rho^2 \langle \Sigma + \Sigma^\dagger \rangle^2 \\
& - W'_8 \rho^2 \langle \Sigma \Sigma + \Sigma^\dagger \Sigma^\dagger \rangle.
\end{aligned} \tag{1.66}$$

Note that including the lattice spacing modifies the pion mass to

$$M_0^2 = 2B'(m_0 - m_{cr}) \tag{1.67}$$

where the mass renormalization  $Z_m$  was absorbed into  $B'$ . We will have to determine the critical mass later on.

Since we restrict our calculation to chiral SU(2), not all operators of  $\mathcal{L}_{\text{NLO}}$  in (1.65) and (1.66) are linearly independent. In appendix A, we derive relations involving traces of operators. With these formulae one can collect all linear dependent operators and, thus, reduce the number of low energy constants. Using (A.20), (A.21) and (A.10) from appendix A we get the following simplifications:

$$\begin{aligned}
& L_1 \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle^2 + L_3 \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \partial_\nu \Sigma \partial_\nu \Sigma^\dagger \rangle \\
& = (L_1 + \frac{1}{2}L_3) \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle^2,
\end{aligned} \tag{1.68}$$

$$\begin{aligned}
& L_4 M_0^2 \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle \langle \Sigma + \Sigma^\dagger \rangle + L_5 M_0^2 \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger (\Sigma + \Sigma^\dagger) \rangle \\
& = (L_4 + \frac{1}{2}L_5) M_0^2 \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle \langle \Sigma + \Sigma^\dagger \rangle,
\end{aligned} \tag{1.69}$$

$$\begin{aligned}
& L_6 M_0^4 \langle \Sigma + \Sigma^\dagger \rangle^2 + L_8 M_0^4 \langle \Sigma \Sigma + \Sigma^\dagger \Sigma^\dagger \rangle \\
& = (L_6 + \frac{1}{2}L_8) M_0^4 \langle \Sigma + \Sigma^\dagger \rangle^2.
\end{aligned} \tag{1.70}$$

With  $\mathcal{L}'_4$  it works analogously. The definitions

$$\begin{aligned}
L_{13} & := L_1 + \frac{1}{2}L_3, & L_{45} & := L_4 + \frac{1}{2}L_5, & L_{68} & := L_6 + \frac{1}{2}L_8, \\
W_{45} & := W_4 + \frac{1}{2}W_5, & W_{68} & := W_6 + \frac{1}{2}W_8, & W'_{68} & := W'_6 + \frac{1}{2}W'_8,
\end{aligned}$$



now allow us to rewrite (1.65) and (1.66) as

$$\begin{aligned} \mathcal{L}_4 = & -L_{13} \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle^2 - L_2 \langle \partial_\mu \Sigma \partial_\nu \Sigma^\dagger \rangle \langle \partial_\mu \Sigma \partial_\nu \Sigma^\dagger \rangle \\ & + L_{45} M_0^2 \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle \langle \Sigma + \Sigma^\dagger \rangle - L_{68} M_0^4 \langle \Sigma + \Sigma^\dagger \rangle^2 \end{aligned} \quad (1.71)$$

$$\begin{aligned} \mathcal{L}'_4 = & W_{45} \rho \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle \langle \Sigma + \Sigma^\dagger \rangle - W_{68} \rho M_0^2 \langle \Sigma + \Sigma^\dagger \rangle^2 \\ & - W'_{68} \rho^2 \langle \Sigma + \Sigma^\dagger \rangle^2 \end{aligned} \quad (1.72)$$

The  $\mathcal{O}(a)$  lattice artifacts at LO are on the same footing as the tree level pion mass  $M_0^2$  respectively the quark mass  $m$ . In terms of the QCD energy scale  $\Lambda_{\text{QCD}}$  this scenario can be formulated as  $m \sim a\Lambda_{\text{QCD}}^2$ . Therefore, we can organize the power counting in the following schematic way:

$$\begin{aligned} \text{LO :} & \quad p^2, m, a \\ \text{NLO :} & \quad p^4, p^2 m, m^2, p^2 a, ma, a^2 \end{aligned} \quad (1.73)$$

We refer to this scenario as the *generic small quark masses* (GSM) regime [7].

# Chapter 2

## Effective theories with $\mathcal{O}(a^2)$ corrections at leading order

In this chapter, we first investigate some properties of the GSM regime where the quark mass is of the same order of magnitude as the  $\mathcal{O}(a)$  lattice artifacts. Then, we extend the framework to a scenario where higher order lattice artifacts become significant and, therefore, the  $\mathcal{O}(a^2)$  corrections have to be considered at leading order. After some simple tree level computations we construct a lagrangian which can be used for a full one-loop calculation in this scenario.

### 2.1 Rewriting the $\mathcal{O}(a)$ LO lagrangian

In the construction of the potential term in  $\mathcal{L}_2$  we found during the spurion analysis two very similar terms:

$$\langle \hat{\chi} \Sigma^\dagger + \Sigma \hat{\chi}^\dagger \rangle \quad \text{and} \quad \langle \hat{\rho} \Sigma^\dagger + \Sigma \hat{\rho}^\dagger \rangle.$$

Since at leading order only *one* spurion enters the traces, the above two terms are at any time linear both in  $\hat{\chi}$  and in  $\hat{\rho}$ . Adding up the two terms to get the potential term preserves linearity too and, hence,  $\hat{\chi}$  and  $\hat{\rho}$  are linearly related at leading order. This allows us to define a new variable  $\hat{\chi}'$

$$\hat{\chi}' = \hat{\chi} + \hat{\rho} \tag{2.1}$$

which merges  $\hat{\chi}$  and  $\hat{\rho}$  to a new parameter. After setting the spurions to its constant value, we can write the LO lagrangian in terms of a shifted pion mass  $\tilde{M}_0^2$

$$\mathcal{L}_2(\tilde{M}_0^2) = \frac{f^2}{4} \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle - \frac{f^2}{4} \tilde{M}_0^2 \langle \Sigma + \Sigma^\dagger \rangle. \tag{2.2}$$

with

$$\tilde{M}_0^2 = M_0^2 + \rho = M_0^2 + 2W_0a, \quad (2.3)$$

or, in terms of a shifted quark mass

$$\tilde{M}_0^2 = 2B' \left( m_0 + \frac{c}{a} \right) + 2W_0a =: 2Bm \quad (2.4)$$

where we have absorbed the linear  $a$  dependence by a redefinition of the quark mass. Expanding  $\mathcal{L}_2(\tilde{M}_0^2)$  in terms of the pion fields leads to

$$\begin{aligned} \mathcal{L}_2 = & \frac{1}{2} \partial_\mu \vec{\pi} \cdot \partial_\mu \vec{\pi} + \frac{1}{2} \tilde{M}_0^2 \vec{\pi}^2 \\ & + \frac{1}{6f^2} \left( (\vec{\pi} \cdot \partial_\mu \vec{\pi})(\vec{\pi} \cdot \partial_\mu \vec{\pi}) - (\partial_\mu \vec{\pi} \cdot \partial_\mu \vec{\pi}) \vec{\pi}^2 \right) - \frac{1}{24f^2} \tilde{M}_0^2 \vec{\pi}^4. \end{aligned} \quad (2.5)$$

This lagrangian differs from the one in the continuum (1.53) only by means of  $\tilde{M}_0^2$  instead of  $M_0^2$ . (The minus sign in front of the mass term is not a principal difference, it occurs because (2.5) is given in Euclidean space and not in Minkowski space.) Therefore, we can conclude that all the leading order computations involving  $\mathcal{L}_2(\tilde{M}_0^2)$  both at tree level and to one loop work in complete analogy to the ones in the continuum with  $\mathcal{L}_2(M_0^2)$ . One simply has to replace  $M_0^2$  by  $\tilde{M}_0^2$ .

Since now both in the propagator and in the vertices  $\tilde{M}_0^2$  appears instead of  $M_0^2$ , we can reason that the divergences can be cured by the same  $\mathcal{L}_4$  as in continuum chiral perturbation theory with the only difference that we have to replace  $M_0^2$  with  $\tilde{M}_0^2$ . The general structure of  $\mathcal{L}_{\text{NLO}} = \mathcal{L}_4(M_0^2) + \mathcal{L}'_4(M_0^2)$  in (1.71) and (1.72), however, does not involve  $\tilde{M}_0^2$ . Therefore, we have to substitute

$$M_0^2 = \tilde{M}_0^2 - \rho \quad (2.6)$$

in  $\mathcal{L}_4(M_0^2)$  as well as in  $\mathcal{L}'_4(M_0^2)$  to get a structure which only depends on  $\tilde{M}_0^2$ . This new lagrangian can now be written as

$$\tilde{\mathcal{L}}_{\text{NLO}} = \tilde{\mathcal{L}}_4(\tilde{M}_0^2) + (\text{terms} \sim \rho \tilde{M}_0^2 \text{ and } \sim \rho^2)$$

with  $\tilde{\mathcal{L}}_4(\tilde{M}_0^2)$  being the lagrangian (1.71) with  $M_0^2$  replaced by  $\tilde{M}_0^2$ . Performing this substitution we get

$$\begin{aligned} \tilde{\mathcal{L}}_4(\tilde{M}_0^2) = & -L_{13} \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle^2 - L_2 \langle \partial_\mu \Sigma \partial_\nu \Sigma^\dagger \rangle \langle \partial_\mu \Sigma \partial_\nu \Sigma^\dagger \rangle \\ & + L_{45} \tilde{M}_0^2 \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle \langle \Sigma + \Sigma^\dagger \rangle - L_{68} \tilde{M}_0^4 \langle \Sigma + \Sigma^\dagger \rangle^2 \end{aligned} \quad (2.7)$$

$$\begin{aligned} \tilde{\mathcal{L}}'_4(\tilde{M}_0^2) = & \bar{W}_{45} \rho \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle \langle \Sigma + \Sigma^\dagger \rangle - \bar{W}_{68} \rho \tilde{M}_0^2 \langle \Sigma + \Sigma^\dagger \rangle^2 \\ & - \bar{W}'_{68} \rho^2 \langle \Sigma + \Sigma^\dagger \rangle^2 \end{aligned} \quad (2.8)$$

where we have introduced the new low energy constants

$$\overline{W}_{45} := W_{45} - L_{45} \quad (2.9)$$

$$\overline{W}_{68} := W_{68} - 2L_{68} \quad (2.10)$$

$$\overline{W}'_{68} := W'_{68} - W_{68} - L_{68} \quad (2.11)$$

as linear combinations of the old ones. Since, now, our NLO lagrangian depends solely on  $\tilde{M}_0^2$ , we will call it shifted mass NLO lagrangian in the proceeding work. As already mentioned, the divergences stemming from the loop integrals are completely cured with  $\tilde{\mathcal{L}}_4(\tilde{M}_0^2)$  in (2.7). Hence, the new low energy constants  $\overline{W}_{45}$ ,  $\overline{W}_{68}$  and  $\overline{W}'_{68}$  are finite and do not get renormalized. If one performs a one loop computation without the above quadratic completion of the NLO lagrangian, one can determine the renormalization coefficients for  $W_{45}$ ,  $W_{68}$  and  $W'_{68}$ . Plugging  $W_{45}$ ,  $W_{68}$  and  $W'_{68}$  with their divergent part into the above definitions of the new low energy constants, one sees indeed that  $\overline{W}_{45}$ ,  $\overline{W}_{68}$  and  $\overline{W}'_{68}$  are finite. The procedure is straightforward but lengthy and, therefore, is not shown here.

This naive quadratic completion works, because  $\mathcal{L}_{\text{NLO}}$  in (1.71) and (1.72) is really the most general lagrangian which includes all possible contributions up to order  $E^4$ . Therefore, throughout the substitution procedure no new structures which were not already part of  $\mathcal{L}_{\text{NLO}}$  could appear. In the next section when we promote the  $\rho^2$  term from NLO to LO, however, we will see that this approach fails, because then the remaining lagrangian is not the most general one any more. We will solve this problem by constructing additional counterterms corresponding to contributions from the  $\mathcal{L}_6$ .

Note that rewriting the lagrangian in terms of the shifted mass  $\tilde{M}_0^2$  does *not* mean the we leave the GSM regime defined in section 1.4 although the lattice spacing does not explicitly appear in the power counting scheme at leading order:

$$\begin{aligned} \text{LO} : & \quad p^2, m \\ \text{NLO} : & \quad p^4, p^2m, m^2, p^2a, ma, a^2 \end{aligned} \quad (2.12)$$

From now on, when we talk about the GSM regime, we always think of the quark mass  $m$  as the corresponding linearly shifted quark mass in the lattice spacing.

## 2.2 Promotion of the $\mathcal{O}(a^2)$ term from NLO to LO

We now discuss the scenario where higher order cutoff effects become significant. Physically, this means that the quark mass is not any more of  $\mathcal{O}(a)$

like in the GSM regime, but at least of  $\mathcal{O}(a^2)$ . In terms of the QCD energy scale, we write this as  $m \sim a^2 \Lambda_{\text{QCD}}^3$ . This regime is called *large cutoff effects* (LCE) contrary to the GSM regime from section 1.4. We accomodate this fact by promoting the NLO  $\mathcal{O}(a^2)$  term to a LO term. The term in question in (2.8) is

$$\mathcal{L}_{\rho^2} = -\rho^2 \overline{W}'_{68} \langle \Sigma + \Sigma^\dagger \rangle^2. \quad (2.13)$$

Promoting this term to leading order,  $\mathcal{L}_{\text{LO}}$  reads

$$\mathcal{L}_{\text{LO}} = \frac{f^2}{4} \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle - \frac{f^2}{4} \tilde{M}_0^2 \langle \Sigma + \Sigma^\dagger \rangle - \rho^2 \overline{W}'_{68} \langle \Sigma + \Sigma^\dagger \rangle^2. \quad (2.14)$$

In the following discussion we refer to the last two terms in (2.14) as the potential term  $\mathcal{L}_{\text{pot}}$  since it does not include any derivatives mediating a kinetic part. Now, we immediately see the difference to our initial approach where we only introduced the  $\mathcal{O}(a)$  correction. There, the continuum part and the lattice part had exactly the same operator structure, i.e. they had the same basis in the LO lagrangian and, therefore, could be merged with a new effective parameter  $\tilde{M}_0^2$ . Now, this approach fails, because  $\langle \Sigma + \Sigma^\dagger \rangle$  and  $\langle \Sigma + \Sigma^\dagger \rangle^2$  do not exhibit the same structure. After expanding the traces up to the fourth power in the pion fields

$$\langle \Sigma + \Sigma^\dagger \rangle = 4 - \frac{2}{f^2} \vec{\pi}^2 + \frac{1}{6f^4} \vec{\pi}^4 \quad (2.15)$$

$$\langle \Sigma + \Sigma^\dagger \rangle^2 = 16 - \frac{16}{f^2} \vec{\pi}^2 + \frac{16}{3f^4} \vec{\pi}^4 \quad (2.16)$$

and dropping the constant terms,  $\mathcal{L}_{\text{pot}}$  in eq. (2.14) can now be written in terms of the pion fields:

$$\begin{aligned} \mathcal{L}_{\text{pot}} &= -\frac{f^2}{4} \tilde{M}_0^2 \langle \Sigma + \Sigma^\dagger \rangle - \rho^2 \overline{W}'_{68} \langle \Sigma + \Sigma^\dagger \rangle^2 \\ &= \frac{1}{2} \tilde{M}_0^2 \vec{\pi}^2 - \frac{1}{4!} \frac{\tilde{M}_0^2}{f^2} \vec{\pi}^4 + 16 \frac{\rho^2}{f^2} \overline{W}'_{68} \vec{\pi}^2 - \frac{16}{3} \frac{\rho^2}{f^4} \overline{W}'_{68} \vec{\pi}^4. \end{aligned} \quad (2.17)$$

Remembering from our definition (1.63) that  $\rho = 2W_0 a$  we introduce the following short hand notation for the various prefactors of the  $\rho^2$  terms:

$$16 \frac{\rho^2}{f^2} \overline{W}'_{68} = 64 \overline{W}'_{68} \frac{W_0^2}{f^2} a^2 = -c_2 a^2. \quad (2.18)$$

This definition of  $c_2$  is chosen in order to match with the one given in [21] and allows us to write

$$\mathcal{L}_{\text{pot}} = \frac{1}{2} (\tilde{M}_0^2 - 2c_2 a^2) \vec{\pi}^2 - \frac{1}{4! f^2} (\tilde{M}_0^2 - 4 \cdot 2c_2 a^2) \vec{\pi}^4 \quad (2.19)$$

where  $c_2 a^2$  has the dimension of a squared mass. It is now self-evident to define a new mass  $\mathcal{M}^2$  as the factor which multiplies the quadratic portion of the potential:

$$\mathcal{M}^2 = \tilde{M}_0^2 - 2c_2 a^2 = 2Bm - 2c_2 a^2 \quad (2.20)$$

Equipped with this new  $\mathcal{M}^2$  we can write

$$\mathcal{L}_{\text{pot}}(\mathcal{M}^2) = \frac{1}{2} \mathcal{M}^2 \vec{\pi}^2 - \frac{1}{4!} \frac{\mathcal{M}^2}{f^2} \vec{\pi}^4 + \frac{3}{4!} \frac{2c_2 a^2}{f^2} \vec{\pi}^4. \quad (2.21)$$

We see in eqs. (2.15) and (2.16) that the pion fields of the same power are weighted with different numerical factors. If we had solely considered the quadratic mass term, we would not have run into troubles, because whatever constant we find in front, it can be absorbed in the new mass. However, when we also consider the  $\vec{\pi}^4$  terms, the factors will “differ differently” from the ones in the quadratic portion. Having already defined  $\mathcal{M}^2$  we would not succeed in contracting the interaction into one single term. In general there remains an additional new interaction term. In our case it is proportional to  $a^2$  and reads

$$\mathcal{L}_{a^2} = \frac{3}{4!} \frac{2c_2 a^2}{f^2} \vec{\pi}^4. \quad (2.22)$$

It has of course its own vertices and produces loop corrections which will, for example, give an additional mass shift in the pion mass  $M_\pi^2$ . Compared to the original lagrangian (2.5) the new leading order lagrangian differs with respect to the mass and this additional interaction term. The fully expanded leading order lagrangian therefore is given by

$$\begin{aligned} \mathcal{L}_{\text{LO}} = & \frac{1}{2} \partial_\mu \vec{\pi} \cdot \partial^\mu \vec{\pi} + \frac{1}{2} \mathcal{M}^2 \vec{\pi}^2 + \frac{1}{6f^2} (\vec{\pi} \cdot \partial_\mu \vec{\pi})(\vec{\pi} \cdot \partial^\mu \vec{\pi}) \\ & - \frac{1}{6f^2} (\partial_\mu \vec{\pi} \cdot \partial^\mu \vec{\pi}) \vec{\pi}^2 - \frac{1}{4!} \frac{\mathcal{M}^2}{f^2} \vec{\pi}^4 + \frac{3}{4!} \frac{2c_2 a^2}{f^2} \vec{\pi}^4. \end{aligned} \quad (2.23)$$

Besides the first two terms which correspond to free theory, we have four interaction terms which all give rise to a distinct interaction vertex. Setting  $a = 0$  and substituting  $\mathcal{M}^2$  with  $M_0^2$  reproduces the lagrangian in the continuum. We therefore expect that computations with (2.23) will reproduce the results from the continuum when we set  $a = 0$  in the calculated observable. Later, we will use this feature to check our results.

## 2.3 Significance of $c_2$

The interesting concern about  $c_2$  is that its sign determines a phase diagram where for certain values of the quark masses parity and flavour symmetry

are spontaneously broken [7]. Let us repeat here the main arguments leading to this conclusion. To determine the condensate  $\langle \Sigma_0 \rangle$  of the theory (i.e. the vacuum expectation value) we do not need to consider the kinetic term in (2.14) and focus solely on the potential

$$\mathcal{L}_{\text{pot}} = -2Bm \frac{f^2}{4} \langle \Sigma + \Sigma^\dagger \rangle + c_2 \frac{f^2 a^2}{16} \langle \Sigma + \Sigma^\dagger \rangle^2 \quad (2.24)$$

that is to be minimized. So far, we assumed that after spontaneous breaking of chiral symmetry no further symmetries are spontaneously broken. This means that the (arbitrarily chosen) ground state is still SU(2) invariant. We express this by writing  $\Sigma = \mathbf{1} e^{\frac{i}{f} \vec{\pi} \vec{\sigma}}$  where, by construction, the  $\mathbf{1}$  corresponds to a symmetric vacuum.<sup>1</sup> More generally, if we allow for a further spontaneous symmetry breaking of SU(2), we are supposed to write

$$\Sigma = \Sigma_0 e^{\frac{i}{f} \vec{\pi} \vec{\sigma}} = A(x) + i \vec{B}(x) \vec{\sigma}, \quad (2.25)$$

where  $\Sigma_0 = A_0 + i \vec{B}_0 \vec{\sigma}$  is a space-time independent SU(2) matrix corresponding to a ground state which is not invariant under SU(2) rotations. In addition, we used the result from appendix A which allows us to parametrize any SU(2) matrix in terms of four real parameters  $A$  and  $\vec{B}$  satisfying  $A^2 + \vec{B}^2 = 1$ , the unit matrix and the Pauli matrices. Plugging (2.25) into the potential leads to a quadratic function in  $A$

$$\mathcal{L}_{\text{pot}} = -2Bm f^2 A + c_2 f^2 a^2 A^2. \quad (2.26)$$

Due to the SU(2) constraint  $A^2 + \vec{B}^2 = 1$ ,  $A$  is forced to lie between  $-1$  and  $+1$  inclusive. The crucial point now is that the action of an SU(2) vector transformation on  $\Sigma$  leaves  $A$  invariant but rotates  $\vec{B}$  by an orthogonal transformation. Applying this statement on  $\Sigma_0$  we see that the vacuum is invariant with respect to SU(2) vector transformations only if  $\vec{B}_0$  vanishes. In case of a non-zero  $\vec{B}_0$ , the vacuum is not invariant any more and the SU(2) flavor symmetry breaks spontaneously down to a U(1) subgroup. To parametrize symmetry breaking, we simply have to determine the phase where the minimum of the potential lies within the interval  $(-1, +1)$  exclusively. Only in this case  $\vec{B}_0$  can achieve a non-zero value.

The extremum of the potential is found to be at  $A_{\text{ex}} = \frac{Bm}{c_2 a^2}$ . For positive values of  $c_2$  this is a minimum. If  $|A_{\text{min}}| > 1$ , then  $A_0$  is constrained to lie on the edge of the interval  $[-1, +1]$  which corresponds to  $\Sigma_0 = \pm \mathbf{1}$ . Then, the

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<sup>1</sup>Very loosely speaking the vacuum corresponds to the origin in flavor space, i.e. to  $\vec{\pi} = 0$ . In the exponential parametrization this is the unit matrix which is invariant under SU(2) rotations of the form  $R \mathbf{1} R^\dagger = \mathbf{1}$ .

symmetry is not spontaneously broken. For  $|A_{\min}| < 1$ , however,  $A_{\min} = A_0$  and spontaneous symmetry breaking occurs. Thus, for positive values of  $c_2$  the variation of the quark mass  $m$  smoothly interpolates the vacuum between two flavor symmetric values. This is precisely a second order phase transition and the phase of broken symmetry is called Aoki phase [22]. The pion masses are straightforwardly determined by expanding  $\Sigma$  in (2.25) around the vacuum. The result is that within the Aoki phase the charged pions become massless and, hence, the Nambu Goldstone Bosons of broken symmetry. The critical point for this transition is at  $2Bm = 2c_2a^2$ . Outside the Aoki phase the pion mass reads  $\mathcal{M}^2 = 2Bm - 2c_2a^2$ , as expected.

Let us now return to the case where  $c_2 < 0$ . In this case the extremum of the potential is a maximum and the necessary minimum for the condensate is forced to lie on the edge of the interval  $[-1, +1]$ . For  $2Bm > 0$  we have  $\Sigma_0 = +1$  respectively the other way round  $\Sigma_0 = -1$  for  $2Bm < 0$ . Hence, there is no  $\vec{B}_0$  in the vacuum and the symmetry remains unbroken. Varying the quark mass the vacuum “jumps” from  $\Sigma_0 = +1$  to  $\Sigma_0 = -1$  at the critical point  $2Bm = 0$ . Therefore, this scenario corresponds to a first order phase transition. The expansion around the vacuum determines again the pion masses. Due to the unbroken symmetry they acquire all the same mass with a minimum for  $2Bm = 0$  that reads

$$\mathcal{M}_{\min}^2 = 2|c_2|a^2. \quad (2.27)$$

Sign and magnitude of  $c_2$  are not yet satisfactorily determined. The ETM collaboration [23] gave a rough estimate for  $c_2$  where within errors  $c_2$  would be negative. However, the statistical uncertainties were rather large. In the present work, we will, therefore, suggest an alternative method to determine the sign of  $c_2$  using pion scattering. The detailed idea will be described in section 2.6. First, however, we have to learn some general aspects about scattering theory.

## 2.4 Scattering theory

**Kinematics:** The most general collision of two particles A and B with mass  $m_A$  and  $m_B$  is of the form

$$A + B \longrightarrow C + D + F + \dots$$

The intention of our analysis, however, is low energy  $\pi\pi$ -scattering, hence we are in the elastic region where the above reaction reads  $A + B \rightarrow A + B$ . Far



away from the scattering process the particles are considered as free particles with on shell conditions

$$p_A^2 = m_A^2, p_B^2 = m_B^2, p_A'^2 = m_A^2, p_B'^2 = m_B^2. \quad (2.28)$$

$p_A$  and  $p_B$  are the particles four-momenta before the collision,  $p_A'$  and  $p_B'$  correspondingly afterwards. Since the total four-momentum is conserved in the collision, we get an additional constraint

$$p_A + p_B + p_A' + p_B' = 0. \quad (2.29)$$

With  $p_A, p_B, p_A'$  and  $p_B'$  ten different Lorentz invariant scalar products can be built. Four of them are already contained in the energy-momentum relations in (2.28). Conservation of the total four-momentum in (2.29) imposes another four constraints. Therefore, the number of independent variables is only two. The common choice of variables are the Mandelstam variables,

$$\begin{aligned} s &= (p_A + p_B)^2 = (p_A' + p_B')^2, \\ t &= (p_A + p_A')^2 = (p_B + p_B')^2, \\ u &= (p_A + p_B')^2 = (p_A' + p_B)^2. \end{aligned} \quad (2.30)$$

The fact that there are only two independent variables is expressed by the relation

$$s + t + u = \sum_{i=1}^4 m_i^2 \quad (2.31)$$

with the particles masses  $m_i$ . It can be derived using (2.28) and (2.29). Our calculations will be performed in the center of mass system. This is the system with vanishing total three-momentum, i.e.

$$\mathbf{p}_A^{\text{c.m.}} = -\mathbf{p}_B^{\text{c.m.}}, \quad \mathbf{p}'_A{}^{\text{c.m.}} = -\mathbf{p}'_B{}^{\text{c.m.}}. \quad (2.32)$$

Since the total three-momentum is zero, only the zeroth component of  $p_A^{\text{c.m.}} + p_B^{\text{c.m.}}$  is nonvanishing. Yet, this component is the energy. Hence, we can conclude that the Lorentz invariant Mandelstam variable  $s$  is the total center of mass energy squared. This means  $E^{\text{c.m.}} = \sqrt{s}$ .

With the assumption of isospin symmetry, all pions have equal masses and we can set  $m_A^2 = m_B^2 = M_\pi^2$ . This immediately dictates, that  $E^{\text{c.m.}}$  is equally distributed on the two particles so that

$$E_A^{\text{c.m.}} = E_B^{\text{c.m.}} = \frac{\sqrt{s}}{2} \quad (2.33)$$

The magnitude of the three momentum is found to be

$$|\mathbf{p}_A^{\text{c.m.}}| = |\mathbf{p}_B^{\text{c.m.}}| = \sqrt{E_A^{\text{c.m.}2} - m_A^2} = \frac{1}{2}\sqrt{s - 4M_\pi^2} := q \quad (2.34)$$

Here we have defined  $q$  as the magnitude of three momentum in the center of mass frame. Due to elastic scattering  $q$  is the same for both the incoming and outgoing particles. Therefore, such a process only rotates the direction of the three momentum around a distinct angle  $\theta$ . We can now express  $t$  in terms of  $\theta$  and  $q$ :

$$\begin{aligned} t &= (p_A - p'_A)^2 = 2M_\pi^2 - 2(E_A E'_A - \mathbf{p}_A \cdot \mathbf{p}'_A) \\ &= 2M_\pi^2 - 2\left(\frac{s^2}{4} - q^2 \cos \theta\right) \\ &= -2q^2(1 - \cos \theta) \end{aligned}$$

With  $u$  we can proceed analogously. For convenience, we summarize the result for  $s, t, u$  in terms of the variables  $q$  and  $\theta$ .

$$s = 4(q^2 + M_\pi^2) \quad (2.35)$$

$$t = -2q^2(1 - \cos \theta) \quad (2.36)$$

$$u = -2q^2(1 + \cos \theta) \quad (2.37)$$

We see that we can choose either  $s$  and  $t$  to describe the process ( $s$  and  $u$  would do it as well, of course), or work with  $\cos \theta$  and  $q$ . An experimentalist usually measures momenta of particles and their angular distribution. Although  $\theta$  and  $q$  are variables of the center of mass system, we will finally use them as our “physical variables”. They can then easily be transformed into the lab system. Due to the functional dependence between  $s$  and  $q$  in (2.35) we will sometimes use  $E^{\text{c.m.}}$  and  $\cos \theta$  as a set of independent variables.

**Two particle states:** Our next task is to describe the dynamics of the scattering process. In a scattering experiment, the experimentalist prepares a state with a definite particle content in the far past, the  $|in\rangle$ -state, and measures the particle content in the far future, described by the  $|out\rangle$ -state. The quantum mechanical transition amplitude for such a process, the S-matrix, is the scalar product of these two states

$$S_{if} = \langle out|in\rangle \quad (2.38)$$

where  $i$  stands for “initial” and  $f$  for “final”. To evaluate matrix elements we assume that both in the far past and far future the particles do not interact

any more and can be considered as free. If we collect all the free particles in the far past in  $|i\rangle$  and correspondingly in the far future in  $|f\rangle$ , we can define an operator  $S$  such that

$$S_{if} := \langle f|S|i\rangle. \quad (2.39)$$

The properties of  $S$  like, for example, unitarity are well discussed in [24].

It is convenient to separate the unity operator from  $S$  which corresponds to no interaction. The dynamics of the process, then, is found completely in the matrix elements of the remaining  $\mathcal{T}$ -Operator.

$$S = 1 + i\mathcal{T} \quad (2.40)$$

Since total four-momentum is conserved in the process we can further extract a four-momentum delta function from the matrix elements

$$\begin{aligned} \langle f|S|i\rangle &= \langle f|i\rangle + i\langle f|\mathcal{T}|i\rangle \\ &= \langle f|i\rangle + i\delta(p_f - p_i)T(i \rightarrow f). \end{aligned} \quad (2.41)$$

$T(i \rightarrow f)$  is called the *scattering amplitude*, it is one main object of interest of the present work. From it, one can extract measurable quantities like the cross section for  $\pi\pi$ -scattering. In [25] it is shown that the differential cross section in the center of mass system for spinless particles with identical masses ( $\pi\pi$ -scattering) is

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{c.m.}} = \frac{\pi^2}{4s}|T|^2. \quad (2.42)$$

As will be explained in appendix C cross sections in low energy scattering become constant for short range interactions. The characteristic measure for such a situation is the *scattering length* which can be extracted from the scattering amplitude  $T$ . How this procedure works is discussed in detail in appendix C.

**Scattering amplitude:** From the LSZ formula [26] we know that the scattering amplitude is essentially the amputated four-point Green's function times a wave function renormalization  $\sqrt{Z}$  for each external leg.

$$\begin{aligned} T^{i,j;k,l}(p_1, p_2; p_3, p_4) &= (p_1^2 - M_\pi^2)(p_2^2 - M_\pi^2)(p_3^2 - M_\pi^2)(p_4^2 - M_\pi^2) \\ &\quad \times G_4^{i,j;k,l}(p_1, p_2; p_3, p_4) \\ &= \left(\sqrt{Z_\pi}\right)^4 G_{4\text{amp}}^{i,j;k,l}(p_1, p_2; p_3, p_4). \end{aligned} \quad (2.43)$$

In principle,  $\sqrt{Z}$  is different for each external field. In our computation, however, we may set all factors equal to  $\sqrt{Z_\pi}$  due to the isospin symmetry.

We will directly compute the amputated four point function in a perturbative way using Feynman diagrams.

What can be said about  $T$  even before it is computed? Strong interaction is parity conserving. The pions are pseudoscalar particles with the property

$$\mathcal{P}\pi(x^0, \vec{x}) = -\pi(x^0, -\vec{x}). \quad (2.44)$$

In order to have a parity conserving theory, the pion fields must enter the lagrangian with even powers and one can write  $\mathcal{L} = f[\pi_i\pi_j]$  where  $f$  denotes a not further specified functional dependence. If we further assume isospin symmetry, we can even say  $\mathcal{L} = f[\vec{\pi}^2]$ , because isospin symmetry means that the theory is invariant with respect to rotations in flavor space. When we now compute the four-point Green's function in a diagrammatic way using Wick pairing, the contraction of the fields to any order only gives contributions different from zero if two of the external fields are equal at any time. The most general way of writing such an amplitude is

$$T^{i,j;k,l} = A(s, t, u)\delta^{ij}\delta^{kl} + B(s, t, u)\delta^{ik}\delta^{jl} + C(s, t, u)\delta^{il}\delta^{kj}. \quad (2.45)$$

On the right hand side, we expressed the amplitudes in terms of the Mandelstam variables (2.30).

In a next step, we apply the theorem of crossing symmetry which states that the S-matrix element stays invariant if one replaces an incoming particle with an outgoing antiparticle of opposite momentum [26]. Starting with a reaction

$$\pi^i(p_1) + \pi^j(p_2) \rightarrow \pi^k(p_3) + \pi^l(p_4) \quad (2.46)$$

this translates to another scattering channel

$$\pi^i(p_1) + \bar{\pi}^k(p_3) \rightarrow \bar{\pi}^j(p_2) + \pi^l(p_4). \quad (2.47)$$

The bar over the pion fields denotes the corresponding antiparticle. (We need not reverse the sign of the momenta, because we define all external lines in our diagrams as incoming particles.) Let us briefly summarize the properties of  $\pi_i$  with respect to charge conjugation  $\mathcal{C}$ . With the definition of  $\pi_i$  in (1.24) we can conclude:

$$\mathcal{C}\pi_1 = \pi_1, \quad \mathcal{C}\pi_2 = -\pi_2, \quad \mathcal{C}\pi_3 = \pi_3. \quad (2.48)$$

Hence, the  $\pi_i$  change at most their sign. Yet, since the  $\pi_i$  enter always paired due to isospin symmetry, we can forget about this problem. If we perform the exchange of the fields at the level of the corresponding momenta in the Mandelstam variables (2.30), we see that this is equivalent to exchanging  $s$

and  $t$ . There is another way to get a third scattering channel, namely to exchange  $s$  and  $u$ , and, in terms of flavor, going from configuration  $\{i, j, k, l\}$  to  $\{i, l, k, j\}$ .

These considerations allow us to conclude that the scattering amplitude is determined by one single function  $A(s, t, u)$ , the functions  $B(s, t, u)$  and  $C(s, t, u)$  in (2.45) are simply obtained by changing  $s$  and  $t$  respectively  $s$  and  $u$  in  $A(s, t, u)$ . The general structure of the scattering amplitude, therefore, simplifies to

$$T^{i,j;k,l} = A(s, t, u)\delta^{ij}\delta^{kl} + A(t, s, u)\delta^{ik}\delta^{jl} + A(u, t, s)\delta^{il}\delta^{kj}. \quad (2.49)$$

This formula agrees with the one given in [12].

## 2.5 Feynman rules

The Feynman rules for Euclidean Green's functions are now deduced from the chiral Lagrangian in (2.23). First, the propagator in momentum space is given by

$$\Delta_E(p) = \frac{1}{p^2 + \mathcal{M}^2} \quad (2.50)$$

The four interaction terms involving four pion fields in (2.23) give rise to the following four vertices:

$$\begin{aligned} V_1^{ijkl}[p_1, p_2, p_3, p_4] = & \frac{1}{3f^2} \left[ \delta^{ij}\delta^{kl} (p_1p_3 + p_2p_4 + p_2p_3 + p_1p_4) \right. \\ & + \delta^{ik}\delta^{jl} (p_1p_2 + p_1p_4 + p_2p_3 + p_3p_4) \\ & \left. + \delta^{il}\delta^{jk} (p_1p_2 + p_1p_3 + p_2p_4 + p_3p_4) \right] \quad (2.51) \end{aligned}$$

$$\begin{aligned} V_2^{ijkl}[p_1, p_2, p_3, p_4] = & -\frac{2}{3f^2} \left[ \delta^{ij}\delta^{kl} (p_1p_2 + p_3p_4) \right. \\ & + \delta^{ik}\delta^{jl} (p_1p_3 + p_2p_4) \\ & \left. + \delta^{il}\delta^{jk} (p_1p_4 + p_2p_3) \right] \quad (2.52) \end{aligned}$$

$$V_3^{ijkl}[p_1, p_2, p_3, p_4] = \frac{\mathcal{M}^2}{3f^2} \left[ \delta^{ij}\delta^{kl} + \delta^{ik}\delta^{jl} + \delta^{il}\delta^{jk} \right] \quad (2.53)$$

$$V_4^{ijkl}[p_1, p_2, p_3, p_4] = -\frac{2c_2a^2}{f^2} \left[ \delta^{ij}\delta^{kl} + \delta^{ik}\delta^{jl} + \delta^{il}\delta^{jk} \right]. \quad (2.54)$$

The latin indices denote pion indices and run from 1 to 3. Each vertex exhibits the same structure in terms of the pion fields with  $\delta^{\{ij\}}\delta^{\{kl\}}$ . This is precisely the structure which we anticipated in (2.45), now on the level of the vertices.

## 2.6 The tree level calculation

We will now perform some simple tree level calculations to get a better physical understanding of the new  $\mathcal{O}(a^2)$  leading order lagrangian. The easiest calculation is the pion mass at tree level. The calculation is trivial since the tree level mass is just the mass in the lagrangian

$$M_\pi^2 = \mathcal{M}^2 = 2Bm - 2c_2a^2. \quad (2.55)$$

The leading order transition amplitude and the scattering lengths extracted thereof are more interesting. The amputated Euclidean 4-point function is just the sum of all interaction vertices. Hence, the amplitude  $A$  is given by

$$\begin{aligned} A(p_1, p_2; p_3, p_4) &= G_{4, \text{amp}}^{i,i;k,k}(p_1, p_2; p_3, p_4) \\ &= \frac{1}{3f^2} \left[ + (p_1p_3 + p_2p_4 + p_2p_3 + p_1p_4) - 2(p_1p_2 + p_3p_4) \right. \\ &\quad \left. + \mathcal{M}^2 - 3 \cdot 2 \frac{c_2}{f^2} a^2 \right]. \end{aligned} \quad (2.56)$$

Here, we set  $Z_\pi^2 = 1$ . As we will see in the next chapter, the wave function renormalization is of the form  $Z_\pi^2 = 1 + \mathcal{O}(\mathcal{M}^2)$  and will, therefore, only contribute when we perform the full one loop computation. Wick-rotating back to Minkowski space, using energy conservation  $p_1 + p_2 + p_3 + p_4 = 0$  and going on-shell we get

$$\begin{aligned} A(p_1, p_2; p_3, p_4) &= \frac{1}{3f^2} \left[ - (p_1p_3 + p_2p_4 + p_2p_3 + p_1p_4) \right. \\ &\quad \left. + 2p_1p_2 + 2p_3p_4 + \mathcal{M}^2 - 3 \cdot 2c_2a^2 \right] \\ &= \frac{1}{3f^2} \left[ 6p_1p_2 + 2M_\pi^2 + \mathcal{M}^2 - 3 \cdot 2c_2a^2 \right]. \end{aligned} \quad (2.57)$$

At tree level without further loop corrections we may set  $M_\pi^2 = \mathcal{M}^2$  and the amplitude can be written as

$$A(s, t, u) = \frac{1}{f^2} (s - \mathcal{M}^2 - 2c_2a^2). \quad (2.58)$$

Here, we expressed the scattering amplitude  $A$  in terms of the Mandelstam variables  $s, t, u$ . Comparing our amplitude with the tree level scattering amplitude first obtained by Weinberg [27] one immediately sees that it differs from the continuum by an extra additive constant  $-2c_2a^2/f^2$ . Its significance will become clear at the end of this section when we will have computed the appropriate scattering lengths.

In a next step we have to relate the amplitude  $A(s, t, u)$  to a scattering amplitude  $T^I(s, t, u)$  of definite isospin  $I$ . The corresponding relations are derived in [28] using projection operators and read

$$T^0(s, t, u) = 3A(s, t, u) + A(t, s, u) + A(u, t, s), \quad (2.59)$$

$$T^1(s, t, u) = A(t, s, u) - A(u, t, s), \quad (2.60)$$

$$T^2(s, t, u) = A(t, s, u) + A(u, t, s). \quad (2.61)$$

With the above amplitude (2.58) they read

$$T^0(s, t, u) = \frac{1}{f^2} (2s - \mathcal{M}^2 - 2 \cdot 2c_2a^2), \quad (2.62)$$

$$T^1(s, t, u) = \frac{1}{f^2} (t - u), \quad (2.63)$$

$$T^2(s, t, u) = \frac{1}{f^2} (s - 4\mathcal{M}^2 - 2 \cdot 2c_2a^2). \quad (2.64)$$

We are now ready to compute the tree level scattering length using the method of partial wave decomposition given in appendix C.1. With the normalization of [1] the expansion in terms of Legendre polynomials reads<sup>2</sup>

$$T^I(s, \theta) = 32\pi \sum_{l=0}^{\infty} (2l+1) T_l^I(s) P_l(\cos \theta). \quad (2.65)$$

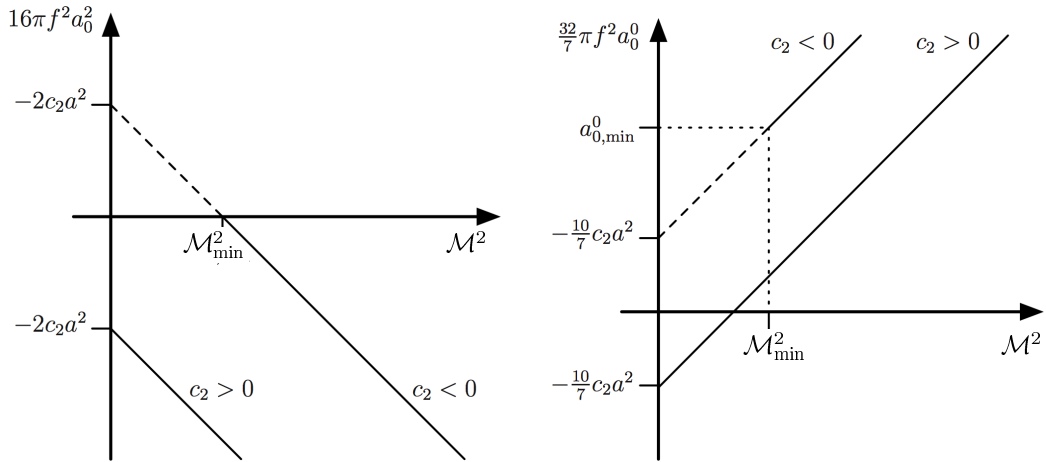
The partial wave amplitudes  $T_l^I$  are found by inverting (2.65) and are given by the integral

$$T_l^I(s) = \frac{1}{64\pi} \int_{-1}^1 d(\cos \theta) P_l(\cos \theta) T^I(s, \cos \theta). \quad (2.66)$$

Expanding the real part of  $T_l^I$  for low momenta we can extract the  $a_0^0, a_0^2$

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<sup>2</sup>The factor of  $32\pi$  is due to the historical normalization used in the book of Martin et al. [29] which has become standard for pion-pion scattering. It can be traced back to a nonrelativistic normalization of the one particle states and a different convention in defining the  $\mathcal{T}$  matrix elements.



**Figure 2.1:** Dependence of the scattering lengths on the pion mass. The dashed lines indicate that one extrapolates to the massless point although it does not exist for  $c_2 < 0$ . The values for both scenarios only differ in the sign, i.e. for  $I = 2$ , the intersection is at  $-2c_2 a^2/16\pi f^2$  for  $c_2 < 0$  and of opposite sign for  $c_2 > 0$ .

and  $a_1^1$  scattering lengths from (C.26):

$$a_0^0 = \frac{7}{32\pi f^2} \left( \mathcal{M}^2 - \frac{5}{7} 2c_2 a^2 \right), \quad (2.67)$$

$$a_1^1 = \frac{1}{24\pi} \frac{\mathcal{M}^2}{f^2}, \quad (2.68)$$

$$a_0^2 = -\frac{1}{16\pi f^2} \left( \mathcal{M}^2 + 2c_2 a^2 \right). \quad (2.69)$$

Setting the lattice spacing equal to zero the continuum tree level result [27] is recovered. However, for finite  $a$ , the scattering lengths  $a_0^0$  and  $a_0^2$  significantly differ by an additive contribution proportional to  $c_2 a^2$ . This is a remarkable result. As a consequence, the scattering lengths do not vanish in the chiral limit, rather, they exhibit a functional dependence on the pion mass<sup>3</sup> of the form

$$a_0^I = A_{00}^I + A_{10}^I M_\pi^2 \quad (2.70)$$

where  $A_{00}^I$  is a constant of  $\mathcal{O}(a^2)$ . As described in detail in section 2.3, the chiral limit is possible only in the scenario where  $c_2 > 0$ . For  $c_2 < 0$ , there is a minimal pion mass and, consequently, also the scattering length will achieve a minimal value. It is obtained by plugging the minimal pion mass (2.27)

<sup>3</sup>We expressed the scattering length in terms of the physical pion mass  $M_\pi^2$  as described in section 1.4. Remember that  $M_\pi^2 = \mathcal{M}^2$  at tree level.



into  $a_0^0$  and  $a_0^2$ :

$$a_{0,\min}^0 = \frac{12}{32\pi f^2} 2|c_2|a^2, \quad a_{0,\min}^2 = 0. \quad (2.71)$$

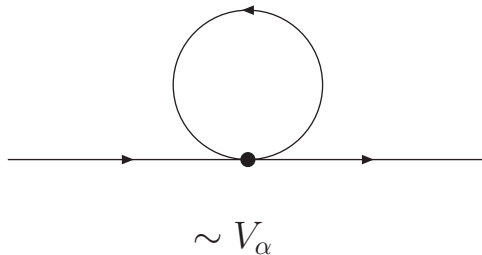
The dependence of the scattering lengths  $a_0^0$  and  $a_0^2$  on the pion mass is shown in figure 2.1, for both scenarios with  $c_2$  positive and negative. This suggests to relate the scattering lengths to  $c_2$  by the following idea: One measures the scattering length at nonzero lattice spacing for different pion masses and then extrapolates the data to the chiral limit. The intersection of the straight line with the axis, i.e. with the massless point, allows one to directly read off the value of  $c_2$ . Hence, we ought to determine which scenario of the phase diagram is actually realized. Note that this procedure works, although the massless point does not exist for  $c_2 < 0$ .

The  $a_1^1$  scattering length does not show any  $c_2 a^2$  dependence and vanishes in the chiral limit. This is because of the minus sign in  $T^1$  which cancels the momentum independent terms present in the scattering amplitude  $A(s, t, u)$ . Therefore, we expect the dependence on lattice artifacts of  $a_1^1$  being comparatively small.

## 2.7 The NLO lagrangian including $\mathcal{O}(a^4)$

With the vertices from section 2.5 we can now perform loop calculations. As we discussed in section 1.3, the NLO lagrangian has to be included too. Yet, by promoting the  $\mathcal{O}(a^2)$  term from NLO to LO we modify the NLO lagrangian and we expect that we must include terms from next to next to leading order (NNLO). In this section, we will now explicitly construct the new counterterms.

Before we determine the counterterms in a systematic way, we will give some hand waving arguments which kind of divergences we will expect and which counterterms we definitely need in order to cancel the infinities. As an example, we consider the pion mass to one loop. The diagram for the one loop two point Green's function is given in figure 2.2. In section 3.1, we will perform the corresponding loop integrals in detail. Anticipating the result we get a singularity proportional to  $\mathcal{M}^2$  for every loop. This is multiplied by  $p^2$ ,  $\mathcal{M}^2$  or  $a^2$  which reflect at any time the content of the corresponding vertices given in section 2.5. Going on shell we end up with two divergent terms: one proportional to  $\mathcal{M}^4$  and the other to  $\mathcal{M}^2 a^2$ . The structure of the  $\mathcal{M}^4$  term is analogous to the continuum where the  $M_0^4$  divergence could be cancelled by the original renormalized NLO lagrangian from Gasser and Leutwyler [1, 2]. Therefore, we expect that it is cancelled with (1.71) if



**Figure 2.2:** One loop two point function.  $V_\alpha$  are the vertices from section 2.5.

we simply replace  $M_0^2$  by  $\mathcal{M}^2$ . The situation, however, is different for the  $\mathcal{M}^2 a^2$  term. Neither in the NLO lagrangian in (1.71) and in (1.72) nor in the shifted mass NLO lagrangian in (2.7) and (2.8) a term of the form  $(\text{mass}^2 \cdot \rho^2)$  appears. This is a first hint that we have to include new structures in our lagrangian. Remembering the definition  $\mathcal{M}^2 = \tilde{M}_0^2 - 2c_2 a^2$  these structures will look like

$$\tilde{M}_0^2 a^2 \quad \text{and} \quad a^4. \quad (2.72)$$

Further, we have to reflect that in  $\tilde{M}_0^2$  a linear  $a$  dependence is hidden. Therefore, we expect the general lagrangian also to depend on a term  $\sim a^3$ .

If we add to the shifted mass lagrangian in (2.7) and (2.8) some new terms in order to get again the most general lagrangian after the promotion of the  $\mathcal{O}(a^2)$  term, we can use the method of quadratic completion outlined in section 2.1. There, we pointed out that it only worked, because the substitution procedure did not create structures which had not already been present before. If we have indeed the most general lagrangian at hand, this cannot happen. Therefore, we simply plug

$$\tilde{M}_0^2 = \mathcal{M}^2 + 2c_2 a^2 \quad (2.73)$$

into this general lagrangian and rewrite it in terms of  $\mathcal{M}^2$  such that the Gasser Leutwyler part (2.7) depends on  $\mathcal{M}^2$  instead of  $\tilde{M}_0^2$ . This will cancel the divergences in analogy to the continuum. The other parts, for example terms proportional to  $\mathcal{M}^2 a^2$ , will be used to cure the new divergences.

The idea for our proceeding now is to construct all the necessary counterterms out of a spurion analysis in complete analogy to the method outlined in sections 1.3 and 1.4. From the beginning on we will use the shifted quark mass. Hence, the spurion field for the mass term is

$$\hat{\chi}' = \hat{\chi} + \hat{\rho} \quad (2.74)$$

and not  $\hat{\chi}$  alone. In order to construct terms  $\sim a^3$  and  $\sim a^4$  we employ again  $\hat{\rho}$  as spurion.

Now, we embark upon the construction of the counterterms. This will be outlined in detail by means of the  $\hat{\chi}'\rho^2$  term. Then, the other ones can be determined analogously. Spurion analysis dictates the following terms:

$$\begin{aligned}
& \langle \hat{\chi}'^\dagger \Sigma + \Sigma^\dagger \hat{\chi}' \rangle \langle \hat{\rho}^\dagger \Sigma + \Sigma^\dagger \hat{\rho} \rangle^2 \rightarrow \tilde{M}_0^2 \rho^2 \langle \Sigma + \Sigma^\dagger \rangle^3 \\
& \langle \hat{\chi}'^\dagger \Sigma \hat{\rho}^\dagger \Sigma \hat{\rho}^\dagger \Sigma + \Sigma^\dagger \hat{\chi}' \Sigma^\dagger \hat{\rho} \Sigma^\dagger \hat{\rho} \rangle \rightarrow \tilde{M}_0^2 \rho^2 \langle \Sigma \Sigma \Sigma + \Sigma^\dagger \Sigma^\dagger \Sigma^\dagger \rangle \\
& \langle \hat{\chi}'^\dagger \Sigma + \Sigma^\dagger \hat{\chi}' \rangle \langle \hat{\rho}^\dagger \Sigma \hat{\rho}^\dagger \Sigma + \Sigma^\dagger \hat{\rho} \Sigma^\dagger \hat{\rho} \rangle \rightarrow \tilde{M}_0^2 \rho^2 \langle \Sigma + \Sigma^\dagger \rangle \langle \Sigma \Sigma + \Sigma^\dagger \Sigma^\dagger \rangle \\
& \langle \hat{\rho}^\dagger \Sigma + \Sigma^\dagger \hat{\rho} \rangle \langle \hat{\chi}'^\dagger \Sigma \hat{\rho}^\dagger \Sigma + \Sigma^\dagger \hat{\chi}' \Sigma^\dagger \hat{\rho} \rangle \rightarrow \tilde{M}_0^2 \rho^2 \langle \Sigma + \Sigma^\dagger \rangle \langle \Sigma \Sigma + \Sigma^\dagger \Sigma^\dagger \rangle \\
& \quad \langle \hat{\rho}^\dagger \hat{\rho} \rangle \langle \hat{\chi}'^\dagger \Sigma + \Sigma^\dagger \hat{\chi}' \rangle \rightarrow \tilde{M}_0^2 \rho^2 2 \langle \Sigma + \Sigma^\dagger \rangle \\
& \quad \langle \hat{\rho}^\dagger \hat{\chi}' + \hat{\chi}'^\dagger \hat{\rho} \rangle \langle \hat{\rho}^\dagger \Sigma + \Sigma^\dagger \hat{\rho} \rangle \rightarrow \tilde{M}_0^2 \rho^2 4 \langle \Sigma + \Sigma^\dagger \rangle \\
& \langle \hat{\chi}'^\dagger \Sigma - \Sigma^\dagger \hat{\chi}' \rangle \langle \hat{\rho}^\dagger \Sigma - \Sigma^\dagger \hat{\rho} \rangle \langle \hat{\rho}^\dagger \Sigma + \Sigma^\dagger \hat{\rho} \rangle \rightarrow \tilde{M}_0^2 \rho^2 \langle \Sigma + \Sigma^\dagger \rangle \langle \Sigma - \Sigma^\dagger \rangle^2 \\
& \quad \langle \hat{\chi}'^\dagger \Sigma + \Sigma^\dagger \hat{\chi}' \rangle \langle \hat{\rho}^\dagger \Sigma - \Sigma^\dagger \hat{\rho} \rangle^2 \rightarrow \tilde{M}_0^2 \rho^2 \langle \Sigma + \Sigma^\dagger \rangle \langle \Sigma - \Sigma^\dagger \rangle^2 \\
& \langle \hat{\chi}'^\dagger \Sigma - \Sigma^\dagger \hat{\chi}' \rangle \langle \hat{\rho}^\dagger \Sigma \hat{\rho}^\dagger \Sigma - \Sigma^\dagger \hat{\rho} \Sigma^\dagger \hat{\rho} \rangle \rightarrow \tilde{M}_0^2 \rho^2 \langle \Sigma - \Sigma^\dagger \rangle \langle \Sigma \Sigma - \Sigma^\dagger \Sigma^\dagger \rangle \\
& \langle \hat{\rho}^\dagger \Sigma - \Sigma^\dagger \hat{\rho} \rangle \langle \hat{\chi}'^\dagger \Sigma \hat{\rho}^\dagger \Sigma - \Sigma^\dagger \hat{\chi}' \Sigma^\dagger \hat{\rho} \rangle \rightarrow \tilde{M}_0^2 \rho^2 \langle \Sigma - \Sigma^\dagger \rangle \langle \Sigma \Sigma - \Sigma^\dagger \Sigma^\dagger \rangle
\end{aligned}$$

On the right hand side, we have set the spurions to their constant value, i.e.  $\hat{\chi}' \rightarrow \tilde{M}_0^2$  and  $\hat{\rho} \rightarrow \rho$ . The last four lines can be dropped, because  $\langle \Sigma - \Sigma^\dagger \rangle = \langle \Sigma \Sigma - \Sigma^\dagger \Sigma^\dagger \rangle = 0$  as shown in appendix A in (A.11) and (A.12). In principle, every term is associated with its own LE constant. With eqs. (A.9) and (A.22) we see, however, that they are not independent from each other and will only occur as a linear combination with fixed coefficients. We finally end up with two independent terms

$$A_1 \frac{\tilde{M}_0^2 \rho^2}{f^2} \langle \Sigma + \Sigma^\dagger \rangle \quad \text{and} \quad A_2 \frac{\tilde{M}_0^2 \rho^2}{f^2} \langle \Sigma + \Sigma^\dagger \rangle^3. \quad (2.75)$$

The factor of  $f^2$  was introduced to keep the  $A_i$  dimensionless. When we expand the traces in terms of pion fields, the fields will be weighted with different numerical factors, depending on whether they stem from the expansion of  $A_1 \langle \Sigma + \Sigma^\dagger \rangle$  or  $A_2 \langle \Sigma + \Sigma^\dagger \rangle^3$ . Yet, the structure of the fields itself is the same: We will always get fields to second and fourth power. We already explicitly determined the factors involved with  $A_1$  in (2.15). Here, however, we are not interested in detailed values. For both  $A_i$  we can write very generally

$$expansion = A_i \frac{\tilde{M}_0^2 \rho^2}{f^2} \left( const + X_{A_i} \frac{\vec{\pi}^2}{f^2} + Y_{A_i} \frac{\vec{\pi}^4}{f^4} \right). \quad (2.76)$$

$X_{A_i}$  and  $Y_{A_i}$  are the undetermined expansion coefficients. After dropping the constant term this allows us to write down the counterterm

$$\begin{aligned}\mathcal{L}_{\tilde{M}_0^2 \rho^2} &= \frac{\tilde{M}_0^2 \rho^2}{f^2} \left( \sum_{i=1}^2 A_i X_{A_i} \frac{\vec{\pi}^2}{f^2} + \sum_{j=1}^2 A_j Y_{A_j} \frac{\vec{\pi}^4}{f^4} \right) \\ &= \frac{\tilde{M}_0^2 \rho^2}{f^2} \left( \tilde{A}_x \frac{\vec{\pi}^2}{f^2} + \tilde{A}_y \frac{\vec{\pi}^4}{f^4} \right).\end{aligned}\quad (2.77)$$

All principally calculable and uninteresting factors have been absorbed into a new LE constant, whose precise value is to be determined by lattice calculations. The renormalization of  $\tilde{A}_x$  will now cancel divergent terms proportional to  $\tilde{M}_0^2 a^2$  stemming from the two point function while  $\tilde{A}_y$  is responsible for the divergences proportional to  $\tilde{M}_0^2 a^2$  from the four point function. This means that we simply add one divergent counterterm of order  $\tilde{M}_0^2 a^2 \cdot \pi^2$  and another one of order  $\tilde{M}_0^2 a^2 \cdot \pi^4$  to our theory. What, if we, for instance, needed an additional six-point vertex? Could we simply add an order  $\pi^6$  counterterm with coefficient  $\tilde{A}_z$ ? Yes, but it would not be independent any more since its coefficient would be a linear combination of  $\tilde{A}_x$  and  $\tilde{A}_y$ . A simple argument can clarify this feature. In our general considerations about the structure of the  $\tilde{M}_0^2 \rho^2$  counterterms we found that the basis consisted of two elements:  $\langle \Sigma + \Sigma^\dagger \rangle$  and  $\langle \Sigma + \Sigma^\dagger \rangle^3$ . Hence, we need exactly two LE constants  $A_1$  and  $A_2$ . Due to the unique linear relation in (2.76) they can be determined from  $\tilde{A}_x$  and  $\tilde{A}_y$  and vice versa. Thus, we will always need two independent quantities as input. All additional constants, then, can be deduced therefrom.

The renormalization program which we apply here is directly fit to our use: Any divergences from two- and four-point functions at one loop are cancelled by appropriate counterterms. The main difference to the method from Gasser and Leutwyler outlined in section 1.3 is that they renormalize the whole generating functional to one loop without specification of a distinct observable. There, one can indeed perform any calculation, no matter which kind of n-point function or observable it involves: Taking the NLO tree level contribution into account one always ends up with a finite result. In principle, one could also perform such a renormalization procedure with (2.14) at leading order. Since we restrict our calculation to the scattering length only, we can fortunately avoid such enormous efforts. The results in the end are the same and much easier obtained.

The  $\rho^4$  case works in complete analogy. Here, we found after a spurion analysis that any  $\rho^4$  term is represented by

$$B_1 \frac{\rho^4}{f^4} \langle \Sigma + \Sigma^\dagger \rangle^2 \quad \text{and} \quad B_2 \frac{\rho^4}{f^4} \langle \Sigma + \Sigma^\dagger \rangle^4 \quad (2.78)$$

which reads in terms of pion fields and redefined LE constants

$$\mathcal{L}_{\rho^4} = \frac{\rho^4}{f^4} \left( \tilde{B}_x \frac{\vec{\pi}^2}{f^2} + \tilde{B}_y \frac{\vec{\pi}^4}{f^4} \right). \quad (2.79)$$

Again, we encounter two low energy constants and the well known structure of pion fields. The same arguments as in the  $\tilde{M}_0^2 a^2$  case announce the independence of the two constants. In the spurion analysis of the  $\rho^4$  term we omitted the chirally invariant term  $\langle \rho^\dagger \rho \rangle \langle \rho^\dagger \rho \rangle$  just as we dropped pure source terms of the form  $\langle \chi^\dagger \chi \rangle$  or  $\langle L_{\mu\nu} L^{\mu\nu} \rangle$  in section 1.3. As long as one does not consider the sources dynamically, they are only constants and have no further influence.

For completeness, we also write down the  $\rho^3$  term. The basis is the same as for the  $\chi' \rho^2$  term and the result is, as expected,

$$\mathcal{L}_{\rho^3} = \frac{\rho^3}{f^2} \left( \tilde{C}_x \frac{\vec{\pi}^2}{f^2} + \tilde{C}_y \frac{\vec{\pi}^4}{f^4} \right). \quad (2.80)$$

The terms  $\sim p^2 a^2$  are, from the point of view of a spurion analysis, a little bit more cumbersome. In the construction of chirally invariant traces we now have to consider  $\partial_\mu \Sigma$  and  $\partial_\mu \Sigma^\dagger$  in addition to  $\Sigma$ ,  $\Sigma^\dagger$ ,  $\rho$  and  $\rho^\dagger$ . The number of chirally invariant combinations is increasing rapidly. Using trace relations again we find the following general structure:

$$D_1 \frac{\rho^2}{f^2} \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle, \quad D_2 \frac{\rho^2}{f^2} \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle \langle \Sigma + \Sigma^\dagger \rangle^2, \quad D_3 \frac{\rho^2}{f^2} \langle \partial_\mu \Sigma + \partial_\mu \Sigma^\dagger \rangle^2. \quad (2.81)$$

The general expansion of these operators in terms of pion fields and newly defined low energy constants reads

$$\mathcal{L}_{p^2 \rho^2} = \frac{\rho^2}{f^2} \left( \tilde{D}_x \frac{1}{f^2} \partial_\mu \vec{\pi} \partial_\mu \vec{\pi} + \tilde{D}_y \frac{1}{f^4} (\vec{\pi} \partial_\mu \vec{\pi})(\vec{\pi} \partial_\mu \vec{\pi}) + \tilde{D}_z \frac{1}{f^4} \vec{\pi}^2 (\partial_\mu \vec{\pi} \partial_\mu \vec{\pi}) \right). \quad (2.82)$$

Now, we have all ingredients at hand to construct the (N)NLO lagrangian. The N in parentheses denotes that elements both from NLO and NNLO are included. Let us summarize once again the elements:  $\mathcal{L}_{(N)\text{NLO}}$  consists of the old  $\tilde{\mathcal{L}}_4(\tilde{M}_0^2)$  from (2.7) and of  $\tilde{\mathcal{L}}'_4(\tilde{M}_0^2)$  from (2.8) without the  $\rho^2$  terms. From now on, we refer to the latter as  $\mathcal{L}_{\tilde{M}_0^2 \rho} + \mathcal{L}_{p^2 \rho}$ . Further, we include all terms which we determined in this section. Finally, we can write:

$$\mathcal{L}_{(N)\text{NLO}} = \tilde{\mathcal{L}}_4(\tilde{M}_0^2) + \mathcal{L}_{p^2 \rho} + \mathcal{L}_{\tilde{M}_0^2 \rho} + \mathcal{L}_{p^2 \rho^2} + \mathcal{L}_{\tilde{M}_0^2 \rho^2} + \mathcal{L}_{\rho^3} + \mathcal{L}_{\rho^4}. \quad (2.83)$$

There is still one remaining point to tackle: As anticipated, we want our lagrangian to depend only on  $\mathcal{M}^2$ , the tree level pion mass which is used in the LO lagrangian for the computation of the loop diagrams. Since our new (N)NLO lagrangian in (2.83) includes all possible terms, the naive quadratic completion mentioned in the beginning of this section should work. Thus, substituting  $\tilde{M}_0^2 = \mathcal{M}^2 + 2c_2a^2$  will not produce any new structure in the power counting scheme. To check this and for later use we write down the concrete result of this procedure although it is a rather lengthy expression.

$$\begin{aligned}
\mathcal{L}_{(\text{N})\text{NLO}} &= \mathcal{L}_4(\mathcal{M}^2) + \mathcal{L}_{p^2\rho} + \mathcal{L}_{\mathcal{M}^2\rho} \\
&+ L_{45} 2c_2a^2 \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle \langle \Sigma + \Sigma^\dagger \rangle && \sim p^2a^2 \\
&- L_{68} 2\mathcal{M}^2 2c_2a^2 \langle \Sigma + \Sigma^\dagger \rangle^2 && \sim \mathcal{M}^2a^2 \\
&- L_{68} 4c_2^2a^4 \langle \Sigma + \Sigma^\dagger \rangle^2 && \sim a^4 \\
&- \bar{W}_{68} \rho 2c_2a^2 \langle \Sigma + \Sigma^\dagger \rangle^2 && \sim a^3 \\
&+ \frac{\mathcal{M}^2\rho^2}{f^2} \left( \tilde{A}_x \frac{\vec{\pi}^2}{f^2} + \tilde{A}_y \frac{\vec{\pi}^4}{f^4} \right) && \sim \mathcal{M}^2a^2 \\
&+ \frac{2c_2a^2}{f^2} \rho^2 \left( \tilde{A}_x \frac{\vec{\pi}^2}{f^2} + \tilde{A}_y \frac{\vec{\pi}^4}{f^4} \right) && \sim a^4 \\
&+ \mathcal{L}_{\rho^3} + \mathcal{L}_{\rho^4} + \mathcal{L}_{p^2\rho^2}.
\end{aligned} \tag{2.84}$$

The first term is the NLO Gasser-Leutwyler lagrangian from continuous chiral perturbation theory, but now with mass  $\mathcal{M}^2$ . The second and third term in the first line give corrections of order  $p^2a$  and  $\mathcal{M}^2a$  corresponding to  $\mathcal{L}_{p^2\rho} + \mathcal{L}_{\tilde{M}_0^2\rho}$  in (2.83). Their LE constants do not contain any infinities as discussed in detail in section 2.1. Then, all further terms which change under the substitution procedure are listed. The column on the right hand side indicates the power counting level at any time. We see that we indeed do not gain any other structures which had not already been part of the lagrangian before the substitution. The terms of the last line remain unchanged. The expansion of the lagrangian in terms of pion fields finally allows one to combine all the terms of the same power counting. We will have to do this when we compute the pion mass.

Finally, we can organize what we have learned in this section in a power counting scheme for the LCE regime:

$$\begin{aligned}
\text{LO} : & \quad p^2, m, a^2 \\
\text{NLO} : & \quad p^2a, ma, a^3 \\
\text{NNLO} : & \quad p^4, p^2m, m^2, p^2a^2, ma^2, a^4
\end{aligned} . \tag{2.85}$$

At NLO, we have collected all the operators, whose LE constants will not get renormalized. At NNLO, all operators which potentially serve to cancel any divergencies are present. Note that NNLO only partially includes operators from the  $\mathcal{L}_6$  given in [15]. We still work to one loop and only adapted the power counting to our special use.

# Chapter 3

## One-loop computation

In the first section of this chapter, the pion mass to one loop in the LCE regime is computed and the differences to the continuum formulae are pointed out. Then, in the second section, we compute the full scattering amplitude to one loop.

### 3.1 The pion mass to one loop

We now embark upon the loop corrections of the pion mass in the LCE regime. For this purpose, we have to calculate the truncated two point Green's function to one loop with the vertices given in section 2.5. The corresponding diagrams were already sketched in the previous section in figure 2.2. Hence, we write down all one loop diagrams leading to the expression

$$G_{2,\text{tr},1\text{-loop}}^{ij}(p, -p) = \frac{1}{2} \int \frac{d^4k}{(2\pi)^4} \frac{1}{(k+p)^2 + \mathcal{M}^2} \sum_{\alpha;r,s} V_{\alpha}^{irjs}[p, p+k, -p, -(p+k)] \quad (3.1)$$

for the truncated 2-point function. This expression factorizes into the loop integral and the vertex sum.  $\alpha$  runs from 1 to 4 and denotes the distinct vertices from section 2.5.  $r$  and  $s$  are flavor indices of internal lines and have to be summed over. Further we have set

$$\begin{aligned} p_1 &= p, & p_3 &= -p, \\ p_2 &= p+k, & p_4 &= -(p+k) \end{aligned} \quad (3.2)$$



which expresses four-momentum conservation at each vertex. For the vertex-sum we find the following result:

$$\sum_{\alpha;r,s} V_{\alpha}^{irjs}[p, p+k, -p, -(p+k)] = \delta^{ij} \frac{1}{3f^2} (4p^2 + 4(p+k)^2 + 5\mathcal{M}^2 - 15 \cdot 2c_2 a^2). \quad (3.3)$$

With this result we can write

$$G_{2,\text{tr}, 1\text{-loop}}^{ij}(p, -p) = \delta^{ij} \frac{1}{6f^2} \left[ (4p^2 + 5\mathcal{M}^2 - 15 \cdot 2c_2 a^2) A_0(\mathcal{M}^2) + 4A_1(\mathcal{M}^2) \right], \quad (3.4)$$

where we defined the two scalar integrals via dimensional regularization

$$A_0(\mathcal{M}^2) = \int \frac{d^D k}{(2\pi)^D} \frac{1}{(k+p)^2 + \mathcal{M}^2} = -\frac{\mathcal{M}^2}{16\pi^2} (\Delta + 1 - \ln \mathcal{M}^2), \quad (3.5)$$

$$A_1(\mathcal{M}^2) = \int \frac{d^D k}{(2\pi)^D} \frac{(k+p)^2}{(k+p)^2 + \mathcal{M}^2} = -\mathcal{M}^2 A_0. \quad (3.6)$$

$\Delta = \frac{2}{\epsilon} - \gamma + \ln(4\pi)$  contains the divergence in  $\epsilon = D - 4$  for  $D = 4$  and  $\gamma = 0.577$  is the Euler-Mascheroni constant. The detailed discussion of integrals in dimensional regularization can be found in appendix B. The truncated one-loop 2-point function in the end reads

$$\begin{aligned} G_{2,\text{tr}, 1\text{-loop}}^{ij}(p, -p) &= \delta^{ij} \frac{1}{6f^2} (4p^2 + \mathcal{M}^2 - 15 \cdot 2c_2 a^2) A_0(\mathcal{M}^2) \\ &= -\delta^{ij} \frac{1}{6f^2} (4p^2 + \mathcal{M}^2 - 15 \cdot 2c_2 a^2) \frac{\mathcal{M}^2}{16\pi^2} (\Delta + 1 - \ln \mathcal{M}^2). \end{aligned} \quad (3.7)$$

We now calculate the tree level contribution of the truncated (N)NLO 2-point function with the (N)NLO lagrangian (2.84) constructed in the previous chapter. The expansion in terms of the pion fields and the determination of the corresponding vertices is shown in appendix D. Thus, the appropriate

truncated 2-point function reads

$$\begin{aligned}
G_{2,\text{tr},(\text{N})\text{NLO}}^{ij}(p, -p) = & -16L_{45} \frac{p^2 \mathcal{M}^2}{f^2} - 32L_{68} \frac{\mathcal{M}^4}{f^2} \\
& -16\bar{W}_{45} \frac{p^2 \rho}{f^2} - 32\bar{W}_{68} \frac{\mathcal{M}^2 \rho}{f^2} \\
& -2\mathcal{M}^2 2c_2 a^2 \frac{1}{f^2} (32L_{68} + \frac{1}{2}A_x) \\
& -2c_2 a^2 p^2 \frac{1}{f^2} (16L_{45} + D_x) \\
& -2c_2 a^2 \rho \frac{1}{f^2} (32\bar{W}_{68} + C_x) \\
& - (2c_2 a^2)^2 \frac{1}{f^2} (32L_{68} + A_x + \frac{1}{2}B_x). \tag{3.8}
\end{aligned}$$

The complete truncated 2-point function finally defines the one loop self energy  $\Sigma$ :

$$-\Sigma \delta^{ij} = G_{2,\text{tr}}^{ij} = G_{2,\text{tr},(\text{N})\text{NLO}}^{ij} + G_{2,\text{tr},1\text{-loop}}^{ij}. \tag{3.9}$$

Since the truncated 2-point function consists of one-particle irreducible diagrams (1PI), we arrive at the full propagator by summing up all reducible diagrams that one can construct out of the 1PI connected with the free propagator [26]. This forms a geometric series:

$$\begin{aligned}
G_2^{ij}(p, -p) &= \frac{1}{p^2 + \mathcal{M}^2} + \frac{1}{p^2 + \mathcal{M}^2} G_{2,\text{tr}}^{ij} \frac{1}{p^2 + \mathcal{M}^2} + \dots = \frac{1}{p^2 + \mathcal{M}^2 - G_{2,\text{tr}}^{ij}} \\
&= \delta^{ij} \frac{1}{p_E^2 + \mathcal{M}^2 + \Sigma_E(p_E^2)}. \tag{3.10}
\end{aligned}$$

The subscript  $E$  in the last line reminds us that we are still in Euclidean space. In order to get physical results, we have to Wick-rotate back to Minkowski space. In our case, this is simply done by changing the sign of  $p^2$ . In terms of the self energy, this means

$$\Sigma_M(p_M^2) = \Sigma_E(-p_E^2). \tag{3.11}$$

The pion mass is defined as the pole of the full propagator (3.10). This dictates us immediately the renormalization condition for the pion mass:

$$p_M^2 - \mathcal{M}^2 - \Sigma_M(p_M^2) = 0 \quad \text{for} \quad p_M^2 = M_\pi^2. \tag{3.12}$$

We can now compute the unrenormalized pion mass to one loop:

$$\begin{aligned}
M_\pi^2 &= \mathcal{M}^2 - \left( \frac{1}{32\pi^2} \frac{\mathcal{M}^4}{f^2} + \frac{5}{32\pi^2} \cdot \frac{2c_2 a^2 \mathcal{M}^2}{f^2} \right) (\Delta + 1 - \ln \mathcal{M}^2) \\
&\quad - \frac{8\mathcal{M}^4}{f^2} [2L_4 + L_5 - 4L_6 - 2L_8] \\
&\quad - \frac{16W_0 \mathcal{M}^2 a}{f^2} [2\bar{W}_4 + \bar{W}_5 - 4\bar{W}_6 - 2\bar{W}_8] \\
&\quad - \mathcal{M}^2 2c_2 a^2 \frac{1}{f^2} [8(2L_4 + L_5 - 8L_6 - 4L_8) + (D_x - A_x)] \\
&\quad + 4W_0 c_2 a^3 \frac{1}{f^2} [32\bar{W}_6 + 16\bar{W}_8 + C_x] \\
&\quad + (2c_2 a^2)^2 \frac{1}{f^2} [32L_6 + 16L_8 + A_x + \frac{1}{2}B_x]. \tag{3.13}
\end{aligned}$$

We used again the full notation in terms of  $L_i$  and  $\bar{W}_i$ , because the linear dependencies of the LE constants will be more obvious in this notation. Further, we set again  $\rho = 2W_0 a$ , to make dependence on the lattice spacing more obvious.

**Wave function renormalization:** For later use, we now compute the wave function renormalization  $Z_\pi$  of the pion fields. It is defined as the residuum of the full propagator (3.10). Using the residuum theorem from complex analysis, one gets for  $Z_\pi$

$$Z_\pi^{-1} = 1 - \frac{d\Sigma}{d(p^2)}. \tag{3.14}$$

Note that we take the derivative with respect to  $p^2$  after we Wick-rotated back to Minkowski space. The concrete determination of  $Z_\pi$  is straight forward and reads

$$\begin{aligned}
Z_\pi &= 1 - \frac{1}{24\pi^2 f^2} \mathcal{M}^2 (\Delta + 1 - \ln \mathcal{M}^2) - 16 L_{45} \frac{\mathcal{M}^2}{f^2} \\
&\quad - 16 \bar{W}_{45} \frac{\rho}{f^2} - (16 L_{45} + D_x) \frac{2c_2 a^2}{f^2}. \tag{3.15}
\end{aligned}$$

Squaring  $Z_\pi$ , neglecting all powers higher than  $\mathcal{M}^2$  which would correspond to higher order loop corrections and using (3.5), we can write

$$\begin{aligned}
Z_\pi^2 &= 1 + \frac{4}{3} \frac{1}{f^2} A_0(\mathcal{M}^2) - 32 L_{45} \frac{\mathcal{M}^2}{f^2} \\
&\quad - 32 \bar{W}_{45} \frac{\rho}{f^2} - (32 L_{45} + 2 D_x) \frac{2c_2 a^2}{f^2}. \tag{3.16}
\end{aligned}$$

As anticipated in section 2.6 we can write  $Z_\pi^2 = 1 + \mathcal{O}(\mathcal{M}^2)$ .

**Renormalization:** In analogy to the Gasser-Leutwyler constants introduced in section 1.3, we now make the ansatz

$$K_i = K_i^r - \mu^{-\epsilon} \frac{\gamma_i}{32\pi^2} (\Delta + 1) \quad (3.17)$$

where  $K_i$  stands for both  $L_i$  and the new LE constants  $A_x$ ,  $B_x$ ,  $C_x$  and  $D_x$ .  $\mu$  denotes the renormalization scale. The renormalization constants  $\gamma_i$  belonging to the  $L_i$  are well known and listed in table 1.1.  $\gamma_{A_x}$ ,  $\gamma_{B_x}$ ,  $\gamma_{C_x}$  and  $\gamma_{D_x}$  must now be chosen such that we end up with a finite result for the one-loop pion mass.

The  $\mathcal{M}^4$  divergence in the first line of (3.13) is canceled by the terms of the second line, exactly like in the continuum. The second divergence, the  $\mathcal{M}^2 a^2$  term, is canceled by the fourth line by properly adjusting the renormalization constants. This gives us a first constraint on  $(D_x - A_x)$ . On the level of the renormalization constants it reads

$$8(2\gamma_4 + \gamma_5 - 8\gamma_6 - 4\gamma_8) + \gamma_{D_x} - \gamma_{A_x} \stackrel{!}{=} 5. \quad (3.18)$$

Since there are no more divergent terms stemming from the leading order loop integrals, we can conclude that all other terms in (3.13) must be finite. The  $\mathcal{M}^2 a$  term in the third line is finite by construction, c.f. section 2.1. All the LE constants of the  $a^3$  term in the fifth line must also be finite since they only involve the finite  $\overline{W}_i$  and the additional constant  $C_x$  which nowhere else pops up and, therefore, we have to choose finite. This is equivalent to  $\gamma_{C_x} = 0$ . In order to keep the  $a^4$  term finite we get a second constraint on the renormalization constants from  $(32L_6 + 16L_8 + A_x + \frac{1}{2}B_x)$ :

$$32\gamma_6 + 16\gamma_8 + \gamma_{A_x} - \frac{1}{2}\gamma_{B_x} \stackrel{!}{=} 0. \quad (3.19)$$

Thus, we are left with two constraints for three unknown parameters. This means that we still can choose one parameter. This is actually not a problem, it is even expected. One encounters the same feature in the continuous case. Going on shell means that one replaces  $p^2$  with  $M_\pi^2$ . At NLO,  $p^2 \mathcal{M}^2$  always reduces to  $\mathcal{M}^4$  since higher powers than  $\mathcal{M}^4$  would correspond to higher order loop corrections. In the continuous theory, this fact is manifest in the linear combination  $[(2L_4 + L_5) - 2(2L_6 + L_8)]$ . The constants *within* parentheses are linear combinations due to the Cayley-Hamilton relations, while the linear combination *between* parentheses expresses the on shell condition. This explains why we encounter an analogous linear combination  $(D_x - A_x)$ .

In our computation, only this specific combination enters and we can think of it as one constant.<sup>1</sup> The most important point for us, however, is that every NLO term in (3.13) consists of linearly independent combinations of LE constants. Although we will not be able to determine all the LE constant separately, we can at least determine certain linear combinations and think of them at any time as one constant. The bottom line is that these constants then are independent from each other.

Having this information in mind, we now arbitrarily choose  $\gamma_{B_x} = 0$ , then  $\gamma_{A_x}$  and  $\gamma_{D_x}$  are determined and we get

$$\gamma_{A_x} = -3, \quad \gamma_{B_x} = 0, \quad \gamma_{C_x} = 0, \quad \gamma_{D_x} = 4. \quad (3.20)$$

Finally, we get for the renormalized pion mass:

$$\begin{aligned} M_\pi^2 &= \mathcal{M}^2 + \frac{1}{32\pi^2} \frac{\mathcal{M}^4}{f^2} \ln\left(\frac{\mathcal{M}^2}{\mu^2}\right) + \frac{5}{32\pi^2} \cdot \frac{2c_2 a^2 \mathcal{M}^2}{f^2} \ln\left(\frac{\mathcal{M}^2}{\mu^2}\right) \\ &\quad - \frac{8\mathcal{M}^4}{f^2} [2L_4^r + L_5^r - 4L_6^r - 2L_8^r] \\ &\quad - 16W_0 \mathcal{M}^2 a \frac{1}{f^2} [2\bar{W}_4 + \bar{W}_5 - 4\bar{W}_6 - 2\bar{W}_8] \\ &\quad - \mathcal{M}^2 2c_2 a^2 \frac{1}{f^2} [8(2L_4^r + L_5^r - 8L_6^r - 4L_8^r) + (D_x^r - A_x^r)] \\ &\quad + 4W_0 c_2 a^3 \frac{1}{f^2} [32\bar{W}_6 + 16\bar{W}_8 + C_x^r] \\ &\quad + (2c_2 a^2)^2 \frac{1}{f^2} [32L_6^r + 16L_8^r + A_x^r + \frac{1}{2}B_x^r]. \end{aligned} \quad (3.21)$$

As we have just discussed, we are free to collect the LE constants in square bracket into new constants. Furthermore, we want the renormalization scale  $\mu$  to be absorbed into scale independent LE constants. For this purpose we define

$$\begin{aligned} \Lambda_3^2 &= \mu^2 \exp\left(8 \cdot 32\pi^2 (2L_4^r + L_5^r - 4L_6^r - 2L_8^r)\right) \\ \Xi_3^2 &= \mu^2 \exp\left(\frac{32\pi^2}{5} (8(2L_4^r + L_5^r - 8L_6^r - 4L_8^r) + (D_x^r - A_x^r))\right) \\ k_1 &= 16 (2\bar{W}_4 + \bar{W}_5 - 4\bar{W}_6 - 2\bar{W}_8) \\ k_3 &= 2 (32\bar{W}_6 + 16\bar{W}_8 + C_x^r) \\ k_4 &= (32L_6^r + 16L_8^r + A_x^r + \frac{1}{2}B_x^r) \end{aligned}$$

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<sup>1</sup>If we had, in addition, computed the pion decay constant  $f_\pi$  to one loop, another linear combination involving  $D_x$  would have entered the calculation and one would have to check carefully the linear independencies.

and the pion mass reads

$$M_\pi^2 = \mathcal{M}^2 \left\{ 1 + \frac{1}{32\pi^2} \frac{\mathcal{M}^2}{f^2} \ln \left( \frac{\mathcal{M}^2}{\Lambda_3^2} \right) + \frac{5}{32\pi^2} \frac{2c_2 a^2}{f^2} \ln \left( \frac{\mathcal{M}^2}{\Xi_3^2} \right) + k_1 \frac{W_0 a}{f^2} \right\} + k_3 \frac{2c_2 W_0 a^3}{f^2} + k_4 \frac{(2c_2 a^2)^2}{f^2}. \quad (3.22)$$

In the pioneering work of Gasser and Leutwyler on ChPT [1], they parameterized the pion fields in the SU(2) square root representation, another non-linear realization of SU(2)×SU(2). Consequently, their low energy constants  $l_i$  as well as the renormalization constants  $\gamma'_i$  (c.f. eq. (9.6) in [1]) differ from the  $L_i$  and  $\gamma_i$  which we have used so far. Their scale independent LE constants  $\bar{l}_i$  are defined as

$$l_i^r(\mu) = \frac{\gamma'_i}{32\pi^2} \left( \bar{l}_i + \ln \frac{\mathcal{M}^2}{\mu^2} \right), \quad (3.23)$$

i.e., at the scale  $\mu = \mathcal{M} \simeq \mathcal{M}_\pi$  the value of  $\bar{l}_i$  is the same as the renormalized low energy constant  $l_i^r$  up to the number  $\gamma'_i/32\pi^2$ . In case of the pion mass, their LE constants are related to our SU(2) matrix representation by  $l_3^r = -4(2L_4^r + L_5^r - 4L_6^r - 2L_8^r)$  and correspondingly  $\gamma'_3 = -4(2\gamma_4 + \gamma_5 - 4\gamma_6 - 2\gamma_8)$ . If we apply these relations to the above definition of  $\Lambda_3^2$  we get precisely

$$\bar{l}_3 = -\ln \left( \frac{\mathcal{M}^2}{\Lambda_3^2} \right). \quad (3.24)$$

Later on, we will therefore often use the notation in terms of  $\bar{l}_i$  due to the simplicity of notation.

**Discussion:** Setting  $a = 0$  we arrive at the continuum result first obtained in [1]. Yet, for finite lattice spacing the continuum result gets modified by an additional chiral logarithm proportional to  $\mathcal{M}^2 a^2$ , as anticipated, and analytic corrections of order  $a^3$ ,  $a^4$  and  $\mathcal{M}^2 a^2$ . In order to estimate the strength of the new logarithm, we rewrite the terms in square brackets such that the dependence on  $\mathcal{M}^2$  lies completely in  $\ln(\mathcal{M}^2/\Lambda_3^2)$ :

$$\left[ 1 + \frac{1}{32\pi^2} \{ \mathcal{M}^2 + 10c_2 a^2 \} \ln \left( \frac{\mathcal{M}^2}{\Lambda_3^2} \right) + \frac{10}{32\pi^2 f^2} c_2 a^2 \ln \left( \frac{\Lambda_3^2}{\Xi_3^2} \right) + k_1 \frac{W_0 a}{f^2} \right]$$

One immediately sees that the factor in front of the chiral logarithm for  $c_2 a^2$  is one order of magnitude larger than for  $\mathcal{M}^2$ . The consequence is that even small contributions of  $\mathcal{O}(a^2)$  strongly affect the curvature which one would

expect due to the continuum chiral logarithm. For negative  $c_2$  which so far seems to be the most likely scenario (c.f. discussion in section 2.3), the value of  $\mathcal{M}^2 + 10c_2a^2$  can become small such that the expected curvature won't be seen.

The other interesting feature is that in the chiral limit the pion mass does not vanish due to the lattice artifacts of the terms  $k_3$  and  $k_4$ . These contributions are of  $\mathcal{O}(a^3, a^4)$ . At this point, it is worth performing the additive mass renormalization outlined in section 1.4, though this time, it is not only restricted to the  $1/a$  term. Hence, we determine the critical quark mass  $\tilde{m}$  such that the pion mass  $M_\pi^2$  again vanishes in the chiral limit:

$$\tilde{\mathcal{M}}^2 = 2B\tilde{m} \equiv 2Bm - 2c_2a^2 + k_3 \frac{2c_2W_0a^3}{f^2} + \left( k_4 \frac{(2c_2a^2)^2}{f^2} - k_1 \frac{W_0}{f^2} k_3 \frac{2c_2W_0a^3}{f^2} \right).$$

The quark masses  $\tilde{m}$  and  $m$  now differ by order  $a^2$  and higher, i.e. the additional contributions of  $\mathcal{O}(a^3, a^4)$  will be cleverly absorbed. With this new definition, the one loop pion mass can be written in terms of  $\tilde{m}$  and finally reads

$$M_\pi^2 = \tilde{\mathcal{M}}^2 \left[ 1 + \frac{1}{32\pi^2} \frac{\tilde{\mathcal{M}}^2}{f^2} \ln \left( \frac{\tilde{\mathcal{M}}^2}{\Lambda_3^2} \right) + \frac{5}{32\pi^2} \frac{2c_2a^2}{f^2} \ln \left( \frac{\tilde{\mathcal{M}}^2}{\Xi_3^2} \right) + k_1 \frac{W_0a}{f^2} \right].$$

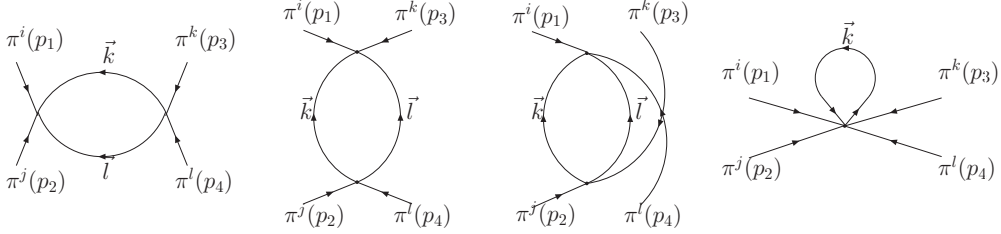
As discussed in section 1.4, our final aim will be to express scattering lengths in terms of the physical pion masses, resp. in terms of the pion mass which one measures on the lattice. Therefore, we essentially do not need the pion mass in terms of the critical quark mass. The above determination has got a more pedagogical intention, namely, to illustrate the principal differences of the lattice observables to those in the continuum. For later use, we now invert the pion mass  $M_\pi^2$  with respect to the tree level pion mass  $\mathcal{M}^2$ . The result is

$$\begin{aligned} \mathcal{M}^2 = M_\pi^2 \left\{ 1 - \frac{1}{32\pi^2} \frac{M_\pi^2}{f^2} \ln \left( \frac{M_\pi^2}{\Lambda_3^2} \right) - \frac{5}{32\pi^2} \frac{2c_2a^2}{f^2} \ln \left( \frac{M_\pi^2}{\Xi_3^2} \right) - k_1 \frac{W_0a}{f^2} \right\} \\ - k_3 \frac{2c_2W_0a^3}{f^2} - k_4 \frac{(2c_2a^2)^2}{f^2} \end{aligned} \quad (3.25)$$

where we neglected all corrections higher than our power counting scheme. The LE constants will now also depend on  $M_\pi^2$  instead of  $\mathcal{M}^2$ , i.e.  $\bar{l}_3(\mathcal{M}^2) \rightarrow \bar{l}_3(M_\pi^2)$ .

## 3.2 The scattering amplitude to one loop

Next, we compute the scattering amplitude  $A(s, t, u)$ . The one loop computation consists of the four diagrams shown in figure 3.1. The first three of



**Figure 3.1:** One loop diagrams contributing to the scattering amplitude. The first one is called s-channel diagram, the second respectively the third one t-channel respectively u-channel diagram. The fourth diagram is referred to as tadpole diagram and involves a six point vertex.

them are related by crossing symmetry which we have discussed in section 2.4. (Therefore, the diagrams are called s-channel, t-channel and u-channel.) We will now use this fact to compute all of the necessary diagrams in a systematic way. The tadpole contribution will be discussed afterwards.

According to (2.49), the amplitude  $A(s, t, u)$  corresponds to the flavor combination  $\delta^{ij}\delta^{kl}$ . This means that we only need to select all vertex combinations of the s-, t- and u-channel leading to the distinct flavor combination  $\delta^{ij}\delta^{kl}$ . In order not to forget any diagrams we precisely investigate how crossing symmetry relates these diagrams to each other: The t-channel diagram with configuration  $\delta^{ij}\delta^{kl}$  in figure 3.1 is obtained from the s-channel with configuration  $\delta^{ik}\delta^{jl}$  simply by exchanging  $p_2 \leftrightarrow p_3$ . Analogously, it works with the u-channel with configuration  $\delta^{ij}\delta^{kl}$  which is obtained from the s-channel with configuration  $\delta^{il}\delta^{kj}$  by interchanging  $p_2 \leftrightarrow p_4$ . The idea now is to write down an expression leading to the truncated four-point Green's function of the s-channel diagram  $G_{4,\text{s-chn}}^{ijkl}[p_1, p_2, p_3, p_4]$  which includes all possible flavor combinations, i.e.  $\delta^{ij}\delta^{kl}$ ,  $\delta^{ik}\delta^{jl}$  and  $\delta^{il}\delta^{kj}$ . From this general s-channel, one can immediately derive the  $\delta^{ij}\delta^{kl}$  contributions of the t- and u-channel and, hence, derive the contributions to the amplitude  $A(s, t, u)$ .

**General s-channel:** The momentum flow is defined by means of the arrows in figure 3.1. All external momenta are defined as incoming resulting in the total momentum conservation

$$p_1 + p_2 + p_3 + p_4 = 0. \quad (3.26)$$

The momentum conservation at each vertex gives

$$\begin{aligned} p_1 + p_2 + l + k &= 0, \\ -l - k + p_3 + p_4 &= 0. \end{aligned} \quad (3.27)$$



With the vertices given in (2.51) - (2.54) the most general one loop s-channel reads

$$G_{4,s\text{-chn}}^{ijkl}[p_1, p_2, p_3, p_4] = \frac{1}{2} \int \frac{d^4 k}{(2\pi)^4} \frac{1}{(k^2 + \mathcal{M}^2)((k + P_{12})^2 + \mathcal{M}^2)} \times \sum_{\alpha, \beta} V_{\alpha}^{ijrs}[p_1, p_2, l, k] V_{\beta}^{rskl}[-l, -k, p_3, p_4] \quad (3.28)$$

where we introduced the short-hand notation

$$P_{ab} = (p_a + p_b), \quad a, b = 1, 2, 3, 4. \quad (3.29)$$

The sum over  $\alpha$  and  $\beta$  runs from 1 to 4 according to the four different vertices. Further, we sum over the repeated indices  $r, s = 1, 2, 3$  of internal pion lines. In order to extract the three different configurations  $\{i, j, k, l\}$  we rewrite the complicated sum in (3.28) such that we can control the Kronecker deltas and the factors which multiply the Kronecker deltas at each vertex separately. For this purpose, we introduce the following short hand notation for the pion configuration:

$$\delta_{[i,j]_M} = \delta^{\{ij\}} \delta^{\{rs\}} \quad \text{and} \quad \delta_{[k,l]_N} = \delta^{\{rs\}} \delta^{\{kl\}}.$$

$M, N = 1, 2, 3$  denotes the appropriate configuration of pion indices, i.e.

$$\begin{aligned} \delta_{[i,j]_1} &= \delta^{ij} \delta^{rs}, & \delta_{[i,j]_2} &= \delta^{ir} \delta^{js}, & \delta_{[i,j]_3} &= \delta^{is} \delta^{rj}, \\ \delta_{[k,l]_1} &= \delta^{rs} \delta^{kl}, & \delta_{[k,l]_2} &= \delta^{rk} \delta^{sl}, & \delta_{[k,l]_3} &= \delta^{rl} \delta^{ks}. \end{aligned}$$

This allows us to write

$$V_{\alpha} = \sum_{M=1}^3 \tilde{V}_{\alpha_M} \delta_{[i,j]_M} \quad \text{and} \quad V_{\beta} = \sum_{N=1}^3 \tilde{V}_{\beta_N} \delta_{[k,l]_N}.$$

$\tilde{V}_{\alpha_M}$  is the factor which multiplies the Kronecker deltas. For  $V_1$  and  $V_2$ , its content is momentum dependent and, therefore, depends on the specific pion configuration. We indicate this fact with an additional subscript  $M$  resp.  $N$  on  $\alpha$  resp.  $\beta$ . Further we collect the momentum configuration in

$$[p_1, p_2, l, k] =: [\text{in}], \quad [-l, -k, p_3, p_4] =: [\text{out}].$$

Now, the sum in (3.28) reads:

$$\begin{aligned}
& \sum_{\alpha,\beta} V_{\alpha}^{ijrs}[p_1, p_2, l, k] V_{\beta}^{rskl}[-l, -k, p_3, p_4] \\
&= \sum_{\alpha,\beta} V_{\alpha}^{ijrs}[\text{in}] V_{\beta}^{rskl}[\text{out}] \\
&= \sum_{\alpha,\beta=1}^4 \sum_{M=1}^3 \tilde{V}_{\alpha M}^{[\text{in}]} \delta_{[i,j]_M} \sum_{N=1}^3 \tilde{V}_{\beta N}^{[\text{out}]} \delta_{[k,l]_N} \\
&= \sum_M \sum_{\alpha} \tilde{V}_{\alpha M}^{[\text{in}]} \delta_{[i,j]_M} \sum_N \sum_{\beta} \tilde{V}_{\beta N}^{[\text{out}]} \delta_{[k,l]_N} \\
&= \sum_M (\tilde{V}_{1M}^{[\text{in}]} + \tilde{V}_{2M}^{[\text{in}]} + \tilde{V}_{3M}^{[\text{in}]} + \tilde{V}_{4M}^{[\text{in}]}) \delta_{[i,j]_M} \\
&\quad \times \sum_N (\tilde{V}_{1N}^{[\text{out}]} + \tilde{V}_{2N}^{[\text{out}]} + \tilde{V}_{3N}^{[\text{out}]} + \tilde{V}_{4N}^{[\text{out}]}) \delta_{[k,l]_N}. \tag{3.30}
\end{aligned}$$

Performing the sum over  $M$  and  $N$  in the last line produces nine different summands. The whole expression is indeed very long. In order to control it systematically we define

$$[M \text{ in}] := (\tilde{V}_{1M}^{[\text{in}]} + \tilde{V}_{2M}^{[\text{in}]} + \tilde{V}_{3M}^{[\text{in}]} + \tilde{V}_{4M}^{[\text{in}]}) \tag{3.31}$$

$$[N \text{ out}] := (\tilde{V}_{1N}^{[\text{out}]} + \tilde{V}_{2N}^{[\text{out}]} + \tilde{V}_{3N}^{[\text{out}]} + \tilde{V}_{4N}^{[\text{out}]}) \tag{3.32}$$

and write the above sum in the following scheme:

$$\begin{aligned}
& \delta^{ij} \delta^{rs} [1 \text{ in}] [1 \text{ out}] \delta^{rs} \delta^{kl} \\
& \delta^{ir} \delta^{js} [2 \text{ in}] [2 \text{ out}] \delta^{rk} \delta^{sl} \\
& \delta^{is} \delta^{rj} [3 \text{ in}] [3 \text{ out}] \delta^{rl} \delta^{ks}
\end{aligned} \tag{3.33}$$

Now, the recipe works as follows: Take at any time one factor of  $[M \text{ in}]$ , pair it with one factor of  $[N \text{ out}]$  and contract the Kronecker deltas with respect to  $r$  and  $s$ . For example

$$\begin{aligned}
& \delta^{ij} \delta^{rs} [1 \text{ in}] [2 \text{ out}] \delta^{rk} \delta^{sl} \\
&= \delta^{ij} \delta^{kl} \frac{1}{3f^2} \left[ (p_1 l + p_2 k + p_2 l + p_1 k) \right. \\
&\quad \left. - 2(p_1 p_2 + lk) + \mathcal{M}^2 - 3 \cdot 2c_2 a^2 \right] \\
&\quad \times \frac{1}{3f^2} \left[ (p_1 p_2 - p_1 k - p_2 l + lk) \right. \\
&\quad \left. + 2(p_1 l + p_2 k) + \mathcal{M}^2 - 3 \cdot 2c_2 a^2 \right].
\end{aligned}$$

### 3.2.1 s-channel

To compute the s-channel contribution to the amplitude  $A(s, t, u)$ , i.e. the s-channel with configuration  $\delta^{ij}\delta^{kl}$ , we have to pick up the following contractions from the above scheme:

$$\begin{aligned}
\delta^{ij} \delta^{rs} \delta^{rs} \delta^{kl} &\longrightarrow 3 \delta^{ij} \delta^{kl}, \\
\delta^{ij} \delta^{rs} \delta^{rk} \delta^{sl} &\longrightarrow \delta^{ij} \delta^{kl}, \\
\delta^{ij} \delta^{rs} \delta^{rl} \delta^{sk} &\longrightarrow \delta^{ij} \delta^{kl}, \\
\delta^{ir} \delta^{js} \delta^{rs} \delta^{kl} &\longrightarrow \delta^{ij} \delta^{kl}, \\
\delta^{is} \delta^{rj} \delta^{rs} \delta^{kl} &\longrightarrow \delta^{ij} \delta^{kl}.
\end{aligned}$$

For the following discussion we define the function

$$H_{ij} = -4p_i p_j - p_i^2 - p_j^2 + \mathcal{M}^2. \quad (3.34)$$

After many pages of algebra the vertex sum can finally be written as

$$\begin{aligned}
[\text{s-vertex sum}] &= \delta^{ij} \delta^{kl} \frac{1}{9f^4} \left\{ 4k^4 + 8k^2(k \cdot P_{12}) + 4(k \cdot P_{12})^2 \right. \\
&\quad + 2k^2 [H_{12} + H_{34} + 6\mathcal{M}^2 - 24 \cdot 2c_2 a^2] \\
&\quad + 2(k \cdot P_{12}) [H_{12} + H_{34} + 6\mathcal{M}^2 - 24 \cdot 2c_2 a^2] \\
&\quad + [H_{12} \cdot H_{34} + (H_{12} + H_{34})(3\mathcal{M}^2 - 12 \cdot 2c_2 a^2) \\
&\quad \left. - 18 \cdot 2c_2 a^2 \mathcal{M}^2 + 63(2c_2 a^2)^2] \right\}. \quad (3.35)
\end{aligned}$$

We are now ready to perform the loop integration with respect to the independent loop momentum  $k$ . The necessary integrals in dimensional regularization are given in appendix B. In order to obtain a physical result we have to Wick-rotate back to Minkowski space setting the scalar products  $p_i \cdot p_j \rightarrow -p_i \cdot p_j$ . Going on shell, we further set  $p_i^2 = \mathcal{M}^2$  (at one loop one can use  $M_\pi^2 = \mathcal{M}^2$  since the difference corresponds to higher order loop corrections) and eventually obtain for the s-channel

$$\begin{aligned}
A_s &= \frac{1}{18f^4} \left\{ (20 p_1 \cdot p_2 + \mathcal{M}^2 - 48 \cdot 2c_2 a^2) A_0(\mathcal{M}^2) \right. \\
&\quad \left( 36 (p_1 \cdot p_2)^2 + 72 p_1 \cdot p_2 \mathcal{M}^2 - 144 p_1 \cdot p_2 \cdot 2c_2 a^2 \right. \\
&\quad \left. \left. + 27\mathcal{M}^4 - 90 \cdot 2c_2 a^2 \mathcal{M}^2 + 63(2c_2 a^2)^2 \right) B_0(-P_{12}^2, \mathcal{M}^2) \right\}. \quad (3.36)
\end{aligned}$$

### 3.2.2 t-channel

To compute the t-channel contribution we have to select in our scheme (3.33) the  $\delta^{ik} \delta^{jl}$  terms

$$\begin{aligned}\delta^{ir} \delta^{js} \delta^{rk} \delta^{sl} &\longrightarrow \delta^{ik} \delta^{jl} \\ \delta^{is} \delta^{rj} \delta^{rl} \delta^{ks} &\longrightarrow \delta^{ik} \delta^{jl}\end{aligned}\quad (3.37)$$

and then exchange the indices  $k \longleftrightarrow j$  as well as the momenta  $p_2 \longleftrightarrow p_3$  in the vertex sum. The momentum conservation at each vertex therefore translates to

$$\begin{aligned}p_1 + p_3 + l + k &= 0, \\ -l - k + p_2 + p_4 &= 0\end{aligned}\quad (3.38)$$

and the loop integral therewith is written as

$$A_t \delta^{ij} \delta^{kl} = \frac{1}{2} \int \frac{d^4 k}{(2\pi)^4} \frac{[\text{t-vertex sum}]}{(k^2 + \mathcal{M}^2) ((k + P_{13})^2 + \mathcal{M}^2)}. \quad (3.39)$$

Defining the two functions

$$F_{ij} = p_i - 2p_j, \quad (3.40)$$

$$G_{ij} = 2p_i p_j + 2p_i^2 - p_j^2 + \mathcal{M}^2 \quad (3.41)$$

the vertex sum reads

$$\begin{aligned}[\text{t-vertex sum}] &= \delta^{ij} \delta^{kl} \frac{1}{9f^4} \left\{ 2k^4 + 4k^2(k \cdot P_{13}) \right. \\ &\quad - 4 \left[ (k \cdot F_{13})(k \cdot F_{24}) + (k \cdot F_{31})(k \cdot F_{42}) \right] \\ &\quad - k^2 \left[ G_{24} + G_{42} + G_{13} + G_{31} - 12 \cdot 2c_2 a^2 \right] \\ &\quad + 2k \cdot \left[ F_{13} G_{24} + F_{31} G_{42} - F_{24} G_{13} - F_{42} G_{31} + 6P_{13} 2c_2 a^2 \right] \\ &\quad + \left[ G_{13} G_{24} + G_{31} G_{42} + 18 \cdot (2c_2 a^2)^2 \right. \\ &\quad \left. - 3 \cdot 2c_2 a^2 (G_{24} + G_{42} + G_{13} + G_{31}) \right] \left. \right\}. \quad (3.42)\end{aligned}$$

Performing the loop integrals, Wick-rotating back to Minkowski space and going on shell, after a very long calculation we get the t-channel amplitude.

$$\begin{aligned}A_t &= \frac{1}{18f^4} \left\{ \left( 24(p_1 \cdot p_3)(p_1 \cdot p_3) + 12(p_1 \cdot p_2)(p_1 \cdot p_3) - 12p_1 \cdot p_2 \mathcal{M}^2 \right. \right. \\ &\quad \left. \left. + 36 \cdot 2c_2 a^2 p_1 \cdot p_3 - 6\mathcal{M}^4 + 18(2c_2 a^2)^2 \right) B_0(-P_{13}^2, \mathcal{M}^2) \right. \\ &\quad \left. + \left( 16p_1 \cdot p_3 + 12p_1 \cdot p_2 + 4\mathcal{M}^2 + 12 \cdot 2c_2 a^2 \right) A_0(\mathcal{M}^2) \right\}\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{72\pi^2 f^4} \left\{ (p_1 \cdot p_3)(p_1 \cdot p_3) + 2(p_1 \cdot p_2)(p_1 \cdot p_3) - p_1 \cdot p_3 \mathcal{M}^2 \right. \\
& \quad \left. - 4 p_1 \cdot p_2 \mathcal{M}^2 - 2 \mathcal{M}^4 \right\}. \tag{3.43}
\end{aligned}$$

Note that the last two lines are not divergent. They stem from the finite part of integral (B.27).

### 3.2.3 u-channel

To compute the u-channel contribution we have to select in our scheme (3.33) the  $\delta^{il} \delta^{kj}$  terms and proceed in complete analogy to the t-channel. The two contributions read

$$\begin{aligned}
\delta^{ir} \delta^{js} \delta^{rl} \delta^{ks} & \longrightarrow \delta^{il} \delta^{kj}, \\
\delta^{is} \delta^{rj} \delta^{rk} \delta^{sl} & \longrightarrow \delta^{il} \delta^{kj}.
\end{aligned}$$

Comparing the above contractions with the ones from the t-channel (3.37), one immediately sees that they are simply related by exchanging the indices  $l \leftrightarrow k$ . This, however, corresponds to interchanging  $p_3 \leftrightarrow p_4$ . Hence, we get the u-channel amplitude from the t-channel amplitude directly by exchanging  $p_3 \leftrightarrow p_4$ . Note that the s- and t-channel resp. the s- and u-channel cannot be related in such a way due to the different way of contracting the pion indices. Hence the u-channel amplitude reads

$$\begin{aligned}
A_u & = \frac{1}{18f^4} \left\{ \left( 24 (p_1 \cdot p_4)(p_1 \cdot p_4) + 12 (p_1 \cdot p_2)(p_1 \cdot p_4) - 12 p_1 \cdot p_2 \mathcal{M}^2 \right. \right. \\
& \quad \left. \left. + 36 \cdot 2c_2 a^2 p_1 \cdot p_4 - 6 \mathcal{M}^4 + 18 (2c_2 a^2)^2 \right) B_0(-P_{14}^2, \mathcal{M}^2) \right. \\
& \quad \left. + \left( 16 p_1 \cdot p_4 + 12 p_1 \cdot p_2 + 4 \mathcal{M}^2 + 12 \cdot 2c_2 a^2 \right) A_0(\mathcal{M}^2) \right\} \\
& \quad + \frac{1}{72\pi^2 f^4} \left\{ (p_1 \cdot p_4)(p_1 \cdot p_4) + 2(p_1 \cdot p_2)(p_1 \cdot p_4) - p_1 \cdot p_3 \mathcal{M}^2 \right. \\
& \quad \left. - 4 p_1 \cdot p_2 \mathcal{M}^2 - 2 \mathcal{M}^4 \right\}. \tag{3.44}
\end{aligned}$$

### 3.2.4 Tadpole contribution

The last loop diagram is the tadpole diagram in figure ???. In order to compute it we have to expand the LO lagrangian in terms of the pion fields up to  $\mathcal{O}(\pi^6)$ . The corresponding six point vertices are given in appendix D.2

and give rise to the following one loop contribution

$$G_{4,\text{TP}}^{ijkl}[p_1, p_2, p_3, p_4] = \frac{1}{2} \int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2 + \mathcal{M}^2} \times \sum_{\alpha} V_{\alpha}^{ijrklr}[p_1, p_2, k, p_3, p_4, -k]. \quad (3.45)$$

The contraction is such that we select all terms leading to

$$\delta^{\{ij\}} \delta^{\{rk\}} \delta^{\{lr\}} \longrightarrow \delta^{ij} \delta^{kl}.$$

Doing the integration, Wick-rotating back to Minkowski space and going on shell leads us to the following one loop tadpole amplitude

$$A_{\text{TP}} = -\frac{1}{18f^4} \left( 40 p_1 p_2 + 9 \mathcal{M}^2 - 63 \cdot 2c_2 a^2 \right) A_0(\mathcal{M}^2). \quad (3.46)$$

### 3.2.5 (N)NLO tree level contribution

We now embark upon the (N)NLO computation of the four point function. The expansion of the appropriate lagrangian (2.84) in terms of pion fields up to fourth order and the corresponding four point vertices  $W_n^{ijkl}$  are given in appendix D.1. Since we consider the (N)NLO contribution at tree level only, we simply have to sum up all four point vertices

$$G_{(\text{N})\text{NLO}}^{ijkl}[p_1, p_2, p_3, p_4] = \sum_{n=3}^7 W_n^{ijkl}[p_1, p_2, p_3, p_4]. \quad (3.47)$$

Selecting again the  $\delta^{ij} \delta^{kl}$  portion we arrive at the contribution for the scattering amplitude

$$\begin{aligned} A_{(\text{N})\text{NLO}} &= 32 L_{13} \frac{1}{f^4} (p_1 \cdot p_2) (p_1 \cdot p_2) \\ &+ 16 L_2 \frac{1}{f^4} \left( (p_1 \cdot p_3) (p_1 \cdot p_3) + (p_1 \cdot p_4) (p_1 \cdot p_4) \right) \\ &+ 2 X_5 (p_1 \cdot p_3 + p_1 \cdot p_4) + 4 X_6 (p_1 \cdot p_2 + p_3 \cdot p_4) - 8 X_7. \end{aligned} \quad (3.48)$$

The  $X_i$  are linear combinations of low energy constants and are defined in appendix D.1. Using momentum conservation, Wick-rotating back to Minkowski space and going on shell the amplitude can be written as

$$\begin{aligned} A_{(\text{N})\text{NLO}} &= 32 L_{13} \frac{1}{f^4} (p_1 \cdot p_2)^2 + 16 L_2 \frac{1}{f^4} \left( (p_1 \cdot p_3)^2 + (p_1 \cdot p_4)^2 \right) \\ &+ 4 X_5 (\mathcal{M}^2 + p_1 \cdot p_2) - 8 X_6 p_1 \cdot p_2 - 8 X_7. \end{aligned} \quad (3.49)$$

### 3.2.6 Wave function renormalization contribution

As anticipated in section 2.6, we have to include the effects of the wave function renormalization on the LO tree level amplitude (2.57) when we perform the full one loop computation. Basically, this means that the tree level scattering amplitude (2.57) will be multiplied by the factor  $Z_\pi^2$  that was given in section 3.1. The  $\mathcal{O}(\mathcal{M}^2)$  contributions of the scattering amplitude multiplied by the  $\mathcal{O}(\mathcal{M}^2)$  corrections from  $Z_\pi^2$  in (3.16) will contribute with additional terms of  $\mathcal{O}(\mathcal{M}^2)$  which we collect in  $A_{\text{FR}}$ . From now on, it is very important to indicate which on shell condition in the tree level scattering amplitude was used. On the one hand, we write  $A_{\text{LO}}(M_\pi^2)$  if we use  $p^2 = M_\pi^2$  like in (2.57), i.e. if it is important that loop corrections to the pion mass are considered. On the other hand, we write  $A_{\text{LO}}(\mathcal{M}^2)$  like in (2.58) if we apply  $p^2 = \mathcal{M}^2$

$$\begin{aligned} Z_\pi^2 A_{\text{LO}}(M_\pi^2) &= A_{\text{LO}}(M_\pi^2) + (Z_\pi^2 - 1)A_{\text{LO}}(M_\pi^2) \\ &= A_{\text{LO}}(M_\pi^2) + (Z_\pi^2 - 1)A_{\text{LO}}(\mathcal{M}^2) \\ &= A_{\text{LO}}(M_\pi^2) + A_{\text{FR}}. \end{aligned} \quad (3.50)$$

The first line is still exact. In the second line we use the fact that we can write  $Z_\pi^2 = 1 + \mathcal{O}(\mathcal{M}^2)$  and that we can neglect terms of higher powers than  $\mathcal{M}^4$ . This allows us to replace  $A_{\text{LO}}(M_\pi^2)$  by  $A_{\text{LO}}(\mathcal{M}^2)$ .  $A_{\text{FR}}$  is a lengthy expression and reads

$$\begin{aligned} A_{\text{FR}} &= -32 L_{45} \frac{\mathcal{M}^2}{3f^4} (6 p_1 p_2 + 3 \mathcal{M}^2 - 3 \cdot 2c_2 a^2) \\ &\quad - 32 \bar{W}_{45} \frac{\rho}{3f^4} (6 p_1 p_2 + 3 \mathcal{M}^2 - 3 \cdot 2c_2 a^2) \\ &\quad - 32 L_{45} \frac{2c_2 a^2}{3f^4} (6 p_1 p_2 + 3 \mathcal{M}^2 - 3 \cdot 2c_2 a^2) \\ &\quad - 2 D_x \frac{2c_2 a^2}{3f^4} (6 p_1 p_2 + 3 \mathcal{M}^2 - 3 \cdot 2c_2 a^2) \\ &\quad + \frac{1}{18f^4} (48 p_1 p_2 + 24 \mathcal{M}^2 - 24 \cdot 2c_2 a^2) A_0(\mathcal{M}^2). \end{aligned} \quad (3.51)$$

Note that the last line contains an explicitly divergent term in  $A_0(\mathcal{M}^2)$  defined in (3.5).

### 3.2.7 Renormalization and cancellation of the divergencies

We are now in the position to write down the full scattering amplitude  $A$  to one loop. It is simply the sum of all the contributions that we have computed

so far

$$A = A_{\text{LO}}(M_\pi^2) + A_s + A_t + A_u + A_{\text{TP}} + A_{\text{FR}} + A_{(\text{N})\text{NLO}}.$$

After the discussion of the individual terms we know that this expression is enormously large. In order not to lose the orientation, we first focus on the renormalization of the divergencies.

Putting all ingredients together we can extract the divergent part of the amplitude. The divergencies arise from the s-, t- and u-channel as well as from the tadpole contribution. Further, we found a divergence in  $A_{\text{FR}}$ . A last divergent structure enters the amplitude when in the leading order amplitude  $A_{\text{LO}}(M_\pi^2)$  the unrenormalized one-loop pion mass  $M_\pi^2$  from (3.13) is substituted.<sup>2</sup> Due to the specific structure of  $M_\pi^2$ , we can write  $A_{\text{LO}}(M_\pi^2) = A_{\text{LO}}(\mathcal{M}^2) + \mathcal{O}(\mathcal{M}^4)$  where  $\mathcal{O}(\mathcal{M}^4)$  includes both the divergencies from the one-loop computation and the (unrenormalized) (N)NLO low energy constants. For the renormalization process, only the  $\mathcal{O}(\mathcal{M}^4)$  contribution is important.  $A_{\text{LO}}(\mathcal{M}^2)$  will be considered in the very end. With this ingredients, the divergent part reads

$$A_{\text{div}} = \frac{1}{96\pi^2 f^4} \left\{ 8 \left( (p_1 \cdot p_2)^2 + (p_1 \cdot p_3)^2 + (p_1 \cdot p_4)^2 \right) - 27 \cdot 2c_2 a^2 \mathcal{M}^2 \right. \\ \left. - 60 \cdot 2c_2 a^2 (p_1 \cdot p_2) + 33 \cdot (2c_2 a^2)^2 \right\} (\Delta + 1 - \ln \mathcal{M}^2). \quad (3.52)$$

These infinities are cancelled by the appropriate counterterms from the (N)NLO lagrangian. They enter our calculation through  $A_{(\text{N})\text{NLO}}$  and  $A_{\text{FR}}$ . Further, we encounter an additional contribution after the substitution of the unrenormalized pion mass (3.13) in the leading order amplitude (see above). Collecting all counterterms we end up with the following structure:

$$A_{\text{CT}} = \frac{1}{f^4} \left\{ (p_1 \cdot p_2)^2 32 L_{13} + \left( (p_1 \cdot p_2)^2 + (p_1 \cdot p_2)^2 \right) 16 L_2 \right. \\ + 2c_2 a^2 \rho \left[ 32 \overline{W}_{45} - \frac{4}{3} C_x - 4 C_y \right] \\ + \mathcal{M}^2 2c_2 a^2 \left[ 32 L_{45} - 4 A_y + 2 D_y - 2 D_x + \frac{4}{3} (D_x - A_x) \right] \\ + (p_1 \cdot p_2) 2c_2 a^2 \left[ 2 D_y - 4 D_z - 4 D_x \right] \\ \left. + (2c_2 a^2)^2 \left[ 32 L_{45} - 2 (2 A_y + B_y) + 2 D_x - \frac{4}{3} (A_x + \frac{1}{2} B_x) \right] \right\}. \quad (3.53)$$

---

<sup>2</sup>One could use the renormalized pion mass as well, where all divergencies are already cancelled. The structure of the whole computation, however, is more obvious in the here described framework since some of the unrenormalized terms cancel each other and need not be carried through the whole process.



Note that neither in  $A_{\text{div}}$  nor in  $A_{\text{CT}}$  any terms proportional to  $\mathcal{M}^2$  or  $a\mathcal{M}^2$  are present. They dropped out during the computation. We now employ the same renormalization procedure that we already used for the pion mass with the ansatz

$$K_i = K_i^r - \mu^{-\epsilon} \frac{\gamma_i}{32\pi^2} (\Delta + 1). \quad (3.54)$$

The renormalization constants for the  $L_i$  were determined in continuous ChPT (see table 1.1). Hence,  $L_{13}$  and  $L_2$  cancel the divergences which solely depend on momentum, i.e. the terms proportional to  $(p_1 \cdot p_2)^2$ ,  $(p_1 \cdot p_3)^2$  and  $(p_1 \cdot p_4)^2$ . The constants  $A_x, B_x, C_x, D_x$  were fixed in the calculation of the pion mass. There, we also saw that the  $\bar{W}_i$  did not get renormalized. The new free parameters of the four point function involving the lattice spacing, therefore, are  $A_y, B_y, C_y, D_y$  and  $D_z$ . Their renormalization constants are now fixed such that we get a finite scattering amplitude. Since there is no divergence proportional to  $a^3$  this gives a first constraint on  $C_y$  and we must choose  $\gamma_{C_y} = 0$ . There are three remaining divergencies: one proportional to  $a^2\mathcal{M}^2$ , one to  $a^2p_1p_2$  and another one to  $a^4$ . However, we have four constants and, hence, can conclude that one of them is not independent. This can be understood as follows: in the construction of the (N)NLO lagrangian we found three independent operators for the term proportional to  $p^2\mathcal{M}^2$ , c.f. (2.82). In the expansion in terms of pion fields, we got a constant  $D_x$  for the 2-point function and another two constants  $D_y$  and  $D_z$  for the four-point function. This means that in such a four-point function, in principle, one could distinguish a part proportional to  $p_1p_2$  and, for instance, a part  $p_1p_3$  (c.f. the discussion of the Mandelstam variables). However, due to the specific form of the vertices one encounters only a part proportional to  $p_1p_2$ . This can be seen in the transition from (3.48) to (3.49) in the discussion of the (N)NLO amplitude: Energy conservation and going on shell reduces one degree of freedom and, hence,  $D_y$  will depend on  $D_z$  or vice versa. We choose arbitrarily  $\gamma_{D_y} = 0$ . The other renormalization coefficients are then easily determined and read

$$\gamma_{A_y} = \frac{1}{12}, \quad \gamma_{B_y} = \frac{46}{3}, \quad \gamma_{C_y} = 0, \quad \gamma_{D_y} = 0, \quad \gamma_{D_z} = -9.$$

The most important point for us is that the terms in square brackets in (3.53) are again linearly independent combinations of low energy constants and, therefore, can be collected in terms of new constants. Substituting  $p_1p_2 = \frac{1}{2}s - \mathcal{M}^2$  in (3.53) modifies the coefficients of the renormalized LE constants, the linear combinations, however, are still linearly independent.

In analogy to the procedure outlined at the pion mass we define:

$$\begin{aligned}
\Lambda_1^2 &= \mu^2 \exp\left(16 \cdot 48\pi^2 L_{13}^r\right), & \Lambda_2^2 &= \mu^2 \exp\left(8 \cdot 48\pi^2 L_2\right), \\
\Xi_4^2 &= \mu^2 \exp\left(\frac{16\pi^2}{5} \left[D_y^r - 2D_z^r - 2D_x^r\right]\right), \\
\Xi_5^2 &= \mu^2 \exp\left(\frac{32\pi^2}{11} \left[32L_{45}^r - 4A_y^r + 4D_z^r - \frac{10}{3}D_x^r - \frac{4}{3}A_x^r\right]\right), \\
\Xi_6^2 &= \mu^2 \exp\left(\frac{32\pi^2}{11} \left[32L_{45}^r - 2(2A_y^r + B_y^r) + 2D_x^r - \frac{4}{3}(A_x^r + \frac{1}{2}B_x^r)\right]\right), \\
k_5 &= 2 \left[32\bar{W}_{45} - \frac{4}{3}C_x - 4C_y\right],
\end{aligned}$$

Using Mandelstam variables the renormalized part of the amplitude reads

$$\begin{aligned}
A_{\text{div}} + A_{\text{CT}} &= \frac{1}{96\pi^2 f^4} \left\{ -2(s - 2\mathcal{M}^2)^2 \ln\left(\frac{\mathcal{M}^2}{\Lambda_1^2}\right) \right. \\
&\quad - 2\left((t - 2\mathcal{M}^2)^2 + (u - 2\mathcal{M}^2)^2\right) \ln\left(\frac{\mathcal{M}^2}{\Lambda_2^2}\right) \\
&\quad + 30 \cdot 2c_2 a^2 s \ln\left(\frac{\mathcal{M}^2}{\Xi_4^2}\right) - 33 \cdot 2c_2 a^2 \mathcal{M}^2 \ln\left(\frac{\mathcal{M}^2}{\Xi_5^2}\right) \\
&\quad \left. - 33 \cdot (2c_2 a^2)^2 \ln\left(\frac{\mathcal{M}^2}{\Xi_4^2}\right) \right\} + k_5 \frac{W_0 2c_2 a^3}{f^4}. \quad (3.55)
\end{aligned}$$

In analogy to the discussion on the pion mass, we introduce the short hand notation for the scale independent low energy constants

$$\bar{l}_i(\mathcal{M}^2) = -\ln\left(\frac{\mathcal{M}^2}{\Lambda_i^2}\right) \quad i = 1, 2, 3, \quad (3.56)$$

$$\bar{\xi}_i(\mathcal{M}^2) = -\ln\left(\frac{\mathcal{M}^2}{\Xi_i^2}\right) \quad i = 3, \dots, 6. \quad (3.57)$$

### 3.2.8 The full one loop amplitude

The last step to do is to collect all analytic terms which we have not considered so far. These are

- the tree level leading order amplitude  $A_{LO}(\mathcal{M}^2)$
- the finite parts from the t- and u-channel which do neither involve  $B_0(\mathcal{M}^2, P^2)$  nor  $A_0(\mathcal{M}^2)$

- the finite parts from the  $B_0(\mathcal{M}^2, P^2)$  integrals which is given in appendix B

Putting all together and doing some algebra, we arrive at the following formula for the one loop amplitude

$$A(s, t, u) = \frac{s - \mathcal{M}^2 - 2c_2a^2}{f^2} + B(s, t, u) + C(s, t, u) \quad (3.58)$$

$$\begin{aligned} B(s, t, u) = \frac{1}{96\pi^2 f^4} & \left\{ 3(s^2 - \mathcal{M}^4)F(s) \right. \\ & + \{t(t-u) - 2\mathcal{M}^2(t-2u) - 2\mathcal{M}^2\}F(t) \\ & + \{u(u-t) - 2\mathcal{M}^2(u-2t) - 2\mathcal{M}^2\}F(u) \\ & + 2c_2a^2 \left[ (42c_2a^2 + 18\mathcal{M}^2 - 24s)F(s) \right. \\ & \quad + (12c_2a^2 - 12\mathcal{M}^2 + 6t)F(t) \\ & \quad \left. \left. + (12c_2a^2 - 12\mathcal{M}^2 + 6u)F(u) \right] \right\} \end{aligned} \quad (3.59)$$

$$\begin{aligned} C(s, t, u) = \frac{1}{96\pi^2 f^4} & \left\{ 2\left(\bar{l}_1 + \frac{2}{3}\right)(s - 2\mathcal{M}^2)^2 + \left(\bar{l}_2 + \frac{7}{6}\right)(s^2 + (t-u)^2) + \mathcal{M}^4 \right. \\ & + 2c_2a^2 \left[ 30s(\bar{\xi}_4 - 1) - 3\mathcal{M}^2(11\bar{\xi}_5 - 6) \right. \\ & \quad \left. \left. - 33 \cdot 2c_2a^2(\bar{\xi}_6 - 1) \right] \right\} + k_5 \frac{W_0 2c_2a^3}{f^4} \end{aligned} \quad (3.60)$$

in which we use the function  $F(x)$  defined in appendix B

$$F(p^2) = \left\{ \begin{array}{ll} \sigma \ln \frac{1-\sigma}{1+\sigma} - i\pi\sigma, & p^2 = s \\ \sigma \ln \frac{\sigma-1}{\sigma+1}, & p^2 = t, u \end{array} \right\} \text{ with } \sigma = \sqrt{1 - \frac{4\mathcal{M}^2}{p^2}}. \quad (3.61)$$

The terms in square brackets in (3.59) and (3.60) and the  $a^3$  term in (3.60) are new with respect to the continuum amplitude [1] which is recovered setting  $a = 0$ .

# Chapter 4

## Scattering lengths

In the first section the  $a_0^0$ ,  $a_0^2$  and  $a_1^1$  scattering lengths to one loop are explicitly computed. This section focuses mainly on the technical aspects of the calculation. In the subsequent section, the application of the formulae to fit lattice data is discussed.

### 4.1 One-loop computation of $a_0^0$ , $a_0^2$ and $a_1^1$

The scattering lengths are computed with the same formalism that we already applied on the tree level amplitude. Let us recapture the most important steps: First, we have to relate the one-loop amplitude  $A(s, t, u)$  from the previous section to amplitudes  $T^I$  of definite isospin  $I = 0, 1, 2$  with the isospin decomposition formulae (2.59), (2.60) and (2.61) given in section 2.6. Then, the partial wave amplitude  $T_l^I$  is projected out by means of the partial wave decomposition (2.66). Finally the scattering lengths are extracted with the low energy expansion (C.26) described in appendix C.

The isospin amplitude  $T^I$  is decomposed in analogy to the scattering amplitude  $A(s, t, u)$  into

$$T^I = T_A^I + T_B^I + T_C^I \quad (4.1)$$

The  $T_A^I$  are the tree level isospin amplitudes which we have already computed in section 2.6.  $T_B^I$  and  $T_C^I$  are obtained by plugging  $B(s, t, u)$  resp.  $C(s, t, u)$  from the previous section into the isospin decomposition formulae of section 2.6. One then extracts the “partial scattering lengths” belonging to  $T_A^I$ ,  $T_B^I$  and  $T_C^I$  and finally adds them up to get the total scattering length

$$a_l^I = a_{l,A}^I + a_{l,B}^I + a_{l,C}^I. \quad (4.2)$$

The scattering lengths  $a_{0,A}^2$  and  $a_{1,A}^1$  are the same like in the tree level calculation given by the formulae (2.69) and (2.68). With  $a_{0,A}^0$  one has to be

careful, because there, the on-shell condition  $p^2 = M_\pi^2$  enters the computation resulting in an additional contribution

$$a_{0,A}^0 = \frac{7}{32\pi f^2} \left( \mathcal{M}^2 - \frac{5}{7} 2c_2 a^2 \right) + \frac{3}{8\pi f^2} \left( M_\pi^2 - \mathcal{M}^2 \right). \quad (4.3)$$

To determine  $a_{i,B}^I$  we replace in the isospin amplitude  $T_{0,B}^I$  the Mandelstam variables by

$$s = 4(q^2 + \mathcal{M}^2), \quad t = -2q^2(1-x), \quad u = -2q^2(1+x) \quad (4.4)$$

where  $x = \cos \theta$  as discussed in detail in section 2.4. This leads to a structure of the form

$$T_{0,B}^I = \frac{1}{96\pi^2 f^4} \left( S(q, x) \cdot F(s) + T(q, x) \cdot F(t) + U(q, x) \cdot F(u) \right) \quad (4.5)$$

$S$ ,  $T$  and  $U$  are lengthy expressions with  $q$  and  $x$  as kinetic variables. Note that  $q$  can appear only with even powers.

Let us now focus on  $a_{0,B}^0$ . In the low energy expansion of the  $a_0^0$  scattering length we consider the limit  $q \rightarrow 0$ . This means that we can neglect all terms which depend on  $q^2$  or higher powers. Performing the partial wave decomposition (2.66) by means of an integral over  $x$  (remember that  $P(x) = 1$  for  $l = 0$ ) we end up with the following expression

$$a_{0,B}^0 = \frac{1}{64\pi} \frac{1}{96\pi^2 f^4} \left\{ \int_{-1}^{+1} dx \left( 147\mathcal{M}^4 + 75 \cdot (2c_2 a^2)^2 - 210 \mathcal{M}^2 2c_2 a^2 \right) F(s) \right. \\ \left. + \int_{-1}^{+1} dx \left( 5\mathcal{M}^4 + 45 \cdot (2c_2 a^2)^2 - 30 \mathcal{M}^2 2c_2 a^2 \right) \left[ F(t) + F(u) \right] \right\}_{q^2 \rightarrow 0}.$$

The expansion of the function  $F(s)$  in powers of  $q^2/\mathcal{M}^2$  using (4.4) gives

$$F(s) = -2 \frac{q^2}{\mathcal{M}^2} - i\pi \left( \frac{q^2}{\mathcal{M}^2} \right)^{\frac{1}{2}} + \dots, \quad (4.6)$$

hence, in the low energy limit, it does not contribute. The remaining now is to compute the integral

$$I_t = \int_{-1}^{+1} dx F(t) = \int_{-1}^{+1} dx \sigma \ln \frac{\sigma - 1}{\sigma + 1} \quad (4.7)$$

and the corresponding integral with respect to  $F(u)$ . The function

$$\sigma(x) = \sqrt{1 - \frac{4\mathcal{M}^2}{t(x)}} = \sqrt{1 + \frac{B}{1-x}} \quad \text{with} \quad B = \frac{2\mathcal{M}^2}{q^2} \quad (4.8)$$

is monotonic on the interval  $(-1, 1)$  and, therefore, can be inverted to

$$x = 1 - \frac{B}{\sigma^2 - 1}. \quad (4.9)$$

This allows us to perform the integral over  $\sigma$  with boundaries

$$\sigma(-1) = \sqrt{1 + \frac{B}{2}} =: \sigma_i, \quad \sigma(+1) = \infty \quad (4.10)$$

and with the transformed measure

$$dx = \frac{dx}{d\sigma} d\sigma = \frac{2B\sigma}{(\sigma^2 - 1)^2} d\sigma. \quad (4.11)$$

The final integral reads

$$I_t = 2B \int_{\sigma_i}^{\infty} d\sigma \frac{\sigma^2}{(\sigma^2 - 1)^2} \ln \frac{\sigma - 1}{\sigma + 1}. \quad (4.12)$$

The integral over  $F(u)$  leads precisely to the same result. This integral can be solved analytically. To do this, we employ the computer algebra system MAPLE and finally expand the result in powers of  $\frac{q^2}{\mathcal{M}^2}$  since we are interested in the low energy behaviour only. The expansion gives

$$I_t = -4 - \frac{2}{3} \frac{q^2}{\mathcal{M}^2} + \mathcal{O}\left(\frac{q^4}{\mathcal{M}^4}\right) \quad (4.13)$$

With this result we compute

$$a_{0,B}^0 = \frac{5}{128} \frac{2c_2 a^2 \mathcal{M}^2}{\pi^3 f^4} - \frac{5}{768} \frac{\mathcal{M}^4}{\pi^3 f^4} - \frac{15}{256} \frac{(2c_2 a^2)^2}{\pi^3 f^4}. \quad (4.14)$$

The computation of  $a_{0,C}^0$  is straightforward and not very illuminating. Since the terms become very lengthy we let again MAPLE do the work. Adding up  $a_{0,A}^0$ ,  $a_{0,B}^0$  and  $a_{0,C}^0$ , we end up with

$$\begin{aligned} a_0^0 = & \frac{7}{32\pi} \frac{\mathcal{M}^2}{f^2} \left( 1 + \frac{5}{84\pi^2} \frac{\mathcal{M}^2}{f^2} \left\{ \bar{l}_1 + 2\bar{l}_2 + \frac{21}{8} \right\} \right. \\ & \left. - \frac{5}{84\pi^2} \frac{2c_2 a^2}{f^2} \left\{ 9\bar{\xi}_4 - \frac{33}{8}\bar{\xi}_5 + \frac{15}{4} \right\} \right) \\ & - \frac{5}{32\pi} \frac{2c_2 a^2}{f^2} \left( 1 - \frac{W_0 a}{f^2} k_5 - \frac{2c_2 a^2}{32\pi^2 f^2} \left\{ 11\bar{\xi}_6 - 1 \right\} \right) \\ & + \frac{3}{8\pi f^2} (M_\pi^2 - \mathcal{M}^2). \end{aligned} \quad (4.15)$$

The determination of  $a_0^2$  works analogously to the  $a_0^0$  case. The result is

$$a_0^2 = -\frac{\mathcal{M}^2}{16\pi f^2} \left( 1 - \frac{\mathcal{M}^2}{12\pi^2 f^2} \left\{ \bar{l}_1 + 2\bar{l}_2 + \frac{3}{8} \right\} - \frac{2c_2 a^2}{32\pi^2 f^2} \left\{ 11\bar{\xi}_5 + 2 \right\} \right) - \frac{2c_2 a^2}{16\pi f^2} \left( 1 - \frac{W_0 a}{f^2} k_5 - \frac{2c_2 a^2}{32\pi^2 f^2} \left\{ 11\bar{\xi}_6 - 7 \right\} \right). \quad (4.16)$$

Setting  $a = 0$  we arrive at the well known continuum result for  $a_0^0$  and  $a_0^2$  to one loop [1]. As anticipated, we get for non-vanishing lattice spacing additional chiral logarithms of order  $a^2 \mathcal{M}^2 \ln \mathcal{M}^2$  and  $a^4 \ln \mathcal{M}^2$ , as well as analytic corrections of order  $a^3$  and  $a^4$ . The remarkable point at this result is that, contrary to the continuum, the scattering lengths do not vanish in the chiral limit. We encountered this feature already at tree level due to a non-vanishing analytic correction of order  $a^2$ . New at one-loop level is that the scattering lengths now even diverge in the chiral limit because of the non-analytic contribution of order  $a^4 \ln \mathcal{M}^2$ .

The calculation of  $a_1^1$  is different with respect to two important points.

1. We must consider the Legendre polynomial  $P_1(x) = x$  in the integrals.
2. The low energy expansion in (C.26) for  $l = 1$  extracts a factor of  $q^2/\mathcal{M}^2$ . Hence the  $a_1^1$  scattering length is essentially what is multiplied by  $q^2$  in the final expansion and we can drop all powers higher than  $q^2$ .

Writing again  $T_{B,1}^1$  in the notation of (4.5), we get for the coefficients

$$\begin{aligned} S(q, x) &= 16 q^4 x \\ T(q, x) &= \left( 30 \cdot 2c_2 a^2 \mathcal{M}^2 + 15(2c_2 a^2)^2 - 17\mathcal{M}^4 \right) + \left( 60 \cdot 2c_2 a^2 - 28 \mathcal{M}^2 \right) q^2 \\ &\quad + \left( 12 \mathcal{M}^2 - 60 \cdot 2c_2 a^2 \right) q^2 x + \mathcal{O}(q^4) \\ &= \mathcal{A} + \mathcal{B} q^2 + \mathcal{C} q^2 x + \mathcal{O}(q^4) \\ U(q, x) &= -\mathcal{A} - \mathcal{B} q^2 + \mathcal{C} q^2 x + \mathcal{O}(q^4). \end{aligned}$$

Dropping all contributions of  $\mathcal{O}(q^4)$  the integral for  $a_{1,B}^1$  reads

$$a_{1,B}^1 = \frac{1}{64\pi} \frac{1}{96\pi^2 f^4} \left\{ \frac{\mathcal{M}^2}{q^2} \left[ \int_{-1}^{+1} dx \left( \mathcal{A} x + \mathcal{B} q^2 x + \mathcal{C} q^2 x^2 \right) F(t) + \int_{-1}^{+1} dx \left( -\mathcal{A} x - \mathcal{B} q^2 x + \mathcal{C} q^2 x^2 \right) F(u) \right] \right\}_{q^2 \rightarrow 0}. \quad (4.17)$$

Following the same arguments that were outlined for  $a_{0,B}^0$  we derive the fol-

lowing formulae for the integrals to perform

$$\begin{aligned}
\int_{-1}^{+1} dx x F(t) &= \int_{\sigma_i}^{\infty} d\sigma \frac{2B\sigma}{(\sigma^2 - 1)^2} \left(1 - \frac{B}{\sigma^2 - 1}\right) \sigma \ln \frac{\sigma - 1}{\sigma + 1} \\
&= - \int_{-1}^{+1} dx x F(u) = \frac{2}{9} \frac{q^2}{\mathcal{M}^2} + \mathcal{O}(q^4), \\
\int_{-1}^{+1} dx x^2 F(t) &= \int_{\sigma_i}^{\infty} d\sigma \frac{2B\sigma}{(\sigma^2 - 1)^2} \left(1 - \frac{B}{\sigma^2 - 1}\right)^2 \sigma \ln \frac{\sigma - 1}{\sigma + 1} \\
&= \int_{-1}^{+1} dx x^2 F(u) = -\frac{4}{3} - \frac{2}{9} \frac{q^2}{\mathcal{M}^2} + \mathcal{O}(q^4). \tag{4.18}
\end{aligned}$$

Plugging these results into (4.17) and taking the  $q \rightarrow 0$  limit we get

$$a_{0,B}^0 = \frac{65}{2304} \frac{2c_2 a^2 \mathcal{M}^2}{\pi^3 f^4} - \frac{89}{13824} \frac{\mathcal{M}^4}{\pi^3 f^4} - \frac{5}{4608} \frac{(2c_2 a^2)^2}{\pi^3 f^4}. \tag{4.19}$$

Evaluating  $a_{1,C}^1$  with MAPLE and adding up all partial scattering lengths we finally arrive at the  $a_1^1$  scattering length

$$\begin{aligned}
a_1^1 &= \frac{\mathcal{M}^2}{24\pi f^2} \left(1 - \frac{\mathcal{M}^2}{12\pi^2 f^2} \left\{\bar{l}_1 - \bar{l}_2 + \frac{65}{48}\right\} - \frac{2c_2 a^2}{16\pi^2 f^2} \left\{5\bar{\xi}_4(\mathcal{M}^2) - \frac{35}{6}\right\}\right) \\
&\quad + \frac{2c_2 a^2}{24\pi f^2} \left(\frac{2c_2 a^2}{16\pi^2 f^2} \left\{\frac{5}{12}\right\}\right). \tag{4.20}
\end{aligned}$$

Setting  $a = 0$ , the continuum result [1] is recovered again. The result for  $a_1^1$  looks different compared with  $a_0^0$  and  $a_0^2$ : There are no analytic corrections of order  $a^2$  and  $a^3$ , and also the term  $a^4 \ln \mathcal{M}^2$  is missing. This is because such contributions cancel when we compute the  $T^1$  amplitude by taking the difference  $A(t, s, u) - A(u, t, s)$ . Like for  $a_0^0$  and  $a_0^2$ , the scattering length  $a_1^1$  does not vanish in the chiral limit, though, the dependence on the lattice spacing is smaller due to the missing terms mentioned above.

## 4.2 Fitting formulae

As explained in section 1.4 we have to express the scattering lengths in terms of the physical pion mass  $M_\pi^2$  only. For this purpose we simply plug the



inverted pion mass (3.25) into the above scattering length and finally obtain:

$$a_0^0 = \frac{7}{32\pi} \frac{M_\pi^2}{f^2} \left( 1 + \frac{5}{84\pi^2} \frac{M_\pi^2}{f^2} \left\{ \bar{l}_1(M_\pi^2) + 2\bar{l}_2(M_\pi^2) - \frac{3}{8}\bar{l}_3(M_\pi^2) + \frac{21}{8} \right\} \right. \\ \left. + \frac{5}{7} k_1 \frac{W_0 a}{f^2} - \frac{5}{84\pi^2} \frac{2c_2 a^2}{f^2} \left\{ \frac{201}{40} \bar{\xi}_3(M_\pi^2) - \frac{33}{8} \bar{\xi}_4(M_\pi^2) + \frac{15}{4} \right\} \right) \\ - \frac{5}{32\pi} \frac{2c_2 a^2}{f^2} \left( 1 - \{k_3 + k_5\} \frac{W_0 a}{f^2} - k_4 \frac{2c_2 a^2}{f^2} - \frac{2c_2 a^2}{32\pi^2 f^2} \left\{ 11\bar{\xi}_5(M_\pi^2) + 1 \right\} \right), \quad (4.21)$$

$$a_0^2 = -\frac{M_\pi^2}{16\pi f^2} \left( 1 - \frac{M_\pi^2}{12\pi^2 f^2} \left\{ \bar{l}_1(M_\pi^2) + 2\bar{l}_2(M_\pi^2) - \frac{3}{8}\bar{l}_3(M_\pi^2) + \frac{3}{8} \right\} \right. \\ \left. - k_1 \frac{W_0 a}{f^2} - \frac{2c_2 a^2}{32\pi^2 f^2} \left\{ 11\bar{\xi}_4(M_\pi^2) - 5\bar{\xi}_3(M_\pi^2) + 2 \right\} \right) \\ - \frac{2c_2 a^2}{16\pi f^2} \left( 1 - \{k_3 + k_5\} \frac{W_0 a}{f^2} - k_4 \frac{2c_2 a^2}{f^2} - \frac{2c_2 a^2}{32\pi^2 f^2} \left\{ 11\bar{\xi}_5(M_\pi^2) - 7 \right\} \right). \quad (4.22)$$

Note that we have explicitly written  $\bar{l}_i(M_\pi^2)$  and  $\bar{\xi}_i(M_\pi^2)$  because the chiral logarithms in the low energy constants also change replacing  $\mathcal{M}^2$  by  $M_\pi^2$ . In principle, one should also replace the pion decay constant  $f$  of the chiral limit with the physical decay constant  $f_\pi$  to one loop. In the continuum, this would generate an explicit dependence on  $\bar{l}_4$ . Though,  $f_\pi$  has not been computed yet with lattice corrections in the LCE regime. It could be done by constructing the appropriate axial vector current and imposing a corresponding renormalization condition. Such a method is outlined in [30]. Here, however, we treat  $f$  simply as a free parameter.

For  $a_1^1$  we get analogously

$$a_1^1 = \frac{M_\pi^2}{24\pi f^2} \left( 1 - \frac{M_\pi^2}{12\pi^2 f^2} \left\{ \bar{l}_1(M_\pi^2) - \bar{l}_2(M_\pi^2) - \frac{3}{8}\bar{l}_3(M_\pi^2) + \frac{65}{48} \right\} \right. \\ \left. - k_1 \frac{W_0 a}{f^2} - \frac{2c_2 a^2}{16\pi^2 f^2} \left\{ -\frac{5}{2}\bar{\xi}_3(M_\pi^2) + 5\bar{\xi}_4(M_\pi^2) - \frac{35}{6} \right\} \right) \\ - \frac{2c_2 a^2}{24\pi f^2} \left( k_3 \frac{W_0 a}{f^2} + k_4 \frac{2c_2 a^2}{f^2} - \frac{2c_2 a^2}{16\pi^2 f^2} \left\{ \frac{5}{12} \right\} \right). \quad (4.23)$$

With this replacement,  $a_1^1$  now also depends on terms of  $\mathcal{O}(a^3)$ .

The above formulae can now be applied to fit scattering lengths obtained from simulations with unphysical pion masses to the physical point of  $M_\pi \simeq 135$  MeV or to the chiral limit. As a coproduct, one obtains numerical values for distinct linear combinations of low energy constants. Of special interest are, of course, the GL constants from the continuum, since they are the

LE constants of the “true” low energy expansion of QCD. Before the era of lattice QCD, these low energy constants could only be determined by phenomenological arguments and are indeed constants corresponding to the uniquely fixed pion mass of  $M_\pi \simeq 135$  MeV. This is the reason why one uses in continuum ChPT the scale independent GL constants  $\bar{l}_i$ . On the lattice where the quark mass and, hence, the pion mass is a variable, it is, therefore, useful to work with the scale dependent GL constants in the manner we have discussed them in (3.23). Expressing the scattering lengths with scale dependent LE constants the chiral logarithm with the renormalization scale  $\mu$  will explicitly appear in our formulae.

To give some practical formulae, we primarily assume to perform measurements at one fixed lattice spacing and we will later give the generalization to different lattice spacings. Focussing first on  $a_0^0$  and  $a_0^2$  the formulae read

$$a_0^0 = \frac{7M_\pi^2}{32\pi f^2} \left( \kappa_{01} + \frac{M_\pi^2}{32\pi^2 f^2} \left\{ 5 \ln \frac{M_\pi^2}{\mu^2} + \frac{10}{21} l_{\pi\pi}^{I=0} \right\} + \frac{2c_2 a^2}{32\pi^2 f^2} \left\{ \frac{32}{21} \ln \frac{M_\pi^2}{\mu^2} \right\} \right) - \frac{5 \cdot 2c_2 a^2}{32\pi f^2} \left( \kappa_{02} + \frac{2c_2 a^2}{32\pi^2 f^2} \left\{ 11 \ln \frac{M_\pi^2}{\mu^2} \right\} \right), \quad (4.24)$$

$$a_0^2 = -\frac{M_\pi^2}{16\pi f^2} \left( \kappa_{21} + \frac{M_\pi^2}{16\pi^2 f^2} \left\{ \frac{7}{2} \ln \frac{M_\pi^2}{\mu^2} - \frac{4}{3} l_{\pi\pi}^{I=2} \right\} + \frac{2c_2 a^2}{16\pi^2 f^2} \left\{ 3 \ln \frac{M_\pi^2}{\mu^2} \right\} \right) - \frac{2c_2 a^2}{16\pi f^2} \left( \kappa_{22} + \frac{2c_2 a^2}{16\pi^2 f^2} \left\{ \frac{11}{2} \ln \frac{M_\pi^2}{\mu^2} \right\} \right). \quad (4.25)$$

In  $l_{\pi\pi}^I$ , we collected the linear combination of GL constants for definite isospin channels:

$$l_{\pi\pi}^{I=0} = l_1 + 2l_2 - \frac{3}{8}l_3 + \frac{21}{8}, \quad l_{\pi\pi}^{I=2} = l_1 + 2l_2 - \frac{3}{8}l_3 + \frac{3}{8}. \quad (4.26)$$

In  $\kappa_{Ij}$ , we further collected analytic terms of  $\mathcal{O}(a)$  and  $\mathcal{O}(a^2)$ . At fixed lattice spacing the  $\kappa_{Ij}$  are constants except for the renormalization scale dependence  $\mu$  which enters through the  $\xi_i(\mu)$ .

Let us summarize qualitatively what we gained with this rewriting of the scattering length for one distinct isospin channel  $I$ : So far, we still have the parameters from continuous ChPT, i.e.  $f$  and  $l_{\pi\pi}^I$ , further, there are the lattice parameters  $c_2$ ,  $\kappa_{I1}$  and  $\kappa_{I2}$ . Hence, there are five independent fitting parameters. This allows us to write down the most general fitting formula in the LCE regime:

$$a_0^I = A_{00} + A_{10}M_\pi^2 + A_{20}M_\pi^4 + A_{30}M_\pi^4 \ln M_\pi^2 + A_{40}M_\pi^2 \ln M_\pi^2 + \tilde{A}_{40} \ln M_\pi^2. \quad (4.27)$$

$\tilde{A}_{40}$  is not an independent fitting parameter any more since, like  $A_{40}$ , it depends only on  $c_2$  and on  $f$  (and on the renormalization scale).

If one simultaneously analyzes data at different lattice spacings one must consider that the  $\kappa_{Ij}$  consist of two independent terms at any time, one of  $\mathcal{O}(a)$  and the other one of  $\mathcal{O}(a^2)$ . Thus, we have to write

$$\kappa_{Ij} = 1 + \kappa_{Ij}^{(1)}a + \kappa_{Ij}^{(2)}a^2. \quad (4.28)$$

In other words, the number of independent fitting parameters is increased from five to seven. In the case that one analyzes scattering lengths for the  $I = 0$  and for the  $I = 2$  channel simultaneously, one sees by comparing (4.21) and (4.22) that the  $\mathcal{O}(a)$  terms  $\kappa_{Ij}^{(1)}$  are correlated by

$$5\kappa_{01}^{(1)} = -7\kappa_{02}^{(1)}, \quad \kappa_{02}^{(1)} = \kappa_{22}^{(1)}. \quad (4.29)$$

One remaining point to tackle is the comparison of the scattering lengths between the GSM regime and the LCE regime. The formulae for the GSM regime are simply obtained by dropping all contributions of  $\mathcal{O}(a^3, a^4, M_\pi^2 a^2)$  in (4.21) and (4.22) since these are not present in the GSM regime.

$$a_0^0 = \frac{7M_\pi^2}{32\pi f^2} \left( 1 + \kappa_{01}^{(1)} + \frac{M_\pi^2}{32\pi^2 f^2} \left\{ 5 \ln \frac{M_\pi^2}{\mu^2} + \frac{10}{21} l_{\pi\pi}^{I=0} \right\} \right) - \frac{5 \cdot 2c_2 a^2}{32\pi f^2}, \quad (4.30)$$

$$a_0^2 = -\frac{M_\pi^2}{16\pi f^2} \left( 1 + \kappa_{21}^{(1)} + \frac{M_\pi^2}{16\pi^2 f^2} \left\{ \frac{7}{2} \ln \frac{M_\pi^2}{\mu^2} - \frac{4}{3} l_{\pi\pi}^{I=2} \right\} \right) - \frac{2c_2 a^2}{16\pi f^2}. \quad (4.31)$$

Now the  $\kappa_{Ij}$  are only of  $\mathcal{O}(a)$ . Together with  $f$ ,  $l_{\pi\pi}^{I=0}$  and  $c_2$ , there are four independent parameters and the fitting formulae exhibit the following functional form

$$a_0^I = A_{00} + A_{10}M_\pi^2 + A_{20}M_\pi^4 + A_{30}M_\pi^4 \ln M_\pi^2. \quad (4.32)$$

For completeness, we outline the discussion for the  $a_1^1$  case: Using the same arguments as above one arrives at

$$a_1^1 = \frac{M_\pi^2}{24\pi f^2} \left( \kappa_{11} - \frac{M_\pi^2}{24\pi^2 f^2} \left\{ \frac{3}{4} \ln \frac{M_\pi^2}{\mu^2} + 2l_{\pi\pi}^{I=1} \right\} + \frac{2c_2 a^2}{24\pi^2 f^2} \left\{ \frac{15}{4} \ln \frac{M_\pi^2}{\mu^2} \right\} \right) - \frac{2c_2 a^2}{24\pi f^2} \kappa_{12}, \quad (4.33)$$

where  $l_{\pi\pi}^{I=1} = l_1 - l_2 - \frac{3}{8}l_3 + \frac{65}{48}$  is defined in analogy to the  $a_0^0$  and  $a_0^2$  case. The structure of the coefficient  $\kappa_{11} = 1 + \kappa_{11}^{(1)}a + \kappa_{11}^{(2)}a^2$  is the same as in the

$I = 0, 2$  case,  $\kappa_{12} = \kappa_{12}^{(1)}a + \kappa_{12}^{(2)}a^2$  is slightly different due to the absence of the  $\mathcal{O}(a^2)$  terms in  $a_1^1$ . For a fixed lattice spacing, there are again five independent parameters:  $f$ ,  $l_{\pi\pi}^{I=1}$ ,  $c_2$ ,  $\kappa_{11}$  and  $\kappa_{12}$ . The corresponding fitting formula reads

$$a_1^1 = A_{01} + A_{11}M_\pi^2 + A_{21}M_\pi^4 + A_{31}M_\pi^4 \ln M_\pi^2 + A_{41}M_\pi^2 \ln M_\pi^2. \quad (4.34)$$

Note that a term  $\tilde{A}_{41} \ln M_\pi^2$  like in (4.27) does not appear. Further,  $A_{01}$  is at least of  $\mathcal{O}(a^3)$  why we expect  $a_1^1$  to become very small in the chiral limit.

If one has data for all three isospin channels one can make use of the fact that the  $\kappa_{I1}^{(1)}$  are all together related by

$$7\kappa_{01}^{(1)} = -5\kappa_{21}^{(1)} = -5\kappa_{11}^{(1)}. \quad (4.35)$$

A corresponding relation for  $\kappa_{12}^{(1)}$  cannot be derived because the relevant low energy constants of the  $\mathcal{O}(a^3)$  contribution are different in the  $a_1^1$  case: while for  $a_0^0$  and  $a_0^2$  their form is always  $\{k_3 + k_5\}$ ,  $k_5$  is completely missing in  $a_1^1$  and a matching is not possible.

It remains to discuss the GSM regime for  $a_1^1$ . We get the appropriate formulae again by dropping the contributions of  $\mathcal{O}(a^3, a^4, M_\pi^2 a^2)$ :

$$a_1^1 = \frac{M_\pi^2}{24\pi f^2} \left( 1 + \kappa_{11}^{(1)} - \frac{M_\pi^2}{24\pi^2 f^2} \left\{ \frac{3}{4} \ln \frac{M_\pi^2}{\mu^2} + 2l_{\pi\pi}^{I=1} \right\} \right) \quad (4.36)$$

Except for a correction of  $\mathcal{O}(aM_\pi^2)$  this is just the  $a_1^1$  scattering length from continuum ChPT.

# Conclusion and outlook

In this diploma thesis, we computed the one-loop scattering lengths  $a_0^0$ ,  $a_0^2$  and  $a_1^1$  in WChPT in order to have analytic expressions at hand to extrapolate numerical data obtained from pion scattering to the physical point.

The remarkable result of our computation in the LCE regime is that the one-loop scattering lengths do not vanish in the chiral limit at non-zero lattice spacing. While this effect is small for  $a_1^1$  due to analytic corrections of  $\mathcal{O}(a^3, a^4)$ , it is substantial for  $a_0^0$  and  $a_0^2$ . There, the remaining analytic terms are of  $\mathcal{O}(a^2)$ , and in addition, there is also a singular chiral logarithm proportional to  $a^4 \ln M_\pi^2$ .

For all isospin channels, there is besides the traditional chiral logarithm from continuum ChPT another chiral logarithm proportional to  $a^2 M_\pi^2 \ln M_\pi^2$ . Hence, using the formulae from continuum ChPT to extrapolate lattice data from larger pion masses to the physical point can easily lead to erroneous results. The careful analysis of the quark mass regime and the appropriate application of the formulae that were developed in this work should lead to a better extrapolation. A future project which employs our formulae to fit the available data from the CP-PACS collaboration [5] would be of great interest.

If one uses pion scattering to numerically determine the GL coefficients, one often misses the expected characteristic logarithmic curvature of continuum ChPT. Our formulae give an explanation how the functional form can easily be deluted. Using our result takes the lattice artifacts directly into account and should give better estimates for the desired constants.

The scattering lengths exhibit a direct dependence on the parameter  $c_2$  which determines the phase diagram of the theory. Therefore, we propose to use pion scattering to get a quantitative picture of this parameter. At least the sign of  $c_2$  is supposed to be determined from an extrapolation to the chiral limit.

It would be interesting to repeat the whole computation for the twisted mass case. Since the presence of a twisted mass term explicitly breaks isospin symmetry, the isospin decomposition of the amplitude has to be modified.

The computation for 2+1 flavors, however, should be the most tempting challenge. In this case, the trace relations that we used to simplify the lagrangian are not valid any more and much more operators must be considered. This means that the number of independent LE constants increases. Further, due to the lack of quark mass degeneracy, the on-shell condition strongly depends on the particle content and is not the same for all “participants” as it was in this work. We hope that these computations will soon be performed.

# Appendix A

## Trace relations

The motivation for the analysis is to find relations between different operators in  $SU(2)$ , for example between  $\langle \Sigma + \Sigma^\dagger \rangle^2$  and  $\langle \Sigma \Sigma + \Sigma^\dagger \Sigma^\dagger \rangle$ .  $\Sigma = \exp(i\vec{\sigma}\vec{\pi}(x)/f)$  is the exponential realization described in chapter 1.3, as usual. As an  $SU(2)$  matrix, it has the unitarity properties  $\Sigma^\dagger \Sigma = \Sigma \Sigma^\dagger = \mathbf{1}$  and  $\det \Sigma = 1$ . This can also be written as

$$\Sigma = A(x) \mathbf{1} + i\vec{B}(x) \cdot \vec{\sigma} \quad (\text{A.1})$$

with the additional constraint

$$A^2 + \vec{B}^2 = 1 \quad (\text{A.2})$$

where  $A(x)$  and  $\vec{B}(x)$  are real space-time dependent parameters. One easily checks that this parametrization indeed fullfills the unitarity conditions:

$$\Sigma^\dagger \Sigma = \Sigma \Sigma^\dagger = A^2 - i^2(\vec{B}\vec{\sigma})(\vec{B}\vec{\sigma}) = A^2 + \vec{B}^2 = 1 \quad (\text{A.3})$$

where we have used  $(\vec{B}\vec{\sigma})(\vec{B}\vec{\sigma}) = \vec{B}^2$  and (A.2). Further, we can write:

$$\det \Sigma = \begin{vmatrix} A + iB_3 & iB_1 + B_2 \\ iB_1 - B_2 & A - iB_3 \end{vmatrix} = A^2 + B_3^2 - (-B_1^2 - B_2^2) = 1. \quad (\text{A.4})$$

First we derive in a direct brute force computation a relation between  $\langle \Sigma + \Sigma^\dagger \rangle^2$  and  $\langle \Sigma \Sigma + \Sigma^\dagger \Sigma^\dagger \rangle$ :

$$\Sigma \Sigma = (A + i\vec{B}\vec{\sigma})^2 = A^2 + 2Ai\vec{B}\vec{\sigma} - \vec{B}^2 \quad (\text{A.5})$$

$$\Sigma^\dagger \Sigma^\dagger = (A - i\vec{B}\vec{\sigma})^2 = A^2 - 2Ai\vec{B}\vec{\sigma} - \vec{B}^2 \quad (\text{A.6})$$

$$\langle \Sigma \Sigma + \Sigma^\dagger \Sigma^\dagger \rangle = \langle 2A^2 - 2B^2 \rangle = 8A^2 - 4 \quad (\text{A.7})$$

$$\langle \Sigma + \Sigma^\dagger \rangle^2 = \langle 2A \rangle^2 = 16A^2 \quad (\text{A.8})$$

and we can conclude:

$$\langle \Sigma \Sigma + \Sigma^\dagger \Sigma^\dagger \rangle = \frac{1}{2} \langle \Sigma + \Sigma^\dagger \rangle^2 - 4. \quad (\text{A.9})$$

This is the desired relation. If we are interested in relations of the lagrangian which involves  $\langle \Sigma \Sigma + \Sigma^\dagger \Sigma^\dagger \rangle$  and  $\langle \Sigma + \Sigma^\dagger \rangle^2$  only separately, i.e. two terms with its own low energy constant, we can drop the additive constant in eq. (A.9) since a constant on lagrangian level does not affect the equations of motion. This is, for example, the case in  $\mathcal{L}_4$  and  $\mathcal{L}'_4$  in eqs. (1.65) and (1.66) and we can write

$$\langle \Sigma \Sigma + \Sigma^\dagger \Sigma^\dagger \rangle = \frac{1}{2} \langle \Sigma + \Sigma^\dagger \rangle^2. \quad (\text{A.10})$$

Yet, if we consider terms like, for example,  $\langle \Sigma \Sigma + \Sigma^\dagger \Sigma^\dagger \rangle \cdot \langle \Sigma + \Sigma^\dagger \rangle$  we must include the constant because otherwise we would loose dynamical information.

At this point, we can convince ourselves that the parity breaking operators  $\langle \Sigma - \Sigma^\dagger \rangle$  and  $\langle \Sigma \Sigma - \Sigma^\dagger \Sigma^\dagger \rangle$  vanish. This can be seen by the direct application of (A.1), (A.5) and (A.6) in

$$\langle \Sigma - \Sigma^\dagger \rangle = 2i\vec{B} \langle \vec{\sigma} \rangle = 0, \quad (\text{A.11})$$

$$\langle \Sigma \Sigma - \Sigma^\dagger \Sigma^\dagger \rangle = 4iA\vec{B} \langle \vec{\sigma} \rangle = 0 \quad (\text{A.12})$$

where we used the fact that the Pauli matrices are traceless.

To get more intricate trace relations we make use of the Cayley–Hamilton theorem [31]. Let  $A$  be a real or complex valued square  $n \times n$  matrix and

$$P(\lambda) = \det(\lambda \mathbf{1} - A) \quad (\text{A.13})$$

its characteristic polynomial. The Cayley–Hamilton theorem states that substituting the matrix  $A$  in the characteristic polynomial results in the zero matrix:

$$P(A) = 0. \quad (\text{A.14})$$

A neat proof of an algorithm to determine the coefficients of the characteristic polynomial is given in [32]. The special feature there is that the coefficients only appear as functions of the traces of its successive powers. One starts with  $n = 1$  and obtains recursively  $P(A)$  for any given  $n$ . Our case of interest is, of course,  $n = 2$ . One obtains:

$$0 = P(A) = A^2 - \langle A \rangle A + \frac{1}{2} \left( \langle A \rangle^2 - \langle A^2 \rangle \right) \mathbf{1}. \quad (\text{A.15})$$



This equation fits perfectly to determine trace relations of matrices. For this purpose, we multiply (A.15) with  $A$  and take the trace of the whole equation to get

$$\langle A^3 \rangle - \frac{3}{2} \langle A^2 \rangle \langle A \rangle + \frac{1}{2} \langle A \rangle^3 = 0 \quad (\text{A.16})$$

Now we make the Ansatz  $A = \lambda_1 A_1 + \lambda_2 A_2 + \lambda_3 A_3$ . After some algebra we end up with the following expression:

$$\sum_{2 \text{ perm}} \langle A_1 A_2 A_3 \rangle - \sum_{3 \text{ perm}} \langle A_1 A_2 \rangle \langle A_3 \rangle + \langle A_1 \rangle \langle A_2 \rangle \langle A_3 \rangle = 0. \quad (\text{A.17})$$

With this equation, we can find explicit relations by substituting  $A_1$ ,  $A_2$ , and  $A_3$  in (A.17) with matrices of our interest. Before doing so, we introduce two useful formulae:

$$(\partial_\mu \Sigma^\dagger) \Sigma = -\Sigma^\dagger (\partial_\mu \Sigma), \quad (\text{A.18})$$

$$\langle \Sigma \partial_\mu \Sigma^\dagger \rangle = 0. \quad (\text{A.19})$$

The first one follows from differentiating the unity operator  $\partial_\mu \mathbf{1} = \partial_\mu (\Sigma^\dagger \Sigma) = 0$ . The second one can be seen in the following short derivation:

$$\begin{aligned} 0 &= \partial_\mu \det \Sigma = \partial_\mu (e^{\log \det \Sigma}) \\ &= e^{\log \det \Sigma} \partial_\mu (\log \det \Sigma) = \partial_\mu (\text{tr} \log \Sigma) \\ &= \text{tr} (\Sigma^\dagger \partial_\mu \Sigma) = \langle \Sigma^\dagger \partial_\mu \Sigma \rangle = \langle \Sigma \partial_\mu \Sigma^\dagger \rangle. \end{aligned}$$

In order to get from the second line to the third line, we used the fact that unitary matrices can be diagonalized and that  $\Sigma^{-1} = \Sigma^\dagger$ .

In a first example, we now set  $A_1 = A_2 = \Sigma \partial_\mu \Sigma^\dagger$  and  $A_3 = \partial_\mu \Sigma \partial_\mu \Sigma^\dagger$ . Using (A.18) and (A.19) and the cyclic property of traces we arrive at the following trace relation:

$$\langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \partial_\nu \Sigma \partial_\nu \Sigma^\dagger \rangle = \frac{1}{2} \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle^2. \quad (\text{A.20})$$

In a second example, we set  $A_1 = A_2 = \Sigma \partial_\mu \Sigma^\dagger$  and  $A_3 = \Sigma + \Sigma^\dagger$ . Using again (A.18) and (A.19) and the cyclic property of traces we arrive at

$$\langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger (\Sigma + \Sigma^\dagger) \rangle = \frac{1}{2} \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle \langle \Sigma + \Sigma^\dagger \rangle. \quad (\text{A.21})$$

Further, we want to evaluate trace relations involving three operators like  $\langle \Sigma \Sigma \Sigma + \Sigma^\dagger \Sigma^\dagger \Sigma^\dagger \rangle$ . Successively substituting  $\{A_1, A_2, A_3\}$  in (A.17) by

$\{\Sigma, \Sigma, \Sigma\}$ ,  $\{\Sigma, \Sigma, \Sigma^\dagger\}$ ,  $\{\Sigma, \Sigma^\dagger, \Sigma^\dagger\}$ , and  $\{\Sigma^\dagger, \Sigma^\dagger, \Sigma^\dagger\}$  we get four independent equations. These resulting four equations can be cleverly combined to

$$\langle \Sigma + \Sigma^\dagger \rangle^3 = 2 \langle \Sigma \Sigma \Sigma + \Sigma^\dagger \Sigma^\dagger \Sigma^\dagger \rangle - 3 \langle \Sigma + \Sigma^\dagger \rangle \cdot \langle \Sigma \Sigma + \Sigma^\dagger \Sigma^\dagger \rangle$$

which by use of eq. (A.9) reads as

$$\langle \Sigma \Sigma \Sigma + \Sigma^\dagger \Sigma^\dagger \Sigma^\dagger \rangle = \frac{5}{4} \langle \Sigma + \Sigma^\dagger \rangle^3 - 6 \langle \Sigma + \Sigma^\dagger \rangle. \quad (\text{A.22})$$

# Appendix B

## Loop integrals in dimensional regularization

The divergent loop integrals which we encountered in chapter 3 are regularized in dimensional regularization. This is done by performing the calculation in a dimension  $D = 4 - \epsilon$  different from four by means of a regulator  $\epsilon$ . With this procedure, one can isolate the singularities as simple poles of analytic functions for  $\epsilon = 0$ , and they can be absorbed into the renormalized LE constants.

The divergent loop integrals exhibit the following general structure:

$$A = \int \frac{d^D k}{(2\pi)^D} \frac{a}{k^2 + \mathcal{M}^2} \quad (\text{B.1})$$

$$B = \int \frac{d^D k}{(2\pi)^D} \frac{b}{(k^2 + \mathcal{M}^2)((k+p)^2 + \mathcal{M}^2)} \quad (\text{B.2})$$

where  $a$  and  $b$  can obtain the values

$$\begin{aligned} a &= 1, k^2, \\ b &= 1, k_\mu, k \cdot p, k^2, (k \cdot p)^2, k^2(k \cdot p), k^4, k_\mu k_\nu. \end{aligned}$$

The direct calculation shows that all of them can basically be expressed by the two scalar integrals

$$A_0(\mathcal{M}^2) = \int \frac{d^D k}{(2\pi)^D} \frac{1}{k^2 + \mathcal{M}^2}, \quad (\text{B.3})$$

$$B_0(p^2, \mathcal{M}^2) = \int \frac{d^D k}{(2\pi)^D} \frac{1}{(k^2 + \mathcal{M}^2)((k+p)^2 + \mathcal{M}^2)}. \quad (\text{B.4})$$

Usually, one includes in the definition of the regularized loop integrals the factor  $\mu^\epsilon$  with  $\mu$  the renormalization scale such that the dimension of the integrals is always an integer which in our case is four. In our case, this factor is already included in the definition of the renormalized Gasser-Leutwyler constants in (1.50) and need not to be considered here. For the computation of the two scalar integrals (B.3) and (B.4) we employ the following general formula (eq. 7.86 in [26])

$$\int \frac{d^D k}{(2\pi)^D} \frac{1}{(k^2 + L)^n} = \frac{1}{(4\pi)^{D/2}} \frac{\Gamma(n - D/2)}{\Gamma(n)} L^{-n + \frac{D}{2}}. \quad (\text{B.5})$$

In order to compute (B.3) we set  $n = 1$  and  $L = \mathcal{M}^2$ , and simply expand (B.5) around  $D = 4$  respectively around  $\epsilon = 0$ . One immediately sees that in this case, the gamma function  $\Gamma(-1 + \frac{\epsilon}{2})$  gets singular. With  $\Gamma(z+1) = z\Gamma(z)$ , we can expand the singularity around  $\epsilon = 0$ :

$$\begin{aligned} \Gamma\left(1 - \frac{D}{2}\right) &= \frac{\Gamma\left(1 - \frac{D}{2} + 1\right)}{\left(1 - \frac{D}{2}\right)} = \frac{\Gamma\left(2 - \frac{D}{2} + 1\right)}{\left(1 - \frac{D}{2}\right)\left(2 - \frac{D}{2}\right)} = \frac{\Gamma\left(1 + \frac{\epsilon}{2}\right)}{\left(-1 + \frac{\epsilon}{2}\right)\frac{\epsilon}{2}} \\ &= -\frac{2}{\epsilon} \left(\Gamma(1) + \frac{\epsilon}{2}\Gamma'(1) + \mathcal{O}(\epsilon^2)\right) = -\frac{2}{\epsilon} - \gamma + \mathcal{O}(\epsilon) \end{aligned} \quad (\text{B.6})$$

where  $\gamma := \Gamma'(1) = 0.577\dots$  is the Euler-Mascheroni constant. Having this result at hand, the expansion of (B.3) around  $\epsilon = 0$  reads

$$\begin{aligned} A_0(\mathcal{M}^2) &= -\frac{\mathcal{M}^2}{16\pi^2} \left(\frac{2}{\epsilon} - \gamma + \ln 4\pi + 1 - \ln \mathcal{M}^2\right) \\ &= -\frac{\mathcal{M}^2}{16\pi^2} (\Delta + 1 - \ln \mathcal{M}^2) \end{aligned} \quad (\text{B.7})$$

where we defined the shorthand notation

$$\Delta = \frac{2}{\epsilon} - \gamma + \ln 4\pi. \quad (\text{B.8})$$

For the evaluation of the  $B_0$  integral (B.4), we use Feynman-parameters to write it in a suitable form in order to apply formula (B.5). With

$$\frac{1}{ab} = \int_0^1 dx \frac{1}{[ax + b(1-x)]^2}, \quad (\text{B.9})$$

the integral can be written as

$$B_0(p^2, \mathcal{M}^2) = \int_0^1 dx \int \frac{d^D k}{(2\pi)^D} \frac{1}{[(k - p(1-x))^2 + p^2 x(1-x) + \mathcal{M}^2]^2}. \quad (\text{B.10})$$

Identifying  $p^2x(1-x) + \mathcal{M}^2 = L(x)$  and performing a shift of the integration variables  $q^2 = (k - p(1-x))^2$  which leaves the measure invariant we arrive at the canonical form

$$\begin{aligned} B_0(p^2, \mathcal{M}^2) &= \int_0^1 dx \int \frac{d^D q}{(2\pi)^D} \frac{1}{(q^2 + L(x))^2} \\ &= \int_0^1 dx \frac{1}{(4\pi)^{D/2}} \frac{\Gamma(2 - D/2)}{\Gamma(n)} L(x)^{-2 + \frac{D}{2}}. \end{aligned} \quad (\text{B.11})$$

An analogous expansion around  $\epsilon = 0$  which we already discussed for the  $A_0(\mathcal{M}^2)$  integral leads to the following analytic expression:

$$B_0(p^2, \mathcal{M}^2) = \frac{1}{16\pi^2} \left( \Delta - \ln \mathcal{M}^2 - I(p^2, \mathcal{M}^2) \right). \quad (\text{B.12})$$

with

$$I(p^2, \mathcal{M}^2) = \int_0^1 dx \ln \left[ \frac{p^2}{\mathcal{M}^2} x(1-x) + 1 \right]. \quad (\text{B.13})$$

The remaining integral  $I(p^2)$  is discussed in detail in [33]. Some subtleties have to be considered when rotating back to Minkowski space concerning the phase definition of the complex logarithm. In the result, then, three different cases need to be distinguished depending on the magnitude of  $p^2$ :

$$I(-p^2, \mathcal{M}^2) = \begin{cases} -2 - \sigma \ln \frac{\sigma-1}{\sigma+1}, & p^2 < 0 \\ -2 + 2\sqrt{\frac{4\mathcal{M}^2}{p^2} - 1} \operatorname{arccot} \left( \sqrt{\frac{4\mathcal{M}^2}{p^2} - 1} \right), & 0 \leq p^2 < 4\mathcal{M}^2 \\ -2 - \sigma \ln \frac{1-\sigma}{1+\sigma} - i\pi\sigma, & 4\mathcal{M}^2 \leq p^2 \end{cases} \quad (\text{B.14})$$

where we defined

$$\sigma = \sqrt{1 - \frac{4\mathcal{M}^2}{p^2}}, \quad p^2 \notin [0, 4\mathcal{M}^2]. \quad (\text{B.15})$$

Important for the present work is the situation in which  $p^2$  is one of the Mandelstam variables. Due to the relation (2.35) one immediately sees that  $s \geq 4M_\pi^2 = 4\mathcal{M}^2$  (the latter equality holds at one loop level) and, hence, the last case in (B.14) has to be applied. Contrarily, we learn from (2.36) and (2.37) that both  $t$  and  $u$  are less than zero, i.e. for them, the first case holds. Defining the function

$$F(p^2) = \begin{cases} \sigma \ln \frac{1-\sigma}{1+\sigma} - i\pi\sigma, & \text{for } p^2 = s \\ \sigma \ln \frac{\sigma-1}{\sigma+1}, & \text{for } p^2 = t, u \end{cases} \quad (\text{B.16})$$

we can write down the expression for  $B_0$  in Minkowski space

$$B_0(-p^2, \mathcal{M}^2) = \frac{1}{16\pi^2} \left( \Delta - \ln \mathcal{M}^2 + 2 + F(p^2) \right) \quad (\text{B.17})$$

All other loop integrals for the distinct choices of  $a$  and  $b$  in (B.1) and (B.2) can now be expressed by means of  $A_0(\mathcal{M}^2)$  and  $B_0(\mathcal{M}^2, p^2)$ . For example, the case  $a = k^2$  is recovered by writing  $k^2 = (k^2 + \mathcal{M}^2) - \mathcal{M}^2$  which leads to two integrals of the form (B.5), one for  $n = 0$  and the other one for  $n = 1$ . The idea is always to write the numerators in such a way that one can, after some algebra or, for example, a partial fraction expansion, apply the already well known formulae. For completeness, we list all the integrals which we will use in our computations. A more detailed description can be found in [33]. For simplicity, we write  $A_0 = A_0(\mathcal{M}^2)$  and  $B_0 = B_0(p^2, \mathcal{M}^2)$ .

1-point integrals:

$$\int \frac{d^D k}{(2\pi)^D} \frac{1}{k^2 + \mathcal{M}^2} = A_0(\mathcal{M}^2) \quad (\text{B.18})$$

$$\int \frac{d^D k}{(2\pi)^D} \frac{k^2}{k^2 + \mathcal{M}^2} = -\mathcal{M}^2 A_0 \quad (\text{B.19})$$

2-point integrals:

$$\int \frac{d^D k}{(2\pi)^D} \frac{1}{(k^2 + \mathcal{M}^2)((k+p)^2 + \mathcal{M}^2)} = B_0 \quad (\text{B.20})$$

$$\int \frac{d^D k}{(2\pi)^D} \frac{k_\mu}{(k^2 + \mathcal{M}^2)((k+p)^2 + \mathcal{M}^2)} = -\frac{p_\mu}{2} B_0 \quad (\text{B.21})$$

$$\int \frac{d^D k}{(2\pi)^D} \frac{kp}{(k^2 + \mathcal{M}^2)((k+p)^2 + \mathcal{M}^2)} = -\frac{p^2}{2} B_0 \quad (\text{B.22})$$

$$\int \frac{d^D k}{(2\pi)^D} \frac{k^2}{(k^2 + \mathcal{M}^2)((k+p)^2 + \mathcal{M}^2)} = A_0 - \mathcal{M}^2 B_0 \quad (\text{B.23})$$

$$\int \frac{d^D k}{(2\pi)^D} \frac{(kp)^2}{(k^2 + \mathcal{M}^2)((k+p)^2 + \mathcal{M}^2)} = \frac{p^2}{2} A_0 + \frac{p^4}{4} B_0 \quad (\text{B.24})$$

$$\int \frac{d^D k}{(2\pi)^D} \frac{k^2(kp)}{(k^2 + \mathcal{M}^2)((k+p)^2 + \mathcal{M}^2)} = -\frac{p^2}{2} (2A_0 - \mathcal{M}^2 B_0) \quad (\text{B.25})$$

$$\int \frac{d^D k}{(2\pi)^D} \frac{k^4}{(k^2 + \mathcal{M}^2)((k+p)^2 + \mathcal{M}^2)} = (p^2 - 2\mathcal{M}^2)A_0 + m^4 B_0 \quad (\text{B.26})$$

$$\begin{aligned}
\int \frac{d^D k}{(2\pi)^D} \frac{k_\mu k_\nu}{(k^2 + \mathcal{M}^2)((k+p)^2 + \mathcal{M}^2)} &= \frac{1}{6} \delta_{\mu\nu} \left( A_0 - \frac{1}{2}(p^2 + 4\mathcal{M}^2)B_0 \right) \\
&+ \frac{1}{3} \frac{p_\mu p_\nu}{p^2} \left( A_0 + (p^2 + \mathcal{M}^2)B_0 \right) + \frac{1}{96\pi^2} (p^2 + 6\mathcal{M}^2) \frac{p_\mu p_\nu - p^2 \delta_{\mu\nu}}{3p^2}
\end{aligned} \tag{B.27}$$

# Appendix C

## Scattering length formalism

### C.1 Partial wave expansion

In this section, we will give a more detailed description how the scattering length and the transition amplitude are related. The derivation is presented according to [25]. First, we want to specialize the asymptotic states  $|i\rangle$  and  $|f\rangle$  from section 2.4. As already mentioned the particles are considered as free long before and long after the collision. Then both  $|i\rangle$  and  $|f\rangle$  are described by a direct product of single particle states  $|p_A, p_B\rangle = |p_A\rangle \otimes |p_B\rangle$  with Lorentz invariant normalization

$$\langle p_A, p_B | p'_A, p'_B \rangle = 2p_{A0} \delta(\mathbf{p}_A - \mathbf{p}'_A) 2p_{B0} \delta(\mathbf{p}_B - \mathbf{p}'_B). \quad (\text{C.1})$$

The states do not exhibit any spin dependence since we are dealing with pions whose spin is zero. In a next step we separate in our two particle state the center of mass motion  $\mathbf{p} = \mathbf{p}_A + \mathbf{p}_B$  from the relative motion  $\mathbf{q} = \frac{1}{2}(\mathbf{p}_A - \mathbf{p}_B)$ . This allows us to write

$$|p_A, p_B\rangle = |\mathbf{p}, \mathbf{q}\rangle = |p, \Omega_{\mathbf{q}}\rangle = |p\rangle \otimes |\Omega_{\mathbf{q}}\rangle \quad (\text{C.2})$$

This notation indicates that the two-particle state is described by six independent parameters. Instead of using  $\mathbf{p}$  and  $\mathbf{q}$  we will use the total four-momentum and the angular variables  $\Omega_{\mathbf{q}}$  since the angular variables fit better for partial wave analysis. Further, we can write:

$$\delta(\mathbf{p}_A - \mathbf{p}'_A) \delta(\mathbf{p}_B - \mathbf{p}'_B) = \delta(\mathbf{p} - \mathbf{p}') \delta(\mathbf{q} - \mathbf{q}') \quad (\text{C.3})$$



Now, we formulate the delta function containing  $\mathbf{q}$  in terms of angular variables and the total energy  $p_0$

$$\begin{aligned}\delta(\mathbf{q} - \mathbf{q}') &= \frac{1}{|\mathbf{q}|^2} \delta(|\mathbf{q}| - |\mathbf{q}'|) \delta(\Omega_{\mathbf{q}} - \Omega_{\mathbf{q}'}) \\ &= \frac{1}{|\mathbf{q}|^2} \mathcal{J}^{-1} \delta(p_0 - p'_0) \delta(\Omega_{\mathbf{q}} - \Omega_{\mathbf{q}'}). \end{aligned} \quad (\text{C.4})$$

Here,  $\delta(\Omega_{\mathbf{q}} - \Omega_{\mathbf{q}'}) = \delta(\cos \vartheta - \cos \vartheta') \delta(\varphi - \varphi')$  are the angular variables of  $\mathbf{k}$  and  $\mathbf{k}'$ , respectively.  $\mathcal{J} = \partial|\mathbf{q}|/\partial p_0$  is the Jacobian for the transformation of the delta function from  $|\mathbf{q}(p_0)|$  to  $p_0$ . It is evaluated in the center of mass system where  $p_0 = (m_A^2 + \mathbf{q}^2)^{1/2} + (m_B^2 + \mathbf{q}^2)^{1/2}$  and reads

$$\mathcal{J} = \frac{\partial|\mathbf{q}|}{\partial p_0} = \frac{p_{A0} p_{B0}}{p_0 |\mathbf{q}|}. \quad (\text{C.5})$$

Plugging the last three equations into (C.1) and using  $p_0^{\text{c.m.}} = \sqrt{s}$  we finally obtain

$$\langle p_A, p_B | p'_A, p'_B \rangle = \langle p, \Omega_{\mathbf{q}} | p', \Omega_{\mathbf{q}'} \rangle = \frac{4\sqrt{s}}{q} \delta^{(4)}(p - p') \delta(\Omega_{\mathbf{q}} - \Omega_{\mathbf{q}'}). \quad (\text{C.6})$$

This is the normalization where we have separated the total momentum conservation from the relative motion. (From now on, we write again  $q$  instead of  $|\mathbf{q}|$  due to simplicity of notation.) In [25] it is shown that one now can define a completeness relation which explicitly takes into account this feature.

$$1 = 1_{\text{c.m.}} \otimes 1_{\text{rel.}}$$

$$1_{\text{c.m.}} = \int d^4 p |p\rangle \langle p| \quad (\text{C.7})$$

$$1_{\text{rel.}} = \frac{q}{4\sqrt{s}} \sum_{l,m} |l, m\rangle \langle l, m|. \quad (\text{C.8})$$

We will use this equation below. With (C.6), we can write eq. (2.41) as follows:

$$\begin{aligned}\langle p_A, p_B | S | p'_A, p'_B \rangle &= \langle p_A, p_B | p'_A, p'_B \rangle + i \delta(p - p') T(i \rightarrow f) \\ &= \delta^{(4)}(p - p') \left\{ 4 \frac{\sqrt{s}}{q} \delta(\Omega_{\mathbf{q}} - \Omega_{\mathbf{q}'}) + i T(i \rightarrow f) \right\}. \end{aligned} \quad (\text{C.9})$$

As pointed out in section 2.4 the scattering process itself depends on two independent variables only. Working with the center of mass energy  $\sqrt{s}$  and

the center of mass scattering angle  $\cos \theta$ , the scattering amplitude can be written

$$T(i \rightarrow f) = T(s, \cos \theta). \quad (\text{C.10})$$

$T(s, \cos \theta)$  is now expanded in Legendre Polynomials

$$T(s, \cos \theta) = \sum_{l=0}^{\infty} (2l+1) P_l(\cos \theta) T_l(s). \quad (\text{C.11})$$

The  $T_l(s)$  are called *partial wave amplitudes*. They depend solely on  $s$  while the angular dependence is completely absorbed in the Legendre polynomials. In a next step we rewrite in (C.9) the part which corresponds to no interaction in terms of legendre polynomials. With the completeness relation and the addition theorem for the spherical harmonics [34]

$$\sum_{l=0}^{\infty} \sum_{m=-l}^{+l} Y_{lm}^*(\vartheta, \varphi) Y_{lm}(\vartheta', \varphi') = \delta(\cos \vartheta - \cos \vartheta') \delta(\varphi - \varphi') \quad (\text{C.12})$$

$$\sum_{m=-l}^{+l} Y_{lm}^*(\vartheta, \varphi) Y_{lm}(\vartheta', \varphi') = \frac{2l+1}{4\pi} P_l(\cos \theta) \quad (\text{C.13})$$

where  $\theta = \sphericalangle(\vartheta\varphi, \vartheta'\varphi')$  is the scattering angle between  $\mathbf{q}$  and  $\mathbf{q}'$  we can write (C.9) as

$$\langle p_A, p_B | S | p'_A, p'_B \rangle = \delta^{(4)}(p - p') \sum_{l=0}^{\infty} (2l+1) P_l(\cos \theta) \left\{ \frac{s^{1/2}}{q\pi} + i T_l(s) \right\}. \quad (\text{C.14})$$

To compare both sides with each other we write

$$\begin{aligned} \langle p_A, p_B | S | p'_A, p'_B \rangle &= \langle p | \otimes \langle \Omega_{\mathbf{q}} | S | \Omega_{\mathbf{q}} \rangle \otimes | p \rangle = \delta^{(4)}(p - p') \langle \Omega_{\mathbf{q}} | S | \Omega_{\mathbf{q}} \rangle \\ &= \delta^{(4)}(p - p') \sum_{l,m} \sum_{l',m'} Y_{lm}^*(\Omega_{\mathbf{q}}) Y_{l'm'}(\Omega_{\mathbf{q}'}) \langle l, m | S | l', m' \rangle \\ &= \delta^{(4)}(p - p') \sum_{l=0}^{\infty} (2l+1) P_l(\cos \theta) \frac{1}{4\pi} S_l. \end{aligned} \quad (\text{C.15})$$

In the first line we have used (C.2) and translation invariance of  $S$ . In the second line we have expanded  $|\Omega_{\mathbf{q}}\rangle$  in terms of  $|l, m\rangle$  and in the third line, we made use of  $\langle l, m | S | l', m' \rangle = S_l \delta_{ll'} \delta_{mm'}$ . This last relation is valid due to the Wigner-Eckhart theorem and the rotational invariance of  $S$ . Details can be found in [35]. Comparing (C.14) and (C.15) we arrive at the following relation:

$$S_l = \frac{4s^{1/2}}{q} + 4\pi i T_l(s). \quad (\text{C.16})$$

This looks nice but it is actually not suitable for getting information about the quantity of interest, the scattering amplitude. There is still one property of  $S$  which we have not used yet: Unitarity, i.e.  $S^\dagger S = 1$ . From (C.6) we can deduce  $(4s^{1/2}/q)\delta_{ll'}\delta_{mm'} = \langle lm|l'm'\rangle$ . Inserting the unitarity relation and using the completeness relation (C.8) we finally get

$$\begin{aligned}
\frac{4s^{1/2}}{q} \delta_{ll'}\delta_{mm'} &= \langle l, m|l', m'\rangle = \langle l, m|S^\dagger S|l', m'\rangle \\
&= \sum_{l'', m''} \langle l, m|S^\dagger \frac{q}{4s^{1/2}}|l'', m''\rangle \langle l'', m''|S|l', m'\rangle \\
&= \frac{q}{4s^{1/2}} \sum_{l'', m''} \langle l'', m''|S|l', m'\rangle^* \langle l'', m''|S|l, m\rangle \\
&= \frac{q}{4s^{1/2}} S_l^* S_l \delta_{ll'}\delta_{mm'}. \tag{C.17}
\end{aligned}$$

This equation is fulfilled if  $S_l^* S_l = (4s^{1/2}/q)^2$ . Therefore, we can write

$$S_l = \frac{4s^{1/2}}{q} e^{2i\delta_l(s)}. \tag{C.18}$$

The factor of 2 in the exponent is convention. The  $\delta_l(s)$  are the *phase shifts*. They depend only on the energy and are specific real numbers for each  $l$ . Plugging (C.18) into (C.16) and performing some simple algebra we obtain the desired expression for the scattering amplitude

$$T_l(s) = \frac{2}{\pi} \frac{s^{1/2}}{q} \sin \delta_l e^{i\delta_l}. \tag{C.19}$$

With this result we can write the partial wave expansion in (C.11) as

$$T(s, \cos \theta) = \frac{2s^{1/2}}{\pi q} \sum_{l=0}^{\infty} (2l+1) P_l(\cos \theta) \sin \delta_l(s) e^{i\delta_l(s)}. \tag{C.20}$$

## C.2 Effective range formalism

In a last step we relate the partial wave amplitudes  $T_l$  to the scattering length. For this purpose we define a function  $\Phi_l$

$$T_l(s) = \frac{4}{\pi} q^{2l} \left\{ \Phi_l - \frac{2i}{s^{1/2}} q^{2l+1} \right\}^{-1}. \tag{C.21}$$

If we express  $\Phi_l(q^2)$  in terms of the phase shift

$$\Phi_l = \frac{2q^{2l+1}}{s^{1/2}} \cot \delta_l, \tag{C.22}$$

equation (C.21) coincides indeed with (C.19). In [36] it is shown very generally that for *interactions with finite range*,  $\Phi_l = \Phi_l(q^2)$  is an analytic function in  $q^2$  and that for real  $q^2$ ,  $\Phi_l(q^2)$  is real, too. The proof of analyticity is very technical and is based on dispersion theory of the S-Matrix. It will not be described here, but simply the result will be used. Since  $\Phi_l$  is analytic we may expand it in a power series and get

$$\Phi_l(q^2) \simeq \frac{2}{s^{1/2}}(a_l^{-1} + \frac{1}{2}r_{0l}q^2 + r_{1l}q^4 + \dots). \quad (\text{C.23})$$

$a_l$  is called  $l$ -wave scattering length while  $r_{nl}$  are called effective range parameters. Of special interest are  $r_{0l}$  which give information of the range of the interaction. If  $r_{0l}$  is infinite, then the expansion of  $\Phi$  fails. This fact reflects the constraint of interactions with finite range. (Plugging the last equation into (C.22) one can derive the effective range formula  $q^{2l+1} \cot \delta_l = a_l^{-1} + \frac{1}{2}r_l q^2$  which is perhaps more familiar to the reader.) If we plug (C.23) into (C.21), we can study the low energy limit for  $q \rightarrow 0$ . Then, only the lowest powers in  $q$  will essentially contribute to the amplitude. This can be seen neatly in the  $l = 0$  case where

$$\lim_{q \rightarrow 0} T_0(s) = \frac{4s^{1/2}}{\pi 2} a_0. \quad (\text{C.24})$$

Using our formula for the scattering cross section (2.42) we get

$$\left( \frac{d\sigma}{d\Omega} \right)_{l=0} = \frac{\pi^2}{4s} \left( \frac{2s^{1/2}}{\pi} a_0 \right)^2 = (a_0)^2. \quad (\text{C.25})$$

We see that the differential cross section for the s-wave becomes a constant in the low energy limit. This is precisely the meaning of the scattering length. Since a cross section is an effective area, the name scattering length is justified.  $a_0$  has indeed the dimension of a length. From dimensional analysis in (C.21), however, one sees that already  $a_1$  does not any more have the dimension of a length. The lowest power of  $T_1$  is  $\propto q^2 a_1$ , hence, the cross section will now be momentum dependent. Since  $\Phi_l(q^2)$  is real, the general procedure to get  $a_l$  is simply to expand the real part of  $T_l$ . We therefore define

$$\text{Re } T_l^I(s) = \left( \frac{q^2}{M_\pi^2} \right)^l \left( a_l^I + b_l^I \frac{q^2}{M_\pi^2} + \dots \right). \quad (\text{C.26})$$

The superscript  $I$  denotes a possible isospin channel. The factor of  $M_\pi^2$  in the denominators in (C.26) is introduced in order to get dimensionless quantities for  $a_l^I$ .

# Appendix D

## Feynmanrules for NLO computations and six point vertices

### D.1 Feynmanrules for the NLO lagrangian

The expansion of the (N)NLO lagrangian (2.84) up to  $O(\pi^4)$  leads to a lagrangian of the form

$$\begin{aligned}
\mathcal{L}_{(N)NLO} = & X_1 \partial_\mu \vec{\pi} \cdot \partial_\mu \vec{\pi} + X_2 \vec{\pi}^2 + X_3 (\partial_\mu \vec{\pi} \cdot \partial_\mu \vec{\pi})(\partial_\mu \vec{\pi} \cdot \partial_\mu \vec{\pi}) \\
& + X_4 (\partial_\mu \pi \cdot \partial_\nu \pi)(\partial_\mu \pi \cdot \partial_\nu \pi) + X_5 (\vec{\pi} \cdot \partial_\mu \vec{\pi})(\vec{\pi} \cdot \partial_\mu \vec{\pi}) \\
& + X_6 (\partial_\mu \vec{\pi} \cdot \partial_\mu \vec{\pi}) \vec{\pi}^2 + X_7 \vec{\pi}^4
\end{aligned} \tag{D.1}$$

where we introduced the shorthand notation

$$\begin{aligned}
X_1 &:= \frac{1}{f^2} \left( 8 L_{45} \mathcal{M}^2 + 8 \overline{W}_{45} \rho + 8 L_{45} 2c_2 a^2 + \frac{1}{2} D_x 2c_2 a^2 \right) \\
X_2 &:= \frac{1}{f^2} \left( 16 L_{68} \mathcal{M}^2 + 16 \overline{W}_{68} \mathcal{M}^2 \rho + 2 \mathcal{M}^2 2c_2 a^2 (16 L_{68} + \frac{1}{4} A_x) \right. \\
&\quad \left. + 2c_2 a^2 \rho (16 \overline{W}_{68} + \frac{1}{2} C_x) + (2c_2 a^2)^2 (16 L_{68} + \frac{1}{2} A_x + \frac{1}{4} B_x) \right) \\
X_3 &:= -\frac{4}{f^4} L_{13} & X_4 &:= -\frac{4}{f^4} L_2 \\
X_5 &:= \frac{1}{f^4} \left( \frac{8}{3} L_{45} \mathcal{M}^2 + \frac{8}{3} \overline{W}_{45} \rho + \frac{8}{3} L_{45} 2c_2 a^2 + c_2 a^2 D_y \right) \\
X_6 &:= \frac{1}{f^4} \left( -\frac{20}{3} L_{45} \mathcal{M}^2 - \frac{20}{3} \overline{W}_{45} \rho - \frac{20}{3} L_{45} 2c_2 a^2 + c_2 a^2 D_z \right)
\end{aligned}$$

$$X_7 := \frac{1}{f^4} \left( -\frac{16}{3} L_{68} \mathcal{M}^4 - \frac{16}{3} \overline{W}_{68} \mathcal{M}^2 \rho - \frac{16}{3} L_{68} (4 \mathcal{M}^2 c_2 a^2 + 4 c_2^2 a^4) \right. \\ \left. - \frac{16}{3} \overline{W}_{68} \rho 2 c_2 a^2 + \mathcal{M}^2 c_2 a^2 A_y + 2 c_2^2 a^4 A_y + c_2^2 a^4 B_y + \rho c_2 a^2 C_y \right).$$

Note that we rescaled the low energy constants of the counterterms from section 2.7 using  $\rho = 2W_0 a$ :

$$A_i := \frac{4W_0^2}{c_2 f^2} \tilde{A}_i, \quad B_i := \frac{16W_0^4}{c_2^2 f^4} \tilde{B}_i, \quad C_i := \frac{4W_0^2}{c_2 f^2} \tilde{C}_i, \quad D_i := \frac{4W_0^2}{c_2 f^2} \tilde{D}_i.$$

The corresponding vertices read

$$W_1^{ij}[p_1, p_2] = 2 X_1 \delta^{ij} p_1 \cdot p_2, \quad (D.2)$$

$$W_2^{ij}[p_1, p_2] = -2 X_2 \delta^{ij}, \quad (D.3)$$

$$W_3^{ijkl}[p_1, p_2, p_3, p_4] = -8 \cdot X_3 \left[ \delta^{ij} \delta^{kl} (p_1 p_2 \cdot p_3 p_4) \right. \\ \left. + \delta^{ik} \delta^{jl} (p_1 p_3 \cdot p_2 p_4) \right. \\ \left. + \delta^{il} \delta^{jk} (p_1 p_4 \cdot p_2 p_3) \right], \quad (D.4)$$

$$W_4^{ijkl}[p_1, p_2, p_3, p_4] = -4 \cdot X_4 \left[ \delta^{ij} \delta^{kl} (p_1 p_3 \cdot p_2 p_4 + p_1 p_4 \cdot p_2 p_3) \right. \\ \left. + \delta^{ik} \delta^{jl} (p_1 p_4 \cdot p_2 p_3 + p_1 p_2 \cdot p_3 p_4) \right. \\ \left. + \delta^{il} \delta^{jk} (p_1 p_2 \cdot p_3 p_4 + p_1 p_3 \cdot p_2 p_4) \right], \quad (D.5)$$

$$W_5^{ijkl}[p_1, p_2, p_3, p_4] = 2 \cdot X_5 \left[ \delta^{ij} \delta^{kl} (p_1 p_3 + p_2 p_4 + p_2 p_3 + p_1 p_4) \right. \\ \left. + \delta^{ik} \delta^{jl} (p_1 p_2 + p_1 p_4 + p_2 p_3 + p_3 p_4) \right. \\ \left. + \delta^{il} \delta^{jk} (p_1 p_2 + p_1 p_3 + p_2 p_4 + p_3 p_4) \right], \quad (D.6)$$

$$W_6^{ijkl}[p_1, p_2, p_3, p_4] = 4 \cdot X_6 \left[ \delta^{ij} \delta^{kl} (p_1 p_2 + p_3 p_4) \right. \\ \left. + \delta^{ik} \delta^{jl} (p_1 p_3 + p_2 p_4) \right. \\ \left. + \delta^{il} \delta^{jk} (p_1 p_4 + p_2 p_3) \right], \quad (D.7)$$

$$W_7^{ijkl}[p_1, p_2, p_3, p_4] = -8 \cdot X_7 \left[ \delta^{ij} \delta^{kl} + \delta^{ik} \delta^{jl} + \delta^{il} \delta^{jk} \right]. \quad (D.8)$$

## D.2 Six point vertex

For the tadpole diagram contributing to the scattering amplitude, the six point vertex must be determined. The expansion of the LO lagrangian (2.14) leads to the following four terms:

$$\begin{aligned} \mathcal{L}_{\text{LO,6-pt}} = \frac{1}{45f^4} & \left( (\partial_\mu \vec{\pi} \cdot \partial_\mu \vec{\pi}) \vec{\pi}^4 - (\vec{\pi} \cdot \partial_\mu \vec{\pi})(\vec{\pi} \cdot \partial_\mu \vec{\pi}) \vec{\pi}^2 \right. \\ & \left. + \frac{1}{16} \mathcal{M}^2 \vec{\pi}^6 - \frac{15}{16} \cdot 2c_2 a^2 \vec{\pi}^6 \right). \end{aligned} \quad (\text{D.9})$$

The corresponding six point vertices read

$$\begin{aligned} V_{1,6\text{-pt}}^{ijklrs} [p_1, \dots, p_6] = \frac{16}{45f^4} & \left[ \delta^{ij} \delta^{kl} \delta^{rs} (p_1 p_2 + p_3 p_4 + p_5 p_6) \right. \\ & \left. + \text{all combinations } \{ij\}\{kl\}\{rs\} \right], \end{aligned} \quad (\text{D.10})$$

$$\begin{aligned} V_{2,6\text{-pt}}^{ijklrs} [p_1, \dots, p_6] = \frac{4}{45f^4} & \left[ \delta^{ij} \delta^{kl} \delta^{rs} [(p_1 + p_2)(p_3 + p_4) \right. \\ & \left. + (p_1 + p_2)(p_5 + p_6) + (p_3 + p_4)(p_5 + p_6)] \right. \\ & \left. + \text{all combinations } \{ij\}\{kl\}\{rs\} \right], \end{aligned} \quad (\text{D.11})$$

$$V_{3,6\text{-pt}}^{ijklrs} [p_1, \dots, p_6] = -\frac{\mathcal{M}^2}{15f^4} \left[ \delta^{ij} \delta^{kl} \delta^{rs} + \text{all combinations } \{ij\}\{kl\}\{rs\} \right], \quad (\text{D.12})$$

$$V_{4,6\text{-pt}}^{ijklrs} [p_1, \dots, p_6] = -\frac{2c_2 a^2}{f^4} \left[ \delta^{ij} \delta^{kl} \delta^{rs} + \text{all combinations } \{ij\}\{kl\}\{rs\} \right]. \quad (\text{D.13})$$

“all combinations  $\{ij\}\{kl\}\{rs\}$ ” means all the remaining configurations which one successively obtains by interchanging the flavor indices and the corresponding momenta.

# Bibliography

- [1] J. Gasser and H. Leutwyler. Chiral perturbation theory to one loop. *Annals of Physics*, 158(1):142–210, November 1984.
- [2] J. Gasser and H. Leutwyler. Chiral perturbation theory: Expansions in the mass of the strange quark. *Nuclear Physics B*, 250(1-4):465–516, 1985.
- [3] Gilberto Colangelo. Theoretical progress on pi pi scattering lengths and phases. *PoS*, KAON:038, 2008.
- [4] H. Leutwyler. On the foundations of chiral perturbation theory. *Ann. Phys.*, 235:165–203, 1994.
- [5] CP-PACS Collaboration, T. Yamazaki, S. Aoki, M. Fukugita, K-I. Ishikawa, N. Ishizuka, Y. Iwasaki, K. Kanaya, T. Kaneko, Y. Kuramashi, M. Okawa, A. Ukawa, and T. Yoshié. I=2 pi pi scattering phase shift with two flavors of  $O(a)$  improved dynamical quarks. *Phys. Rev. D*, 70(7):074513–, October 2004.
- [6] A. Ukawa. Computational cost of full QCD simulations experienced by CP-PACS and JLQCD Collaborations. *Nuclear Physics B - Proceedings Supplements*, 106-107:195–196, March 2002.
- [7] Stephen Sharpe and Robert Singleton. Spontaneous flavor and parity breaking with Wilson fermions. *Phys. Rev. D*, 58(7):074501, Aug 1998.
- [8] Gautam Rupak and Noam Shoresh. Chiral perturbation theory for the Wilson lattice action. *Phys. Rev. D*, 66(5):054503–, September 2002.
- [9] Oliver Bär, Gautam Rupak, and Noam Shoresh. Chiral perturbation theory at  $O(a^2)$  for lattice QCD. *Phys. Rev.*, D70:034508, 2004.
- [10] Michael I. Buchoff. Isotropic and anisotropic lattice spacing corrections for I = 2 pi pi scattering from effective field theory. *Phys. Rev. D*, 77(11):114502–9, June 2008.



- [11] David J. Gross and Frank Wilczek. Ultraviolet Behavior of Non-Abelian Gauge Theories. *Phys. Rev. Lett.*, 30(26):1343–, June 1973.
- [12] John F. Donoghue, Eugene Golowich, and Barry R. Holstein. *Dynamics of the Standard Model*. Cambridge University Press, 1992.
- [13] C. Amsler et al. (Particle Data Group). *PL*, B667:1, 2008.
- [14] Steven Weinberg. Phenomenological Lagrangians. *Physica A: Statistical and Theoretical Physics*, 96(1-2):327–340, April 1979.
- [15] Johan Bijnens, Gilberto Colangelo, and Gerhard Ecker. The mesonic chiral lagrangean of order  $p^6$ . *Journal of High Energy Physics*, 1999(02):020–020, 1999. ISSN 1126-6708.
- [16] J. Bijnens, G. Colangelo, and G. Ecker. Renormalization of Chiral Perturbation Theory to Order  $p^6$ . *Annals of Physics*, 280(1):100–139, February 2000.
- [17] Luigi Del Debbio, Leonardo Giusti, Martin Lüscher, Roberto Petronzio, and Nazario Tantalo. QCD with light Wilson quarks on fine lattices (I): first experiences and physics results. *Journal of High Energy Physics*, 2007(02):056–056, 2007. ISSN 1126-6708.
- [18] Kenneth G. Wilson. Confinement of quarks. *Phys. Rev. D*, 10(8):2445–2459, Oct 1974. doi: 10.1103/PhysRevD.10.2445.
- [19] K. Symanzik. Continuum limit and improved action in lattice theories: (I). Principles and  $\phi^4$  theory. *Nuclear Physics B*, 226(1):187–204, September 1983.
- [20] B. Sheikholeslami and R. Wohlert. Improved continuum limit lattice action for QCD with Wilson fermions. *Nuclear Physics B*, 259(4):572–596, September 1985.
- [21] Sinya Aoki and Oliver Bär. Twisted mass QCD,  $O(a)$  improvement, and Wilson chiral perturbation theory. *Phys. Rev. D*, 70(11):116011, 2004.
- [22] Sinya Aoki. New phase structure for lattice QCD with Wilson fermions. *Phys. Rev. D*, 30(12):2653–, December 1984.
- [23] Christopher Michael and Carsten Urbach. Neutral mesons and disconnected diagrams in Twisted Mass QCD. *PoS*, LAT2007:122, 2007.

- [24] Steven Weinberg. *The Quantum Theory of Fields, Volume I*. Cambridge University Press, 1995.
- [25] Francisco J. Yndurain. *Relativistic Quantum Mechanics and Introduction to Field Theory*. Springer, 1996.
- [26] Michael E. Peskin and Daniel V. Schroeder. *An Introduction to Quantum Field Theory*. Westview, 1995.
- [27] Steven Weinberg. Pion Scattering Lengths. *Phys. Rev. Lett.*, 17(11): 616–621, Sep 1966. doi: 10.1103/PhysRevLett.17.616.
- [28] J. L. Petersen. Meson-meson scattering. *Physics Reports*, 2(3):155–251, November 1971.
- [29] B.R. Martin, D. Morgan, and G. Shaw. *Pion-Pion Interactions in Particle Physics*. Academic Press, 1976.
- [30] Sinya Aoki and Oliver Bär. The vector and axial vector current in Wilson ChPT. *PoS LATTICE2007*, 062, 2007.
- [31] Klaus Jänich. *Lineare Algebra*. Springer, 2002.
- [32] Hong-Hao Zhang, Wen-Bin Yan, and Xue-Song Li. Trace formulae of characteristic polynomial and Cayley- Hamilton’s theorem, and applications to chiral perturbation theory and general relativity. *Commun. Theor. Phys.*, 49:801, 2008.
- [33] Stefan Scherer. Introduction to chiral perturbation theory. *Adv. Nucl. Phys.*, 27:277, 2003.
- [34] Wolfgang Nolting. *Grundkurs: Theoretische Physik Band 3, Elektrodynamik*. Springer, 2002.
- [35] Hartmut M. Pilkuhn. *Relativistic particle physics*. Springer, 1979.
- [36] M. Goldberger and Kenneth M. Watson. *Collision Theory*. Wiley, 1964.

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# Selbständigkeitserklärung

Hiermit erkläre ich, die vorliegende Arbeit selbständig ohne fremde Hilfe verfaßt und nur die angegebene Literatur und Hilfsmittel verwendet zu haben.

Bendikt Biedermann

Berlin, den 19. August 2008