Quark-Mass Dependence of the Nucleon-Nucleon Interaction in QCD and Chiral Effective Field Theory

Diploma Thesis

by

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1 Introduction

The interaction between nucleons is of great interest for nuclear physicists and has a long history. Yukawa [Yuk35] introduced the idea that pions could be the force carriers of the nuclear force and field-theoretic investigations to explain the nucleon-nucleon (NN) interaction were attempted. While one-pion exchange was very useful to describe scattering data and properties of the deuteron, multi-pion exchange failed to improve the theory [ME11]. The experimental discovery of heavier mesons such as the $\rho(770)$ motivated the phenomenological one-boson exchange (OBE) models. They contain an isoscalar $\sigma$-meson, which is experimentally controversial. There are some phenomenological two-pion exchange models, such as the Paris [LLR+80] or the Bonn potential [MHE87], which give a good quantitative description for the NN interaction.

Although the experimental data are described very well by these potentials, there are some conceptual deficiencies. In particular, the construction of consistent nuclear many-body force can only be meaningfully defined in a consistent scheme with a given two-body NN interaction [Epe10].

The development of Quantum Chromodynamics (QCD) as the underlying theory of the strong interactions motivated physicists to derive the force between nucleons from a new point of view because the connection between QCD and the OBE is only loose [Epe06]. Due to the non-perturbative features of QCD at low energies, a direct derivation of the nuclear force from QCD with quarks and gluons as degrees of freedom is quite involved.

However, the concept of effective field theories (EFTs) was developed and nucleons and pions became once again the effective degrees. The crucial difference to Yukawa’s original idea are symmetries: Weinberg [Wei79] stated that the effective theory has to fulfill the (spontaneously broken) chiral symmetry of QCD. This constrains multi-pion exchange and is the reason why the earlier attempts in the 1950s to describe the nuclear force with pions failed.

Another approach to the non-perturbative region of QCD at low energies is lattice QCD. Recently the HAL-QCD collaboration [IAH07] and Beane et al. [BBOS06] set up lattice simulations that describe the nucleon-nucleon interaction, but because of limitations of computational time their calculations have been performed for non-physical current-quark masses.

In this diploma thesis we investigate the quark-mass dependence of the nucleon-nucleon interaction in chiral effective field theory and compare resulting potentials and phase shifts with the most recent results from lattice QCD. Therefore, in chapter 2, we start with the foundation of the chiral effective field theory, its symmetries and symme-
1 Introduction

try breaking pattern. Using these symmetry we construct chiral effective Lagrangians in chapter 3. For clarity we first present the Lagrangian for a theory containing only pions and include nucleons later on. In chapter 4 the perturbative and non-perturbative aspects of the NN interaction are discussed in the framework of the EFT: the chiral N^3LO potential as well as scattering phase shifts from the chiral N^2LO potential are shown and the phase shifts are compared to data from the Nijmegen phase shift analysis [SKRdS93]. At the beginning of chapter 5 some recent results from lattice QCD are presented: the NN central and tensor potential and phase shifts in the 1S_0 channel. We consider the pion-mass dependence of these potentials in the EFT and compare the chiral and lattice tensor potential. In the end of this chapter we choose the only pion-mass dependent parameter in the 1S_0 potential to fit the lattice phase shifts and discuss the consequences of this choice. Finally, in chapter 6 we summarize our results and give a brief outlook. Conventions and technical details on the numerical solution of the Lippmann-Schwinger equation are displayed in the appendix.
2 Quantum Chromodynamics

2.1 General remarks about QCD

2.1.1 SU(3)$_C$ and the QCD Lagrangian

In the 1960s particles like the nucleon resonances $\Delta^{++}, \Delta^-$ and the hyperon $\Omega^-$ were known to be fermions, but before the introduction of the color quantum number, the s-wave states could not be explained as the flavor ($uud/ddd/sss$), spin ($S = 3/2$) and orbital ($L = 0$) wave functions are symmetric. Experiments showed that the ratio $R = \sigma(e^+e^- \rightarrow \text{Hadrons})/\sigma(e^+e^- \rightarrow \mu^+\mu^-)$ was too small by a factor of three. Han and Nambu (1965), Greenberg (1965), and Gell-Mann (1972) proposed that quarks carry an additional quantum number, later called color, such that besides this quantum number there are three kinds of identical quarks. The fermionic Lagrangian

$$\mathcal{L}_{\text{Dirac}} = \bar{q}_f (i\gamma^\mu \partial_\mu - m_f) q_f \quad (2.1)$$

(with $q_f = (q_f^{\text{red}}, q_f^{\text{green}}, q_f^{\text{blue}})$ denoting the quark fields of the flavor $f \in \{u,d,s,c,b,t\}$ and including the color quantum numbers) is invariant under a global SU(3)$_C$ symmetry.

The strong interaction still had to be explained at that time and people knew that gauging a U(1) symmetry introduces photons and can explain electrodynamics. Promoting the group SU(3)$_C$ to a local gauge symmetry also introduces spin-1 exchange bosons, the gluons, and an interaction between color-charged particles. The main difference compared to the U(1) symmetry of electrodynamics is the non-Abelian character of SU(3) that leads to three- and four-gluon vertices expressing self interactions between the gluons. The quarks transform in the fundamental (3) representation of SU(3), i.e., $q(x) \rightarrow U(x)q(x)$, with

$$U(x) = \exp \left[ -i \sum_{a=1}^{8} \frac{\lambda^a}{2} \theta^a(x) \right] \quad (2.2)$$

being an element of SU(3) generated by $t^a = \lambda^a/2$ and $\lambda^a$ the 8 Gell-Mann matrices given in Eq. (A.2). The gluon fields are introduced by the substitution of the normal derivative with the covariant derivative

$$D_\mu = \partial_\mu - ig t^a A^a_\mu(x). \quad (2.3)$$

The Lagrangian (2.1) is invariant under a local SU(3) transformations, if the fields transform according to

$$A_\mu(x) \equiv t^a A^a_\mu(x) \rightarrow U(x)A_\mu(x)U^\dagger(x) + \frac{i}{g} U(x)\partial_\mu U^\dagger(x)$$

$$D_\mu q_f(x) \rightarrow U(x)D_\mu q_f(x). \quad (2.4)$$
The gluon dynamics is described by a field-strength tensor defined as
\[
G_{\mu\nu} = \frac{i}{g} [D_{\mu}, D_{\nu}] = \partial_\mu A_\nu - \partial_\nu A_\mu - ig \left[ \frac{\lambda^b}{2}, \frac{\lambda^c}{2} \right] A^b_\mu A^c_\nu
\]
where the commutator relation of SU(3) from Eq. (A.3) was used and \( f^{abc} \) are the structure constants of SU(3). The field-strength tensor transforms like the covariant derivative according to the adjoint (8) representation of SU(3). Therefore the trace in color space is necessary to make the term \( G_{\mu\nu} G^{\mu\nu} \) invariant. The full QCD Lagrangian then reads:
\[
\mathcal{L}_{\text{QCD}} = \bar{q}_f (i\gamma^\mu - m_f) q_f - \frac{1}{2} \text{Tr}C [G_{\mu\nu} G^{\mu\nu}].
\]
(2.6)

The restrictions imposed by Lorentz and gauge invariance and renormalizability (in the meaning that operators cannot have mass dimension greater than 4) only allow one more term in the Lagrangian, the so called “\( \theta \)-term”:
\[
\mathcal{L}_\theta = -\frac{\theta g^2}{32\pi} \epsilon^{\mu
u\rho\tau} G^a_{\mu\nu} G^a_{\rho\tau}.
\]
(2.7)

This term however would give rise to both C and CP violation of the strong interaction and, e.g., lead to a nonvanishing electric dipole moment of the neutron. The upper bound for this dipole moment is currently \(|d| < 2.6 \cdot 10^{-26} \) \( [\text{B}^+06] \). As this should not be the topic of this thesis, \( \theta \) will be set to 0 throughout this work.

### 2.1.2 Quantization

The quantization of SU(3)\(_C\) using the Fadeev-Popov [FP67] formalism introduces unphysical ghost fields that couple to gluons. The procedure applied to the Yang-Mills case is as follows: start from the functional integral
\[
\int \mathcal{D}A \exp \left[ -i \int d^4x \frac{1}{4} G^a_{\mu\nu} G^{\mu\nu,a} \right]
\]
and choose a gauge-fixing condition \( F[A] = 0 \) to split \( \mathcal{D}A \) into an integral over all gauge-inequivalent configurations and a second integral over all possible gauge transformations. Applying the identity
\[
1 = \int \mathcal{D}\theta(x) \delta(F[A^{(\theta)}]) \det \left( \frac{\delta F[A^{(\theta)}]}{\delta \theta} \right)
\]
(2.9)
to the generalized Lorentz gauge condition \( F^a[A] = \partial_\mu A^{\mu,a}(x) - \omega^a(x) = 0 \) we can calculate the determinant using the infinitesimal form of Eqs. (2.2) and (2.4). Using the functional integral representation for the determinant then yields
\[
\det \left( \frac{\delta F[A^{(\theta)}]}{\delta \theta} \right) = \int \mathcal{D}\bar{\eta} \mathcal{D}\eta \exp \left[ i \int d^4x \bar{\eta}^a \left( -\partial_\mu \partial^\mu \delta^{ab} - g \partial_\mu f^{abc} A^{\mu,b} \right) \eta^c \right],
\]
(2.10)
where $\eta$ and $\bar{\eta}$ are scalar anticommuting (Grassmann-)fields. These fields are called ghost fields and are unphysical. After a Gaussian integration over the weight functions $\omega^a(x)$ the gauge-fixed Yang-Mills Lagrangian reads

$$L_{YM} = -\frac{1}{2} \text{Tr}_c [G_{\mu\nu} G^{\mu\nu}] - \frac{1}{2\kappa} (\partial_{\mu} A^{\mu,a})^2 + \bar{\eta}^a \left( -\partial_{\mu} \partial^{\mu} \delta^{ab} - g \partial_{\mu} f^{abc} A_{\mu,b} \right) \eta^c$$

(2.11)

where $\zeta$ is a freely adjustable gauge-parameter. The inclusion of fermions does not change the argumentation and we only need to add the fermionic term of Eq. (2.6) to end up with a gauge-fixed QCD Lagrangian.

We now want to show how to derive the Feynman rules of QCD using Feynman’s path-integral formalism [Fey65],[PS95]. The Feynman rules of any theory are computed from the $n$-point correlation or Green functions which for arbitrary fields $\phi$ have the path-integral representation

$$G^{(n)}(x_1,..x_n) = \langle 0| T \{ \phi(x_1)...\phi(x_n) \} |0 \rangle = \frac{\int D\phi \phi(x_1)...\phi(x_n) \exp[iS]}{\int D\phi \exp[iS]}.$$  

(2.12)

A formal way of calculating these correlation functions makes use of external fields. The idea is to define one functional from which all correlators of a theory can be deduced by functional derivatives. Therefore, we introduce the generating functional

$$Z[\Phi] \equiv Z[J,\bar{\chi},\chi,\bar{\xi},\xi] = \int DAD\bar{q}DqD\bar{\eta}D\eta \exp \left[ i \int d^4x \left( L_{QCD} + L_{GF} + L_{source} \right) \right],$$

(2.13)

where we have introduced source terms

$$L_{source} = \int d^4x \ J^{a,a} A^{a}_{\mu} + \bar{\chi}q + \bar{q}\chi + \bar{\xi}^a \eta^a + \bar{\eta}^a \xi^a.$$  

(2.14)

When turning the sources off, $L_{QCD}+L_{GF}+L_{source}$ describes the gauge-fixed Lagrangian of the original theory. In a perturbative theory it is possible to rewrite the Lagrangian without the external fields into a free ($L_0$) and an interaction Lagrangian ($L_{int}$) and expand the interaction part of the generating functional $\exp[iS_{int}] = 1 + iS_{int} + \ldots$ as a power series in the couplings. Starting from the generating functional of the free theory,

$$Z_0[\Phi] = \int DAD\bar{q}DqD\bar{\eta}D\eta \exp \left[ i \int d^4x \left( L_0 + L_{source} \right) \right],$$

(2.15)

we obtain the same power series using functional derivatives of the external sources and therefore Eq. (2.13) can be rewritten as

$$Z[\Phi] = \exp \left[ i \int d^4x \ L_{int} \left( -i \frac{\delta}{\delta J^{a,a}(x)} , -i \frac{\delta}{\delta \bar{\chi}(x)} , i \frac{\delta}{\delta \chi(x)} , -i \frac{\delta}{\delta \bar{\xi}^a(x)} , i \frac{\delta}{\delta \xi^a(x)} \right) \right] Z_0[\Phi].$$

(2.16)

The different signs are due to the anticommuting property of the fermion and ghost fields. For practical calculations in perturbation theory the power series of $\exp[iS_{int}]$ is truncated at the desired order. This procedure is well established for QCD and we refer the reader to textbooks like [PS95] for the actual Feynman rules.
2 Quantum Chromodynamics

2.1.3 The Running Coupling and its Consequences

In a quantum field theory there are loop corrections to the tree level results. These loop corrections show divergences which we want to regularize in order to isolate the singularities. There are different regularization schemes, but in this work we will use dimensional regularization throughout as it preserves the underlying symmetries. The calculations are performed in \( D = 4 - 2\epsilon \) dimensions such that appearing integrals are convergent. We want to mention that there are some subtleties with the total antisymmetric tensor \( \epsilon_{\mu\nu\rho\tau} \) and therefore the definition of \( \gamma_5 \) in \( D \) dimensions which have been pointed out in by t’Hooft and Veltman [tHV72]. The results of the computations are then expanded in \( \epsilon \) and the singularities are parametrized as poles in \( \epsilon \). The demand of a dimensionless action \( S = \int d^Dx \mathcal{L} \) requires the Lagrangian to be of mass dimension \( D \), making it necessary to replace the dimensionless coupling \( g \) by \( g\mu^\epsilon \) where \( \mu \) is an arbitrary scale-parameter of mass dimension 1. After isolating the singularities one still needs to give physical meaning to the infinite amplitudes. This is done by renormalization conditions which set the computed amplitudes at a fixed scale \( \mu \) equal to physical amplitudes, thus renormalizing the parameters and wave functions of the theory:

\[
Z_g(\mu)\mu^\epsilon g(\mu) = g_0 \quad Z_m(\mu)m(\mu) = m_0 \quad Z_A^{1/2}(\mu)A_{\mu}^{\alpha} = A_0^{\alpha}.
\]

The subscript “0” denotes the bare parameters or wave functions of the original Lagrangian. Their scale-dependent counterparts on the left-hand side are the renormalized quantities and the \( Z \) are called renormalization factors. The choice of the renormalization conditions is not unique, but a frequently used method is the modified minimal subtraction (\( \overline{\text{MS}} \)) scheme, that does not only subtract the \( 1/\epsilon \) poles, but few other summands that always appear in connection with it in dimensional regularization. In this work scale-dependent results are understood to be given in the modified \( \overline{\text{MS}} \) scheme.

Noting that the right-hand side of Eqs. (2.17) is scale independent, the \( \mu \) dependence of the renormalized quantities can be expressed by differential equations, the renormalization-group equations. For the coupling \( g(\mu) \) one has

\[
\frac{d}{d\ln \mu} g(\mu) = \beta(\mu, g(\mu)) - \epsilon g(\mu),
\]

where the \( \beta \)-function describes the scale dependence of the vertex renormalization factor \( Z_g \):

\[
\beta(\mu, g(\mu)) = -\frac{g(\mu)}{Z_g(\mu)} \frac{d}{d\ln \mu} Z_g(\mu).
\]

Eq. (2.18) describes the “running” of the coupling \( g(\mu) \). In the limit \( \epsilon \to 0 \) the second summand vanishes and the scale dependence of \( g(\mu) \) is dictated by the \( \beta \)-function. At one-loop level there are two contributions with different signs: as in QED the fermionic degrees of freedom act with a screening effect, i.e., enlarge the \( \beta \)-function, whereas gluon loops have an anti-screening effect. At this order the \( \beta \)-function of QCD reads

\[
\beta(g) = \left(-11 + \frac{2n_f}{3}\right) \frac{g^3}{16\pi^2},
\]

\[n_f \text{ is the number of active fermion flavors.}\]
2.1 General remarks about QCD

<table>
<thead>
<tr>
<th>flavor</th>
<th>$u$</th>
<th>$d$</th>
<th>$s$</th>
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</thead>
<tbody>
<tr>
<td>$m_q$ [MeV]</td>
<td>1.7–3.3</td>
<td>4.1–5.8</td>
<td>80–130</td>
</tr>
<tr>
<td>$m_q$ [GeV]</td>
<td>1.18–1.34</td>
<td>4.10–4.37</td>
<td>170–172</td>
</tr>
</tbody>
</table>

Table 2.1: Current quark masses in $\overline{\text{MS}}$ scheme at $\mu = 2$ GeV from PDG \([N^+10]\)

where $n_f$ is the number of active quark flavors ($m_f < \mu$) and the $\mu$ dependence was suppressed. Even if all six quark-flavors are effective degrees of freedom, the $\beta$-function is negative and the coupling $g(\mu)$ decreases with rising scales. With this $\beta$-function we are able to solve the differential equation (2.18) and with the definition of the strong coupling strength $\alpha_s = g^2/(4\pi)$ we obtain

$$
\alpha_s(\mu) = \frac{\alpha_s(\mu_0)}{1 + \frac{\alpha_s(\mu_0)}{4\pi}(11 - \frac{2}{3}n_f) \ln(\frac{\mu^2}{\mu_0^2})}.
$$

From this it follows that for sufficiently small number of fermions ($n_f \leq 16$) the running coupling decreases for larger scales and $\lim_{\mu \to \infty} \alpha_s(\mu) = 0$. Theories with the latter attribute are called asymptotically free. Frank Wilczek and David Gross [GW73], and David Politzer [Pol74] discovered the asymptotic freedom in QCD and won the Nobel Prize in Physics for their work in 2004.

On the other hand, going to smaller scales increases the coupling strength and there exists an intrinsic scale $\Lambda_{\text{QCD}}$ at which $\alpha_s(\Lambda_{\text{QCD}})$ diverges at one-loop level. The one-loop calculation is not trustworthy as $\alpha_s$ grows because we leave the regime of perturbative QCD. We can estimate $\Lambda_{\text{QCD}}$ from the one-loop calculation to get a feeling at which momentum scale QCD cannot be treated perturbatively anymore. Inserting the central value of $\alpha_s(m_{Z^0}) = 0.1184 \pm 0.0007$ at the scale $m_{Z^0} = 91.2$ GeV [Bet09] and $n_f = 5$ (neglecting that at lower scales we should decrease the active flavors) we can calculate that the divergence of Eq. (2.21) arises at $\Lambda_{\text{QCD}} \approx 0.1$ GeV. Perturbation theory already breaks down for scales where $\alpha_s$ approaches unity and therefore we need nonperturbative methods to describe QCD in the region of $\mu < 1$ GeV. In this thesis we will analyze the low-energy behavior of the nucleon-nucleon interaction for energy scales in this nonperturbative region.

Table 2.1 shows that only the three light quarks ($u, d, s$) possess current quark masses of below 1 GeV. Hence we can work with a reduced number of active quark flavors in low-energy QCD, where we treat processes with external momenta far below this scale. In this work the two-flavor case $q = (u, d)$ is preferred because strange-quarks are not necessary to describe the valence quarks of nucleons ($uud/duu$) and pions ($du, (\bar{u}u - \bar{d}d)/\sqrt{2}, \bar{u}d$) and chiral symmetry is a better approximation in the two flavor case.

\(^1\)from direct observations of top events
2 Quantum Chromodynamics

2.1.4 QCD on the Lattice

The Green functions (2.12) determine a quantum field theory as all relevant physical quantities can be described by them. In QCD we are not able to approximate them in the low energy region \( \mu < 1 \text{ GeV} \) using perturbation theory and therefore other means are necessary. Kenneth Wilson described a new approach [Wil74] by discretizing the spacetime and working on a discrete and finite lattice. This limits the infinite dimensional integral measure \( D\phi(x) \) to a finite number of degrees of freedom for integration. The lattice spacing naturally acts as a UV-cutoff because the momenta are restricted to the first Brillouin zone (\( |k_\mu| \leq \pi/a \)). Actual computations can only be performed on a finite lattice which imposes an infrared cutoff. Hence, the finite-volume behavior of calculated quantities should also be examined.

In his paper Wilson also proposed to work in an Euclidian space-time instead of the Minkowski space \( (x_0 \to -ix_4) \) because the phase factors then become exponential damping factors \( \exp[iS] \to \exp[-S_E] \). This has the advantage that large action contributions are unimportant from the beginning whereas in Minkowski space they have to average with nearby paths to exponentially small contributions, which is numerically not as stable.

If we start with the Euclidian Dirac action,

\[
S_{\text{Dirac}} = \int d^4x_E \bar{q}(x_E)(\partial_E + m_q)q(x) := \int d^4x_E \bar{q}(x_E)Kq(x_E),
\]

where we defined the quark matrix \( K \) for later use, we already notice that we have to define the “derivative” on the lattice. The symmetric difference operator

\[
\partial_\mu q(x) = \frac{1}{2a} (q(x + \hat{\mu}) - q(x - \hat{\mu}))
\]

makes \( \bar{q}(x_E)Kq(x_E) \) a nonlocal operator (\( \hat{\mu} = ae_\mu \) and \( e_\mu \) denotes a unit vector in \( \mu \)-direction). The concept of parallel transport from differential geometry is helpful to gauge such nonlocal operators. Let \( O_1(x)O_2(y) \) be a nonlocal operator, then the parallel-transport operator

\[
U(x, y) = \mathcal{P} \exp \left[ ig \int_{\gamma(x,y)} ds^\mu \frac{\Lambda^a}{2} A^a_\mu(s) \right]
\]

makes \( O_1(x)U(x, y)O_2(y) \) a building block that can be used for gauge-invariant theories. \( \gamma(x, y) \) denotes a path connecting \( x \) and \( y \), \( \mathcal{P} \) indicates path ordering and \( A^a_\mu(x) \) are the gluon fields. It is convenient to define link variables that connect two neighboring sites (e.g., \( n \) and \( n + \hat{\mu} \)) on the four-dimensional Euclidian lattice

\[
U_\mu(n) = U(n + \hat{\mu}, n).
\]

Any path \( \gamma \) along the lattice sites is then given by a path-ordered product of these link variables. While in continuum calculations we use the gauge fields, in lattice QCD the set of all link variables, elements of the gauge group itself, represent the lattice gauge
2.1 General remarks about QCD

The smallest closed loops on the lattice are called plaquettes and the corresponding transporter
\[ U_p(n) = U_{-\mu}(n + \mu)U_{-\nu}(n + \mu + \nu)U_{\mu}(n + \nu)U_{\nu}(n) \]  

(2.26)
denotes the plaquette variable starting from lattice site \( n \) in the \( \mu-\nu \) plane. It turns out that the pure gauge-field action is given by the sum over all distinct plaquette variables on the lattice [Rot05]:

\[ S_{\text{gauge}} = \frac{6}{g_0^2} \sum_p \left( 1 - \frac{1}{6} \text{Tr}C(U_p + U_p^\dagger) \right). \]  

(2.27)

In lattice convention the parameter \( \beta = 6/g^2 \) is introduced and used as the input parameter instead of the bare coupling \( g_0 \).

After ensuring gauge invariance and describing lattice gauge-field dynamics we turn back to the fermions. We notice that the naive fermion action of Eq. (2.22) with the difference operator of Eq. (2.23) suffers from the so called fermion-doubling, i.e., instead of the description of one quark, we describe \( 2^4 = 16 \) degenerate “quark tastes”. There are several possibilities to handle that problem, but there exist a theorem by Nielson and Ninomiya that states that in a Hermitian, local and translational invariant lattice gauge theory one cannot solve the doubler problem without breaking chiral symmetry for vanishing quark masses [NN81]. Wilson’s original approach was to add a term to the action that explicitly breaks chiral symmetry but vanishes for \( a \to 0 \) such that 15 of the 16 fermions would become infinitely heavy in the continuum limit. For more details and different fermion actions that have been developed over the past 40 years we refer the reader to the lattice literature, e.g., introductions like [Rot05] or [Gup].

Finally, we want to make a remark on the so called quenched approximation\(^2\). For this purpose we recall that the action in lattice QCD takes the form

\[ S[U, \bar{q}, q] = S_{\text{gauge}}[U] + S_q[U, \bar{q}, q], \]  

(2.28)

where \( S_q \) is the fermion action of the quarks coupled to the link variables. When calculating the vacuum expectation value of some physical quantity \( \mathcal{O}[U, \bar{q}, q] \)

\[ \langle \mathcal{O} \rangle = \frac{\int DUD\bar{q}Dq \mathcal{O}[U, \bar{q}, q]e^{-S[U,\bar{q},q]}}{\int DUD\bar{q}Dq e^{-S[U,\bar{q},q]}}, \]  

(2.29)

we can formally integrate out the quarks (Grassmann fields) and receive an effective operator \( \mathcal{O}_{\text{eff}}[U] \) and an effective action

\[ S_{\text{eff}}[U] = S_{\text{gauge}}[U] - \ln(\det K[U]). \]  

(2.30)

The problem is that the computation of the fermion determinant \( \det K[U] \) is very expensive in terms of computing time. Neglecting the dependence of this determinant of

\(^2\)We follow the idea from Ref. [TW01].
the link variables makes the path integral independent of it and the vacuum expectation value can be approximated by

\[ \langle O \rangle \approx \int \mathcal{D}U \, \mathcal{O}_{\text{eff}}[U] e^{-S_{\text{gauge}}[U]} \].

(2.31)

In a pictorial way, the quenched approximation neglects the quantum fluctuations of quark loops.

### 2.2 Symmetries

After this brief introduction of lattice QCD we want to work in the direction of an effective field theory based on symmetries of QCD to describe the nonperturbative low-energy regime. Taking only the two lightest quarks into account, the QCD Lagrangian reads

\[ \mathcal{L}_{\text{QCD}} = \bar{q} (i \slashed{D} - \mathcal{M}) q - \frac{1}{2} \text{Tr} [G_{\mu\nu} G^{\mu\nu}] . \]

(2.32)

We want to investigate the symmetries of this Lagrangian and therefore recall Noether’s theorem.

#### 2.2.1 Noether’s Theorem

Noether’s theorem tells us that every global continuous symmetry generates a conserved current. It also tells us about the relation of this current with the symmetry breaking part of a Lagrangian if the symmetry is only an approximate symmetry. Let \( \phi \rightarrow \phi + \delta \phi = \phi + \epsilon \, it \phi \) be an infinitesimal symmetry transformation (with \( t \) the generator of a symmetry group) under which the action is invariant or, equivalently, the Lagrangian only changes (if at all) by a total derivative of a function vanishing at the limits of integration

\[ \mathcal{L}_0[\phi] \rightarrow \mathcal{L}_0' = \mathcal{L}_0[\phi] + \epsilon \partial_\mu J^\mu[\phi] . \]

(2.33)

On the other hand, one can expand

\[ \mathcal{L}_0' = \mathcal{L}_0[\phi + \delta \phi] = \frac{\partial \mathcal{L}_0}{\partial \phi} \delta \phi + \frac{\partial \mathcal{L}_0}{\partial (\partial_\mu \phi)} \partial_\mu \delta \phi + \epsilon \partial_\mu J^\mu[\phi] . \]

(2.34)

By exploiting the equations of motion the first bracket vanishes. Hence, we conclude that for all points in Minkowski space there is a conserved current

\[ \partial_\mu j^\mu \equiv \partial_\mu \left( \frac{\partial \mathcal{L}_0}{\partial (\partial_\mu \phi)} \, it \phi - J^\mu \right) = 0 . \]

(2.35)

From this conserved current we find a conserved charge \( Q = \int d^3r \, j^0 \) with

\[ \partial_0 Q = \partial_0 \int d^3r \, j^0 = \int d^3r \, \nabla \cdot j = 0 . \]

(2.36)
Using the canonical formalism for quantization we note that \([H, Q] = 0\) is equivalent to Eq. (2.36). Furthermore, it can be shown that the charges generate the symmetry transformations on the Hilbert space:

\[
\Pi(x) = \frac{\partial L_0}{\partial (i\partial_0 \phi)} \quad \Rightarrow \quad [\Phi(x), \Pi(y)]|_{x_0 = y_0} = i\delta^{(3)}(x - y)
\]

\[
Q = \int d^3r \, \Pi(x) i t \Phi(x) \quad \Rightarrow \quad [Q, \Phi(x)] = t \Phi(x).
\]  

(2.37)

Let us explore the case when there is a part of the Lagrangian, \(L_1\), that explicitly breaks this symmetry. Then, there is a \(\delta L_1\) for an infinitesimal transformation that is not a total derivative:

\[
L_1 \rightarrow L_1 + \delta L_1.
\]  

(2.38)

The above reasoning of Eqs. (2.34)–(2.35) is still valid, but there is an additional part from the explicit breaking now and therefore we can see that

\[
\partial_\mu j^\mu = \left. \frac{\partial L_1}{\partial \epsilon} \right|_{\epsilon = 0}.
\]  

(2.39)

### 2.2.2 Symmetries of QCD

After this brief digression we want to explore the global continuous symmetries of QCD and start with rewriting the fermionic part Eq. (2.32) as

\[
L_{\text{ferm}} = \left[\bar{q}_L(i\slashed{D})q_L + \bar{q}_R(i\slashed{D})q_R\right] - \left[\bar{q}_L M q_R - \bar{q}_R M q_L\right],
\]  

(2.40)

where we have introduced the projection operators

\[
P_R = \frac{1}{2} (1 + \gamma_5), \quad P_L = \frac{1}{2} (1 - \gamma_5)
\]  

(2.41)

acting in spinor space. They project the quark fields on their left- and right-handed components \(q_R/L = P_R/L q\) and satisfy the relations

\[
1_4 = P_R + P_L, \quad P_R^2 = P_L^2 = P_R/L, \quad P_R \cdot P_L = 0.
\]  

(2.42)

The quark mass term mixes the left- and right-handed quarks and only allows for a combined symmetry transformation of both fields

\[
q(x) \rightarrow \exp[-i\varphi V]q(x) = \begin{pmatrix} \exp[-i\varphi V] & 0 \\ 0 & \exp[-i\varphi V] \end{pmatrix} \begin{pmatrix} q_L(x) \\ q_R(x) \end{pmatrix}.
\]  

(2.43)

This U(1)_V symmetry creates a conserved charge, \(B = \frac{1}{3} \int d^3x \, \bar{q}^\dagger q\), called baryon number. It is the only exact symmetry of QCD and so far consistent with all experiments.

To find symmetries that are “barely” broken in the Lagrangian, we look at the hadron spectrum and see that besides eight very light pseudoscalars the hadronic scale is in the region of 1 GeV. For instance, the mass of the nucleons is around 939 MeV [N+10],

15
whereas the combined current quark mass of its three valence quarks is below 20 MeV. The mass of these hadrons has to be generated dynamically and we can assume that the small current quark mass itself is not the main generator of the hadron masses. Hence we expect symmetries for $M \to 0$ (chiral limit) to be approximate symmetries. In this limit the QCD Lagrangian reads
\begin{align}
L^0_{\text{QCD}} = \left[ \bar{q}_L(i\not{D})q_L + \bar{q}_R(i\not{D})q_R \right] - \frac{1}{2} \text{Tr}_C[G_{\mu\nu}G^{\mu\nu}] .
\end{align}

Besides the still existing $U(1)_V$ symmetry another $U(1)$ appears because
\begin{align}
q(x) \to \exp[-i\varphi_A] \gamma_5 q(x) = \begin{pmatrix} \exp[+i\varphi_A] & 0 \\ 0 & \exp[-i\varphi_A] \end{pmatrix} \begin{pmatrix} q_L(x) \\ q_R(x) \end{pmatrix}
\end{align}
is now a symmetry transformation. This axial $U(1)_A$ symmetry is only manifest on the classical level but is broken anomalously by quantum effects where a finite divergence is generated for the axial current [Adl69].

The chiral Lagrangian $L^0_{\text{QCD}}$ is also invariant under global chiral transformations, which are transformations in the two-dimensional flavor space $q = (u, d)$:
\begin{align}
q_L(x) &\to L \ q_L = \exp[-i\Theta_L \cdot \frac{\tau}{2}] q_L(x) \\
q_R(x) &\to R \ q_R = \exp[-i\Theta_R \cdot \frac{\tau}{2}] q_R(x) .
\end{align}

The $\tau^i$ are called isospin matrices and are the Pauli matrices given in Eq. (A.1) and the according symmetry group of these transformations is $\text{SU}(2)_L \times \text{SU}(2)_R$. An infinitesimal transformation of $\text{SU}(2)_L$ can be parametrized as $L = 1 - i\Theta_L \cdot \tau/2 + \mathcal{O}(\Theta^2_L)$. The respective conserved currents are given by
\begin{align}
L^{\mu,a}(x) &= \bar{q}_L(x) \gamma^\mu \frac{\tau^a}{2} q_L(x) \\
R^{\mu,a}(x) &= \bar{q}_R(x) \gamma^\mu \frac{\tau^a}{2} q_R(x) .
\end{align}

We can also write these currents as a vector, $V_\mu(x) = R_\mu(x) + L_\mu(x)$, and an axialvector current, $A_\mu(x) = R_\mu(x) - L_\mu(x)$. The appropriate charges can then be calculated and are conserved in the chiral limit:
\begin{align}
V^a &= \frac{1}{2} \int d^3x \ q^\dagger(x) \tau^a q(x) \\
A^a &= \frac{1}{2} \int d^3x \ q^\dagger(x) \tau^a \gamma_5 q(x) .
\end{align}

An important point to note here is that the vector and axialvector current have different parity. The charges derived from them have positive (vector charge $V^a$) and negative (axial charge $A^a$) parity. Finally, the left- and right-handed charges fulfill two independent $\text{su}(2)$ algebras, while the vector and axial charges do not fulfill these and do not
2.2 Symmetries

commute:

\[ [V^a, V^b] = [R^a, R^b] + [L^a, L^b] = i\epsilon^{abc} V^c \]
\[ [A^a, A^b] = [R^a, R^b] + [L^a, L^b] = i\epsilon^{abc} A^c \]
\[ [V^a, A^b] = [R^a, R^b] - [L^a, L^b] = i\epsilon^{abc} A^c. \] (2.49)

The chiral limit is only an approximation to nature and we investigate how the quark mass term \( \mathcal{L}_{\text{QCD}} = -\bar{q}_L M q_R - \bar{q}_R M q_L \) explicitly breaks chiral symmetry and how the divergences of the just mentioned currents change. Therefore we perform an infinitesimal SU(2)\(_L\) transformation:

\[ \bar{q}_L M q_R \rightarrow \bar{q}_L M q_R + i\theta_L \bar{q}_L \frac{\tau^a}{2} M q_R + O(\theta^2_L) \]
\[ \bar{q}_R M q_L \rightarrow \bar{q}_R M q_L - i\theta_L \bar{q}_R \frac{\tau^a}{2} M q_L + O(\theta^2_L). \] (2.50)

An analogous calculation can be done for an infinitesimal transformation of SU(2)\(_R\) and using Eq. (2.39) one derives for the divergences of the left- and right-handed quark currents

\[ \partial_\mu L^{\mu,a} = -i \left( \bar{q}_L \frac{\tau^a}{2} M q_R - \bar{q}_R \frac{\tau^a}{2} q_L \right) \]
\[ \partial_\mu R^{\mu,a} = -i \left( \bar{q}_R \frac{\tau^a}{2} M q_L - \bar{q}_L \frac{\tau^a}{2} q_R \right). \] (2.51)

Writing Eq. (2.51) in terms of a vector and an axialvector current we end up with

\[ \partial_\mu V^{\mu,a} = i\bar{q} [\mathcal{M}, \frac{\tau^a}{2}] q \]
\[ \partial_\mu A^{\mu,a} = i\bar{q} \{\mathcal{M}, \frac{\tau^a}{2}\} \gamma_5 q. \] (2.52)

The mass of up and down quarks is nearly the same and since we treat their whole mass as an perturbation, it is a justified approximation to work in the isospin limit where \( \mathcal{M} = m_q 1_2 \). We will work in this limit throughout the thesis. If the reader is interested in isospin breaking effects in the nucleon-nucleon sector, we refer to [FvKPC03]. Inserting the isospin limit in Eqs. (2.52) we end up with a conserved vector current and a relation for the no longer conserved axialvector current with a pseudoscalar density:

\[ \partial_\mu A^{\mu,a}(x) = im_q \bar{q}(x) \tau^a \gamma_5 q(x). \] (2.53)

2.2.3 Chiral Symmetry in the Presence of External Fields

The effective field theory which we want to construct later is based on chiral symmetry. It is convenient to include external fields in both the original QCD as well as in the effective Lagrangian and demand that these external fields transform the same way under chiral transformations. This demand makes it possible to find all operators of the
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effective theory that are allowed by the symmetry. We will also see that external fields can be used to find a systematic way to incorporate the explicit symmetry breaking by the quark-masses. We define vector, axialvector, scalar and pseudoscalar fields which are Hermitian $2 \times 2$ matrices in flavor space and introduce them into a new Lagrangian, 

$$
\mathcal{L}_{\text{ext}} = \mathcal{L}^0_{\text{QCD}} + \bar{q} \gamma_\mu \left( \frac{1}{2} v^\mu + \frac{\tau^a}{2} (v^\mu + \gamma_5 a^\mu) \right) q - \bar{q} (s - i \gamma_5 p) q,
$$

(2.54)

where $s = \frac{1}{2} s^0 + \tau^a s^a$ and $p = \frac{1}{2} p^0 + \tau^a p^a$. We can define a generating functional

$$
\exp\left[ i Z^0_{\text{QCD}}[v,a,s,p] \right] = \int \mathcal{D}A \mathcal{D}\bar{q} \mathcal{D}q \exp \left[ i \int d^4x \mathcal{L}_{\text{ext}}(A, \bar{q}, q; v, a, s, p) \right] \quad (2.55)
$$

that describes the dynamics of QCD in the chiral limit in the presence of external fields. We are able to calculate vacuum expectation values of certain operators by the means of functional derivatives. There are relations between divergences of these Green’s functions and other Green’s functions (e.g., Eq (2.53)) that represent the underlying symmetry, called Ward identities. Leutwyler proved an “invariance theorem” \cite{Leu94} that states that all chiral Ward identities, which are local relations, can be deduced from the generating functional of Eq. (2.55) if we promote the global chiral symmetry of QCD to a local symmetry of the Lagrangian $\mathcal{L}_{\text{ext}}$. Using the left- and right-handed projectors $P_{R/L}$ and the relation $P_{R/L} \gamma_5 = \pm P_{R/L}$ we can rewrite Eq. (2.54) as:

$$
\mathcal{L}_{\text{ext}} = \bar{q}_L (i\not{\partial}) q_L + \bar{q}_R (i\not{\partial}) q_R - \frac{1}{2} \text{Tr}[G_{\mu\nu}G^{\mu\nu}] \\
+ \bar{q}_L \gamma^\mu \left( \frac{1}{2} v^\mu + \frac{\tau^a}{2} (v^\mu - a^\mu) \right) q_L + \bar{q}_R \gamma^\mu \left( \frac{1}{2} v^\mu + \frac{\tau^a}{2} (v^\mu + a^\mu) \right) q_R \\
- \bar{q}_R (s + ip) q_L - \bar{q}_L (s - ip) q_R.
$$

(2.56)

The requirement of local invariance under transformations $q \rightarrow [L(x)P_L + R(x)P_R]q$ dictates the chiral transformation behavior of the external fields. We define left- and right-handed vector fields $l_\mu = \frac{\tau^a}{2} (v^\mu - a^\mu)$ and $r_\mu = \frac{\tau^a}{2} (v^\mu + a^\mu)$ and see that they are the gauge fields of the local chiral symmetry. $v^\mu$ is not acting in flavor space and therefore it does not transform under chiral transformations. In summary, the external fields have the following chiral transformation behavior:

$$
\begin{align*}
v^\mu &\rightarrow v^\mu \\
l_\mu &\rightarrow L (l_\mu + i\partial^\mu) L^\dagger \\
r_\mu &\rightarrow R (r_\mu + i\partial^\mu) R^\dagger \\
s + ip &\rightarrow R (s + ip) L^\dagger \\
s - ip &\rightarrow L (s - ip) R^\dagger.
\end{align*}
$$

(2.57)

At this point it should be mentioned that the gluonic part of the Lagrangian is not affected by chiral transformations and therefore it was omitted from the discussion. We also did not discuss an isoscalar axialvector current as an external field because
the corresponding $U(1)_A$ symmetry is anomalously broken and therefore the generating functional is not invariant under a local axial transformation \cite{Leu94}.

Finally, we note that the connection between the Lagrangian with external fields which we defined in the chiral limit to the full QCD Lagrangian is given by setting all external fields equivalent to 0 besides $s = \mathcal{M}$. This connection will be used to include the explicit breaking of chiral symmetry in the effective Lagrangian.

### 2.3 Spontaneous Symmetry Breaking

#### 2.3.1 Signature of a Symmetry Breakdown

The hadron spectrum is approximately built of multiplets of SU(2). However these states do not have degenerate parity partners which is a sign that the chiral symmetry group $SU(2)_L \times SU(2)_R$ is broken down to its vectorial subgroup $SU(2)_V$ as the axial generators would otherwise change the parity of states: let $|m, p, n\rangle$ be a state with mass $m$ and parity $p = \pm 1$ and possible other quantum numbers collected in $n$:

$$H|m, p, n\rangle = m|m, p, n\rangle, \quad P|m, p, n\rangle = p|m, p, n\rangle.$$  

If the axial symmetry were a symmetry of the ground state, i.e.,

$$A^a|0\rangle = 0 \quad \text{(Wigner-Weyl mode)}, \quad \text{(2.58)}$$

then the charges of the symmetry generate new states,

$$A^a|m, a, n\rangle = (A^a, a^\dagger_{m,p,n} + a^\dagger_{m,p,n}A^a)|0\rangle = a^\dagger_{m',p',n'}|0\rangle = |m', p', n'\rangle,$$

with the same mass ($m' = m$) but different parity ($p' = -p$):

$$[H, A^a]|m, p, n\rangle = 0 = (m' - m)|m', p', n'\rangle$$

$$P|m', p', n'\rangle = PA^aP^{-1}P|m, p, n\rangle = -A^aP|m, p, n\rangle = -p|m', p', n'\rangle. \quad \text{(2.59)}$$

In the case of a spontaneously broken symmetry the ground state does no longer respect the full symmetry and in our case the 3 axial charges generate new states

$$|\pi^a\rangle = A^a|0\rangle \neq 0 \quad \text{(Nambu-Goldstone mode)}. \quad \text{(2.60)}$$

According to the Goldstone theorem these states are massless bosons carrying the same quantum numbers as the broken generators. Looking at the hadron spectrum we see that there exists a large mass gap between the pseudoscalar and the scalar mesons, e.g., the neutral pion ($I = 1, J^P = 0^-, m_{\pi^0} \approx 135 \text{ MeV}$) is nearly massless compared to its scalar counterpart $a_0$ ($I = 1, J^P = 0^+, m_{a_0} = 980 \text{ MeV}$) \cite{N+10}. Since the current quark mass is nonzero and chiral symmetry is only approximate realized, the Goldstone bosons will acquire a small mass which justifies the pions as the Goldstone bosons of the broken
2 Quantum Chromodynamics

approximate chiral symmetry. The relation between the quark and pion masses is given by the Gell-Mann–Oakes–Renner relation \[GMOR68\],

\[ f_0^2 m_\pi^2 = m_q \langle 0 | \bar{q} q | 0 \rangle. \] (2.61)

This relation will be derived in chapter 2.3.2 using current and charge algebra and in chapter 3.2.2 in the context of the effective theory. The other hadrons (consisting of up and down quarks) all possess a mass in the chiral limit, and chiral extrapolations show that, e.g., the nucleon mass in the chiral limit is \( 884 \pm 6 \) MeV [PMW06] and therefore not that different from its physical value of around \( 939 \) MeV [N+10]. This strengthens the picture that the quark masses can be treated as perturbations to the chiral limit.

2.3.2 The PCAC Hypothesis and the Gell-Mann–Oakes–Renner relation

Goldstone’s theorem tells us that pions have the quantum numbers of the broken generators and that \( A^a | 0 \rangle \) is nonzero. We can deduce that a pion can be generated out of the ground state via an axial current, and because of T-invariance also decay. Because of Lorentz covariance we can parametrize

\[ \langle 0 | A^{\mu,a}(x) | \pi^b(p) \rangle = i p^\mu f_0 \delta^{ab} e^{-ipx}. \] (2.62)

\( f_0 \) is called the pion decay constant and its experimental value is \( f_\pi = (92.4 \pm 0.3) \) MeV (e.g., in \( \pi^+ \to \mu^+ \bar{\nu}_\mu \)). Taking the divergence of this relation implies because of \( p^2 = m_\pi^2 \)

\[ \langle 0 | \partial_\mu A^{\mu,a}(x) | \pi^b(p) \rangle = m_\pi^2 f_0 \delta^{ab} e^{-ipx}. \] (2.63)

The partially conserved axial-vector current (PCAC) hypothesis promotes this relation on the operator level:

\[ \partial_\mu A^{\mu,a}(x) = m_\pi^2 f_0 \pi^a(x), \] (2.64)

where \( \pi^a(x) \) is the pion field operator. This field operator can either create or destroy exactly one pion state, and therefore we only need to include one-pion intermediate states

\[ \sum_c \int \frac{d^3p}{(2\pi)^3 2E_p} |\pi^c(p)\rangle \langle \pi^c(p)| \]

to achieve completeness for an intermediate state in \( \langle 0 | [A^a, \partial_\mu A^{\mu,b}(x)] | 0 \rangle \). Furthermore we write the charge as a spatial integral over the 0-component of the current and use Eqs. (2.62) and (2.63) to evaluate

\[ -i \langle 0 | [A^a, \partial_\mu A^{\mu,b}(x)] | 0 \rangle = m_\pi^2 f_0^2 \delta^{ab}. \] (2.65)

We want to stress that Eq. (2.64) is not exact as the axial-vector current cannot only create one-pion states, but all states that share the same quantum numbers. But as pions are the lightest of these particles the spectrum will be dominated by them.
Now we look at the commutator \([A^a, \partial_\mu A^{\mu b}(x)]\) on the operator level. Eqs. (2.48) and (2.53) relate them to composite Hermitian operators of QCD and we can compute them on this level:

\[
- i[A^a, \partial_\mu A^{\mu b}(x)] = \frac{m_q}{2} \int d^3y \left[ q_{\alpha,i}^\dagger(y) (\gamma_5 \tau^a)_{\alpha\beta} q_{\beta,j}(y), q_{\nu,k}^\dagger(x) (\gamma_0 \gamma_5 \tau^b)_{\nu\rho} q_{\rho,l}(x) \right]
\]

\[
= \frac{m_q}{2} q_{\alpha,i}^\dagger(x) [\gamma_5 \tau^a, \gamma_0 \gamma_5 \tau^b] q(x) = -\frac{m_q}{2} \bar{q}(x) \{\tau^a, \tau^b\} q(x)
\]

\[
= -m_q \bar{q} q \delta^{ab}.
\]

(2.66)

\{
\alpha, \beta, \nu, \rho\} are spinor indices, \{i, j, k, l\} denote the isospin indices of the matrices and equal-time canonical anticommutator relations \(\{q_{\alpha,i}(x), q_{\beta,j}(y)\} = \delta^{(3)}(x - y) \delta_{\alpha\beta} \delta_{ij}\) are used. Finally, inserting Eq. (2.66) into Eq. (2.65) leads to the Gell-Mann–Oakes–Renner relation Eq. (2.61). We will use this relation throughout the present work in order to express the current-quark-mass dependence in terms of the pion mass. This has the advantage that observables scale with the pion mass and we have a well-defined physical limit at \(m_\pi \approx 138\) MeV (average pion mass).

2.3.3 Group Theoretical Considerations for Pion-Field Transformations

We now want to derive the nonlinear transformation behavior of the pions from a group theoretical point. Let us assume that there is a symmetry group \(G\) broken down to a subgroup \(H\). That means that \(h|0\rangle = 0 \forall h \in H\) and \(g|0\rangle \neq 0 \forall g \notin H\). We can see that the coset space \(gH\) plays a crucial role because all elements of one coset generate the same transformations on the ground state:

\[
g|0\rangle = gh|0\rangle = g'|0\rangle \iff g' \in gH.
\]

(2.67)

We can identify the cosets \(gH\) (besides \(H\) itself) with the broken generators as they describe the possible transformations that do not annihilate the ground state.

We collect the pion fields in an SU(2)-matrix \(U\)

\[
U = \frac{1}{f_0} (\sigma_{12} + i\tau \cdot \pi) = \frac{1}{f_0} \left( \sqrt{f_0^2 - \pi^2} 1_{12} + i\tau \cdot \pi \right).
\]

(2.68)

To find a nonlinear realization we define the operation of an element \(g = (L, R)\) of the chiral group \(G = SU(2)_L \times SU(2)_R\) on the set \(M = SU(2) \times SU(2)\) in the following way:

\[
(A, B) \overset{g=(L,R)}{\rightarrow} (L, R)(A, B) \equiv (LA, RB) \quad \forall (A, B) \in M.
\]

(2.69)

The remaining symmetry \(H = SU(2)_V\) consists of all transformations, where left- and right-handed fields are transformed in the same way (\(\{g = (V, V)|V \in SU(2)\}\)). Therefore it is always possible to find a representative of \(gH\) in the set \(M\), that has the unit matrix in the second argument:

\[
(A, B) = (AB^\dagger, 1_2)(B, B) \in (AB^\dagger, 1_2)H.
\]

(2.70)
Letting a chiral transformation act on the representative containing the pion matrix \( U \), we find that
\[
(U, 1_2) \xrightarrow{\gamma=(L,R)} (LU, R) \in (LUR^\dagger, 1_2)H
\]
and the pion matrix therefore transforms as
\[
U \rightarrow LUR^\dagger. \tag{2.72}
\]
The restriction on transformations of SU(2)_V shows that the pion matrix transforms in the 3-dimensional adjoint representation of SU(2), which is locally isomorphic to the fundamental vector representation of SO(3).

The definition of the pion fields in an SU(2) matrix of Eq. (2.68) is not unique. Another frequently used parametrization is
\[
U = \exp \left[ \frac{1}{f_0} \tau \cdot \pi' \right]. \tag{2.73}
\]
The pion fields of the two matrices are connected by a nonlinear field redefinition
\[
\pi^a(x) = \pi'^a(x) + \mathcal{O}(|\pi'|^3) \tag{2.74}
\]
as can best be seen when expanding both \( U \) matrices in terms of pion fields:
\[
U(\pi) = 1 + \frac{1}{f_0} \tau \cdot \pi - \frac{1}{2f_0^2} \pi^2 + \mathcal{O}(|\pi|^3). \tag{2.75}
\]
In general, there is an infinite amount of parametrizations as unitarity and unit determinant only fix the first three summands of the expansion. Independent of the way the pion fields are collected in an SU(2) matrix \( U(\pi) \), the behavior under chiral transformations is according to Eq. (2.72).
3 Chiral Perturbation Theory

3.1 Effective-Field-Theory Approach

In the previous chapter we explored the approximate chiral symmetry of the QCD Lagrangian, its breaking pattern, and the transformation properties of the resulting Goldstone bosons. In the 1960’s the Ward identities related to the spontaneously broken chiral symmetry were explored in the context of current algebra [AD68]. However, the inclusion of quantum effects required the concept of an effective field theory (EFT).

The idea behind EFTs is similar to a multipole expansion in electrodynamics: for a sufficiently large distance to the charge density one does not need to know its exact form, but can approximate the potential by the multipole moments in an expansion of the charge density radius over the large distance. In a quantum field theory this idea is used for systems with different intrinsic scales $\lambda \ll \Lambda$. Observables can then be expanded in $\lambda/\Lambda$. It is evident that such an expansion breaks down for $\lambda \to \Lambda$ and an EFT is only a low-energy approximation of the underlying theory. An EFT makes the expansion in $\lambda/\Lambda$ on the level of the Lagrangian using symmetry principles. The relation between tree-level EFT and current algebra was established by the works of Dashen and Weinstein [DW69], Weinberg [Wei68] and Callen, Coleman, Wess and Zumino [CWZ69],[CCWZ69]. Weinberg showed the systematic inclusion of loop effects in his seminal paper [Wei79] in which he stated the following well-known theorem:

“If one writes down the most general possible Lagrangian, including all terms consistent with assumed symmetry principles, and then calculates matrix elements with this Lagrangian to any given order in perturbation theory, the result will simply be the most general possible S-matrix consistent with analyticity, perturbative unitarity, cluster decomposition, and the assumed symmetry principles.”

The method was systematized by Gasser and Leutwyler for the flavor-SU(2) [GL84] and SU(3) [GL85] cases. In the case of two-flavor low-energy QCD pions and nucleons are the effective degrees of freedom. Gasser, Sainio and Svarc [GSS88] showed that the inclusion of nucleons is not straightforward because the nucleon mass does not vanish in the chiral limit and hence a new scale is introduced to the problem. Because $M_N \sim 1$ GeV, the four-momentum of a nucleon can never be small. However, we treat processes in which their 3-momenta and the pion mass are of comparable size. We use them as the small expansion parameters whereas the symmetry breaking scale $\Lambda = 4\pi f_\pi \approx 1$ GeV is the hard scale. We could also identify the mass of the $\rho(770)$ as the breakdown scale since we expect the dynamics of this lightest non-Goldstone-boson particle (consisting of only $u$ and $d$ quarks) to become important around its mass scale. The energy region of interest is far below scales where QCD is perturbative, hence a matching calculation
3 Chiral Perturbation Theory

Table 3.1: Transformation properties of the external fields

<table>
<thead>
<tr>
<th>Field</th>
<th>Transformation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\chi$</td>
<td>$L\chi R^\dagger$</td>
</tr>
<tr>
<td>$r_\mu$</td>
<td>$R(r_\mu + i\partial_\mu)R^\dagger$</td>
</tr>
<tr>
<td>$l_\mu$</td>
<td>$L(l_\mu + i\partial_\mu)L^\dagger$</td>
</tr>
</tbody>
</table>

Table cannot be done. Instead the coefficients for the effective operators, the so-called low energy constants, are fitted to physical data.

We first present chiral perturbation theory (ChPT) including only pions. This has the advantage that all momenta and masses are of the size of the small scale and we say they are of order $p$ ($\mathcal{O}(p)$) or chiral dimension one. Later, we will incorporate nucleons into the theory.

3.2 Chiral Perturbation Theory for Pions

3.2.1 Construction of Chiral Lagrangians

Following Weinberg’s statement we try to find all possible Hermitian operators allowed by the symmetries of massless QCD: chiral symmetry, parity, charge conjugation. At lowest chiral order the Lagrangian can be found by noting that all derivatives acting on the pion matrix $U$ rise the chiral order by one and checking for all linear independent terms. For higher orders, however, we want to look for a more systematic way. Gasser and Leutwyler [GL84] first derived a chiral Lagrangian up to order $\mathcal{O}(p^4)$ using the so-called external fields method. In this work we follow the way outlined in Ref. [Sch03]. The idea is to construct a generating functional

$$\exp[iZ^0[v,a,s,p;\pi]] = \int DU \exp \left[ i \int d^4x \mathcal{L}_{\text{eff}}(U;v,a,s,p) \right]$$

which approximates the generating functional of QCD from Eq. (2.55). The effective Lagrangian $\mathcal{L}_{\text{eff}}$ then has to be Hermitian, Lorentz-invariant, invariant under charge conjugation, has to possess positive parity and, finally, must be invariant under local chiral transformations. These demands allow us to look for all possible “building blocks” out of which we can generate all allowed operators in the desired chiral dimension.

The transformations of the external fields and the pion matrix under (local) chiral transformations have been worked out in the previous chapter and given in Eqs. (2.57) and (2.72). The transformations under parity ($P$) and charge conjugation ($C$) can be calculated for the external fields from Eq. (2.54) considering that $q(x,t) \overset{P}{\rightarrow} \gamma_0 q(\mathbf{x},t)$ under parity and $q \overset{C}{\rightarrow} -i(\bar{q}\gamma_0\gamma_2)^T$ under charge conjugation and the overall Lagrangian is even under both transformations separately. We define $\chi = 2B(s-i\rho)$ [GL84] and collect all transformation properties of the external fields in Table 3.1. Goldstone’s
3.2 Chiral Perturbation Theory for Pions

Theorem shows that pions inherit the quantum numbers and transformation properties from the broken charges, hence \( \pi(x) \stackrel{P}{\rightarrow} -\pi(-x) \) and \( \pi \stackrel{C}{\rightarrow} \pi^T \). We can conclude that \( U(x) \stackrel{P}{\rightarrow} U^\dagger(-x) \) and \( U \stackrel{C}{\rightarrow} U^T \).

The next step is to find a chiral covariant derivative for the pion fields. We demand that the covariant derivative of the pion matrix transforms as the pion matrix itself:

\[
D_\mu U(x) \rightarrow D'_\mu L(x)U(x)R^\dagger(x) \equiv L(x)D_\mu U(x)R^\dagger(x). \tag{3.2}
\]

This is fulfilled by

\[
D_\mu U \equiv \partial_\mu U - il_\mu U + iUr_\mu \tag{3.3}
\]

with the transformation properties

\[
\begin{align*}
\partial_\mu U & \rightarrow L(\partial_\mu U)R^\dagger + (\partial_\mu L)UR^\dagger + LU(\partial_\mu R^\dagger) \\
il_\mu U - iUr_\mu & \rightarrow Li_\mu UR^\dagger - (\partial_\mu L)UR^\dagger - LiUr_\mu R^\dagger - LU(\partial_\mu R^\dagger),
\end{align*}
\]

where we used \((\partial_\mu L)L^\dagger = -L(\partial_\mu L^\dagger)\) in the second line. Using the properties of the external fields from Table 3.1 we compute that \(D_\mu U\) also has the same transformation properties as \(U\) under \(C\) and \(P\). For completeness we also introduce the field-strength tensors for the gauge fields \(r_\mu\) and \(l_\mu\):

\[
f^{L}_{\mu\nu} = \partial_\mu l_\nu - \partial_\nu l_\mu - i[l_\mu, l_\nu] \tag{3.4}
\]

and analogously for the right-handed fields. These field-strength tensors transform in the adjoint representation of the corresponding SU(2) Lie group \((f^{L}_{\mu\nu} \rightarrow Lf^{L}_{\mu\nu}L^\dagger)\) and inherit the \(C\) and \(P\) transformations from \(l_\mu\) and \(r_\mu\), respectively.

We now take the pion momentum as an expansion parameter and therefore assign \(O(p)\) to \(D_\mu U\). Any further covariant derivative raises the chiral dimension by one unit. For consistency, \(U\) is of chiral dimension zero, \(l_\mu\) and \(r_\mu\) are of order one and \(f^{L/R}_{\mu\nu}\) are of chiral dimension 2. We have already discussed the connection of the external field \(s\) with the quark mass matrix \(M\) and because of the Gell-Mann–Oakes–Renner relation (Eq. (2.61)) we can deduce that \(\chi = O(p^2)\).

We collected all these attributes of the building blocks in Table 3.2. We notice that the first three behave as \(L(\ldots)R^\dagger\) under chiral transformations. Let \(A, B\) be two of these building blocks, then \(\text{Tr}[AB^\dagger]\) (trace over two-dimensional flavor space) is chiral invariant:

\[
\text{Tr}[AB^\dagger] \rightarrow \text{Tr}[LAR^\dagger RB^\dagger L^\dagger] = \text{Tr}[AB^\dagger]. \tag{3.5}
\]

We can combine four, six, etc. building blocks together in the form \((AB^\dagger)(CD^\dagger)\ldots\) and the trace will still be invariant. Furthermore, the product of invariant traces is invariant as well.

We now derive the lowest order pion Lagrangian. At \(O(p^0)\) there is only the term \(\text{Tr}[UU^\dagger] = \text{Tr}[1_2] = 2\) which is an irrelevant constant and does not contribute to the dynamics. Because of Lorentz-invariance we can only raise the chiral dimension in steps of two:

\[
\mathcal{L}_\pi = \mathcal{L}_\pi^{(2)} + \mathcal{L}_\pi^{(4)} + \mathcal{L}_\pi^{(6)} + \ldots \tag{3.6}
\]
Table 3.2: Building blocks for a ChEFT including only pions and their attributes.

where the superscript denotes the chiral dimension. The next chiral invariant contributions appearing at $\mathcal{O}(p^2)$ are: $\text{Tr}[(D_\mu U)(D^\mu U)^\dagger]$, $\text{Tr}[(D_\mu D^\mu U)U^\dagger]$, $\text{Tr}[U(D_\mu D^\mu U)^\dagger]$, $\text{Tr}[\chi U^\dagger]$ and $\text{Tr}[U\chi^\dagger]$. The relation

$$ (D_\mu U)U^\dagger = -U(D_\mu U)^\dagger $$

shows that the first three candidates are linearly dependent. The common choice is to use $\text{Tr}[(D_\mu U)(D^\mu U)^\dagger]$ and discard the other two. From Table 3.2 we see that this choice has the correct transformation behavior under parity and charge conjugation as well. The demand of even $P$ makes it necessary to combine the remaining two candidates to $\text{Tr}[\chi U^\dagger + U\chi^\dagger]$. The lowest order chiral effective Lagrangian then reads:

$$ \mathcal{L}_\pi^{(2)} = \frac{f_0^2}{4} \left( \text{Tr}[(D_\mu U)(D^\mu U)^\dagger] + \text{Tr}[\chi U^\dagger + U\chi^\dagger] \right). $$

Note that we can use the same prefactor $f_0^2/4$ to both operators because the definition of $\chi = 2B(s - ip)$ carries another independent parameter $B$ – a low energy constant (LEC) – which we will later relate to the scalar quark condensate.

Finally, we set the external fields to $v = a = p \equiv 0$ and $s = M$. The covariant derivatives are substituted by normal derivatives and $\chi = \chi^\dagger = 2B M$. The lowest-order chiral Lagrangian including only pions is:

$$ \mathcal{L}_\pi^{(2)} = \frac{f_0^2}{4} \left( \text{Tr}[(\partial_\mu U)(\partial^\mu U)^\dagger] + 2B\text{Tr}[MU^\dagger + U\mathcal{M}] \right). $$

The same procedure can be applied to construct the higher-order Lagrangians. The elimination of linearly dependent terms becomes more tedious, though. We refer the reader to [GL84] and [FS96] for the effective Lagrangians of chiral order four and six. For the sake of completeness we cite the fourth Lagrangian with the above described external fields:

$$ \mathcal{L}_\pi^{(4)} = \frac{l_1}{4} \left( \text{Tr}[(\partial_\mu U)(\partial^\mu U)^\dagger] \right)^2 + \frac{l_2}{4} \text{Tr}[(\partial_\mu U)(\partial_\nu U^\dagger)] \text{Tr}[(\partial^\mu U)(\partial^\nu U^\dagger)]
 + \frac{l_3}{4} \left( 2B\text{Tr}[MU^\dagger + U\mathcal{M}] \right)^2
 - \frac{l_7}{4} \left( 2B\text{Tr}[MU^\dagger - U\mathcal{M}] \right)^2. $$

We see that the number of operators increases and that we need to introduce additional LECs to raise the chiral order. These low-energy constants have the structure $l_i = \cdots$
\[ \bar{l}_i + l_i^{\inf} \] where \( l_i^{\inf} \) is used to renormalize the divergences from loop diagrams. The finite contributions \( \bar{l}_i \) can be fitted to \( \pi\pi \) scattering data or estimated by resonance saturation [EGPdR89]. The heavier resonances possess derivative couplings to pions and when integrating them out, the momentum-independent part of the propagators (which are local operators in coordinate space) generate pion couplings. This procedure allows for an estimation of the LECs [BKM95].

### 3.2.2 Gell-Mann–Oakes–Renner relation (II)

We have already noted that the Gell-Mann–Oakes–Renner relation (Eq. (2.61)) is not exact. In the previous derivation we have made the assumption that the pseudoscalar states are saturated by one-pion states. We now want to show that the relation between the pion mass and quark masses is correct up to linear order in the quark masses.

The LEC \( B \) is related to the chiral quark condensate as can be seen by a comparison of

\[ \frac{\partial}{\partial m_q} \langle 0| \mathcal{H}_{\text{QCD}} |0 \rangle = \langle 0| \bar{q}q |0 \rangle \] (3.11)

with its counterpart in the effective theory

\[ \frac{\partial}{\partial m_q} \langle 0| \mathcal{H}_{\text{eff}} |0 \rangle = \frac{\partial}{\partial m_q} \langle 0| \bar{q}q |0 \rangle - \frac{f_0^2 B m_q}{2} \text{Tr}[U + U^\dagger] + \ldots |0 \rangle = -2f_0^2 B + \mathcal{O}(m_q). \] (3.12)

Connecting the two equations by the demand that the effective theory describes the underlying QCD for small scales, we obtain

\[ B = -\frac{1}{2f_0^2} \langle 0| \bar{q}q |0 \rangle + \mathcal{O}(m_q). \] (3.13)

We expand the Lagrangian (3.9) in powers of pion fields and consider the two-pion contributions (with \( \mathcal{M} = m_q \mathbf{1}_2 \))

\[ \mathcal{L}_{\pi}^{(2)} |_{2\pi} = \frac{1}{2} (\partial_\mu \pi)(\partial^\mu \pi) - B m_q \pi^2. \] (3.14)

We notice the canonical form for scalar fields of the derivative term and use this to explain the parametrization in Eq. (3.8). We define the pion mass as the constant coefficient to the operator \( -\pi^2/2 \). From Eq. (3.14) we deduce

\[ m_\pi^2 = 2B m_q + \mathcal{O}(m_q^2). \] (3.15)

Inserting Eq. (3.13) into this equation shows that the squared pion mass is linearly dependent on the quark-mass and that there are corrections starting at \( \mathcal{O}(m_q^2) \):

\[ f_0^2 m_\pi^2 = -m_q \langle 0| \bar{q}q |0 \rangle + \mathcal{O}(m_q^2). \] (3.16)
3 Chiral Perturbation Theory

3.2.3 Power Counting and Rescaling

We are now going to classify Feynman diagrams in order to get a consistent result at a particular order in perturbation theory. We therefore look for the power $\nu$ of the soft scale (chiral dimension) associated with a diagram or amplitude. According to Weinberg [Wei79] the only quantities entering in a transition amplitude $\mathcal{M}$ that have a non-vanishing dimensionality are the common energy scale $E$, the renormalization scale $\mu$ and the couplings $g$. Since the couplings factorize any amplitude can be written in the form

$$\mathcal{M} = \mathcal{M}(E, \mu, g) = E^\nu f(E/\mu, g).$$  \hspace{1cm} (3.17)

For small pion energies, $\mu$ can be chosen of the size of $E$. Hence $\nu$ will determine the importance of a given diagram and the dominant graphs will be those with the smallest $\nu$. The chiral power $\nu$ of a given diagram is determined as follows: every internal line represents a propagator, which carries chiral dimension $-2$, every pion vertex stemming from $L(2n)\pi$ increases the power by $2n$, and finally every loop gives rise to a $D$-dimensional momentum integration, thus increasing the chiral dimension by $D = 4 - 2\epsilon$. In summary, we arrive at

$$\nu = DL - 2I + \sum_n 2nV_{2n},$$  \hspace{1cm} (3.18)

where $L$ is the number of loops, $I$ the number of internal lines and $V_{2n}$ the number of vertices from $L(2n)\pi$. Setting $\epsilon \to 0$ and using the topological relation $L = I - \sum_n V_{2n} + 1$ we can find a formula independent of the internal lines [Wei79]:

$$\nu = 2 + 2L + \sum_n (2n - 2)V_{2n}.$$  \hspace{1cm} (3.19)

We make the important observation that diagrams with $n$ meson loops are suppressed by $2n$ powers of the small momenta with respect to the leading term.

We now want to comment on contributions from virtual pions. Eq. (3.17) implicitly and the counting in Eq. (3.18) explicitly assume that virtual momenta $l$ scale to $tl$ if we rescale all small scales ($p \to tp$ and $m_\pi \to tm_\pi$). Because the hard scale only enters in the LECs and factorizes out, the integrands only contain the soft scale. After dimensional regularization and Feynman parametrization any meson loop integral can be written in the form

$$\int \frac{d^Dl}{(2\pi)^4} \frac{i}{[l^2 - p^2 f(m_\pi/p, p_i/p) + i\epsilon]^n},$$  \hspace{1cm} (3.20)

where $f$ is some dimensionless function of the pion mass and the external momenta $p_i$ and $p$ stands for a small external momentum. Now a rescaling of all external momenta and the pion mass can be compensated for by a substitution $l \to tl$, which is the rescaling of the virtual momentum. Thus we are allowed to account for the $D$-dimensional loop-momentum integration by raising the chiral dimension by $D$.  

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3.3 Chiral Perturbation Theory with Pions and Nucleons

In this chapter we extend the constructed chiral EFT (with Lagrangian $\mathcal{L}_\pi$) by the inclusion of nucleons $\Psi = (u, d)$ as possible external states: $\mathcal{L}_{\text{eff}} = \mathcal{L}_\pi + \mathcal{L}_{\pi N} + \mathcal{L}_N$. We will treat processes in which the nucleons have three-momenta of the size of the pion mass, i.e., essentially non-relativistic nucleons. At such low energies the constituents of the nucleon are not resolved and we do not have to treat the nucleon as a composite particle. This feature allows us to describe these spin-1/2 particles with Dirac fields:

$$\mathcal{L}_N = \Psi (i\partial_\mu - M_N)\Psi.$$  \hfill (3.21)

The mass of the nucleons $M_N = 938.9$ MeV (average nucleon mass) is comparable with the hard scale and therefore we can neglect any nucleon-loop effects. We stress that the nucleon mass is not vanishing in the chiral limit. The Dirac Lagrangian is not invariant under local chiral transformations and chiral symmetry will play a crucial role to include the nucleons in the EFT.

3.3.1 Construction of Chiral Pion-Nucleon Lagrangians

We need to find a realization of the SU(2)$_L \times$ SU(2)$_R$ symmetry group for the nucleon field. This realization will in general be nonlinear, but it becomes linear when restricting to the parity-conserving subgroup SU(2)$_V$ (proton and neutron build an isospin doublet). Callan, Coleman, Wess and Zumino [CCWZ69] derived that

$$\begin{pmatrix} U \\ \Psi \end{pmatrix} \rightarrow g(L, R, U) \begin{pmatrix} U \\ \Psi \end{pmatrix} = \begin{pmatrix} LUR^\dagger \\ K(U, L, R)\Psi \end{pmatrix}$$  \hfill (3.22)

is a realization that becomes linear for $L = R$ if we define $K = \sqrt{LU\tilde{R}^\dagger}L\sqrt{U}$. $K = K(U, L, R)$ not only depends on the group elements $L$ and $R$, but also on the pion-field matrix $U$. Because the pion fields are functions of the space-time coordinate $x$, the transformation in Eq. (3.22) becomes a local transformation. We define $\xi = \sqrt{U} \rightarrow \xi' = \sqrt{LU\tilde{R}^\dagger}$, such that we can write $K = \xi'^\dagger L\xi$. We want to check that the map $g(L, R, U)$ in Eq. (3.22) indeed is a realization of chiral symmetry, i.e., the homomorphism property is fulfilled:

$$\begin{pmatrix} U^u \\ \Psi^u \end{pmatrix} = [g(L_2, R_2) \circ g(L_1, R_1)]\begin{pmatrix} U \\ \Psi \end{pmatrix} = g(L_2, R_2)\begin{pmatrix} L_1UR_1^\dagger \\ \xi_1^\dagger L_1\xi \Psi \end{pmatrix}$$

$$= \begin{pmatrix} L_2L_1UR_1^\dagger R_2^\dagger \\ \xi_2^\dagger L_2\xi_1^\dagger L_1\xi \Psi \end{pmatrix} = \begin{pmatrix} (L_2L_1)U(R_2R_1)^\dagger \\ \xi_2^\dagger (L_2L_1)\xi \Psi \end{pmatrix}$$

$$= g(L_2L_1, R_2R_1)\begin{pmatrix} U \\ \Psi \end{pmatrix}.$$  \hfill (3.23)

We have used the abbreviations $\xi_1 = \sqrt{L_1UR_1^\dagger}$ and $\xi_2 = \sqrt{(L_2L_1)U(R_2R_1)^\dagger}$ and the fact that the $\xi$ matrices are SU(2)-valued matrices because $\xi^\dagger\xi = \sqrt{U^\dagger U} = 1$. 

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We still need to show that $g(V,V)$ is a linear representation. We use the relation $\sqrt{\xi^\dagger V} = \sqrt{(VUV^\dagger)(VUV^\dagger)}$ to deduce $\xi^\dagger V = \pm V \xi V^\dagger$ and see from the definition of the compensating field $K$

$$K(U,V,V) = \pm (V\xi V^\dagger)^V \xi = \pm V.$$ 

Thus, this construction ensures that the pions transform as triplet and the nucleons as doublet under SU(2)$_V$ transformations. At this point we need to find building blocks for the nucleon-, pion- and external fields such that $L_{\text{eff}} = L_{\pi} + L_{\pi N} + L_{N}$ is locally chiral invariant, has even parity and is invariant under charge and Hermitian conjugation. We will follow Refs. [FMMS00] and [Mei01] to explain how the chiral nucleon-pion Lagrangians $L_{\pi N}$ can be constructed and refer to this paper for the actual higher order Lagrangians. To find the chiral invariant building blocks we rewrite the transformation of $\xi = \sqrt{U}$ and $\xi^\dagger$ as

$$\xi \rightarrow L \xi K^\dagger, \quad \xi^\dagger \rightarrow K \xi^\dagger L^\dagger = R \xi^\dagger K.$$

The transformation properties of the external fields were summed up in Table 3.1. We first want to form a covariant derivative to make the Dirac Lagrangian $\bar{\Psi}(i\gamma^\mu - M_N)\Psi$ locally chiral invariant. We can check that

$$D_\mu = \partial_\mu + \Gamma_\mu, \quad \Gamma_\mu = \frac{1}{2} (\xi^\dagger (\partial_\mu - il_\mu) \xi + \xi (\partial_\mu - ir_\mu) \xi^\dagger)$$

has the defining attribute

$$D_\mu \Psi \rightarrow (\partial_\mu K) \Psi + K (\partial_\mu \Psi) + \Gamma_\mu K \Psi = KD_\mu \Psi,$$

because the so-called chiral connection $\Gamma_\mu$ transforms as

$$\Gamma_\mu K = \frac{1}{2} \left( K \xi R^\dagger R (\partial_\mu - ir_\mu) (\xi^\dagger K^\dagger) + K \xi L^\dagger L (\partial_\mu - il_\mu) (\xi K^\dagger) \right) = \frac{1}{2} \left( K \Gamma_\mu - \partial_\mu K \right).$$

This means that the covariant derivative itself transforms as $D_\mu \rightarrow KD_\mu K^\dagger$. $\Gamma_\mu$ is built of both left- and right-handed fields to transform as a vector under a parity transformation. There also exists another object with one derivative. It transforms as an axial vector and is denoted by $u_\mu$. The building blocks for chiral pion-nucleon Lagrangians,

$$u_\mu = i (\xi^\dagger (\partial_\mu - il_\mu) \xi - \xi (\partial_\mu - ir_\mu) \xi^\dagger),$$

$$\chi^\pm = \xi^\dagger \chi \xi^\dagger \pm \xi^\dagger \chi \xi^\dagger,$$

$$F^\pm_{\mu\nu} = \xi^\dagger f^R_{\mu\nu} \xi \pm \xi^\dagger f^L_{\mu\nu} \xi^\dagger,$$

all incorporate the transformation properties $X \rightarrow KXX^\dagger$ under chiral symmetry. Chiral invariant terms therefore take the form $\bar{\Psi} X_1 \cdots X_N \Psi$. There are two ways to construct Lorentz-invariant terms out of the building blocks: either we contract the Lorentz-indices of building blocks with themselves, or with Dirac matrices that act on the nucleons. After that, we still have to check for parity, charge conjugation and Hermitian
3.3 Chiral Perturbation Theory with Pions and Nucleons

\[ D_\mu \quad u_\mu \quad \chi_+ \quad \chi_- \quad F^+_{\mu\nu} \quad F^-_{\mu\nu} \]

\[ \mathcal{O}(p^2) \]

| \( D_\mu \) | + | − | + |
| \( u_\mu \) | − | + | + | 1 |
| \( \chi_+ \) | + | + | + | 2 |
| \( \chi_- \) | − | + | − | 2 |
| \( F^+_{\mu\nu} \) | + | − | + | 2 |
| \( F^-_{\mu\nu} \) | − | + | + | 2 |

Table 3.3: Chiral dimension and transformation properties of the building blocks (left) and the structures for Lorentz contractions (right) under charge conjugation \( X \overset{C}{\rightarrow} \pm X^T \), Hermitian conjugation \( X \overset{H}{\rightarrow} \pm X \) and parity transformation \( P \) (+ assigned to scalar and vector)

We did not assign a chiral dimension to the covariant derivative because it is of \( \mathcal{O}(p) \) when acting on any other building block, but because of the large nucleon mass can also be of \( \mathcal{O}(1) \) when acting on a nucleon field.

Any invariant contribution to a Lorentz-invariant chiral Lagrangian can be written as

\[ \bar{\Psi} A^{\mu\nu...} \Theta_{\mu\nu...} \Psi + h.c. \, , \quad (3.28) \]

where \( A^{\mu\nu...} \) consists of pion and external fields and their covariant derivatives and \( \Theta_{\mu\nu...} \) of Dirac matrices and a totally symmetric product of covariant derivatives acting on the nucleon field: \( \Theta_{\mu\nu...} = \Sigma^{(n)}_{\mu\nu...} D_{\alpha\beta...} \) \( \Sigma^{(n)}_{\mu\nu...} \) can be expanded in the standard basis \((1, \gamma_5, \gamma_\mu, \gamma_\mu\gamma_5, \sigma_{\mu\nu})\) and in terms of the metric tensor and Levi-Civita tensor. We only need to include the totally symmetric product of covariant derivatives because \( D_\mu D_\nu = (\{D_\mu, D_\nu\} + [D_\mu, D_\nu])/2 \) and the so-called curvature relation

\[ [D_\mu, D_\nu] = \frac{1}{4} [u_\mu, u_\nu] - \frac{i}{2} F^+_{\mu\nu} \, . \quad (3.29) \]

The covariant derivatives \( D^{(n)}_{\alpha\beta...} \) are not contracted with elements of the Clifford algebra because from \( \bar{D} \Psi = -im\Psi + \mathcal{O}(p) \) one can replace \( \bar{D} \Psi \) by \( -im\Psi \) at a given chiral order. With the same reasoning we can neglect \( \eta^{\mu\nu} \{D_\mu, D_\nu\} \Psi \) because \( \sigma^{\mu\nu} = \gamma^\mu \gamma^\nu - i\eta^{\mu\nu} \).

To find the complete list of \( A^{\mu\nu...} \) at a given chiral order we note that every Lorentz index \( \mu, \nu, \ldots \) increases the chiral order by one. Since the matrix fields do not commute all possible orderings of the buildings blocks are imaginable, but to keep simple transformation properties under \( P, C \) and \( H \) we only have to consider commutators and anticommutators of the building blocks in \( A^{\mu\nu...} \). Considering all these terms the relations

\[ A^l = (-1)^{(l\lambda)} A \, , \, A^C = (-1)^{(c\lambda)} A^T \quad \text{(3.30)} \]

From now on we will combine \( \mathcal{L}_\pi N + \mathcal{L}_N \) in \( \mathcal{L}_\pi N \) for a more convenient notation.
are fulfilled one uses the transformation behavior from Table 3.3 and takes a factor of \((-1)\) into account for every commutator. For the Clifford algebra we can deduce the similar relations
\[
\Sigma^\dagger = (-1)^{(h_\Sigma)} \gamma_0 \Sigma \gamma_0, \quad \Sigma^C = (-1)^{(c_\Sigma)} \Sigma^T.
\] (3.31)
The monomials now take the generic form
\[
\bar{\Psi} A_{\mu \nu \ldots \alpha \beta \ldots} \Sigma_{\mu \nu \ldots} D^{(n)}_{\alpha \beta \ldots} \Psi + (-1)^{h_A + h_\Sigma} \bar{\Psi} D^{(n)}_{\alpha \beta \ldots} \Sigma_{\mu \nu \ldots} A_{\mu \nu \ldots} \Psi.
\] (3.32)
Using integration by parts and neglecting total derivatives and higher order terms from the derivatives acting on external or pion fields we can bring the covariant derivatives to the right. This procedure leads to the prescription \(\bar{D}^{(n)} \rightarrow (-1)^n D^{(n)}\) and the second term has the same form as the first one but with the sign \((-1)^{h_A + h_\Sigma + n}\). This means that the Hermitian conjugate cancels the first term if \(h_A + h_\Sigma + n\) is odd (modulo higher-order terms). With the same reasoning, we can deduce that terms cancel if \(c_A + c_\Sigma + n\) is odd because of charge conjugation (again modulo higher-order terms).²

The list of the remaining monomials \(\bar{\Psi} A_{\mu \nu \ldots} \Theta_{\mu \nu \ldots} \Psi + \text{h.c.}\) includes terms that are linearly dependent because they are connected by general identities or by using the equations of motion which connects two terms modulo higher order terms. For more details on how to eliminate terms and arrive at the minimal set of terms for the Lagrangian we refer to [FMMS00].

Using this formalism we can derive the relativistic chiral Lagrangian in presence of external fields. Setting \(l = r = 0\) changes \(\Gamma_\mu\) and \(u_\mu\) to
\[
\Gamma_\mu \xrightarrow{l=r=0} \frac{1}{2} \left( \xi^\dagger \partial_\mu \xi + \xi \partial_\mu \xi^\dagger \right),
\] (3.33)
\[
u \left( \xi^\dagger \partial_\mu \xi - \xi \partial_\mu \xi^\dagger \right).
\] (3.34)
We can expand these two objects in pion fields and see that \(\Gamma_\mu\) contains at least two, but always an even number, of fields while \(u_\mu\) always yields an odd number of pion fields and therefore at least one. The lowest order Lagrangian with the \(s = M, l = r = p = 0\) configuration of the external fields then includes a coupling between nucleons and an even number of pions by the covariant derivative and an axial coupling between nucleons and one pion (or another odd number):
\[
\mathcal{L}^{(1)}_{\pi N} = \bar{\Psi} \left( i \not{\partial} - M_N + \frac{g_\mu}{2} \gamma_5 \right) \Psi
\] (3.35)
There are four independent terms at the next order:
\[
\mathcal{L}^{(2)}_{\pi N} = \sum_{i=1}^{4} c_i \bar{\Psi} \psi_i \Psi.
\] (3.36)

²Fettes et. al. [FMMS00] therefore assigned the covariant derivative acting on a nucleon formally with a "-" for charge and Hermitian conjugation. This neglects contributions that are anyway canceled by their Hermitian conjugated from the start. With this convention they can define \(h_\Theta = h_\Sigma + n\) and \(c_\Theta = c_\Sigma + n\). Then all invariant monomials fulfill the two conditions \((-1)^{h_A + h_\Theta} = 1\) and \((-1)^{c_A + c_\Theta} = 1\).
The independent operators in Eq. (3.36) are the following:

\[ \mathcal{O}_1 = \text{Tr}[\chi_+] , \quad \mathcal{O}_2 = -\frac{1}{8M_N^2} \text{Tr}[u_\mu u_\nu] D^{\mu\nu} , \quad \mathcal{O}_3 = \frac{1}{2} \text{Tr}[u \cdot u] , \quad \mathcal{O}_4 = \frac{i}{4} [u_\mu, u_\nu] \sigma^{\mu\nu} . \]

The operator \( \mathcal{O}_1 = \text{Tr}[\chi_+] \) is the only one of them related to the explicit symmetry breaking by non-vanishing quark masses. The LECs \( c_1 - c_4 \) can either be fitted to N\( \pi \) scattering data or be estimated from resonance saturation noting that the main contribution to \( c_3 \) and \( c_4 \) stems from the \( \Delta \)-resonance and \( \rho \)-exchange \[BKM97\]. The third-order Lagrangian

\[ \mathcal{L}^{(3)}_{\pi N} = \sum_{i=1}^{23} d_i \bar{\Psi} \mathcal{O}_i^{(3)} \Psi \]  

contains 23 independent terms in the presence of external fields listed in \[FMMS00\]. For the \( s = M, l = r = p = 0 \) configuration only the operators 1–5 and 10–18 are nonzero. We can split these into three types according to the minimal number of pion fields needed for a vertex. This number is dictated by the number of fields \( u_\mu \) because it is the only building block that necessarily consists of at least one pion field. \( d_5 \), and \( d_{16} - d_{18} \) contribute to one-pion exchange, \( d_1 - d_3 \) and \( d_{14}, d_{15} \) contribute to two-pion exchange while the others cannot contribute below three-pion exchange. The LECs \( d_i \) decompose into a finite part \( \tilde{d}_i \) and an infinite part \( d_i^\infty \) which is used for renormalization of loop diagrams.

### 3.3.2 Heavy-Baryon Approach

Having the chiral pion-nucleon Lagrangians at hand, we notice that the nucleon mass \( M_N \) in \( \mathcal{L}_{\pi N}^{(1)} \) introduces a new mass scale. The derivative acting on a nucleon field does not have a chiral order. Consider a nucleon almost at rest \( (p \approx 0) \), then \( \partial_0 \Psi \) is of chiral order zero, while \( \partial_i \Psi \) \( (i = 1, 2, 3) \) and \( (i\partial - M_N) \Psi \) are of chiral order one. As a consequence, the free nucleon propagator cannot be assigned a constant chiral dimension either. Power counting should sort diagrams according to their chiral dimensions, but as they do not have a fixed power from the start a method is needed that solves this problem. If one assigned each diagram the minimal possible order each nucleon propagator would contribute the chiral dimension \(-2\). However, using this way of counting the loop expansion would not coincide with the chiral expansion and, e.g., an infinite number of diagrams would count to \( \mathcal{O}(p^2) \) in \( \pi N \) scattering \[BKM95\].

The heavy-baryon (HB) projection introduced in Refs. \[JM91\] and \[BKKM92\] was the first scheme that allowed for a consistent power counting with nucleons. The basic idea is that the nucleon mass is very heavy and only small nucleon momenta relative to this mass are considered in amplitudes:

\[ \mathcal{M}(E, M_N, \mu, g) = E^\nu f \left( \frac{E}{\mu} \frac{E}{M_N}, g \right) . \]  

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If $f$ does not include negative powers of $E/M_N$, we can expand it in the small parameter $x = E/M_N$:

$$\mathcal{M} = E^x f \left( \frac{E}{\mu}, 0, g \right) + E^{x+1} f_x \left( \frac{E}{\mu}, 0, g \right) + \ldots$$  \hspace{1cm} (3.39)

Again, the order of the small scale $E$ dictates the importance of contributions. An expansion in $1/M_N$ amounts for the non-relativistic limit and in the heavy-baryon formalism this expansion is performed on the level of the Lagrangian$^3$. We separate the mass term from the four-momentum $k_\mu = M_N v_\mu + p_\mu$ where the residual momentum $p_\mu$ will be of the size of the small scale and $v^2 = 1$. We introduce the velocity projection operators $P_+^v = (1 + \not\! v)/2$ to define the two velocity-dependent fields

$$H = e^{iM_N v^2} P_+^v \Psi, \ h = e^{iM_N v^2} P_-^v \Psi.$$ \hspace{1cm} (3.40)

These two fields can be interpreted in the rest-frame $(k_\mu = (M_N, 0))$ as the large component $H$ and the small component $h$ of a Dirac spinor in the Dirac basis $[\text{Sch03}]$:

$$H = \sqrt{E + M_N} \begin{pmatrix} \chi \\ 0 \end{pmatrix} \exp[-i(E - M_N)t + ipx]$$

$$h = \sqrt{E + M_N} \begin{pmatrix} \sigma \cdot p \\ E + M_N \chi \end{pmatrix} \exp[-i(E - M_N)t + ipx].$$ \hspace{1cm} (3.41)

It is useful to rewrite the free Dirac Lagrangian in terms of these fields:

$$\bar{\Psi}(i\not\! \partial - M_N)\Psi = \bar{H}(iv \cdot \partial)H - \bar{h}(iv \cdot \partial + 2M_N)h + \bar{H}(i\not\! \partial^\perp)h + \bar{h}(i\not\! \partial^\perp)H,$$ \hspace{1cm} (3.42)

where $\not\! \partial^\perp$ is the transverse part of $\not\! \partial = \not\! v(\not\! \partial) + \not\! \partial^\perp$. We notice that the large mass term is absorbed in the field $h$. This feature will also appear if we rewrite the Lagrangian $L_{\pi N}$ with these new fields. We will now use a path-integral approach to eliminate this heavy field $h^4$. The generating functional in terms of the velocity-dependent fields will take the form

$$\exp\left[iZ[\bar{R}, R, \bar{\rho}, \rho]\right] = \int [D\bar{U}D\bar{H}DHD\bar{h}Dh] \exp[i(S_\pi + S_{\pi N} + S_{\text{src}})].$$ \hspace{1cm} (3.43)

$S_{\text{src}} = \int d^4x \left( \bar{R}H + \bar{H}R + \bar{\rho}h + \bar{h}\rho \right)$ contains the source terms, the pure Goldstone boson action is given by $S_\pi = \int d^4x \left( L_{\pi N}^{(2)} + L_{\pi N}^{(4)} + \ldots \right)$ and the pion-nucleon action by $S_{\pi N} = \int d^4x \ L_{\pi N}$. The pion-nucleon Lagrangian $L_{\pi N}$ has the generic form

$$L_{\pi N} = \bar{H}\gamma_0\partial_{HH}H - \bar{h}\gamma_0\partial_{hh}h + \bar{h}\gamma_0\partial_{hh}^2h + \bar{H}\gamma_0\partial_{hh}^2\gamma_0h$$ \hspace{1cm} (3.44)

and every operator is expanded at low energies

$$\bar{\partial}_X = \bar{\partial}_X^{(1)} + \bar{\partial}_X^{(2)} + \ldots, \quad X \in \{HH, hh\}$$

$$\partial_{hh} = \partial_{hh}^{(0)} + \partial_{hh}^{(1)} + \ldots.$$ \hspace{1cm} (3.45)

$^3$We used the argumentation with amplitudes as a concrete motivation for an $1/M_N$ expansion. Actually there can be a difference between the two approaches as soon as loop-integrations are involved because they do not always commute with the mass-expansion$^{[BL99]}$.

$^4$Alternatively, one can use the equations of motion.
where $O_{hh}^{(0)} = 2M_N$. After shifting the variables $h \rightarrow h - O_{hh}^{-1}(h_{hh}H + \rho)$ we complete
the square and integrate over the heavy $h$ fields. This results in a determinant $\Delta_h$ which
is assumed to be constant\cite{BKM95}, thus neglecting the propagation of the heavy field.
Because of the variable shift we end up with a changed pion-nucleon action

$$S'_{\pi N} = \int d^4 x \, \bar{H} \left( \sigma_{HH}H + \gamma_0 \sigma_{hH}^{\dagger} \gamma_0 \sigma_{hh}^{-1} h_{hh} H \right) H. \quad (3.46)$$

The next step is to express $O_{hh}^{-1}$ in terms of a series of operators with rising chiral
dimensions which corresponds to an expansion in $O_{hh}^{-1} = 1/(2M_N)$:

$$O_{hh}^{-1} = \frac{1}{2M_N} - \frac{O_{hh}^{(1)}}{(2M_N)^2} + \ldots . \quad (3.47)$$

Finally, the effective pion-nucleon action in Eq. (3.46) up to third order in small momenta
is given by

$$S'_{\pi N} = \int d^4 x \bar{H} \left( \sigma_{HH}^{(1)} + \sigma_{HH}^{(2)} + \sigma_{HH}^{(3)} + \gamma_0 \sigma_{hH}^{(1)\dagger} \gamma_0 \sigma_{hh}^{-1} \sigma_{hh}^{(1)} 
+ \frac{\gamma_0 \sigma_{hH}^{(1)\dagger} \gamma_0 \sigma_{hh}^{(2)}}{2M_N} \sigma_{hh}^{(1)} \right) H + \mathcal{O}(p^4). \quad (3.48)$$

We note that the small momenta are suppressed by inverse powers of $\Lambda_\chi = 4\pi f_\pi$ or $M_N$.
Because of their comparable size we treat both of them on the same footing and only
count the powers of small momenta $O(p)$.

The heavy-mass formulation allows for a simplification of the Dirac algebra. All
bilinears $\bar{H}\Sigma H$ with $\Sigma \in \{1, \gamma_\mu, \gamma_5\gamma_\mu, \sigma_{\mu\nu}\}$ can be written in terms of the velocity $v_\mu$ and
the covariant spin operator $S_\mu = i\gamma_5\sigma_{\mu\nu}v^\nu/2$ (in the convention $\epsilon_{0123} = 1$):

$$\bar{H}\gamma_\mu H = v_\mu \bar{H}H, \quad \bar{H}\gamma_5 H = 0, \quad \bar{H}\gamma_\mu\gamma_5 H = 2\bar{H}S_\mu H, \quad \bar{H}\sigma_{\mu\nu}H = 2\epsilon_{\mu\nu\rho\sigma}v^\rho \bar{H}S^\sigma H. \quad (3.49)$$

The covariant spin operator contains the totally antisymmetric Levi-Civita tensor in
four dimensions and we therefore have to be careful when extending the algebra to $D$
dimensions in dimensional regularization. However, $S_\mu$ satisfies the relations

$$S \cdot v = 0, \quad S^2 = \frac{1-d}{4}, \quad \{S_\mu, S_\nu\} = (v_\mu v_\nu - \eta_{\mu\nu}), \quad [S_\mu, S_\nu] = i\epsilon_{\alpha\beta\gamma\delta}v^\gamma S^\delta \quad (3.50)$$

and reduces to

$$S^\mu = \left( 0, \begin{pmatrix} \sigma/2 & 0 \\ 0 & \sigma/2 \end{pmatrix} \right)$$

in the nucleon rest frame. In this frame the non-relativistic nucleon field $N(x)$ is defined
by

$$H(x) = \left( \begin{array}{c} N(x) \\ 0 \end{array} \right). \quad (3.51)$$
Using these fields the leading order Lagrangians read

\begin{align*}
\hat{\mathcal{L}}_{\pi N}^{(1)} &= \bar{N} (iv \cdot D + g_A S \cdot u) N \\
\hat{\mathcal{L}}_{\pi N}^{(2)} &= \frac{1}{2M_N} \bar{N} \left( (v \cdot D)^2 - D \cdot D - ig_A \{ S \cdot D, v \cdot u \} \right) N + \sum_{i=1}^{4} \hat{c}_i \bar{N} \hat{\Theta}_i N. \tag{3.53}
\end{align*}

For the heavy-baryon projected operators \( \hat{\Theta}_i \) and the third-order pion-nucleon Lagrangian \( \hat{\mathcal{L}}_{\pi N}^{(3)} \) we refer to [FMMS00] again. The Feynman rules for Heavy-Baryon-ChPT are collected in Refs. [ME11] (from \( \hat{\mathcal{L}}_{\pi N}^{(1)} \) and \( \hat{\mathcal{L}}_{\pi N}^{(2)} \)) and [FMS98] (\( \hat{\mathcal{L}}_{\pi N}^{(3)} \)).

We close this section by a look at the heavy-baryon propagator. From Eq. (3.52) we deduce the free nucleon propagator

\begin{equation}
S(p) = \frac{i}{v \cdot p + i\eta}. \tag{3.54}
\end{equation}

The propagator is independent of the nucleon mass which now enters in amplitudes through vertices. The space-time representation of Eq. (3.54) shows that the nucleon is treated as an infinitely heavy static source. The heavy-baryon propagator is of chiral dimension \(-1\), but is infrared divergent for \( v \cdot p = 0 \). In a relativistic treatment this singularity corresponds to contributions of the type \( M_N/p^2 \), which reduce the chiral dimension by two:

\begin{equation}
\frac{i(k + M_N)}{k^2 - M_N^2 + i\epsilon} \overset{v \cdot p = 0}{=} \frac{i(M_N(1 + \not{p}) + \not{p})}{p^2 + i\epsilon}. \tag{3.55}
\end{equation}

It is important to keep this statement in mind for amplitudes that are infrared divergent in the HB approach.

### 3.3.3 Heavy-Baryon Power Counting in Pion-Nucleon Sector

Using the HB approach enables us to treat the mass in terms of a series of couplings. This allows us to write amplitudes as

\begin{equation}
\mathcal{M}(E, M_N, \mu, g) = E^\nu f \left( \frac{E}{\mu}, g' \right), \tag{3.56}
\end{equation}

where \( g' \) includes all couplings generated by the nucleon mass. Loop integrands then only depend on the small scale and therefore we are allowed to count loop momenta of the small scale once again. The chiral dimension \( \nu \) then is increased by four for every loop integration and by \( n \) for every vertex from either \( \mathcal{L}_{\pi}^{(n)} \) or \( \mathcal{L}_{\pi N}^{(n)} \). It is decreased by two for every meson propagator and by one for every nucleon propagator:

\begin{equation}
\nu = 4L - 2I_\pi - I_N + \sum_n nV_n. \tag{3.57}
\end{equation}

In the one-nucleon sector there is one nucleon line running through the diagram and therefore the topological relations \( I_N = \sum_n V_N^n \) and \( L = I_\pi + I_N + \sum_n V_n + 1 \) hold,
where \( V_n^{\pi N} \) denotes vertices from \( \mathcal{L}_{\pi N}^{(n)} \). Eq. (3.57) can then be rewritten as

\[
\nu = 2L + 1 + \sum_m (2m - 2)V_{2m}^\pi + \sum_n (n - 1)V_n^{\pi N}.
\] (3.58)

Notice that \( 2m - 2 \geq 0 \) for pion vertices and \( n - 1 \geq 0 \) for pion-nucleon vertices. Hence, \( \nu \geq 2L + 1 \) and the chiral dimension increases with the number of loops and only a finite number of diagrams contribute at a certain order. HB-ChPT works for \( \pi N \) scattering and phase shifts can be described up to momenta of 200 MeV in HB-ChPT of order \( \mathcal{O}(p^3) \) [FMS98]. We will notice some difficulties of the HB approach and power counting in the NN interaction, but defer this discussion to chapter 4.

### 3.4 Nucleon-Nucleon Contact Interactions

We now turn to the last necessary component of the Lagrangian that is needed to describe the full NN interaction in a chiral effective field theory, namely the contact terms. These contact terms consist of four nucleon fields and no meson fields. They are needed to renormalize loop integrals and to parametrize unresolved short-distance dynamics. When integrating out the heavier meson degrees of freedom, the meson propagator, e.g. of the \( \rho(770) \)-meson, can be expanded in a power series

\[
\frac{i}{m_\rho^2 + q^2} = \frac{i}{m_\rho^2} \left( 1 - \frac{q^2}{m_\rho^2} + \frac{q^4}{m_\rho^4} - \ldots \right).
\] (3.59)

This expansion suggests that the short distance dynamics are described by polynomials in the momenta. The denominators \( m_\rho \) fit very well in the overall power expansion as \( \Lambda_\chi \approx m_\rho \) and they also suggest a “natural” value for the coupling constants we later associate to each contact term. In the Lagrangian the contact terms take the form

\[
C_{12}(\bar{N}\sigma_1N)(\bar{N}\sigma_2N),
\] (3.60)

where \( \sigma \) can be a combination of Pauli spin- and isospin-matrices \( \sigma, \tau \) and derivatives \( \nabla \). The derivatives generate small three-momenta for the nucleon fields and therefore increase the chiral dimension of the term. Because of parity invariance, the contact interactions only come in even powers of derivatives:

\[
\hat{\mathcal{L}}_{NN} = \hat{\mathcal{L}}_{NN}^{(0)} + \hat{\mathcal{L}}_{NN}^{(2)} + \hat{\mathcal{L}}_{NN}^{(4)} + \ldots.
\] (3.61)

There are two terms without derivatives and 14 terms with two derivatives. However, only seven of the subleading terms and 15 terms at \( \mathcal{O}(p^4) \) are independent [EGM05]. Girlanda et al. [GPSV10] recently showed that the number of independent contact terms at \( \mathcal{O}(p^2) \) is actually given by relativity constraints.

These contact terms generate amplitudes that are polynomials in \( q^2 = p^2 + p^2 - 2pp'z \) and \( k^2 = \frac{1}{4}(p^2 + p'^2 + 2pp'z) \), where \( z = \cos(\hat{p} \cdot \hat{p}') \). Thus any linear combination of \( q^{2n} \) and \( k^{2n} \) is a polynomial of order \( n \) in \( z \). The partial-wave decomposition of such terms (see App. A.2 for details) is zero for all partial waves with sufficiently large angular momentum \( L \), e.g., the two-lowest order contact terms only act on the two \( S \)-waves.
4 The Nucleon-Nucleon Interaction in Chiral Effective Field Theory

4.1 Potential Approach to the NN Interaction

4.1.1 Weinberg’s Approach

We have constructed all the needed parts of the Lagrangian $\mathcal{L}_{\text{eff}} = \mathcal{L}_\pi + \mathcal{L}_{\pi N} + \mathcal{L}_{NN}$ in order to compute NN scattering amplitudes and describe the nuclear force. The long and intermediate ranges are described by chiral one- and two-pion exchange. The higher partial waves ($L > 3$) probe these ranges, and ChPT describes the nucleon-nucleon interaction without free parameters\(^1\) already accurately at $\mathcal{N}^2$LO up to laboratory energies of more than 100 MeV [KBW97]. However, for lower partial waves perturbation theory does not apply as there exists a bound state (the deuteron) and there are large scattering lengths in the $S$-waves. Weinberg [Wei91] pointed out the necessity for the power counting given in Eq. (3.58) to fail because it cannot generate a bound state. In this spirit it is fortunate that supposedly non-leading terms in HBChPT stemming from ladder diagrams are afflicted with infrared divergences that require a modified power counting. As already pointed out these infrared divergences stem from the heavy-baryon propagator, which in a relativistic approach generates terms proportional to $M_N/p^2$ as could be seen in Eq. (3.55). The divergence in HBChPT can be absorbed by a nucleon kinetic energy term, but the important point is that the loop diagrams are of smaller chiral order than the usual power counting would suggest. Weinberg suggested that instead of keeping track of these nearly infrared-divergent graphs (reducible graphs with purely nucleonic intermediate states), it is much more convenient to calculate the NN potential $V$ (i.e. the irreducible graphs) in ChPT and apply this potential in the Lippmann-Schwinger equation to obtain the NN $T$-matrix:

$$T(p, p') = V(p, p') - \int \frac{d^3p''}{(2\pi)^3} V(p, p'') \frac{M_N}{p'^2 - p''^2 + i\epsilon} T(p'', p'). \tag{4.1}$$

We follow Kaiser’s convention here; Epelbaum and Machleidt use different conventions and their partial-wave decomposed potentials are multiplied by a factor of $-4\pi$ and $-(2\pi)^3$ compared to our potentials, respectively. Hence their equivalent Lippmann-Schwinger equation is multiplied by these factors as well and takes a different form. For very weak potentials $V$ this equation can be solved iteratively: In Born approximation $T = V$, and higher orders can be obtained by the substitution of $T$ by the result of the

\(^1\)There are no free parameters if the LECs $c_1$, $c_3$ and $c_4$ are taken from fits of $\pi N$ scattering.
lower order, e.g. the second order approximation reads $T = V - VGV$ and the third order approximation is given by $T = V - VGV(V - VGV)$, where $G$ denotes the nucleon-propagator and an implicit momentum integration. This perturbative method for solving the Lippmann-Schwinger equation can be applied in the higher partial waves, but not for the lower partial waves which are nonperturbative. Because of the large scattering lengths and the bound state, Eq. (4.1) has to be solved nonperturbatively. In order to get a finite result we need to regularize the potential $V$. The standard procedure in the NN interaction is to multiply the potential $V$ with a regulator function $f_n(p,p')$:

$$V(p,p',z) \rightarrow V(p,p',z) f_n^A(p,p')$$

If we expand $f_n$ in small momenta, we see that for sufficiently large $n$, e.g. $n \geq 3$ for $N^3$LO, the changes due to the regulator are higher order corrections, which hardly affect the potential in the low momentum range but act as a cutoff for large momenta. We therefore call $\Lambda$ the cutoff scale and typical choices are $800 - 1000$ MeV for chiral $N^2$LO and $\Lambda \approx 600$ MeV for $N^3$LO NN potentials, which is below the chiral symmetry breaking scale $\Lambda_\chi \approx 1$ GeV. This is in the spirit of Lepage [Lep97] who pointed out that it makes little sense to take the momentum cutoff beyond the range of validity of the effective theory.

4.1.2 Chiral NN Potentials from Pion Exchange

We consider elastic nucleon-nucleon scattering $N(p) + N(-p) \rightarrow N(p') + N(-p')$ in the center-of-mass frame. The momentum transfer is given by $q = p' - p$ and the average momentum is given as $k = (p' + p)/2$. We will summarize the chiral nucleon-nucleon potentials up to $O(p^3)$ as the analytic expressions are given in Ref. [KBW97] with explicit pion-mass dependence. The nucleon-nucleon potential takes the general form

$$V = U_C + U_S \sigma_1 \cdot \sigma_2 + U_{SO} \frac{i}{2} (\sigma_1 + \sigma_2) \cdot (q \times k)
+ U_T (\sigma_1 \cdot q)(\sigma_2 \cdot q) + U_{\sigma L} \sigma_1 \cdot (q \times k) \cdot \sigma_2 \cdot (q \times k),$$

where the complex functions $U_X = V_X + \tau_1 \cdot \tau_2 W_X$ are functions of the initial and final relative momenta $p, p'$ and the cosine of the angle between them $z = \cos(\theta)$.

The leading-order one-pion exchange (OPE) potential is given by

$$W_T^{(0)} = \frac{g_A^2}{4f_\pi^2(q^2 + m_\pi^2)},$$

where $q^2 = |q|^2$ and the index of the potential denotes the chiral dimension. There are no contributions of $O(p)$ to the nucleon-nucleon potential, because loops raise the chiral

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2This procedure is used in both of the chiral $N^3$LO descriptions of the two-nucleon system [EM03],[EGM05].

3Epelbaum and Gegelia showed this in an example, see Ref. [EG09] for details.
order by two and the one-loop diagrams with vertices from the lowest order Lagrangians then appear at $\mathcal{O}(p^2)$, which is next-to-leading order (NLO). There are two different kinds of diagrams: either two- or one-pion-exchange diagrams. The latter only contribute to a renormalization of the nucleon and pion masses and the coupling constant [KBW97] and as long as we keep the physical values, we can identify $g_A$ and $f_\pi$ as the physical axial coupling and pion decay constant respectively after renormalization.

The two-pion-exchange contributions can be separated into irreducible and reducible components. As mentioned, the reducible part can be calculated starting from the relativistic amplitude picking the nucleon poles in the energy-component of the loop momentum integration. For the chiral nucleon-nucleon potential we can neglect this contributions because they are generated in the Lippmann-Schwinger equation for the transition amplitude. Nevertheless it is important to know their origin because these nucleon poles have to be excluded when computing the irreducible two-pion-exchange potential. Considering this separation of the iterated part, one finds from the graphs in Fig. 4.1 the following renormalized contributions at second order in small momenta [KBW97]:

$$W_{C}^{(2)} = \frac{1}{384\pi^2 f_\pi^4} \left\{ 6m_\pi^2(15g_A^2 - 6g_A^2 - 1) + q^2(23g_A^4 - 10g_A^2 - 1) \right\} \ln \left( \frac{m_\pi}{\mu} \right)$$

$$+ 4m_\pi^2(4g_A^2 + g_A^2 + 1) + \frac{q^2}{6}(5g_A^4 + 26g_A^2 + 5)$$

$$+ \left[ 4m_\pi^2(5g_A^4 - 4g_A^2 - 1) + q^2(23g_A^4 - 10g_A^2 - 1) + \frac{48g_A^4m_\pi^4}{4m_\pi^2 + q^2} \right] L(q) \right\} , \quad (4.5)$$

$$V_{T}^{(2)} = -\frac{1}{q^2} V_{S}^{(2)} = \frac{3g_A^4}{64\pi^2 f_\pi^2} \left\{ \ln \left( \frac{m_\pi}{\mu} \right) - \frac{1}{2} + L(q) \right\} , \quad (4.6)$$

where the logarithmic loop function $L(q)$ is given by

$$L(q) = \frac{\sqrt{4m_\pi^2 + q^2}}{q} \ln \left( \frac{\sqrt{4m_\pi^2 + q^2} + q}{2m_\pi} \right) . \quad (4.7)$$

The next order in small momenta (N^2LO) is given by the same diagrams, except with one vertex replaced by a higher order vertex from $\mathcal{L}_{\pi^N}^{(2)}$. These can either be terms proportional to the LECs $c_i$ or $1/M_N$. We notice that all contributions at this order are free of divergences, which is an important fact because there are no contact terms at this order. We furthermore note that the football diagram (the leftmost diagram in Fig. 4.1) vanishes. We cite the potential at this order from Ref. [KBW97]:

$$V_{C}^{(3)} = \frac{3g_A^2}{16\pi f_\pi^4} \left\{ 4(c_1 - c_3)m_\pi^3 - \frac{g_A^2m_\pi}{16M_N}(m_\pi^2 + 3q^2) - \frac{g_A^2m_\pi^5}{16M_N(4m_\pi^2 + q^2)} - c_3m_\pi q^2 \right\} + \left\{ 2m_\pi^2(2c_1 - c_3) - q^2 \left( c_3 + \frac{3g_A^2}{16M_N} \right) \right\} (2m_\pi^2 + q^2)\ln(q), \quad (4.8)$$

$$W_{C}^{(3)} = \frac{g_A^2}{128\pi M_N f_\pi^4} \left\{ (8 - 11g_A^2)m_\pi^3 + (2 - 3g_A^2)m_\pi q^2 - \frac{3g_A^2m_\pi^5}{4m_\pi^2 + q^2} \right\} \ln(q), \quad (4.9)$$

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Figure 4.1: Irreducible two-pion-exchange diagrams at one-loop order. The vertices can represent terms from both $\hat{L}^{(1)}_{\pi N}$ and $\hat{L}^{(2)}_{\pi N}$.

\[
V_T^{(3)} = -\frac{1}{q^2} V_S = -\frac{9 g_A^4}{512 \pi M_N f^4_\pi} \left\{ m_\pi + (2 m_\pi + q^2) A(q) \right\}, \tag{4.10}
\]
\[
W_T^{(3)} = -\frac{1}{q^2} W_S = \frac{g_A^2}{32 \pi f^2_\pi} \left\{ \left( c_4 + \frac{2 - 3 g_A^2}{8 M_N} \right) m_\pi 
+ \left[ \left( c_4 + \frac{1}{4 M_N} \right) (4 m^2_\pi + q^2) - \frac{g_A^4}{8 M_N} (10 m^2_\pi + 3 q^2) \right] A(q) \right\}, \tag{4.11}
\]
\[
V_{SO}^{(3)} = \frac{3 g_A^4}{64 \pi M_N f^4_\pi} \left\{ m_\pi + (2 m^2_\pi + q^2) A(q) \right\}, \tag{4.12}
\]
\[
W_{SO}^{(3)} = \frac{g_A^4 (1 - \frac{g_A^2}{M_N})}{64 \pi M f^4_\pi} \left\{ m_\pi + (4 m^2_\pi + q^2) A(q) \right\}. \tag{4.13}
\]

A new loop function $A(q)$ appears:

\[
A(q) = \frac{1}{2q} \arctan \left( \frac{q}{2 m_\pi} \right). \tag{4.14}
\]

Finally, we turn to the fourth order in small momenta. At this order two-loop diagrams with leading-order vertices enter in the potential. It is analytically not possible to evaluate these two-loop diagrams, but using Cutkosky’s cutting rule we are able to determine the imaginary part of NN amplitudes from $\pi N$ scattering. From this imaginary part, contributions to the NN potential can be obtained using subtracted dispersion relations. Furthermore there are one-loop contributions with $\hat{L}^{(3)}_{\pi N}$ vertices that are needed to renormalize the two-loop divergences stemming from $\pi N$ loop graphs. Additionally there are diagrams with two vertex insertions from $\hat{L}^{(2)}_{\pi N}$: terms proportional to $c_i c_j$, $c_i/M_N$ and $1/M_N^2$. Kaiser computed all pion-exchange contributions to the nucleon-nucleon potential in next-to-next-to-next-to-leading order [Kai00], [Kai01b], [Kai01a], [Kai02]. A summary of all N^3LO terms is given in appendix D of Ref. [ME11]. However, no polynomial contributions are given.
4.1 Potential Approach to the NN Interaction

4.1.3 Contact Potentials

The final parts of the nucleon-nucleon potential are generated by the contact Lagrangians from Eq. (3.61). A pictorial way of understanding the contact potential is shown in Fig. 4.2. The short-distance dynamics behind these four-nucleon vertices are parametrized by

\[ V_{\text{cont}} = V_{\text{cont}}^{(0)} + V_{\text{cont}}^{(2)} + V_{\text{cont}}^{(4)} + \ldots. \]  

Figure 4.2: Contact potential up to $O(p^4)$.

In the center-of-mass system with initial and final nucleon momenta $p$ and $p'$, respectively, the first two potentials take the form

\[ V_{\text{cont}}^{(0)} = \tilde{C}_S + \tilde{C}_T \sigma_1 \cdot \sigma_2 \]  
\[ V_{\text{cont}}^{(2)} = C_1 q^2 + C_2 k^2 + (C_3 q^2 + C_4 k^2) \sigma_1 \cdot \sigma_2 + C_5 i \frac{1}{2} (\sigma_1 + \sigma_2) \cdot (q \times k) + C_6 (\sigma_1 \cdot q)(\sigma_2 \cdot q) + C_7 (\sigma_1 \cdot k)(\sigma_2 \cdot k). \]

For the 15 fourth-order terms we refer to [EGM05]. We note that the chosen operator basis is not unique, but a one-to-one correspondence between any other basis and this one can be given upon antisymmetrization of the potential.

In the given operator basis there is no expansion in the pion-mass because as a constant its contributions numerically count as a constant. This means that, e.g.,

\[ \tilde{C}_S = \hat{C}_S + C_S^{\text{mp}} m^2 \]

in practice is treated as one term and fitted to the scattering phase shifts. The fastest way for the numerical implementation of the full NN potential is to absorb all polynomials in $q^2$ (including constants) from dimensional regularization of pion-loops into the contact terms and then perform the fit. In this work we are interested in the pion-mass dependence of the NN interaction and did not absorb these pion-mass-dependent terms but left them explicitly in the pion-exchange potentials.

4.1.4 Spectral Function and Regularization

We want to introduce the concept of the spectral function representation for later use. Furthermore this representation was used as another way of regularizing the chiral potential for the Lippmann-Schwinger equation. The regulator function $f_n^\Lambda$ in Eq. (4.2)
limits the momenta of the nucleons, but the meson loops are usually dimensionally regularized and therefore need no cutoff. Epelbaum, Glöckle and Meißner [EGM04] went one step further and suggested that pion momenta above the hard scale should not contribute and devised a scheme for cutting off the meson loops using the spectral function representation of the potentials. We explain the procedure briefly:

The mathematical basis is the Kramers-Kronig relation

\[ \Re[f(x)] = \frac{1}{\pi} \mathcal{P} \left( \int dx \frac{\Im[f(x)]}{x - x} \right), \tag{4.19} \]

which is valid for any analytic function (in the upper plane) that falls off to zero as \(|z| \to \infty\) and connects the real part \(\Re\) with the imaginary part \(\Im\) of a function. The chiral NN potentials \(V(t)\) in general have polynomial contributions, and therefore the applicability condition for the Kramers-Kronig relation is not met. However, we can subtract those polynomials, i.e. neglect the unresolved short distance dynamics, and then apply the Kramers-Kronig relation to those subtracted functions. The subtracted potentials \(\tilde{V}(t)\) are real for \(t = -q^2 < 4m_n^2\), and the mass spectrum entering in this representation is given by the imaginary part of the potential as a function of the momentum transfer analytically continued to time-like momenta \(t = \mu^2\):

\[ \tilde{V}(q) = \frac{1}{\pi} \int_{2m_n}^{\infty} d\mu 2\mu \frac{\Im[\tilde{V}(i\mu - 0^+)]]}{\mu^2 + q^2}. \tag{4.20} \]

The spectral function regularization suppresses the large \(\mu\) contributions by a sharp cutoff \(\tilde{\Lambda}\) as upper integration boundary, hence regularizing short-distance pion-loop contributions. In coordinate space the omission of the large \(\mu\)-components lead to a less singular potential at the origin \(r = 0\). E. g., the isoscalar central potential \(V_C\) shows a \(1/r\) singularity with the spectral-function cutoff compared to a \(1/r^6\) behavior with dimensional regularization (see Fig. 4.3). However, this cutoff procedure also brings a disadvantage, namely the integrals must be numerically solved and there is no closed coordinate-space representation. In principle the cutoffs \(\tilde{\Lambda}\) from spectral-function regularization and \(\Lambda\) from the Lippmann-Schwinger equation are independent cutoffs, but
they both should be taken below the symmetry breaking scale $\Lambda_X$. Because we subtracted the polynomial terms from the potentials (which anyway could be absorbed into contact terms), the only difference between dimensional regularized and spectral-function regularized potentials are the high-momentum two-pion exchange contributions. Thus deviations can mostly be seen in the intermediate-range of the potential, characterized by partial waves with $L \approx 2$. The advantage of the spectral-function cutoff in comparison to e.g. a Pauli-Villars cutoff is that all symmetries stay conserved because the symmetry-conserving dimensionally-regularized potentials enter into the mass-spectrum.

We will not use this procedure because the difference from dimensional regularization can be compensated by higher-order contact terms and we prefer the analyticity of the dimensionally regularized expressions. Nevertheless we wanted to explain the principle of the spectral-function representation because it will be useful for the transformation into coordinate space in section 4.3.

### 4.2 Phase Shifts and Scattering Length

The chiral NN potential (4.3) is given in momentum space in the helicity basis. The Lippmann-Schwinger equation and the phase shifts are commonly evaluated in the $|LSJ\rangle$ basis, hence a partial wave decomposition of the chiral potential is necessary. The formalism and needed formulas are shown in appendix A.2. The transition amplitudes ($T$ matrix elements) computed with the Lippmann-Schwinger equation are related to the $S$ matrix by

$$S_{LL'}(p) = \delta_{LL'} + \frac{i}{2\pi} \frac{pM_N^2}{\sqrt{M^2 + p^2}} T_{LL'}(p).$$  \hspace{1cm} (4.21)

The operators $(\sigma_1 \cdot q)(\sigma_2 \cdot q)$ and $\sigma_1 \cdot (q \times k) \sigma_2 \cdot (q \times k)$ can couple $|LSJ\rangle$ states to those with orbital angular momenta $J \pm 1$. For given $J > 0$ there are two uncoupled channels with $L = J$ and $S \in \{0, 1\}$ and one coupled channel with $L = J \pm 1$ and $S = 1$. In the uncoupled channels the phase shifts are defined by

$$\exp[2i\delta_{JLSJ}(p)] := S_{JJ}(p).$$  \hspace{1cm} (4.22)

We do not consider coupled channels in this work, but for completeness we give the so called Stapp parametrization [SYM57] of the $S$-matrix in the coupled channels ($S = 1$ and $J$ suppressed for clarity):

$$\begin{pmatrix} S_{j-1j-1} & S_{j-1j+1} \\ S_{j+1j-1} & S_{j+1j+1} \end{pmatrix} = \begin{pmatrix} \cos(2\epsilon) \exp[2i\delta_{j-1}] & i\sin(2\epsilon) \exp[i\delta_{j-1} + i\delta_{j+1}] \\ i\sin(2\epsilon) \exp[i\delta_{j-1} + i\delta_{j+1}] & \cos(2\epsilon) \exp[2i\delta_{j+1}] \end{pmatrix}. $$  \hspace{1cm} (4.23)

In Ref. [KBW97] the peripheral phase shifts ($L \geq 2$) were computed perturbatively up to third order in small momenta $(N^2LO)$ in Born approximation $T = V$. Kaiser states that the perturbative formula

$$\delta_{LSJ} = \frac{M_N^2p}{4\pi\sqrt{M^2 + p^2}} \mathcal{R}e\langle LSJ|V|LSJ \rangle.$$  \hspace{1cm} (4.24)

\footnote{The $S$-matrix is then in the same convention as in Machleidt’s and Epelbaum's works.}
is valid only as long as the difference between $\delta$ and $\sin(\delta) \cos(\delta)$ is small and therefore $|\delta| < 30^\circ$. In third order in small momenta we computed the phase shifts for all partial waves with $L > 0$ perturbatively and compare the results with the phase shifts obtained by the full Lippmann-Schwinger equation (4.1). The numerical solution of this integral equation and the code used are given in appendix A.3 and A.4.

In the following we use the pion decay constant $f_\pi = 92.4$ MeV, the average pion mass $m_\pi = 138$ MeV and the average nucleon mass $M_N = 938.9$ MeV. We use the value $g_A = 1.26$ throughout this work and explicitly treat the pion-mass dependent Goldberger-Treiman discrepancy for the one-pion exchange in chapter 5.2.3. The LECs $c_i$ and $d_i$ are taken from Ref. [EGM05]: $c_1 = -0.81$ GeV$^{-1}$, $c_2 = 3.28$ GeV$^{-1}$ and $c_4 = 3.40$ GeV$^{-1}$ are the central values from a $Q^3$-analysis of the $\pi N$ system. For the LEC $c_3$, however, the value $c_3 = -3.40$ GeV$^{-1}$ is used, which is on the lower side but still consistent with $\pi N$-scattering data\footnote{Machleidt [ME11] used different values with $c_3 = -3.20$ GeV$^{-1}$ and $c_4 = 5.40$ GeV$^{-1}$.}. The LECs associated with the dimension three Lagrangian are $\bar{d}_1 + \bar{d}_2 = 3.06$ GeV$^{-2}$, $\bar{d}_3 = -3.27$ GeV$^{-2}$, $\bar{d}_5 = 0.45$ GeV$^{-2}$ and $\bar{d}_{14} - \bar{d}_{15} = -5.65$ GeV$^{-2}$.

In Fig. 4.4 we show the phase shifts of two peripheral waves, namely the $^1G_4$- and $^1F_3$-waves computed from the chiral N$^3$LO potential. Because we chose the LECs $c_i$ from $\pi N$ scattering, there are no free parameters and this is a check for chiral symmetry. The phase shifts are smaller than $5^\circ$ and the perturbative result approximates the phase shifts obtained by the Lippmann-Schwinger equation very well. This means that the phase shifts are essentially given by the on-shell (momentum-space) matrix elements of the potential and the results are almost cutoff-independent. The computed phase shifts are in good agreement with the partial-wave analysis of the Nijmegen group [SKRdS93]. The sign change and an approximate factor of 3 between the phase shifts from $^1L_L$ to $^1L_L'$ with $L' = L - 1$ is characteristic for the higher partial waves because the dominant one-pion exchange contribution is an isovector quantity and the operator $\tau_1 \cdot \tau_2$ reduces...
to $4I - 3$ with $I \in \{0, 1\}$ in NN scattering.

The $^1D_2$-wave phase shifts are shown in Fig. 4.5. In the left figure it can be seen that the dimensionally-regularized perturbatively-computed phase shifts are growing too rapidly with the laboratory energy $T_{\text{lab}}$. As pointed out in chapter 4.1.4 the high-momentum two-pion exchange contributions are most significant in this channel. Therefore we also plotted the phase-shifts from the spectral-function regularized chiral potential with cutoffs between 600 MeV $\leq \tilde{\Lambda}_S \leq$ 800 MeV (red band). Perturbative and nonperturbative phase shifts (right) with notation from Fig. 4.4. The lower plot shows the dependence on the cutoff from the Lippmann-Schwinger equation; the red-dashed line denotes $\Lambda = 900$ MeV, the full blue line $\Lambda = 1030$ and the yellow dotted line $\Lambda = 1100$ MeV.

Figure 4.5: $^1D_2$-wave NN phase shifts. The left figure shows perturbative phase shifts from chiral N$^2$LO potentials in dimensional regularization (full blue line) and spectral cutoff-regularization with cutoffs between 600 MeV $\leq \tilde{\Lambda}_S \leq$ 800 MeV (red band). Perturbative and nonperturbative phase shifts (right) with notation from Fig. 4.4. The lower plot shows the dependence on the cutoff from the Lippmann-Schwinger equation; the red-dashed line denotes $\Lambda = 900$ MeV, the full blue line $\Lambda = 1030$ and the yellow dotted line $\Lambda = 1100$ MeV.
Finally, we turn to the two lowest spin-singlet partial waves, the $^1P_1$ and $^1S_0$ waves. After the partial wave decomposition there are three unknown parameters $\tilde{C}(^1S_0)$, $C(^1S_0)$ and $C(^1P_1)$ stemming from the contact potentials Eqs. (4.16) and (4.17):

\[
\tilde{C}(^1S_0) := \langle 000 | V_{\text{cont}}^{(0)} | 000 \rangle = (C_S - 3C_T)
\]
\[
C(^1S_0)(p^2 + p'^2) := \langle 000 | V_{\text{cont}}^{(2)} | 000 \rangle = \frac{1}{2} (4C_1 + C_2 - 12C_3 - 3C_4 - 4C_6 - C_7)
\]
\[
C(^1P_1)pp' := \langle 101 | V_{\text{cont}}^{(2)} | 101 \rangle = \frac{1}{6} (-4C_1 + C_2 + 12C_3 - 3C_4 + 4C_6 - C_7).
\]

This has the huge advantage that the contact terms can be separated from the chiral potential and no further integrations have to be done\(^7\). The parameters are then fitted to the scattering data \cite{SKRdS93} to minimize $\chi^2$ taken for laboratory energies of 1, 5, 10, 25, 50 and 100 MeV. The estimations

\[
\tilde{C} \sim \frac{4\pi}{f^2_\pi} \sim 10^{-3} \text{ MeV}^{-2}, \quad C_i \sim \frac{4\pi}{f^2_\pi \Lambda^2} \sim 10^{-9} \text{ MeV}^{-4}
\]

help to limit the parameter space and define a natural size for the LECs \cite{EGM05}. Though the estimation (4.26) for $\tilde{C}$ suggests no $\Lambda$-dependence, it is in fact very cutoff-dependent. This can easily be seen by, e.g., a fit of the scattering length for different $\Lambda$ with $C(^1S_0)$ set to zero.

In Fig. 4.6 the fits of the phase shifts from the chiral N\(^2\)LO potential are shown. In the $^1P_1$-wave the Born approximation still agrees with the empirical phase shifts for small laboratory energies ($T_{\text{lab}} < 25$ MeV), but pion-exchange iterations change the result strongly at higher energies. A different picture appears in the $^1S_0$-wave: the contact terms dominate over the pion-exchange contributions, create large off-shell $K$-matrix elements and nearly make it singular\(^8\). These off-shell contributions provide for the large discrepancy between the phase shifts from Born approximation and

\(^7\)This procedure in fact saves a lot of time when performing a fit. See appendix A.4 for details.

\(^8\)See appendix A.3 why the real $K$-matrix is used instead of the $T$-matrix.

Figure 4.6: $^1P_1$- (left) and $^1S_0$-wave (right) NN phase shifts. For notation see Fig. 4.4.
the full Lippmann-Schwinger equation. Epelbaum [EGM05] shows the dependence of the best fitted contact terms on the chosen cutoffs \( \Lambda \) (Lippmann-Schwinger equation) and \( \tilde{\Lambda}_S \) (two-pion exchange): \( \tilde{C}(^{1S_0}) \) varies by a factor of 3 for cutoff combinations \((\Lambda[\text{MeV}], \tilde{\Lambda}_S[\text{MeV}]) = (450, 700) \) and \((600, 700)\). With the cutoff choice of \( \Lambda = 1030 \) for the chiral N\(^2\)LO potential as input the parameters \( \tilde{C}(^{1S_0}) = -1.31 \cdot 10^{-2} \) and \( C(^{1S_0}) = 1.0 \cdot 10^{-9} \) resulted in the fit shown in Fig. 4.6. The different values for the contact parameters is a sign that a fine-tuning of the contact parameters is necessary in order to achieve the strong attraction in this channel.

We can also see this fine tuning in an other important observable in scattering experiments, the scattering length. The \( S \)-wave scattering length \( a \) is defined as the leading term in the effective range expansion\(^9\):

\[
p \cot \delta = -\frac{1}{a} + \frac{1}{2r_{\text{eff}}} p^2 + \sum_{i=2}^{\infty} v_i p^{2i}.
\]

This expansion is only valid for \( p \leq |1/a| \). In the \(^1S_0\) channel the experimental value for the neutron-proton (np) scattering length is \(-23.739 \text{ fm} \) [EGM05]. This is an unnaturally large value for the scattering length leading to a breakdown of the expansion around \( p \sim 8 \text{ MeV} \) corresponding to less than 0.02 MeV laboratory energy. Therefore the scattering length is a measure of the slope of the phase shift near zero energy and for the overall attraction or repulsion at very low energies. The term “unnaturally large” means that one would usually expect the scattering length to be the inverse of the breakdown scale of an effective theory, such that the expansion in Eq. (4.27) is valid for the whole range \( p \lesssim \Lambda \) of the EFT [KSW98]. In Fig. 4.7 we show the dependence of the scattering length to the constant contact parameter for a fixed \( (p^2 \text{ and } p^2\text{-dependent}) \) parameter \( C(^{1S_0}) \): for a wide range of parameters \( \tilde{C}(^{1S_0}) \) the scattering length is very small and in a small range the scattering length rises and changes sign. This also shows that one has a nearly bound state in the \(^1S_0\) channel because for slightly higher \( \tilde{C}(^{1S_0}) \) there are - as in the \(^3S_1\)-channel - large positive scattering lengths.

\(^9\)For the scattering length we use the same sign convention as Epelbaum. Hence a negative scattering length means attraction.
4.3 Chiral Potentials in Coordinate Space

4.3.1 Transformation Rules

The chiral potential from chiral effective field theory is naturally given in momentum space. However, it is also interesting to have a coordinate space potential in mind because the potential at a certain relative distance is an instructive quantity. We want to use this graphic clarity to see how the chiral potential is built up order by order. Therefore a Fourier transformation of the potential is necessary. For example the isoscalar central potential is given in coordinate space by

$$\tilde{V}_C(r) = -\int \frac{d^3q}{(2\pi)^3} V_C(q)e^{-iqr}.$$  \hspace{1cm} (4.28)

In general these integrals are not convergent. We will use the subtracted dispersion relations (4.20) to generate either polynomials in \(q^2\) or expressions

$$q^{2n}\int f(q) = \frac{q}{\pi} \int d\mu \frac{\mathcal{I}m[f(i\mu - 0^+)]}{\mu^{2n}(\mu^2 + q^2)}.$$ \hspace{1cm} (4.29)

The constant terms \((q^0)\) Fourier transforms into \(\delta^3(r)\)-functions and higher polynomials into derivatives of it because

$$\int \frac{d^3q}{(2\pi)^3} q^2 e^{-iqr} g(q) = -\Delta_r \int \frac{d^3q}{(2\pi)^3} e^{-iqr} g(q).$$ \hspace{1cm} (4.30)

Likewise we transform the polynomials in \(q^2\) in Eq. (4.29) into Laplacians. After this trick the integrals are finite and we can change the order of integration \(\int d^3q \leftrightarrow \int d\mu\).

Finally, we note that

$$y(r) := \int \frac{d^3q}{(2\pi)^3} \frac{4\pi}{q^2 + \mu^2} e^{-iqr} = \frac{e^{-\mu r}}{r},$$

$$-\Delta_r y(r) = -\frac{1}{r} \frac{d^2}{dr^2} e^{-\mu r} = -\mu^2 \frac{e^{-\mu r}}{r}.$$ \hspace{1cm} (4.31)

The last relation allows one to substitute factors of \(q^2\) with \(-\mu^2\). All in all the following relation holds:

$$\tilde{V}_C(r) = -\left[ V_C(q^2 = 0) - \frac{dV_C}{dq^2} \bigg|_{q^2=0} \Delta_r + \ldots \right] \delta^{(3)}(r) - \frac{1}{2\pi^2 r} \int_{2m_n}^{\infty} d\mu \mu^2 e^{-\mu r} \mathcal{I}m[V_C(i\mu - 0^+)],$$ \hspace{1cm} (4.32)

where the ellipsis denotes possible further subtracted terms.

In momentum space the large scale defines a natural limit of applicability of the effective field theory. In coordinate space there is no clear connection to the large scale.

\[10\] Note that we are using a sign convention in which \(V_C(q) > 0\) means attraction.
but a simple estimate for the range of applicability is \( r \lesssim 2\pi/\Lambda_\chi \sim 1 \text{ fm} \). We therefore will show no plots with \( r < 1 \text{ fm} \).

Eq. (4.32) shows that only the imaginary part \( \mathcal{I}m[V_C(i\mu - 0^+)] \) of the momentum space potential enters in the peripheral part of the coordinate space potential and we do not have to keep track of the subtractions. In this chapter we will work with the \( \text{N}^3\text{LO} \) chiral potential and the following imaginary parts are computed for the transformation into coordinate space:

\[
\begin{align*}
\mathcal{I}m \left[ (4m_\pi^2 - \mu^2)^{-1} \right] &= \frac{\pi}{2\mu} \delta(\mu - 2m_\pi) \\
\mathcal{I}m \left[ L(i\mu - 0^+) \right] &= -\frac{\pi}{2\mu} \sqrt{\mu^2 - 4m_\pi^2} \theta(\mu - 2m_\pi) \\
\mathcal{I}m \left[ A(i\mu - 0^+) \right] &= \frac{\pi}{4\mu} \theta(\mu - 2m_\pi) \\
\mathcal{I}m \left[ L^2(i\mu - 0^+) \right] &= -\frac{\pi}{\mu^2} (\mu^2 - 4m_\pi^2) \ln \left( \frac{\mu - \sqrt{\mu^2 - 4m_\pi^2}}{2m_\pi} \right) \theta(\mu - 2m_\pi) \\
\mathcal{I}m \left[ A^2(i\mu - 0^+) \right] &= -\frac{\pi}{8\mu^2} \ln \left( \frac{\mu - 2m_\pi}{\mu + 2m_\pi} \right) \theta(\mu - 2m_\pi), \quad (4.33)
\end{align*}
\]

where \( L(q) \) and \( A(q) \) are given in Eqs. (4.7) and (4.14). As expected all imaginary parts only contribute for \( \mu > 2m_\pi \).

Furthermore the \( q \)-dependent operator basis has to be transformed as well:\(^{11}\):

\[
\hat{U}(r) = \hat{U}_C(r) + (\hat{\sigma}_1 \cdot \hat{\sigma}_2) \hat{U}_S(r) + S_{12}(\hat{r}) \hat{U}_T(r) + \frac{1}{2} (\hat{\sigma}_1 + \hat{\sigma}_2) L \hat{U}_{SO}(r). \quad (4.34)
\]

The rank-2-tensor operator \( S_{12}(\hat{r}) \) is given by \( 3(\hat{\sigma}_1 \cdot \hat{r})(\hat{\sigma}_2 \cdot \hat{r}) - \hat{\sigma}_1 \cdot \hat{\sigma}_2 \). Using the relation

\[
\int \frac{d^3q}{(2\pi)^3} q e^{-iqr} g(q) = -i \nabla \int \frac{d^3q}{(2\pi)^3} e^{-iqr} g(q) \quad (4.35)
\]

we obtain the following transformation rules for the chiral potentials (with \( U_X = V_X + (4I - 3)W_X \)):

\[
\begin{align*}
\hat{U}_C(r) &= -\frac{1}{2\pi r} \int_{2m_\pi}^{\infty} d\mu \mu \mathcal{I}m[U_C(i\mu)] e^{-\mu r} \\
\hat{U}_S(r) &= -\frac{1}{2\pi r} \int_{2m_\pi}^{\infty} d\mu \mu \mathcal{I}m[U_S(i\mu)] e^{-\mu r} \\
&\quad + \frac{1}{6\pi^2 r} \int_{2m_\pi}^{\infty} d\mu \mu^3 \mathcal{I}m[U_T(i\mu)] e^{-\mu r} \\
\hat{U}_T(r) &= \frac{1}{6\pi^2 r^3} \int_{2m_\pi}^{\infty} d\mu [\mu r]^2 + 3\mu r + 3] \mathcal{I}m[U_T(i\mu)] e^{-\mu r} \\
\hat{U}_{SO}(r) &= \frac{1}{\pi^2 r^3} \int_{2m_\pi}^{\infty} d\mu [1 + \mu r] \mathcal{I}m[U_{SO}(i\mu)] e^{-\mu r}. \quad (4.36)
\end{align*}
\]

\(^{11}\)Note that \( \hat{U}_T(r) \) is not the Fourier transform of \( U_T(q) \)!

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4.3.2 Peripheral Chiral Potential

All integrals in Eqs. (4.36) up to third order in small momenta can be computed analytically and are given in Ref. [KBW97]. Kaiser used Cutkovsky’s cutting rules to determine the imaginary part of the chiral N^3LO potential. As we showed in the previous chapter the knowledge of this part of the potential is sufficient to determine the peripheral potential in coordinate space. In some of the potentials appearing at N^3LO the Feynman-parameter integral cannot be solved analytically and we therefore transform the potentials numerically\textsuperscript{12}.

A comment is in place about the energy dependence of the nucleon-nucleon potential. Besides the contact terms, the only energy-dependent contributions stem from $k^2$-dependent $1/M_N^2$ corrections, where $\mathbf{k} = (\mathbf{p} + \mathbf{p}')/2$ is the average center of mass momentum. Because these contributions are nearly zero, we neglect the almost non-existent energy-dependence of the chiral potential.

\textsuperscript{12}Besides the unsolvable Feynman-parameter integrals, all coordinate space potentials can be computed analytically.
4.3 Chiral Potentials in Coordinate Space

Central Potential: Fig. 4.8 shows the order-by-order evolution of the isoscalar and isovector central potentials generated by chiral two-pion exchange. In the isoscalar channel the fourth-order contributions weaken the attraction, but they can be seen as very small corrections, which is a good sign of convergence of the chiral expansion in this potential. The parameters are taken as in chapter 4.2. The LEC $c_3$ has a large influence on the isoscalar central potential $\tilde{V}_C$. While in Ref. [KBW97] $c_3 = -5.3 \text{ GeV}^{-1}$ leads to a large isoscalar central potential, e.g. $\tilde{V}_C(r = 1/m_\pi) = -35.9$ MeV (N$^2$LO), the smaller choice of $c_3$ leads to $-22.4$ MeV and $-19.0$ MeV at N$^2$LO and N$^3$LO, respectively. These values are more in agreement with the attraction produced by the fictitious $\sigma(550)$ boson of the phenomenological Bonn potential [EW88]. We notice that the isoscalar central potential is much stronger than its isovector counterpart, though one should not forget about the isospin factor $\tau_1 \cdot \tau_2$ taking the values 1 ($I = 1$) or $-3$ ($I = 0$). Hence the isovector central potential is attractive in isospin triplet and repulsive in isospin singlet channels. The chiral expansion in the potential has good convergence properties: the contributions become smaller the higher the order and we observer that they alternate the signs from one order to the next.

Another picture emerges from the isoscalar spin-spin potential $\tilde{V}_S$: the N$^3$LO contributions are stronger than the $1/M_N$-corrections. It is a general attribute of all realistic chiral NN potentials that the $1/M_N$ expansion is suppressed against the chiral expansion. Epelbaum et. al therefore count $1/M_N$-contributions to the two-pion exchange as N$^3$LO and do not consider $1/M_N^2$ or $c_i/M_N$ terms in the chiral potential [EGM05]. The similar size of $\tilde{V}_S$ and $\tilde{U}_C$ causes a near cancellation of the two potentials in channels with odd orbital angular momentum $L$ because of the Pauli-principle $L + S + I = \text{odd}$. The momentum-space operator $(\sigma_1 \cdot \mathbf{q})(\sigma_2 \cdot \mathbf{q})$ does not transform as a rank-two tensor under Fourier transformations (unlike $S_{12}$) and therefore the one-pion exchange contributes to the isovector spin-spin potential in coordinate space

$$\tilde{W}_S^{1\pi}(r) = \frac{g_A^2 m_\pi^2}{48\pi f_\pi^2} e^{-m_\pi r}.$$ (4.37)

From Eqs. (4.33) and (4.36) we deduce that all two-pion exchange contributions possess the exponential factor $\exp[-2m_\pi r]/r$. Consequently one-pion exchange is the dominant contribution for large $r$, and two-pion exchange becomes increasingly important for smaller $r$. We evaluate the two exponential factors for some distances $r$ in Table 4.1 to illustrate this statement. We generally plot the potentials for $r \in [1 \text{ fm}, 2 \text{ fm}]$ because in this interval one- and two-pion exchange become equally important while for $r > 2 \text{ fm}$ the two-pion exchange is negligible. The strengths of $\tilde{W}_S(r)$ is about the same as its isoscalar counterpart, but one has to consider that a factor of 9 is generated by the operators $(\sigma_1 \cdot \sigma_2)(\tau_1 \cdot \tau_2)$ for $I = 0$, $S = 0$, thus making the contributions comparable to those from the isoscalar central potential, but repulsive.

Finally, we define a combined central potential

$$\tilde{V}_{\text{central}}(r) = \tilde{U}_C(r) + (4S - 3)\tilde{W}_S(r).$$ (4.38)

Because of the above mentioned factor of 9 from the spin and isospin operators the isovector spin-spin potential overcompensates the attraction from the isoscalar central
potential in the iso-singlet spin-singlet channels for $r > 1.2$ fm while in all other channels the attraction from $\tilde{V}_C(r)$ is dominant for all $r$. The large enhancement of $\tilde{W}_S(r)$ for $I = 0, S = 0$ is also seen in the long range part in Fig. 4.9 because the two-pion exchange contributions are strongly suppressed compared to the one-pion exchange contribution. However, the lower plot shows that the asymptotic of the one-pion exchange is not yet reached for $r = 3$ fm: the relation of one-pion exchange in the central potential is $9 : (-3) : (-3) : 1$ for $(I, S) = (0, 0), (0, 1), (1, 0)$ and $(1, 1)$. For $r > 4$ fm the enhancement of one-pion exchange compared to two-pion exchange is large enough to see that ratios.

<table>
<thead>
<tr>
<th>$r$ [fm]</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\exp[-m_\pi r]/r$ [fm$^{-1}$]</td>
<td>0.50</td>
<td>0.25</td>
<td>0.12</td>
<td>0.061</td>
<td>0.030</td>
</tr>
<tr>
<td>$\exp[-2m_\pi r]/r$ [fm$^{-1}$]</td>
<td>0.25</td>
<td>0.061</td>
<td>0.015</td>
<td>0.0037</td>
<td>0.00092</td>
</tr>
</tbody>
</table>

Table 4.1: Coordinate space Yukawa-factors of one- and two-pion exchange.
4.3 Chiral Potentials in Coordinate Space

Figure 4.10: Peripheral part of the isoscalar (left) and isovector (right) NN tensor potential in coordinate space. The lower plot shows the reduced isovector tensor potential \((m_\pi r)^3\tilde{W}_T\). For notation see Fig. 4.8.

**Tensor Potential:** The tensor operator \(S_{12}(\hat{r})\) can be rewritten in the NN-sector as 
\(6(S \cdot \hat{r}) - 2S^2\), where \(S = (\sigma_1 + \sigma_2)/2\) is the total spin of the two-nucleon system. Consequently, spin-singlet states \((S = 0)\) do not get any contributions from the tensor force (with the operator \(S_{12}\)). The non-vanishing partial-wave matrix elements of \(S_{12}(\hat{r})\) are given in Ref. [EW88]:

\[
\begin{array}{c|ccc}
L & L' & J + 1 & J & J - 1 \\
\hline
J + 1 & -2(J+2) & 0 & 6\sqrt{J(J+1)} & 2J+1 \\
J & 0 & 2 & 0 \\
J - 1 & 6\sqrt{J(J+1)} & 0 & -2(J-1) & 2J+1 \\
\end{array}
\]

Table 4.2: Matrix elements \(\langle L1J|S_{12}(\hat{r})|L'1J\rangle\).

The tensor potential is the dominant potential for large \(r\) because of the one-pion exchange tensor potential

\[
\tilde{W}_T^{1\pi}(r) = \frac{g_\pi^2 m_\pi^2 e^{-m_\pi r}}{48\pi f_\pi^2} \left(1 + \frac{3}{m_\pi r} + \frac{3}{(m_\pi r)^2}\right).
\] (4.39)
In Fig. 4.10 we see that the N^2LO two-pion contributions reduce the strength of the one-pion exchange in the isovector tensor potential, but at the next order a part of the strength is restored. In the lower plot we show the reduced isovector tensor potential for a comparison to the phenomenological Paris potential\[13\]. This comparison shows that the isovector tensor potential from the chiral N^3LO computation and the Paris model agree better than at N^2LO, e.g. at r = 1 fm the chiral N^3LO potential has the value 5.23 MeV which agrees well with the Paris potential. In the isoscalar tensor potential there is, again, the case that at third order in small momenta there are only 1/M_N contributions which are smaller than the contributions at fourth order in small momenta. This leads to an increase from the NLO result of around 50% which suggests a slow convergence of the chiral expansion in this potential. While the isovector part of the potential is stronger for larger r, the slope of the isoscalar part is larger. Consequently for smaller distances r the isoscalar part becomes increasingly important. In Fig. 4.11 we show that the combined tensor potential \( \tilde{U}_T(r) \) is attractive in the full range (at least for r > 1 fm, where the effective theory is applicable) for coupled-channels with I = 0 such as \( ^3S_1 - ^3D_1 \) etc., while in the isospin 1 channels it changes the sign and is not as strong. In contrast to the central potentials the one-pion exchange asymptotic for the different

\[13\] See e.g. [EW88]
4.3 Chiral Potentials in Coordinate Space

Spin-Isospin States

Spin-Isospin states is already reached for \( r > 3 \) fm in the tensor potentials: for \( r = 3 \) fm the potential in the \( I = 0 \) channel has an absolute value of 1.8 MeV, whereas in the \( I = 1 \) channel the value is 0.6 MeV.

Spin-Orbit Potential

The operator \( S \cdot L \) can be evaluated using the relation \( S \cdot L = (J^2 - L^2 - S^2)/2 \) in the \( |LSJ\rangle \) basis. For \( S = 0 \) this operator is zero and for \( S = 1 \) is diagonal in the orbital angular momentum. The spin-orbit potentials all stem from the expansion in \( 1/M_N \). The \( c_1/M_N \) and \( 1/M_N^2 \) contributions are not considered in Epelbaum’s work [EGM05], but in Fig. 4.12 one sees that the contributions from the fourth order terms are not suppressed against the \( 1/M_N \) terms. This justifies the counting of \( c_1/M_N \) and \( 1/M_N^2 \) as \( N^3\)LO terms, but on the other hand, it again raises the question of adequate convergence. In both the isoscalar and isovector cases the fourth-order terms change sign and even increase the strength of the potential. Because we will only treat the phase shifts in spin-singlet channels, we will not further comment on the spin-orbit potential.

4.3.3 Short-Range Potential and Schrödinger Equation

We now give attention to the short-range part, that is, the polynomials we subtracted from the potentials and absorbed into the contact terms. As mentioned previously, \( q^0 \) Fourier transforms into \( \delta^{(3)}(r) \) and polynomials in \( q^2 \) into derivatives of it. This, however, leads to a coordinate space potential, which is physically hard to interpret: the chiral potentials we transformed in the previous chapter are at least \( 1/r^3 \)-singular at the origin and \( \delta \)-functions parametrize the short-distance dynamics. We know that the range of the EFT is limited in momentum space and therefore short-distance dynamics play a role out to \( 2\pi/\Lambda \sim 1 \) fm. Different approaches have been taken to describe the NN interaction in coordinate space. Ordonez, Ray and van Kolck [ORvK96] used cutoffs \( \exp[-(l/\Lambda)^2] \) in loop integrals and \( \exp[-(q/\Lambda)^2] \) for the momentum transfer in potentials to regularize the chiral potential before the Fourier transformation was performed numerically. However, these cutoffs change the behavior of the chiral potential in the partial waves because

Figure 4.12: Peripheral part of the isoscalar (left) and isovector (right) NN spin-orbit potential in coordinate space. For notation see Fig. 4.8.
\( q^2 = p^2 + p'^2 - 2pp'\cos(\theta) \). Hence even a constant term which should only contribute in the \( S \)-wave generates contributions in all higher partial waves\(^{14}\). Instead of solving the Lippmann-Schwinger equation in momentum space, one then meets the problem of solving the Schrödinger equation

\[
H\psi(r) = E\psi(r)
\]

(4.40)

in coordinate space. In 2002 Beane et al. [BBSvK02] suggested another method to regularize and renormalize the coordinate space potential. Their idea was to smear the delta-function over some interval

\[
\delta^{(3)}(r) \rightarrow \frac{3}{4\pi R^3} \theta(R - r),
\]

(4.41)

with \( R = 1/\Lambda \) and similarly cut the chiral potential at \( R \).

We will later compare NN potentials from lattice QCD with the ones derived from chiral effective field theory. As we saw in this chapter, a comparison in coordinate space is troublesome because the short range behavior is not accessible from the EFT. We further want to stress that the phase shifts and the scattering length are even better quantities for a comparison because - unlike the potential - they are observables.

\(^{14}\)One can compensate for this behavior by higher order terms though.
5 The Nucleon-Nucleon Interaction at Non-Physical Quark Masses

5.1 The Nucleon-Nucleon Interaction in Lattice QCD

We briefly summarize how the nucleon-nucleon interaction is treated in lattice QCD. We follow the review [Ish09] and refer the interested reader to Ref. [AHI10] for a more detailed description.

The Bethe-Salpeter (BS) wave function, defined by
\[ \psi_p(x, y) := Z_N^{-1} \langle 0 | T \{ N(x)N(y) \} | N(p)N(-p) \rangle \] (5.1)
can be generated in the nucleon-nucleon center-of-mass frame on the lattice. Here \( p \) is the asymptotic relative momentum of the two initial nucleon states and therefore describes the energy in the system. The composite interpolating field for a nucleon is denoted by \( N(x) \), which however is not unique. The phase shifts are encoded in the long distance asymptotic form of the equal-time BS wave-function, e.g., for the \( S \)-wave:
\[ \psi_p(r) := \lim_{x_0 \to y_0} \psi_p(x, y) \sim e^{i\delta(p)} \frac{\sin(pr + \delta(p))}{pr} + \ldots , \] (5.2)
where \( r = y - x \). Finally, the nucleon-nucleon potential is introduced by demanding that the Schrödinger equation reproduces the BS wave functions for energies below the pion-production threshold:
\[ \left( \frac{p^2}{M_N} - H_0 \right) \psi_p(r) = \frac{1}{M_N} (p^2 + \Delta) \psi_p(r) = \int d^3r' U(r, r') \psi_p(r') . \] (5.3)

The potential \( U(r, r') \) can be chosen energy-independent, but is in general non-local. The functional form of the NN potential defined in this way depends on the choice of the interpolating field \( N(x) \). The particular form of the interpolating field is given in Ref. [AHI10]. In Ref. [Ish11] it is stated that the difference between such phase-shift equivalent potentials only appears in the off-shell behavior and that a bad choice for the interpolating fields results in larger non-localities. Finally, the non-local potential \( U(r, r') \) is treated in a derivative expansion
\[ U(r, r') = V_{NN}(r, \nabla) \delta(r - r') , \] (5.4)
which is valid for low momenta. In Ref. [MIAH09] Aoki et al. find that the energy-dependence of the generated potentials is weak, almost constant within statistical errors.
The Nucleon-Nucleon Interaction at Non-Physical Quark Masses

Figure 5.1: 2+1 flavor QCD results for nuclear potentials with three different values of quark masses (from Ref. [Ish11]). (a) $V_C(r)$ in the $^1S_0$ channel, (b) $V_C(r)$ in the $^3S_1 - ^3D_1$ coupled channel, (c) $V_T(r)$ for the $^3S_1 - ^3D_1$ coupled channel.

In the $^1S_0$ and the coupled $^3S_1 - ^3D_1$ channels the leading order terms in the derivative expansions read:

\[
^1S_0 : V_{NN}(r, \nabla) = V_C^{L=1}(r) + \mathcal{O}(\nabla^2) \\
^3S_1 - ^3D_1 : V_{NN}(r, \nabla) = V_C^{L=0}(r) + V_T S_{12}(\hat{r}) + \mathcal{O}(\nabla).
\]  

(5.5)

The $\mathcal{O}(\nabla)$-term in the coupled channel stems from a spin-orbit term $V_{LS}(r)\mathbf{L} \cdot \mathbf{S}$ which vanishes in the $S$-wave channels. The two central potentials can be compared with the central potential $\hat{U}_C + \sigma_1 \cdot \sigma_2 \hat{U}_S$ from Eq. (4.38). Although they are sometimes both called $V_C$ within the lattice community, it is important to remember that they are not identical.

In Figs. 5.1 and 5.2 we show some results from Ref. [Ish11]. The two central potentials show a very similar behavior: both possess a hard core, are attractive at ranges between 0.5 and 1.2 fm and for $r > 1.2$ fm the errors are quite large compared to the central values. In the central potentials we notice the trend that for lower pion-masses the attractive part of the potential extends further in space and is slightly stronger. In the tensor potential there is an increase in the strength visible for smaller pion masses,
5.2 Pion-Mass Dependences in the Chiral NN Potential

Figure 5.2: Scattering phase shifts from 2+1 flavor QCD NN potentials for three different values of quark masses (from Ref. [Ish11]).

while the position of the minimum stays mostly fixed between 0.1 and 0.2 fm. The tensor potential will be further discussed in chapter 5.3.

Any values of the potential at NN distances below one lattice unit $a$ are not trustworthy because the derivative in Eq. (5.3) is evaluated in a discrete form and combines the potential at $x$ with the BS wave function at $x - a$. In the data given above the lattice spacing $a$ is 0.092 fm, so the potentials becomes reliable for distances significantly larger than 0.1 fm.$^1$

We close this section with a look at the phase shifts in Fig. 5.2. The phase shifts are very small compared to the physical NN phase shifts, and the result that the phase shifts for 570 MeV are smaller than for 700 MeV seem inverted, but Ishii [Ish11] explains this with the observation that in this pion-mass region the repulsive core grows faster than the attractive part of the potential. The lowest pion mass of around 400 MeV has the largest phase shifts, but the peak around 10° seems rather small compared to the value $\delta \sim 60^\circ$ degrees at the physical pion mass. This also means that the scattering length decreases substantially with increasing pion mass. This result is confirmed by the Seattle group$^2$ which did not generate NN potentials but only considered the scattering length.

5.2 Pion-Mass Dependences in the Chiral NN Potential

5.2.1 Contact Terms

We motivated the contact terms by integrating out heavier particles. Thus the contact terms are driven by the hard scale, and should not depend too strongly on the change of the pion mass. We therefore assume that the contact terms are hardly changing with the pion mass and we set them as constant. This conforms with the statement

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$^1$Private conversation with Y. Ikeda.

$^2$See [BOS08] for their formalism and [BBOS06] for latest results on NN scattering length.
of Epelbaum [EMG03] that the renormalization of contact terms is independent of the pion mass. However, the series of chiral contact terms consists of two terms of the form $C^m m^2$ up to third order in small momenta\(^3\). As already mentioned after Eq. 4.18 it is not possible to fit this parameter independently from the contact parameters $\tilde{C}_S$ and $\tilde{C}_T$. Furthermore there are contact terms of the form $D^m m^4$ and $D^m q^2 m^2$ at fourth order in small momenta. Epelbaum et al. [EMG03] and Beane et al. [BS03] separately looked at the pion-mass dependence up to NLO and made different so-called naturalness assumptions for $C^m$:

\[
C_{\text{Ep}}^m = \frac{4\pi\alpha}{f^2 m^2} \quad \alpha \in [-3, 3]
\]

\[
C_{\text{Be}}^m = \eta \frac{\tilde{C}}{m^2} \quad \eta \in \left[\frac{1}{15}, \frac{1}{5}\right]. \tag{5.6}
\]

The estimation of Beane is a bit wider, but both are in the range $10^{-7}$-$10^{-9}$ MeV\(^{-4}\) and therefore similar to other NLO contact terms (see Eq. (4.26)).

We will not make any estimates now, but rather keep in mind that only the constant contact terms are pion-mass dependent up to third order in small momenta. We can write these in the form $C_S^m + C_T^m \mathbf{\sigma}_1 \cdot \mathbf{\sigma}_2$ or, alternatively, take one for the $^1S_0$ and one for the $^3S_1$ wave.

### 5.2.2 Chiral Extrapolations of $g_A$, $f_\pi$ and $M_N$

Regarding the axial coupling, the pion decay constant and the nucleon mass we will take a different approach than Epelbaum et al. and Beane et al. Beane argues that any pion-mass dependence in the pion-exchange potentials are negligible because pion exchange itself is subleading in the $S$-waves (KSW-counting [KSW98]). Epelbaum on the contrary takes the pion-mass dependent renormalization of $g_A$ and $f_\pi$ into account, but only for the one-pion exchange. He justifies this approach for his NLO work with the argument that all corrections to two-pion exchange are higher order. Though this

\(^3\)We will denote an arbitrary pion-mass with $m$ and the physical with $m_\pi$. 

Figure 5.3: Chiral expansions of $f_\pi$ (left) and $M_N$ (right). Black dots from lattice data [Ish11].
renormalization procedure works well for decreasing pion masses\(^4\), an unexpected effect happens for increasing the pion mass: the one-pion exchange term changes its sign at about 260 MeV.

Unlike Epelbaum we are more interested in higher pion masses and therefore choose to work with chiral extrapolations for \(g_\Lambda\), \(f_\pi\) and \(M_N\) to lattice data. Hemmert, Procura and Weise [HPW03] show that for the chiral extrapolation of \(g_\Lambda\) it is necessary to include the \(\Delta\)-isobar degree of freedom. They also show that \(g_\Lambda\) is only very slightly decreasing in our region of interest (\(m < 500\) MeV) and for simplicity we will treat it as constant.

For the pion decay constant we refer to Ref. [N+08] for chiral extrapolations to lattice data. They state that

\[
f_\pi(m) = f_0 \left( 1 - \frac{m^2}{(4\pi f_\pi)^2} \ln \left( \frac{m}{4\pi f_\pi} \right) \right) + \text{const} \cdot \frac{m^2}{(4\pi f_\pi)^2} \tag{5.7}
\]

best fits the current lattice data. We chose \(f_0 = 88\) MeV [GL89] and fitted the constant to reproduce \(f_\pi(m_\pi) = 92.4\) MeV. As can be seen seen in Fig. 5.3, the curve agrees very well with the value \(f_\pi(m \sim 410\) MeV) \(\sim 115\) MeV\(^5\).

We now consider the nucleon mass. It both appears in the third order in the chiral potentials and in the Lippmann-Schwinger equation in the propagator. The changes in the chiral potential are negligible because the \(1/M_N\) contributions are already small. We will nevertheless include these effects as well for consistency. Epelbaum discards changes of the nucleon mass with the pion mass in his NLO work in the propagator as well because he argues that they are higher order effects. Because he decreases the pion mass and the slope \(\partial M_N/\partial m\) is rather small for smaller pion masses (see e.g. Fig. 5.3) this approach seems reasonable. However, for larger pion masses we choose to change the nucleon mass according to Ref. [PHW04]:

\[
M_N(m) = M_0 - 4c_1m^2 - \frac{3g_\pi^2m^3}{32\pi f_\pi^2} + m^4 \left\{ -\frac{3g_\pi^2}{64\pi^2f_\pi^2M_0} \left[ 1 + 2\ln \left( \frac{m}{4\pi f_\pi} \right) \right] + 5.5 \cdot 10^{-9} \text{MeV}^{-3} \right\} \tag{5.8}
\]

We changed the numerical value \(3.5 \cdot 10^{-9}\) to \(5.5 \cdot 10^{-9}\) MeV\(^{-3}\) to fit a nucleon mass of 1197 MeV at 380 MeV pion mass [Ish11].

\[5.2,3\] Chiral Pion Exchange

In this section we present the pion-mass dependence in the chiral potential generated by pion-exchange. We work in coordinate space because all polynomial short-range terms are subtracted. First, we investigate the convergence behavior in the central potentials for a pion mass three times the physical one (414 MeV). Comparing Fig. 5.4 to the corresponding plot at physical pion mass, Fig. 4.8, we notice that in the isoscalar central

\(^4\)Epelbaum was mostly interested in the chiral limit in his work [EMG03];

\(^5\)Y. Ikeda, private conversation.
and spin-spin potentials the chiral expansions show generic behavior. The difference between these potentials for different pion masses is the energy scale that is smaller by more than a factor of 10 at \( r = 1 \) fm. Because of the exponentials we expect the two-pion-exchange potentials to be weaker by a factor of about \( \exp[-2m_\pi r]/\exp[-2(3m_\pi)r] \) for pion masses around 414 MeV which is approximately 16 and 269 at \( r = 1 \) fm and \( r = 2 \) fm, respectively. The exponential factor is also the main reason why, in the isovector spin-spin potential, the importance of one-pion exchange increases for distances between 1 and 2 fm.The isovector central potential is the only one of the four central potentials for which the fourth-order correction becomes more important for the larger pion mass due to the contributions from diagrams with vertices from \( \tilde{\mathcal{L}}^{(3)}_{\pi N} \) and from two-loop diagrams.

The increased importance of one-pion exchange for distances larger than 1 fm in the chiral central potentials for larger pion masses can also be seen in Fig. 5.5. The asymptotics of one-pion exchange \( 9 : (-3) : (-3) : 1 \) for \( (I, S) = (0, 0), (1, 0), (0, 1) \) and \( (1, 1) \) are reached already at \( r = 2.5 \) fm for \( m = 2m_\pi \), and at \( r = 2 \) fm for \( m = 414 \) MeV (compared to 4 fm for the physical pion mass). Though the exponential factors dominate the relation between one- and two-pion exchange, they cannot explain the position of the zero appearing in the potential in the \( I = 0, S = 0 \) channel. One-
5.2 Pion-Mass Dependences in the Chiral NN Potential

\[ m = 2m_\pi = 276 \text{ MeV} \]

\[ m = 3m_\pi = 414 \text{ MeV} \]

Figure 5.5: Chiral central potentials \( \tilde{V}_{\text{Central}}(r) \) in different channels for pion masses of 276 and 414 MeV.
pion exchange is repulsive in this potential while two-pion exchange, which becomes stronger for smaller distances compared to one-pion exchange, causes attraction, hence the exponential suppression suggests that this zero root would be found at smaller $r$. This is the case if we compare the pion masses of 276 and 414 MeV, but not for a comparison between the physical and twice the physical pion mass.

Next we discuss the influence of the contributions from the $c_1$ term to the isoscalar central potential. The LEC $c_1$ is associated with the explicit symmetry breaking term in the Lagrangian up to second order in small momenta and therefore vanishes in the chiral limit. Fig. 5.6 shows that the overall influence on the NN isoscalar central potential is increasing for larger pion masses and larger distances. For the physical pion mass the $c_1$ contributions amount to 1.9% of the overall potential at $r = 1$ fm while at $r = 2$ fm this fraction increases to 7.5%. For a pion mass $m = 3m_\pi$ the symmetry breaking term becomes more significant as can be seen from the fractions of 6.6% and 14.4% at $r = 1$ fm and $r = 2$ fm, respectively.

The relation between contributions from one- and two-pion exchange are also visible in the tensor channels. For channels with $I = 0$ there are cancellations of the two-pion exchange contributions from the isoscalar and isovector tensor potentials ($V^{(2\pi)}_T \sim 3W^{(2\pi)}_T$ for $r > 1$ fm) such that the potential is dominated by one-pion exchange for $m = m_\pi$, $2m_\pi$ and $3m_\pi$ at all distances larger than 1 fm. The size of the cancellations can be deduced from the right side of Fig. 5.7, where the $I = 1$ tensor potential $U^{I=1}_T = V_T + W_T$ is shown: here the two-pion contributions from the isoscalar and isovector tensor add to each other and act against the one-pion exchange. The balance between one- and two-pion exchange contributions is moved towards one-pion exchange at larger distances and to two-pion exchange at smaller distances. For the physical pion mass, two-pion exchange effects become significant for $r \lesssim 2$ fm and even stronger than one-pion exchange at distances below 1.2 fm. When increasing the pion mass the balance is moved to the left on the distance-axis: two-pion exchange becomes visible for $r \lesssim 1.7$ fm and stronger than one pion exchange below $r \sim 0.9$ fm for $m = 2m_\pi$. For $m = 3m_\pi$ two-pion exchange is not important for $r > 1.4$ fm and the tensor potential generated by two-pion exchange is
5.2 Pion-Mass Dependences in the Chiral NN Potential

Figure 5.7: One-pion exchange (black dotted lines) and subtracted N^3LO chiral tensor (blue full lines) potentials for $I = 0$ (left) and $I = 1$ (right) for different pion masses.
5.3 Chiral and Lattice NN Tensor Potential

The dominance of one-pion exchange (and therefore the suppression of higher orders) in the chiral tensor potential for motivate us to compare with lattice QCD results at the level of the tensor potential. We first want to investigate the tensor potential from lattice QCD further before we compare it with the one obtained from chiral EFT. Aoki, Hatsuda and Ishii published a tensor potential for $I = 0$ ($^3S_1 - ^3D_1$ channel) from quenched QCD in Ref. [AHI10] and gave the parametric fit

$$V_T(r) = b_1 \left(1 - e^{-b_2 r^2}\right)^2 \left(1 + \frac{3}{M r} + \frac{3}{(Mr)^2}\right) \frac{e^{-Mr}}{r} + b_3 \left(1 - e^{-b_4 r^2}\right)^2 \left(1 + \frac{3}{m r} + \frac{3}{(mr)^2}\right) \frac{e^{-mr}}{r}$$

(5.9)

to describe their data. They motivated this functional form by tensor potentials generated by one-pion and $\rho$-meson exchange ($M = M_\rho$) and used some form factors to describe the short-range physics. Unfortunately they did not give their fitting parameters $b_1$ to $b_4$. The functional form of the dominant one-pion exchange is given in Eq. (4.39) in coordinate space. Hence we fixed

$$b_3 = -\frac{3g_A^2m^2}{48\pi f_\pi^2}$$

with chiral extrapolated axial coupling and pion decay constant. The $\rho$-meson mass for a pion mass of 380 MeV was given by 838 MeV. For large $r$ the pion-exchange potential still much weaker than $W_T^{(1\pi)}$ at $r = 1$ fm.
is dominant, hence positive data points from the lattice for $V_T$ are not meaningful and were ignored for the fit. We reproduced Aoki’s fit with the parameters $b_1 = 15.2276$, $b_2 = (1.1 \text{ fm})^{-2}$ and $b_4 = (0.6 \text{ fm})^{-2}$ almost identically. The values of $b_2$ and $b_4$ determine the range for which the form factors affect the potential and where the maximum of the potential is located while $b_1$ gives the parametrizes the coupling to the $\rho$-meson. The form factor is chosen such that the pion-exchange-potential will have a minimum depending on $b_4$ and goes to 0 for $r \to 0$. The potential that Aoki parametrized with a $\rho$-meson exchange compensates for the difference between the chiral pion-exchange potential and the lattice data. This $\rho$-meson potential causes visible deviations already for distances around 1.5 fm.

Ishii published the NN tensor potential from lattice QCD with 2+1 dynamical flavors for a pion mass of 411 MeV in Ref. [Ish11]. We used the same parametric form (5.9) to perform a fit. Because in full QCD quark- and antiquark-loop exchange dominate for small distances, we do not associate $M$ with the $\rho$-meson mass but leave it as a free parameter to fit. We obtained in Fig. 5.8 the shown curve with the parameters $b_1 = 1.0271$, $b_2 = (0.29 \text{ fm})^{-2}$, $M = 621.206 \text{ MeV}$ and $b_4 = (0.28 \text{ fm})^{-2}$. There are probably better suited functional forms for a fit to the full QCD data because there are large cancellations between the positive and negative contributions. Nevertheless we are able to fit the short-range data with the parametric form (5.9) and the long-range part is given by one-pion-exchange, thus ignoring all positive lattice data points.

A comparison of the quenched and full QCD tensor potentials in coordinate space (Fig. 5.9) shows that quark-antiquark loops account for differences at distances smaller than 1.5 fm. Especially below 0.5 fm the effect is drastic and the overall strength of the tensor force is more than three times as large due to the quark-antiquark loops. Furthermore the minimum is reached for $r \sim 0.27 \text{ fm}$ which is more than one fm less than in the quenched simulation. The small difference in the long-distance part can be explained by the different pion masses of 380 MeV for the quenched and 411 MeV for the full QCD simulation.

Comparing the chiral potential from subtracted dispersion relations to the lattice potentials, we notice that one-pion exchange dominates for $r > 1.5 \text{ fm}$. Because we
choose $b_3$ from the parametrization (5.9) accordingly, all three potentials agree in this region. For smaller distances, however, the potentials start to deviate. The subtracted chiral potential shows a singular behavior and as explained in chapter 4.3.3 we do not know how far contact potentials smear out in coordinate space. These contact potentials parametrize the short-distance physics that Aoki et al. described by both the form-factors as well as the tensor potential with mass parameter $M$.

Since we fitted the short-distance part of the lattice data and used a parametrization that describes the long-distance part by pion-exchange, the Fourier-transformed lattice potential is well defined. The chiral EFT is naturally described in momentum space and short-distance physics are described by constants and polynomials in $q^2$. We know the chiral expansion of these contact terms and therefore the short-distance physics are much better under control in this approach. In Fig. 5.10 we see the dominance of one-pion exchange in the tensor potential $U_T(q)$ for a pion mass of 411 MeV: we plot the tensor potential once with the contact parameters taken from Machleidt’s N³LO fit to scattering phase shifts [ME11] and once without the $D_{11} q^2$ and $D_{12} k^2$ contact-term contributions. These N³LO contact terms are associated with the operator $(\sigma_1 \cdot q)(\sigma_2 \cdot q)$ and build the main difference between the N³LO and one-pion exchange potential. For a comparison of the chiral and lattice tensor potential we can keep in mind though that these terms do not represent peripheral pion-exchange but describe short-distance dynamics.

In Fig. 5.11 we show the comparison of the chiral N³LO potential with the lattice tensor potential in momentum space for a pion mass of 411 MeV. The upper plots include the contact terms $D_{11}$ and $D_{12}$ with numerical values taken from Ref. [ME11]. After a total shift in strength (which is the only possible effect of the single pion-mass dependent contact term $D_{6}^3 m^2 (\sigma_1 \cdot q)(\sigma_2 \cdot q)$ at N³LO) we notice that the chiral tensor potential rises faster with $q$ than the one obtained from the lattice. This behavior can be explained by the contact terms $D_{11}$ and $D_{12}$, though, as shown in the lower plots. Neglecting these two contact terms, the chiral and the lattice tensor potentials agree for momentum transfers up to 200 MeV.
5.4 Pion-mass dependence in the $^1S_0$-Channel

Finally, we will investigate the behavior in the $^1S_0$ channel. Because we include the chiral N$^2$LO potential in the Lippmann-Schwinger equation, we will consider the chiral potential up to this order as well. We can compare chiral and lattice data on the level of phase-shifts or potentials, but since phase shifts are observables while the potential is not, we will focus most of our attention on phase shifts. Nevertheless it is useful to consider the pion-mass dependence of the chiral potential. In Fig. 5.12 the potentials from one- and two-pion exchange are shown after the angular momentum integration is performed. Because the pion-mass dependent polynomials from the regularization of two-pion exchange are included, there is a small overall shift that increases the potential for larger pion masses. This overall shift can be fitted very well by a parabola, thus the pion-mass dependent terms proportional to $q^0$ could be absorbed by the pion-mass dependent contact term $C(^1S_0)m^2$. For a comparison of the slopes, we also show shifted potentials at the same value for $T_{\text{lab}} = 0$ and notice that the potentials also rise faster at larger pion masses. This can also be explained because of the pion-mass dependent terms proportional to $q^2$ from dimensional regularization that outweigh the decreased slope of the loop functions. Therefore without any compensation from the contact term $Cm(^1S_0)m^2$ the chiral potential becomes more attractive. The non-perturbative aspect of the NN interaction is evident in this channel because the behavior of the chiral potential

Figure 5.11: Lattice (blue full line) and shifted chiral (black dotted line) tensor potentials $U_T(q)$ (left) and $q^2U_T(q)$ in $S = 1$, $I = 0$ channel for pion mass of 411 MeV with $D_{11}$ and $D_{12}$ contact potential (upper figs.) and without (lower figs.).
and phase shifts are inverted. Changes in the potential affect the phase shifts in a nonlinear way due to the iterations. Furthermore the contact terms are large in the $S$-waves and change the potential considerably. Hence it is difficult to deduce consequences from Fig. 5.12 on the phase shifts.

Up to $N^2$LO there is only one free parameter that depends on the pion mass, namely the contact parameter $C(1S_0)m^2$. Together with $\hat{C}(1S_0)$ it is constrained by

$$\hat{C}(1S_0) + C^m(1S_0)m^2 = \tilde{C}(1S_0) = -1.31 \cdot 10^{-2} \text{ MeV}^{-2}.$$  

(5.10)

We performed a fit for laboratory energies below 25 MeV for the phase shifts at a pion mass of 411 MeV to the phase shifts obtained by Ishii in lattice QCD [Ish11]. This resulted in a value of $1.052 \cdot 10^{-7}$ MeV$^{-4}$ for $C^m(1S_0)$ which is in the range of Beane’s estimate (5.6). In Fig. 5.13 we show the consequences of this pion-mass dependent contact parameter on the phase shifts for various values. For pion masses of 411, 276 and 220 MeV the phase shifts are between 15 and $-20$ degrees. We want to stress that even though this is in the region of phase shifts where $\sin(\delta) \cos(\delta) \approx \delta$, one should not use a perturbative approximation. As the pion mass decreases from 220 to 170...
5.4 Pion-mass dependence in the $^1S_0$-Channel

Figure 5.13: Scattering phase shifts in the $^1S_0$ channel for different pion masses [MeV]: in the left diagram 411 (blue full line), 276 (red dashed line), 220 (yellow dotted) and 170 (green dash-dotted) and in the right diagram 150 (blue full line), 140 (red dashed line), 130 (yellow dotted) and 120 (green dash-dotted). The black dots in the left diagram denote phase shifts from lattice QCD [Ish11].

<table>
<thead>
<tr>
<th>$m_\pi$ [MeV]</th>
<th>120</th>
<th>130</th>
<th>140</th>
<th>150</th>
<th>170</th>
<th>220</th>
<th>276</th>
<th>411</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta C(^1S_0)$ [fm$^2$]</td>
<td>-19.0</td>
<td>-8.78</td>
<td>2.28</td>
<td>14.2</td>
<td>40.4</td>
<td>120</td>
<td>234</td>
<td>624</td>
</tr>
</tbody>
</table>

Table 5.1: The difference $\Delta C(^1S_0) = C^m(^1S_0)(m^2 - m_\pi^2)$ created by the pion-mass dependent contact term for different pion masses.

MeV the phase shifts rise strongly and for smaller pion masses this tendency continues. The attraction becomes stronger, and for a pion mass of 120 MeV it is strong enough to generate a bound state. This can be seen from the phase shifts that start at large negative values and jump from $-90^\circ$ to $90^\circ$ for some small energy. As in the $^3S_1$ channel, the negative values are then added to 180° to create a continuous curve. This corresponds to a phase jump over $90^\circ$ for negative energies, hence a bound state.

The phase shifts for different pion masses approximately differ by an almost constant value (the phase shifts for 411 MeV pion mass excluded) which is already given for very small laboratory energies. This is not surprising because a change of the pion mass mostly affects the constant contact term $C(^1S_0)$ which shifts the potential. In Table 5.1 we give the numerical values of these shifts for several pion masses. Comparing them to the change in the chiral potential (see Fig. 5.12) shows that this is the dominant effect. If we leave out the pion-mass dependent polynomial and logarithmic contributions from $2\pi$ exchange and refit $C^m(^1S_0)$ to the lattice data at 411 MeV, we obtain very similar results as in Fig. 5.13. The reasons for this behavior is that the logarithmic, linear, quadratic and cubic terms in the pion mass from the central potentials, which are causing the overall shift of the potential, can be fitted by a parabola very well (as shown in lower diagram of Fig. 5.12) and therefore mostly absorbed into $C^m(^1S_0)$ and that the discrepancies are orders smaller than the changes induced by the fitted $C^m(^1S_0)$ term.

The phase shifts largely differ by an almost constant value, this will show up in a
strong pion-mass dependence of the scattering length. This analysis reveals a region of pion masses where we could expect bound di-neutrons (one would have to check the phase shifts explicitly though). In Fig. 5.14 we see that the scattering length is small compared to the physical one for pion masses above 200 MeV and then it significantly decreases from there to its physical value. For a pion mass of approximately 130 MeV the scattering length diverges and for smaller pion masses there are large positive scattering lengths, the signature of a bound state.

Epelbaum [EMG03] and Beane [BS03] find a quite different result: in their work a bound di-neutron could only appear for larger pion-masses. However, they did not fit the contact term $C^m(1S_0)$ to lattice data, but made the estimates (5.6) for it and, as mentioned in chapter 5.3, both of their NLO analysis used different assumptions for the extrapolations of $g_A$, $f_\pi$ and $M_N$ than the ones used here.
6 Summary

We have presented a description of the nucleon-nucleon interaction using chiral effective field theory. Due to the non-perturbative features of the NN interaction we have numerically solved the Lippmann-Schwinger equation for the chiral N^2LO potential to generate the phase shifts in the spin-singlet channels. We have confirmed the statement from Ref. [KBW97] that in the partial waves with \( L > 2 \) the effects of iterations are small and a perturbative treatment is a sufficient approximation. A fit of the contact parameters up to N^2LO in the spin-singlet S- and P-wave channels has been performed.

The chiral N^3LO potential has been transformed from momentum to coordinate space using subtracted dispersion relations. We have shown the order-by-order evolution of the peripheral chiral potentials and noted that the N^3LO corrections generally affect the potentials with opposite sign as compared to the N^2LO contributions. These corrections improve the agreement with scattering data, e.g. for the case of the reduced isovector potential. With all two-pion exchange contributions up to fourth order in small momenta taken into account, the chiral potentials fulfill the asymptotic ratios of one-pion exchange for \( r > 4 \) fm in the central potentials and for \( r > 3 \) fm in the tensor potentials.

Recent lattice QCD results have been examined. In this context the pion-mass dependence of the chiral potential in the effective theory has been investigated in detail. Apart from the explicit \( m_\pi \)-dependencies in the contact terms and the peripheral potentials, we have taken chiral extrapolations of the axial coupling \( g_A \), the pion-decay constant \( f_\pi \) and the nucleon mass \( M_N \) into account. We have shown that the convergence of the chiral expansion in the central potentials for \( m_\pi = 414 \) MeV is qualitatively similar as the one at physical pion mass in the an order-by-order evolution of the potentials. Furthermore the relation between one- and two-pion exchange has been investigated in both the central and tensor potentials: in both cases the exponential factors \( \exp[-mr] \) (one-pion exchange) and \( \exp[-2mr] \) (two-pion exchange) move the balance into the direction of one-pion exchange at distances larger than 1 fm. This is reflected in the distances at which the asymptotic ratios of one-pion exchange are reached: in the central potentials this distance moves from \( r = 4 \) fm (physical pion mass) to \( r = 2 \) fm (\( m_\pi = 3m_\pi^{\text{phys}} \)).

We have compared the chiral and lattice NN tensor potential for \( m_\pi = 411 \) MeV, the lowest value of the pion mass used in the lattice QCD computations, in both coordinate and momentum space. In coordinate space the chiral potential is almost entirely given by one-pion exchange for \( r > 1.0 \) fm for this large pion mass. In momentum space we have found that the contact terms \( D_{11} \) and \( D_{12} \) become increasingly important for the shape of the potential. We have performed a fit with the parametric form given in Ref. [AHI10] to the 2+1 flavor lattice simulations. The unknown range and size of the subtracted short-distance dynamics in the chiral potential complicate a comparison in coordinate space. Therefore we have carried out a Fourier transformation of the lattice...
tensor potential into momentum space and found agreement of both potentials for small momentum transfers, especially if contributions from $D_{11}$ and $D_{12}$ would cancel. Finally, we have performed a fit of the $^1S_0$ phase shifts for the only pion-mass-dependent contact term in the chiral $N^2$LO potential to lattice data and discussed the consequences for the pion-mass dependence of the phase shifts and the scattering length in this channel. We have found a bound state for pion masses below the physical one. The absolute value of the scattering length decreases rapidly with increasing pion mass and becomes stable at a small value for pion masses above 220 MeV.
A Appendix

A.1 Conventions

Notation

- Minkowski-space metric $\eta = \text{diag}(1, -1, -1, -1)$, Greek letters for Lorentz-indices
- $a$ for three-vector $\vec{a}$
- $\hat{a}$ for a unit-vector in direction of $\vec{a}$
- $\text{Tr}_C$ trace over 3-dimensional color space, $\text{Tr}$ trace over 2-dimensional flavor space
- integrals without boarders are generally from $-\infty$ to $\infty$ (if not otherwise stated or boarders clear from context)
- $q = a_\mu \gamma^\mu$

Important matrices

- Pauli matrices:
  \[
  \tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tau_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{A.1}
  \]

- Gell-Mann matrices:
  \[
  \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix} \\
  \lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\
  \lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix} \\
  \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \tag{A.2}
  \]
A Appendix

These matrices have the following properties:

\[ \text{Tr}[\lambda_a] = 0, \, \lambda_a^\dagger = \lambda_a, \text{Tr}[\lambda_a \lambda_b] = \delta_{ab}, \left[ \frac{\lambda_a}{2}, \frac{\lambda_b}{2} \right] = i f_{abc} \frac{\lambda_c}{2} \]  

(A.3)

- Dirac matrices:

\[ \gamma_0 - \gamma_4 \text{ fulfill the Clifford Algebra } \{ \gamma^\mu, \gamma^\nu \} = 2 \eta^{\mu\nu}. \]  

There is a fifth \( \gamma \)-matrix \( \gamma_5 = i \gamma_0 \gamma_1 \gamma_2 \gamma_3 \), which anticommutes with all other gamma matrices. The gamma matrices are mostly used in the chiral Weyl basis or the Dirac basis. In the chiral Weyl basis with \( \Psi = \langle \phi_L, \eta_R \rangle \) they are given by:

\[ \gamma_0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \gamma_j = \begin{pmatrix} 0 & \sigma^j \\ -\sigma^j & 0 \end{pmatrix}, \quad \gamma_5 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \]  

(A.4)

The Dirac basis can be gained by a basis transformation of the spinor \( \Psi \) such that

\[ \gamma_0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \gamma_j = \begin{pmatrix} 0 & \sigma^j \\ -\sigma^j & 0 \end{pmatrix}, \quad \gamma_5 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \]  

(A.5)

A.2 Partial-Wave Decomposition of NN potential

The NN potential \( V \) can be parametrized as

\[ V = U_C + U_S \sigma_1 \cdot \sigma_2 + U_{SO} \frac{i}{2} (\sigma_1 + \sigma_2) \cdot (q \times k) + U_T (\sigma_1 \cdot q)(\sigma_2 \cdot q) + U_{\sigma L} \sigma_1 \cdot (q \times k) \sigma_1 \cdot (q \times k), \]  

where the convention of Epelbaum et al. [EGM05] was used. The functions \( U_C, U_S, U_{SO}, U_T \) and \( U_{\sigma L} \) depend on the isospin matrices \( T \), the initial and final center of mass momenta \( p \) and \( p' \) and the cosine of the angle between these two momenta \( z = \cos(\theta) \). These functions and the operators in Eq. (A.6) can be evaluated in the helicity state representation \( |\tilde{p} \lambda_1 \lambda_2 \rangle \), but the Lippmann-Schwinger equation is written in terms of partial waves. We note that all operators in Eq. (A.6) commute with \( J^2, J_z \) and \( S^2 \) and only the tensor operators \( (\sigma_1 \cdot q)(\sigma_2 \cdot q) \) and \( \sigma_1 \cdot (q \times k) \sigma_1 \cdot (q \times k) \) do not commute with \( L^2 \) as there are transition matrix elements from \( L = J \pm 1 \) to \( L = J \mp 1 \) due to the tensor force. Because all operators commute with \( J_z \) and \( J^2 \) it is sufficient to evaluate \( \langle L S J m_j | V | L' S J m,i \rangle \) for one \( m_j \), e.g. \( m_j = 0 \). Starting from the coupled basis \( |LSJ\rangle \) we uncouple the orbital angular momentum and the helicities:

\[ |LSJm_j\rangle = \sum_{\lambda_1, \lambda_2} T_1 |Jm_J \lambda_1 \lambda_2\rangle \]

\[ T_1 = \left( \frac{2L + 1}{2J + 1} \right)^{1/2} C^J_{LS}(m_l, \lambda; m_J) C^{S}_{S_1S_2}(\lambda_1, -\lambda_2; \lambda). \]  

(A.7)

\( C^X_{X_1X_2}(x_1, x_2; x) \) are the Clebsch-Gordan coefficients from coupling two angular momenta \( X_1 \) and \( X_2 \) with \( z \)-components \( x_1 \) and \( x_2 \) to an angular momentum \( X \) with \( z \)-projection \( x \).
They are proportional to $\delta(x_1 + x_2 - x)$ and therefore $m_1$ in Eq. (A.7) is determined when $\lambda_1$, $\lambda_2$ and $m_J$ are fixed. The matrix elements of the potential are naturally evaluated as $\langle \hat{p} \lambda'_1 \lambda'_2 | V | \hat{p} \lambda_1 \lambda_2 \rangle$. Because of the invariance of $J$ and $m_J$ this can be written in the form [EAH71]

$$
\langle \hat{p} \lambda'_1 \lambda'_2 | V | \hat{p} \lambda_1 \lambda_2 \rangle = \frac{1}{4\pi} \sum_J (2J + 1) d^J_{\lambda \lambda'}(\theta) \langle Jm_J \lambda'_1 \lambda'_2 | V | Jm_J \lambda_1 \lambda_2 \rangle,
$$

(A.8)

where $d^J_{\lambda \lambda'}$ is a Wigner $d$-function, $\lambda = \lambda_1 - \lambda_2$ and $\lambda' = \lambda'_1 - \lambda'_2$. Using the orthogonality of the $d$-functions allows us to invert the former equation. Finally there are relations between these $d$-functions and the Legendre polynomials. The matrix elements of the operators from Eq. (A.6) were evaluated in Ref. [EAH71] and following the outlined procedure one obtains the following partial-wave matrix elements [EGM05]:

$$
\langle J0J | V | J0J \rangle = \frac{1}{2} \int_{-1}^{1} dz \left[ U_C - 3U_S + p^2 p^2 (z^2 - 1) U_{\sigma L} - q^2 U_T \right] P_J(z)
$$

(A.9)

$$
\langle J1J | V | J1J \rangle = \frac{1}{2} \int_{-1}^{1} dz \left\{ \left[ U_C + U_S + 2p' p z U_{SO} - p^2 p^2 (1 + 3z^2) U_{\sigma L} + 4k^2 U_T \right] P_J(z)
+ \left[-p' p U_{SO} + 2 p^2 p^2 z U_{\sigma L} - 2p' p U_T \right] (P_{J-1}(z) + P_{J+1}(z)) \right\}
$$

(A.10)

$$
\langle J \pm 1, 1, J | V | J \pm 1, 1, J \rangle = \frac{1}{2} \int_{-1}^{1} dz \left\{ p' p \left[ -U_{SO} \pm \frac{2}{2J + 1} (-p' p z U_{\sigma L} + U_T) \right] P_J(z)
+ \left[ U_C + U_S + p' p z U_{SO} + p^2 p^2 (1 - z^2) U_{\sigma L} \right]
\pm \frac{1}{2J + 1} \left(2p^2 p^2 U_{\sigma L} - (p^2 + p^2) U_T \right) P_{J \pm 1}(z) \right\}
$$

(A.11)

$$
\langle J \pm 1, 1, J | V | J \mp 1, 1, J \rangle = \frac{\sqrt{J(J+1)}}{2J + 1} \frac{1}{2} \int_{-1}^{1} dz \left\{ -4p' p U_T P_J(z)
+ \left[ \pm \frac{2p^2 p^2}{2J + 1} U_{\sigma L} + 2p^2 U_T \right] P_{J \pm 1}(z) + \left[ \pm \frac{2p^2 p^2}{2J + 1} U_{\sigma L} + 2p^2 U_T \right] P_{J \pm 1}(z) \right\}
$$

(A.12)

Eqs. (A.9) and (A.10) describe the uncoupled channels, while Eqs. (A.11) and (A.12) display the coupled channels. We want to mention that the factors of $4\pi$ have been chosen appropriately to the used convention in the Lippmann-Schwinger equation (4.1).


A Appendix

A.3 Numerical Solution of Lippmann-Schwinger Equation

A.3.1 General Procedure

We want to introduce briefly a method to numerically solve the Lippmann-Schwinger equation\(^1\). We start with a single channel equation

\[
T(p, p') = V(p, p') - \int \frac{d^3p''}{(2\pi)^3} V(p, p'') \frac{M_N}{p'^2 - p''^2 + i\epsilon} T(p'', p'),
\]

(A.13)

where \(p'\) is the initial, \(p\) the final and \(p''\) the intermediate center of mass momentum. Furthermore we use the regularized potential \(V\) from Eq. (4.2). We use the symmetry of the potential and the \(T\)-matrix in the two momenta and define for a fixed initial momentum \(p'\) the following quantities:

\[
V(p, p') = V(p), \quad T(p, p') = T(p), \quad -V(p, p'') \frac{M_N p''^2}{2\pi^2 (p'^2 - p''^2 + i\epsilon)} = g(p, p'').
\]

(A.14)

For a fixed initial momentum Eq. (A.13) reduces to a integral equation of Fredholm Type II [C+90]:

\[
T(p) = V(p) + \int_0^\infty dp'' g(p, p'') T(p'').
\]

(A.15)

This equation is in general not analytical solvable. As it is a physical motivated equation, we refer the mathematical problems concerning existence and uniqueness of a solution to mathematical books. We approximate the physical solution by discretizing the momenta \(p\) and \(p''\). The integral will be represented by a finite sum with weights \(\omega_j\):

\[
T(p_i) = V(p_i) + \sum_j g(p_i, p_j) \omega_j T(p_j).
\]

(A.16)

We now define the vectors \(y\) and \(x\) by \(y_i = T(p_i)\) and \(x_i = V(p_i)\) and the matrix \(A\) by \(A_{ij} = g(p_i, p_j) \omega_j\) and reduce the integral equation to the linear equation

\[
(1 - A) y = x.
\]

(A.17)

We solve this equation to \(y\) and can interpolate \(T(p, p')\) for fixed initial momentum \(p'\). As we are only interested in the physical on-shell value \(T(p', p')\) we can alternatively pick \(p'\) to be one of the discretized momenta.

It is not possible to directly implement this into a code because of the singularity at \(p'^2 = p^2\). The way to solve this problem is to use the real \(K\)-matrix [Ait72] instead of the \(T\)-matrix. The Lippmann-Schwinger equation for it reads

\[
K(p, p') = V(p, p') - \mathcal{P} \left( \int dp'' \frac{1}{p'^2 - p''^2} \left[ V(p, p'') \frac{4\pi p''^2 M_N}{(2\pi)^3} K(p'', p') \right] \right),
\]

(A.18)

\(^1\)Thanks to Jeremy Holt, who provided a Fortran code and helped me whenever necessary.
A.3 Numerical Solution of Lippmann-Schwinger Equation

where \( \mathcal{P} \) denotes for the principal value. We can eliminate the singularity by subtracting

\[
0 = \left[ V(p, p') \frac{4\pi p'^2 M_N}{(2\pi)^3} K(p', p') \right] \mathcal{P} \left( \int dp'' \frac{1}{p'^2 - p''^2} \right) \tag{A.19}
\]

from Eq. (A.18). We can follow the steps of Eqs. (A.14) - (A.17) to compute an approximation of \( K(p, p') \). The connection between the phase shifts \( \delta(p) \) [in degrees] with the \( K \)-matrix is then given by [Mac01]:

\[
\delta(p) = \frac{180^\circ}{\pi} \arctan \left( \frac{M_N}{4\pi p} K(p, p) \right). \tag{A.20}
\]

Finally, using the effective range expansion in Eq. (4.27) at zero energy we obtain the scattering length as

\[
a = -\frac{M_N}{4\pi} K(0, 0). \tag{A.21}
\]

A.3.2 Coupled Channels

An extension to coupled channels is in principle an extension of the matrix dimension. To see this, we start with \( K \)-matrix and follow the procedure given in the previous section to obtain the 2x2 matrix-valued equation

\[
\begin{bmatrix}
1 - \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} & \begin{pmatrix} y_{11} & y_{12} \\ y_{21} & y_{22} \end{pmatrix} \\
0 & \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix}
\end{bmatrix} = \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix}, \tag{A.22}
\]

where the upper indices denote the two orbital angular momenta \( J \pm 1 \) which are connected by the tensor force in Eq. (A.12). We define the matrices \( B_{xy} \) component-wise by \( B_{xy} = \delta_{xy} - A_{xy} \), the potential vector \( \tilde{x} = (x_{11}, x_{12}, x_{21}, x_{22})^T \) and the solution vector analog. Using this notation Eq. (A.22) simplifies to

\[
\begin{pmatrix}
B_{11} & 0 & B_{12} & 0 \\
0 & B_{11} & 0 & B_{12} \\
B_{21} & 0 & B_{22} & 0 \\
0 & B_{21} & 0 & B_{22}
\end{pmatrix} \begin{pmatrix} y_{11} & y_{12} \\ y_{21} & y_{22} \end{pmatrix} = \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix}, \tag{A.23}
\]

Thus the matrix dimension is 16 times as large as in the single coupled channel, but the problem at hand - namely solving a linear equation system - stays the same.

Finally we state the relations between the on-shell \( K \)-matrix and the eigenphases \( \delta^\pm \) and mixing angle \( \varepsilon \) (in the convention of Blatt and Biedenharn [BB52][Mac01]):

\[
\delta^\pm = \frac{180^\circ}{\pi} \arctan \left( \frac{M_N p}{8\pi} \left( K^{11} + K^{22} \pm \frac{K^{11} - K^{22}}{\cos(2\varepsilon)} \right) \right)
\]

\[
\varepsilon = \frac{1}{2} \arctan \left( \frac{2K^{12}}{K^{11} - K^{22}} \right). \tag{A.24}
\]
A Appendix

A.4 Matlab Codes

We decided to implement the code for the numerical solution of the Lippmann-Schwinger equation in Matlab. It is a powerful numerical computing environment with very sophisticated algorithms for numerical integration and the solution of linear equation systems. We used these algorithms for the numerical integration of the angular momentum in the potential matrix elements and the solution of the equation system (A.17).

The code is written in a way that it can compute the phase shifts for a potential and all parameters given in fm or in MeV. The numerical errors can thus be tested by a comparison of both computations and we found that the numerical errors were negligible in all channels. There are some subroutines that are called in the following code:

- **mpar** calculates the coupling, the pion decay constant and the nucleon mass for different values of the pion mass according to chapter 5.2.2.
- **grid** generates the momentum space points and weights for the Gaussian integration of the Lippmann-Schwinger equation. The code is given in A.4.2.
- **Vspin0** computes the partial wave matrix element \( \langle L0|V|L0\rangle(p,p') \) for the momentum space points \( xp(i) \) and \( xp(j) \).

We furthermore want to stress that for fits (e.g. to the scattering length or \( \chi^2 \)), it is advantageous to evaluate the chiral potential independently from the contact potential. This has the advantage that the angular momentum integrals (with the chiral potential as integrand) only need to be performed once per laboratory energy and the partial-wave decomposed contact potential can be added linearly. For a parameter space of, e.g., 1000 parameters and 100 momentum space points for the Gaussian integration this saves \( 100 \cdot 100 \cdot 999 \sim 10^7 \) evaluations of the chiral potential and as many integrations.

Here we give the code used to generate the phase shifts for different values of the pion-mass \( m \), the angular momentum \( l \) and \( N^2\text{LO} \) spin-singlet contact parameters \( c_1 \) - \( c_4 \) (where \( c_1 \) denotes \( \hat{C}(1S_0) \), \( c_2 \) \( C^m(1S_0) \), \( c_3 \) \( C(1S_0) \) and \( c_4 \) \( C(1P_1) \)):

### A.4.1 Lippmann-Schwinger Equation for Fixed Energy

````matlab
function [phase, pertphase] = LSeq(m, l, Tlab, c1, c2, c3, c4, fm)
% solves Lippmann-Schwinger equation for given laboratory energy in [MeV]
% in spin singlet channel, additionally gives pert. phase shifts T=V
% input parameters:
% contacts c1-c4 [MeV^x]
% orbital angular momentum l
% pion mass m [MeV].
% computation in fm [fm==1] or MeV [fm~=1]

% parameters
% regularization
lambda=1030;
````
n=2; % number of mesh points and weights
points=100;
% others
hc = 197.327;
Pi = 3.14159;
% m,c1–c4 are always in MeV [input] and have to be changed for fm-comp.
if fm==1
    mp=m/hc;
c1p=c1*hc^2;
c2p=c2*hc^4;
c3p=c3*hc^4;
c4p=c4*hc^4;
    lambda=lambda/hc;
else
    mp=m;
c1p=c1;
c2p=c2;
c3p=c3;
c4p=c4;
end
% computation of m–dependent parameters
[g,f,MN] = mpar(mp, fm);
% computation of relative momentum plab
if fm==1
    plab = sqrt(Tlab*MN/(2*hc));
else
    plab = sqrt(Tlab*MN/2);
end
% factor between T(p) and delta(p)
fac1 = MN^2*plab/(4*Pi^2*(plab^2-xp(i)^2));
fac2 = 180 / Pi;

% initializations
V=zeros(points,points);
A=eye(points,points);

% call grid for momentum space points and weights
[xp,w] = grid(plab,fm);
% trick for pole
% multiply factors of M^2 pj^2/(2*Pi^2 (plab^2−pj^2)) into weights
wk=0.0;
for i=1:(points−1)
    wk = wk+w(i)*MN*plab^2/(2*Pi^2*(plab^2−xp(i)^2));
    w(i) = w(i)*MN*xp(i)^2/(2*Pi^2*(plab^2−xp(i)^2));
end
w(points)=wk;

% read in potential on momentum space grid,
% calculate perturbative phase shift,
% regularize potential and generate matrix A for linear equation system
for i=1:points
\textbf{A Appendix}

\begin{verbatim}
for j=1:points
    V(i,j) = Vspin0(xp(i),xp(j),l,c1p,c2p,c3p,c4p,mp,MN,f,g,fm);
    if (i==points && j==points)
        pertphase = fac1*fac2*V(i,j);
    end
    V(i,j) = V(i,j)*exp(-(xp(i)/lambda)^(2*n)-(xp(j)/lambda)^(2*n));
    if j<points
        A(i,j) = A(i,j) + V(i,j)*w(j);
    else
        A(i,j) = A(i,j) - V(i,j)*w(j);
    end
end

% define V(xp(i)) as Vhalf and solve A.Khalf = Vhalf
Vhalf = V(1:points,points);
Khalf = linsolve(A,Vhalf);

% nonperturbative phase shift
phase = fac2*atan(fac1*Khalf(points));
end

A.4.2 Momentum Space Points and Weights for Gaussian Integration

function [pj,wj] = grid(plab.fm)
% defines 100 gauss–weighed points and weights from 0 to inf
% computation in fm [fm==1] or MeV[fm~1]

% last momentum space point
if fm==1
    max=1;
else
    max=3000;
end

% initializations
pj=zeros(100,1);
wj=zeros(100,1);
pj(100)=plab;
wj(100)=0.0;
% interval length
d=plab/8;

% start
A=0;
B=d;
% 33 intervals: 32 finite and one till infinity
\end{verbatim}
for i=1:32
    [sp,sw] = gausspoints(A,B);
    k=3*i-2;
    pj(k)=sp(1);
    wj(k)=sw(1);
    k=k+1;
    pj(k)=sp(2);
    wj(k)=sw(2);
    k=k+1;
    pj(k)=sp(3);
    wj(k)=sw(3);
    % 22 different intervals from 10/8 plab to 3000 MeV
    if (i==10)
        d=(max-10*d)/22;
    end
    A=B;
    B=B+d;
end
% last interval from 3000 MeV to infinity
[sp,sw]=gaussinf(A);
pj(97:99)=sp;
wj(97:99)=sw;
end

function [xi,wi] = gausspoints(A,B)
% generates gaussian (3point) integration points xi with
% weights wi between A and B
% gauss defined on [-1,1]
    xh(1) = -0.7745966;
    xh(2) = 0.0;
    xh(3) = 0.7745966;
    vi(1) = 0.55555555;
    vi(2) = 0.88888888;
    vi(3) = vi(1);
% transformation to [A,B]
    xi = (B-A)*xh/2 + (B+A)/2;
    wi = (B-A)*vi/2;
end

function [xi,wi] = gaussinf(A)
% generates gaussian (3point) integration points xi with
% weights wi between A and infinity
% parameter pi
Pi=3.14159;
% gauss defined on [-1,1]
    xh(1) = -0.7745966;
    xh(2) = 0.0;
    xh(3) = 0.7745966;
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\[
\begin{align*}
\text{vi}(1) &= 0.5555555; \\
\text{vi}(2) &= 0.8888888; \\
\text{vi}(3) &= \text{vi}(1); \\
\end{align*}
\]

80 \texttt{% transformation to } [A, inf[ \texttt{

\[
Y = (1.0 + xh) \times \pi / 4; \\
\text{xi} = A + \tan(Y); \\
\text{wi} = \text{vi} \times \pi / 4 / (\cos(Y)^2); \\
\]
\texttt{end}


Bibliography


Bibliography


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Bibliography


Bibliography


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