Faculty of Physics Adam Mickiewicz University Poznań, Poland

Ph.D. Thesis

Lattice QCD with chirally invariant fermions

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Contents

Introduction						
1	The	eoretical principles				
	of L	attice QCD	11			
	1.1	The QCD Lagrangian	11			
	1.2	Discretizing gauge fields	20			
	1.3	Discretizing fermions	22			
		1.3.1 Naive discretization	22			
		1.3.2 Wilson fermions	23			
		1.3.3 Wilson twisted mass fermions	26			
	1.4	Chiral symmetry on the lattice	29			
		1.4.1 Ginsparg-Wilson relation	29			
		1.4.2 Overlap fermions	30			
		1.4.3 Other kinds of chiral fermions	32			
		1.4.3.1 Domain wall fermions	32			
		1.4.3.2 Creutz fermions	33			
		1.4.4 Topology on the lattice	34			
	1.5	Observables in Lattice QCD	35			
2	Tree	e-level scaling test	41			
	2.1	Fermion propagators	41			
		2.1.1 Overlap fermions	41			
		2.1.2 Wilson twisted mass fermions	42			
		2.1.3 Creutz fermions	43			
	2.2	Observables	43			
	2.3	Test setup	45			
	2.4	Comparison of overlap, twisted mass and Creutz fermions	45			
	2.5	Matching twisted mass and overlap fermions	52			
		2.5.1 Unmatched quark masses	54			
		2.5.2 Effects in the case of matched pion masses	57			

3	Alg	orithmic and technical details	61
	3.1	Simulating QCD	61
		3.1.1 General idea	61
		3.1.2 Hybrid Monte Carlo	62
	3.2	Computation of the overlap operator $\ldots \ldots \ldots \ldots \ldots \ldots$	64
	3.3	Reducing the condition number of $A^{\dagger}A$	66
		3.3.1 Eigenvalue deflation	66
		3.3.2 HYP smearing of gauge fields	68
	3.4	Inverting the Dirac operator	69
		3.4.1 Stochastic sources	70
		3.4.2 The SUMR solver	72
4	Inve	estigations of the continuum limit scaling properties of	
	\mathbf{the}	mixed action setup	75
	4.1	Mixed action approach	75
	4.2	Scaling test – light sea quark mass	78
		4.2.1 Simulation parameters	79
		$4.2.2 \text{Locality} \dots \dots \dots \dots \dots \dots \dots \dots \dots $	80
		4.2.3 Matching the pion mass	83
		4.2.4 Pion decay constant – scaling test	85
	4.3	Chiral zero modes and their contribution to mesonic correlators	88
		4.3.1 Chiral zero modes	88
		4.3.2 The contribution of the zero modes to mesonic correlators	90
		4.3.3 Comparison of correlation functions	93
	4.4	The role of the zero modes – small volume, light sea quark mass	96
	4.5	The role of the zero modes – finite volume effects analysis 1	01
		4.5.1 Simulation parameters	01
		4.5.2 Matching the pion mass – PP correlator	01
		4.5.3 Pion decay constant – PP correlator	02
	4.6	The role of the zero modes – small volume, heavier sea quark	
		mass	04
		4.6.1 Motivation and simulation setup	04
		4.6.2 Pion decay constant – scaling test	06
	4.7	The role of the zero modes – conclusion	09
	4.8	Explicit subtraction of zero modes	11
		4.8.1 Subtraction procedure	11
		4.8.2 Effects of explicit zero modes subtraction	12
		4.8.3 Pion decay constant – scaling test – PP subtr. correlator1	16

5	Various further results	121			
	5.1 Unitarity violations	. 121			
	5.1.1 Motivation \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots	. 121			
	5.1.2 Small volume analysis	. 124			
	5.2 Light baryon masses	. 128			
	5.3 Topological charge and susceptibility	. 131			
Conclusions and prospects 13					
A	Acknowledgements				
Α	Wilson gauge action	141			
в	Tree-level scaling test	143			
	B.1 Overlap fermions	. 143			
	B.2 Creutz fermions	. 145			
	B.3 Correlation functions	. 147			
С	Improvements of the HMC algorithm	149			
D	Tree-level test of zero modes subtraction	151			
	D.1 Analytical formula	. 152			
	D.2 GWC code – point sources	. 153			
	D.3 GWC code – stochastic sources	. 155			
Bibliography 1					

Introduction

The strong force plays a fundamental and crucial role in nature. It is responsible for the formation of all hadrons, which can be classified into mesons and baryons. Examples of the former are the pion and the ρ meson and of the latter the proton and the neutron, which in turn form the nuclei of all atoms. The theory of the strong interaction is believed to be Quantum ChromoDynamics (QCD). It postulates that all hadrons are not elementary themselves but they have an inner structure and are built from constituent particles. Scattering experiments revealed that the constituents are pointlike objects and we now have a large amount of evidence that they can be identified with quarks, which are spin-1/2 fermions and whose interaction is mediated by spin-1 bosons known as gluons. In order to understand the interaction among quarks and gluons and comprehend how it can lead to the formation of hadrons a new quantum number, called the colour charge, had to be introduced. However, all hadrons observed in experiment do not carry this colour charge, but are colourless. This means that the quarks and gluons can not be isolated and do not exist as free particles – they are *confined* into colour-neutral composite hadrons. This fundamental confinement property of QCD results from the fact that at large distances (or at low energies) the QCD coupling constant determining the interaction strength between the quarks and the gluons is large. However, we know from perturbation theory analyses of QCD that at small distances (or at high energies) the QCD coupling constant becomes small and the quarks behave as almost free particles. This property of QCD is called *asymptotic freedom* and has been tested by confronting experimental results with perturbative QCD predictions. It is one of the most amazing characteristics of QCD that it should describe both phenomena, confinement and asymptotic freedom, simultaneously. Clearly, in order to test this theoretical expectation, a method is needed where QCD can be evaluated both in the perturbative regime at small distances and in the non-perturbative regime at large distances, where we enter the world of the observed hadrons.

However, many interesting and relevant phenomena are consequences of

the low-energy properties of QCD. To investigate these issues (e.g. to calculate the hadron spectrum and many structural properties of hadrons, like form factors or parton distribution functions), non-perturbative methods have to be employed. The only method which fulfills the above criterion and allows for precise quantitative predictions is Lattice QCD (LQCD). It consists in discretizing space-time and formulating QCD on a 4-dimensional Euclidean space-time grid with a lattice spacing a. In this way, the theory is fully regularized and mathematically well defined, which led to many conceptual and theoretical developments in our understanding of QCD. On the other hand, by using Feynman's path integral formulation of quantum field theory, LQCD can be interpreted as a kind of a statistical mechanical system which allows an evaluation with numerical methods. LQCD was first proposed in a seminal paper by Wilson in 1974 [1] and shortly after Creutz indeed performed such numerical simulations using Markov chain Monte Carlo methods [2]. It has to be said that over many years LQCD simulations were performed in unphysical setups with much too heavy and even infinite quark masses. However, in the last few years a tremendous progress has been achieved when new algorithmic developments provided a breakthrough in the performance of the used simulation algorithms. At the same time, the increasing computer power made it possible to simulate on large lattices with fine lattice spacings and pion masses approaching the physical pion mass. Lattice QCD computations still require very large computer resources, particularly for fully dynamical simulations, but its prospects are steadily improving with a new generation of supercomputers in the PetaFlop range. The algorithmic and computer improvements were also accompanied by conceptual developments such as ones leading to a faster approach to the continuum limit $(a \rightarrow 0)$ and the formulation of non-perturbative renormalization schemes.

Another important aspect of QCD is chiral symmetry, i.e. the invariance of the theory under the exchange of massless left- and right-handed quarks. It is a continuous symmetry and we believe that it is spontaneously broken in nature, thus giving rise to the appearance of Goldstone bosons. In QCD we identify these Goldstone bosons with the pions, whose mass is much smaller than the mass of any other observed hadron. Assuming such spontaneous breaking of chiral symmetry in QCD, many phenomenological investigations can be performed to interpret experimental data, the most notable of which is chiral perturbation theory.

In principle, LQCD should be able to deduce the phenomenon of spontaneous chiral symmetry from the QCD Lagrangian itself and one would not have to rely on assumptions. However, for many years, it seemed impossible to preserve chiral symmetry on the lattice. Only in the late 1990s it was shown that an alternative approach to chiral symmetry can be followed. This was inspired by the so-called Ginsparg-Wilson relation, which implies that a lattice fermion can be chiral, provided that we allow for a latticemodified version of chiral symmetry. This discovery led to the introduction of so-called overlap fermions, a kind of lattice fermion which respects this lattice modified chiral symmetry. Overlap fermions have many appealing properties, but are much more computationally demanding than other popular fermion discretizations, such as Wilson fermions, modifications thereof or staggered fermions. This makes the use of overlap fermions still a challenge, especially in dynamical simulations. As such, alternatives to dynamical overlap fermions are being looked for to keep chiral symmetry. The goal is is to profit from the good chiral properties of overlap fermions, but at the same time avoid the high computational cost of generating dynamical overlap gauge field configurations. One such approach is called mixed action and it consists in using overlap fermions only as valence quarks and for the sea sector a cheaper fermion discretization is used.

The aim of this thesis is to investigate the mixed action setup of overlap valence fermions and Wilson twisted mass sea quarks. One may suspect that using different lattice fermion formulations in the sea and in the valence sector leads to unphysical effects. And, as we will show in this thesis, this is indeed the case. As we will demonstrate, in order to have a "safe" simulation, where such effects can be avoided, a careful tuning of the physical setup has to be performed. It is one of the main goals of this thesis to specify the regime of parameter values (such as the lattice volume and the pion mass) that allows to perform such safe simulations. Knowing these parameters will then allow to address physical questions and compute physical observables without being affected by possible unphysical effects. Therefore, providing the parameters for safe simulations opens the way for future simulations with chirally invariant overlap fermions in the valence sector to compute important physical quantities.

The outline of the thesis is the following.

In **Chapter 1**, we review the theoretical principles of Lattice QCD. We start by introducing the continuum QCD Lagrangian and discussing its symmetries, particularly the chiral symmetry. Next, we show how the continuum theory is discretized and we introduce different fermion discretizations, including the chirally-symmetric overlap formalism. We also shortly discuss the ways of extracting physical observables from a simulation.

Chapter 2 presents the results of a lattice spacing scaling test of different fermion discretizations at tree-level of perturbation theory. For this we use overlap, twisted mass and Creutz fermions. We also investigate the effects of matching of twisted mass and overlap fermions, which is relevant for considerations in Chapter 4. In **Chapter 3** we discuss some of the algorithmic and technical details of QCD simulations. We review the HMC algorithm and the techniques used to effectively deal with overlap fermions, in particular the method of computation of the overlap Dirac operator, ways of reducing the condition number of its kernel and the use of stochastic sources.

The main results of the thesis are reported in **Chapter 4**. First, the motivation and the general idea of a mixed action simulation are discussed. Then, a continuum limit scaling test of the pion decay constant is performed. This test motivates the analysis of the role of chiral zero modes of the overlap operator. We show that this is a very important effect in the case of a chirally-symmetric valence and non-chirally-symmetric sea quarks discretization. This chapter concludes with the aforementioned range of parameter values that are necessary for a simulation safe against these effects.

In **Chapter 5** we discuss some further results, including the unitarity violations present in the mixed action setup, light baryon masses computation and some topological aspects that can be probed with overlap fermions.

Chapter 1

Theoretical principles of Lattice QCD

1.1 The QCD Lagrangian

Quantum ChromoDynamics (QCD) is a gauge theory of strong nuclear interactions between the constituents of hadrons. The hadrons are a class of particles including baryons (e.g. the nucleon) and mesons (e.g. the pion). The theory is based on the principle of local gauge invariance with a non-Abelian SU(3) gauge group [3, 4]. The fundamental degrees of freedom of the theory are quarks and gluons. The Lagrangian density of QCD can be written as:

$$\mathcal{L}_{QCD} = \mathcal{L}_{quark} + \mathcal{L}_{gluon} + \mathcal{L}_{int}, \qquad (1.1)$$

where \mathcal{L}_{quark} is the purely fermionic (quark) part, \mathcal{L}_{gluon} the purely bosonic (gluon) part and \mathcal{L}_{int} the interaction part that couples quarks and gluons.

Let us now consider the different parts that constitute the QCD Lagrangian. The quark term is^1 :

$$\mathcal{L}_{quark} = \sum_{f=1}^{N_f} \bar{\psi}_f(x) (i\gamma^\mu \partial_\mu - m_f) \psi_f(x), \qquad (1.2)$$

where N_f is the number of flavours², $\psi_f(x)$ is the quark (spinor) field corresponding to flavour f and m_f is the f-flavour bare quark mass and the

¹Throughout the thesis, we employ the Einstein summation convention for Dirac indices (denoted by Greek letters) and SU(3)-group generator indices (denoted by Latin letters).

²The Standard Model incorporates 6 flavours of quarks (up, down, strange, charm, bottom, top). However, investigating the low-energy properties of QCD with Lattice QCD methods, one usually restricts oneself to the lightest 2, 3 or 4 flavours.

gamma matrices satisfy:

$$\{\gamma^{\mu}, \gamma^{\nu}\} = 2\eta^{\mu\nu}, \qquad (1.3)$$

where $\eta^{\mu\nu} = \text{diag}(1, -1, -1, -1)$ is the metric tensor.

The gluon part reads:

$$\mathcal{L}_{gluon} = -\frac{1}{4} F^a_{\mu\nu}(x) F^{\mu\nu}_a(x), \qquad (1.4)$$

where $F^a_{\mu\nu}(x)$ is the field strength tensor, which is related to the gluon field components $A^a_{\mu}(x)$:

$$F^{a}_{\mu\nu}(x) = \partial_{\mu}A^{a}_{\nu}(x) - \partial_{\nu}A^{a}_{\mu}(x) - gf^{abc}A^{b}_{\mu}(x)A^{c}_{\nu}(x), \qquad (1.5)$$

where g is the bare coupling constant and f^{abc} are the structure constants of SU(3), satisfying the commutation relations:

$$[t^a, t^b] = i f^{abc} t^c, (1.6)$$

where t^a are the generators of the group SU(3).

The purely bosonic part of the Lagrangian is invariant with respect to the local gauge transformation. If we want the fermionic part to obey the local gauge symmetry as well, we have to introduce a term that couples the fermions and bosons, i.e. describes the interaction between them. This is the basic building principle of all local gauge theories. It was first discovered in the case of the electromagnetic interaction, where a term that couples electrons and photons is necessary to guarantee the local gauge invariance. In the case of QCD, the sum $\mathcal{L}_{quark} + \mathcal{L}_{gluon}$ is not invariant with respect to the local SU(3) transformation and the way to guarantee this invariance is to introduce the interaction term \mathcal{L}_{int} that couples the quark fields ψ and gluon fields A_{μ} :

$$\mathcal{L}_{int} = g \sum_{f=1}^{N_f} \bar{\psi}_f(x) \gamma^{\mu} A_{\mu}(x) \psi_f(x), \qquad (1.7)$$

where the gluon field A_{μ} is related to its components in the following way:

$$A_{\mu}(x) = t^{a} A^{a}_{\mu}(x). \tag{1.8}$$

Conventionally, one writes the terms \mathcal{L}_{quark} and \mathcal{L}_{int} together, introducing the covariant derivative D_{μ} :

$$D_{\mu}(x) = \partial_{\mu} - igA_{\mu}(x). \tag{1.9}$$

Thus:

$$\mathcal{L}_{QCD} = \sum_{f=1}^{N_f} \bar{\psi}_f(x) (i\gamma^{\mu} D_{\mu} - m_f) \psi_f(x) - \frac{1}{4} F^a_{\mu\nu}(x) F^{\mu\nu}_a(x).$$
(1.10)

Let us also define the (classical) QCD action, which is the integral of the Lagrangian density over space-time:

$$S_{QCD} = \int d^4x \, \mathcal{L}_{QCD}. \tag{1.11}$$

An elegant (and relevant from the point of view of Lattice QCD) way to quantize a classical theory, like the one given by the classical QCD action (1.11), is to use the Feynman path integral formalism [5]. The expectation value of any observable \mathcal{O} is given by:

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int D\bar{\psi} D\psi DA \ \mathcal{O}[\psi, \bar{\psi}, A] e^{iS_{QCD}[\psi, \bar{\psi}, A]}, \qquad (1.12)$$

with the partition function:

$$Z = \int D\bar{\psi}D\psi DA \ e^{iS_{QCD}[\psi,\bar{\psi},A]}.$$
(1.13)

It is worth to emphasize that all fields in the path integral are classical. Such path integral can not be evaluated analytically (except for few special cases much simpler than QCD) and one has to switch to approximate methods. For many theories, like Quantum ElectroDynamics (QED), a very successful method is perturbation theory. It consists in expanding the path integral with respect to a small parameter (e.g. the fine structure constant $\alpha \approx$ 1/137.036 in QED) and dropping terms beyond some order. For example, the most recent calculation of the anomalous magnetic moment of the electron (usually parametrized in terms of the so-called g-factor) up to fourth-order in α agrees with experiment up to 10 significant digits, making it one of the most precisely verified prediction of physics – the electron g-factor is $g_e = 2a_e + 2$, where the theoretical value: $a_e^{\text{th}} = 1\,159\,652\,182.79(7.71) \times 10^{-12}$ and the experimental one: $a_e^{\text{exp}} = 1\,159\,652\,180.73(0.28) \times 10^{-12}$ [6]. However, for perturbative methods to work, there has to be a small parameter with respect to which one expands the path integral. In the case of QCD, the coupling constant of the colour interaction depends on energy and one has to consider two regimes. For high energy or large momentum transfer, the QCD coupling constant is small enough for perturbative methods to work. In this regime, the interaction of quarks and gluons can be arbitrarily weak and

hence it is termed asymptotic freedom. This property of QCD was discovered by Gross, Politzer and Wilczek. However, in the case of low energy or small momentum transfer, this coupling constant becomes of the order of unity and perturbation theory is bound to fail – the strong interactions become strong indeed. Quantitatively, the energy scale when it happens $\Lambda_{\text{strong}} \approx 250$ MeV, where the value is not precisely defined and depends on the chosen observable. Anyway, its approximate value implies that a vast number of relevant phenomena in QCD, such as the confinement of quarks and gluons into hadrons, happen in the non-perturbative regime. Thus, one needs nonperturbative methods, such as Lattice QCD, which is the only known method of extracting quantitative predictions about the low-energy regime of QCD. This approach consists in discretizing the QCD path integral. In this way, one obtains a fully regularized and well-defined theory, which can be studied numerically, but also analytically – the discretized version of QCD enabled many relevant conceptual developments and led to important insight into the nature of strong interactions.

However, the oscillating exponential $e^{iS_{QCD}[\psi,\bar{\psi},A]}$ renders the numerical evaluation of the QCD path integral unfeasible from the practical point of view. Fortunately, integrals like (1.12) are tractable, if one switches from Minkowski space-time with metric tensor $\eta^{\mu\nu}$ with signature e.g. (+ - --)to Euclidean space-time with signature (++++). This is achieved by analytic continuation (Wick rotation of the time direction: $t \rightarrow -i\tau$). In order that the Euclidean formulation can be continued back to physical (Minkowski) space, the Euclidean correlation functions have to satisfy a certain condition, called the Osterwalder-Schrader reflection positivity [7, 8]. This condition ensures that the transition probabilities between gauge-invariant states are non-negative and the quantum mechanical Hamiltonian has only real and positive eigenvalues [9].

The QCD Lagrangian density in Euclidean space reads [10]:

$$\mathcal{L}_{QCD}^{E} = \sum_{f=1}^{N_f} \bar{\psi}_f(x) (\gamma_{\mu}^{E} D_{\mu} + m_f) \psi_f(x) - \frac{1}{4} F_{\mu\nu}^a(x) F_a^{\mu\nu}(x)$$
(1.14)

and the Euclidean gamma matrices satisfy:

$$\{\gamma^{\mu}, \gamma^{\nu}\} = 2\delta^{\mu\nu}, \qquad (1.15)$$

where $\delta^{\mu\nu} = \text{diag}(1, 1, 1, 1)$ is the Euclidean metric tensor. The expectation value of any observable \mathcal{O} is then given by:

$$\langle \mathcal{O} \rangle = \frac{1}{Z^E} \int D\bar{\psi} D\psi DA \ \mathcal{O}[\psi, \bar{\psi}, A] e^{-S^E_{QCD}[\psi, \bar{\psi}, A]}, \qquad (1.16)$$

where $S_{QCD}^E = \int d^4x \mathcal{L}_{QCD}^E$ is the Euclidean action and the Euclidean partition function reads:

$$Z^E = \int D\bar{\psi}D\psi DA \ e^{-S^E_{QCD}[\psi,\bar{\psi},A]}.$$
(1.17)

The oscillating exponential in (1.12) is replaced by the well-behaved factor $e^{-S_{QCD}^E}$ and thus the multi-dimensional integral (1.16) can be evaluated numerically, at least in principle, e.g. with Monte Carlo methods. Formally, the quantum field theory defined by the partition function (1.17) can be interpreted as a statistical mechanical system and the exponential $e^{-S_{QCD}^E}$ plays the role of a Boltzmann factor.

From now on, we will work only with the Euclidean formulation of SU(3) non-Abelian gauge theory (QCD) and hence we drop the superscript E and the subscript QCD that remind us of it.

Now, we will discuss a few important features of continuum QCD that are relevant from the point of view of further considerations, especially the role of chiral symmetry and spontaneous chiral symmetry breaking [10, 11, 4].

To be specific, let us restrict ourselves to two flavours of quarks (u and d quarks). The classical QCD Lagrangian can be rewritten as:

$$\mathcal{L} = \bar{u}\gamma_{\mu}D_{\mu}u + \bar{d}\gamma_{\mu}D_{\mu}d + \bar{u}m_{u}u + \bar{d}m_{d}d - \frac{1}{4}F^{a}_{\mu\nu}F^{\mu\nu}_{a} \equiv$$

$$\equiv \mathcal{L}_{u} + \mathcal{L}_{d} + \mathcal{L}_{m_{u}} + \mathcal{L}_{m_{d}} + \mathcal{L}_{gluon}, \qquad (1.18)$$

where $u \equiv \psi_u$ and $d \equiv \psi_d$ are the corresponding spinors and we have separated the mass terms in the fermionic Lagrangian. We can decompose the quark Lagrangian further by defining left-handed and right-handed quark spinor fields:

$$q_R \equiv \mathcal{P}_+ q, \quad q_L \equiv \mathcal{P}_- q, \qquad q = u, d,$$
 (1.19)

where:

$$\mathcal{P}_{\pm} = \frac{1 \pm \gamma_5}{2}.\tag{1.20}$$

Eq. (1.19) implies for the conjugate spinor fields:

$$\bar{q}_R = \bar{q}\mathcal{P}_-, \quad \bar{q}_L = \bar{q}\mathcal{P}_+. \tag{1.21}$$

Thus, the first two terms in Lagrangian (1.18) become:

$$\mathcal{L}_{u} + \mathcal{L}_{d} = \bar{u}_{L} \gamma_{\mu} D_{\mu} u_{L} + \bar{u}_{R} \gamma_{\mu} D_{\mu} u_{R} + \bar{d}_{L} \gamma_{\mu} D_{\mu} d_{L} + \bar{d}_{R} \gamma_{\mu} D_{\mu} d_{R} = (1.22)$$
$$= \left(\bar{u}_{L} \, \bar{d}_{L} \right) \begin{pmatrix} \gamma_{\mu} D_{\mu} & 0 \\ 0 & \gamma_{\mu} D_{\mu} \end{pmatrix} \begin{pmatrix} u_{L} \\ d_{L} \end{pmatrix} + \left(\bar{u}_{R} \, \bar{d}_{R} \right) \begin{pmatrix} \gamma_{\mu} D_{\mu} & 0 \\ 0 & \gamma_{\mu} D_{\mu} \end{pmatrix} \begin{pmatrix} u_{R} \\ d_{R} \end{pmatrix},$$

i.e. the left- and right-handed fields are decoupled. However, for the mass terms we obtain:

$$\mathcal{L}_{m_u} + \mathcal{L}_{m_d} = m_u (\bar{u}_L u_R + \bar{u}_R u_L) + m_d (d_L d_R + d_R d_L) = (1.23)$$
$$= (\bar{u}_L \bar{d}_L) \begin{pmatrix} m_u & 0\\ 0 & m_d \end{pmatrix} \begin{pmatrix} u_R\\ d_R \end{pmatrix} + (\bar{u}_R \bar{d}_R) \begin{pmatrix} m_u & 0\\ 0 & m_d \end{pmatrix} \begin{pmatrix} u_L\\ d_L \end{pmatrix},$$

i.e. the mass terms couple fields of opposite chiralities.

Let us now consider the massless terms \mathcal{L}_u and \mathcal{L}_d in the Lagrangian. They are invariant with respect to the following transformations, respectively:

$$\begin{pmatrix} u_L \\ d_L \end{pmatrix} \to L \begin{pmatrix} u_L \\ d_L \end{pmatrix}, \qquad \begin{pmatrix} u_R \\ d_R \end{pmatrix} \to R \begin{pmatrix} u_R \\ d_R \end{pmatrix},$$
(1.24)

where L and R are unitary 2×2 matrices, i.e. elements of the (flavour) group U(2). This means that the Lagrangian $\mathcal{L}_u + \mathcal{L}_d$ is invariant with respect to the group U(2)_L×U(2)_R.

Let us take a closer look at the possible forms of transformations. The massless quark Lagrangian is invariant under four $SU(2) \times U(1)$ vector transformations:

$$\begin{pmatrix} u \\ d \end{pmatrix} \to e^{i\alpha u_i} \begin{pmatrix} u \\ d \end{pmatrix}, \qquad (\bar{u} \ \bar{d}) \to (\bar{u} \ \bar{d}) e^{-i\alpha u_i}, \qquad (1.25)$$

where the subscript $i = 0, 1, 2, 3, u_0$ is the identity matrix in flavour space and u_i (i = 1, 2, 3) are flavour SU(2) group generators. There are 4 conserved (vector) Noether currents j_i^{μ} associated with these 4 transformations and hence 4 conserved charges $Q_i = \int d^3x j_i^0$ – the baryon number (i = 0) and the isospin (i = 1, 2, 3).

In addition, there are transformations involving γ_5 , called chiral rotations:

$$\begin{pmatrix} u \\ d \end{pmatrix} \to e^{i\alpha\gamma_5 u_i} \begin{pmatrix} u \\ d \end{pmatrix}, \qquad (\bar{u} \ \bar{d}) \to (\bar{u} \ \bar{d}) e^{i\alpha\gamma_5 u_i}. \tag{1.26}$$

Together with transformations (1.25), the massless quark Lagrangian $\mathcal{L}_u + \mathcal{L}_d$ is invariant under the symmetry group $\mathrm{SU}(2)_R \times \mathrm{SU}(2)_L \times \mathrm{U}(1)_V \times \mathrm{U}(1)_A$.

However, it can be shown that the fermion integration measure in the quantized theory is not invariant under the transformation (1.26) for i = 0, which reduces the full symmetry to $SU(2)_R \times SU(2)_L \times U(1)_V$. This is the so-called axial anomaly and it has important consequences e.g. for the meson spectrum – the chiral flavour singlet symmetry can not be broken spontaneously and hence there is no Goldstone boson associated with spontaneous breaking of this symmetry. This implies that the mass of the flavour singlet η' meson does not vanish in the limit of vanishing quark masses (as

opposed to the mass of the η meson, which is one of the pseudo-Goldstone bosons), but it is related to topological fluctuations of the QCD vacuum via the Witten-Veneziano formula [12, 13]:

$$\frac{f_{\pi}^2}{2N_f} \left(m_{\eta}^2 + m_{\eta'}^2 - 2m_K^2 \right) = \chi_{top}, \qquad (1.27)$$

where f_{π} is the pion decay constant, m_x the mass of the x meson and χ_{top} the topological susceptibility, which will be defined later.

Let us now consider the mass terms of the QCD Lagrangian $\mathcal{L}_{m_u} + \mathcal{L}_{m_d}$. They are invariant with respect to the transformation (1.25) for i = 0, so the baryon number is conserved also in the massive theory. For i = 1, 2, 3 the transformation (1.25) is a symmetry only if the quark masses are equal $m_u =$ m_d . Hence, the isospin is conserved in the massive theory, but only for massdegenerate quarks. However, the mass terms $\mathcal{L}_{m_u} + \mathcal{L}_{m_d}$ are not invariant under chiral rotations (1.26), which is caused by the fact that the exponential in (1.26) is the same for the spinor $(u \ d)^T$ and the conjugate spinor $(\bar{u} \ \bar{d})$, which is, in turn, due to the anticommutation relation $\{\gamma_{\mu}, \gamma_5\} = 0$. Thus, the symmetry of the quantum QCD Lagrangian is broken to $\mathrm{SU}(2)_V \times \mathrm{U}(1)_V$ in the mass-degenerate case and to $\mathrm{U}(1)_V \times \mathrm{U}(1)_V$ if $m_u \neq m_d$.

In the case of arbitrary number N_f of quark flavours, the analysis is easily generalized (the matrices u_i are now the $N_f \times N_f$ identity matrix and $N_f^2 - 1$ generators of the flavour group $\mathrm{SU}(N_f)$) and the full symmetry of the quantized massless QCD Lagrangian is $\mathrm{SU}(N_f)_R \times \mathrm{SU}(N_f)_L \times \mathrm{U}(1)_V$, which is reduced to $\mathrm{SU}(N_f)_V \times \mathrm{U}(1)_V$ in the mass-degenerate case and further to $\mathrm{U}(1)_V \times \ldots \times \mathrm{U}(1)_V$ (with N_f factors $\mathrm{U}(1)_V$) in the case of different quark masses. Thus, in the latter case, the only exact symmetry is the baryon number conservation.

However, since the isospin symmetry is only slightly broken for the lightest two quarks, it is often treated as exact³, while the heavier quarks are treated separately. Moreover, since the up and down quarks are so light, compared to the heavier quarks ($m_u \approx m_d \approx$ a few MeV, whereas already $m_s \approx 100$ MeV), the full symmetry of the massless Lagrangian with $N_f = 2$ flavours $SU(2)_R \times SU(2)_L \times U(1)_V$ remains an important approximate symmetry and is the basis of $N_f = 2$ chiral perturbation theory (χ PT). At low energy, the quarks and gluons are confined into hadrons and hence one can define an effective field theory, in which the fundamental degrees of freedom are not quarks and gluons, but light hadrons. Two-flavour χ PT was formulated by Gasser and Leutwyler [14]. The Lagrangian of this theory is constructed from fields describing the pions (π^{\pm} , π^0) in a way which is consistent with

³In Lattice QCD one usually simulates the lightest two quarks as mass-degenerate.

chiral symmetry. The chiral expansion of such Lagrangian can then be organized in terms of expansion parameters p/Λ_{χ} and m_{π}/Λ_{χ} , where p is the momentum, m_{π} the pion mass and $\Lambda_{\chi} = (4\pi f)^2$ the typical hadronic scale \approx 1 GeV, with f – the pion decay constant in the chiral limit. There are many applications of χPT in the analysis of the low-energy regime of QCD, e.g. pion scattering experiments. Moreover, it is also essential in the analysis of Lattice QCD data, since most of contemporary Lattice QCD simulations are performed at unphysical values of the pion $mass^4$ – hence an extrapolation to the physical point (physical pion mass) is necessary and is performed by fitting χPT formulas. What is more, even though the strange quark mass is much larger than the mass of the up and down quarks, it is still relatively small compared to the typical QCD scale of ≈ 1 GeV and the symmetry $SU(3)_R \times SU(3)_L \times U(1)_V$ of the massless $N_f = 3$ Lagrangian is also an approximate symmetry and forms the basis of $N_f = 3$ chiral perturbation theory, which is also of use in the analysis of low-energy QCD experiments, e.g. including the kaons (also in kaon physics from Lattice QCD). Three-flavour χPT was also introduced by Gasser and Leutwyler [15] as a generalization of the two-flavour case to include the strange quark. The three-flavour Lagrangian includes, besides the pion fields, also other light pseudoscalar meson fields (of the remaining pseudo-Goldstone bosons – the kaons K^{\pm} , K^0 , \bar{K}^0 and the η meson). Quantitatively, the explicit breaking of chiral symmetry by the quark masses can be expressed by the ratios $m_{\pi}^2/(4\pi f)^2 \approx 0.007$ and $m_K^2/(4\pi f)^2 \approx 0.09$. In this sense, the explicit breaking by the strange quark mass is roughly a 10% effect, while for the lightest quarks it is a < 1% effect. Obviously, it is not possible to treat the $N_f = 4$ symmetry as approximately valid, since the charm quark is already heavy ($m_c \approx 1.3 \text{ GeV}$) and the mesons containing it are much heavier than the scale Λ_{γ} .

However, if chiral symmetry was broken only explicitly, we would observe degenerate multiplets of hadrons – e.g. there should be scalar mesons with masses very similar to the pseudoscalar ones. Also, in this case one should not expect such big difference between the masses of the pions and kaons. The explanation of these phenomena can be provided by an assumption that the chiral symmetry of QCD is not only explicitly broken by the quark masses, but also spontaneously broken. We speak of spontaneous symmetry breaking if a symmetry which is present at the Lagrangian level is absent in the physical ground state⁵. If a continuous symmetry is broken spontaneously, then

 $^{^4\}mathrm{Some}$ collaborations have recently started or are preparing simulations at the physical pion mass.

⁵A clear example is provided by ferromagnets. Even though the Hamiltonian of such system is invariant with respect to a simultaneous flip of all spins, in an experiment all spins are aligned, i.e. only one of two degenerate ground states must be chosen – the

massless modes, called the Goldstone bosons, appear. In QCD the pions are interpreted as the "would be"-Goldstone bosons of chiral symmetry breaking, where the prefix "would be"- refers to the fact that they are not massless, but have a small mass (compared to the masses of other hadrons) that is due to (small) explicit breaking of chiral symmetry by the quark masses.

Also, spontaneous breaking of chiral symmetry can be observed in the mass difference of particles that are chiral partners and should have the same mass, if chiral symmetry was exact. Since chiral symmetry is explicitly broken by the quark masses, the experimental mass values of chiral partners should not be equal, but they should be close to each other, because the masses of the light quarks are so small. This is not observed. For example, the vector mesons ρ and a_1 have masses equal to, respectively, 770 and 1260 MeV, which is a much larger difference than one would expect from the small explicit breaking of chiral symmetry [16]. Another example is the nucleon and its negative-parity partner, usually denoted by N^* [11, 17]. The experimental value of the nucleon mass is $m_N \approx 940$ MeV, while $m_{N^*} \approx 1535$ MeV.

Spontaneous chiral symmetry breaking is signalled by a non-zero value of the chiral condensate $\langle 0|\bar{u}u|0\rangle$, where $|0\rangle$ is the vacuum state. This quantity emerges in chiral perturbation theory as an important low-energy constant B_0 :

$$B_0 = -f^{-2} \langle 0 | \bar{u}u | 0 \rangle, \qquad (1.28)$$

where the tree-level pion decay constant f is another low-energy constant. A well-known relation that involves the chiral condensate is the Gell-Mann, Oakes, Renner (GMOR) relation [18]:

$$f^2 m_\pi^2 = -(m_u + m_d) \langle 0 | \bar{u} u | 0 \rangle, \qquad (1.29)$$

which can be derived in χPT . As such, it is desirable to assess the value of the chiral condensate from experiment – thus the value of B_0 would be known. It has been argued that the best estimate can be obtained from the low-energy pion-pion scattering [19, 20]. However, the calculation of the condensate from empirical data requires some model assumptions, i.e. one in fact has to assume that spontaneous chiral symmetry breaking takes place.

Therefore, an important check would be to calculate the condensate nonperturbatively from first principles, without any additional assumptions. One such way is provided by Lattice QCD. Indeed, Lattice QCD simulations confirm that it is non-zero at zero temperature (a review of results on this topic is provided e.g. in. [21]). However, there exists a temperature where the chiral condensate vanishes, thus signalling chiral symmetry restoration. Moreover,

spin-flip symmetry is spontaneously broken.

it has been hypothesized that this temperature is the same as the deconfinement temperature, i.e. the temperature at which the quark-gluon plasma forms and quarks and gluons are no longer confined into hadrons. Up to the present day, this issue has not been resolved completely, but it is a strong hint that Lattice QCD calculations point to the fact that both temperatures are equal, up to statistical error. This strongly suggests that spontaneous chiral symmetry breaking is related to confinement and confirms that understanding chiral symmetry and spontaneous chiral symmetry breaking is essential to fully comprehend QCD. However, much more precise results are needed to unambiguously resolve this question. In Lattice QCD investigations of these phenomena it is therefore essential to take chiral symmetry properly into account, i.e. fermions with good chiral properties have to be used. This is one of the motivations for employing overlap fermions, which will be the main subject of this thesis.

1.2 Discretizing gauge fields

In this section and the next one, we show how QCD can be formulated in a non-perturbative way on a Euclidean 4-dimensional hypercubic lattice with lattice spacing denoted by a [22].

The basic relationship between the continuum and lattice formulation of gauge fields is given by the following equation:

$$U(x, x + a\hat{\mu}) = e^{igaA_{\mu}(x)}, \qquad (1.30)$$

where $U(x, x + a\hat{\mu})$ represents the gauge field on the lattice (it is a variable defined on the link connecting sites x and $x + a\hat{\mu}$, where $\hat{\mu}$ is the unit vector in the μ -direction) and $A_{\mu}(x)$ is the continuum gauge field. This expression also implies that the link variables are SU(3) matrices, since it involves the generators of SU(3), according to eq. (1.8).

We now discuss the simplest gauge field lattice action, called the Wilson action [1], and show that in the continuum limit it is equivalent to the continuum gauge action. It is worth to emphasize that the choice of the lattice action is non-unique. In principle, any lattice action can be used, provided that it has the correct continuum limit. The Wilson action reads:

$$S_{\text{Wilson}}[U] = \frac{\beta}{3} \sum_{x} \sum_{1 \le \mu < \nu \le 4} \left(1 - \operatorname{ReTr} U_P(x, \mu, \nu) \right), \quad (1.31)$$

where U_P is called the plaquette variable and is defined as:

$$U_P(x,\mu,\nu) \equiv U(x,x+a\hat{\mu})U(x+a\hat{\mu},x+a\hat{\mu}+a\hat{\nu})$$
(1.32)

$$\times U(x+a\hat{\mu}+a\hat{\nu},x+a\hat{\nu})U(x+a\hat{\nu},x).$$

To simplify notation, one usually defines $U(x, x + a\hat{\mu}) \equiv U_{x,\mu}$ and $U(x, x - a\hat{\mu}) \equiv U_{x-a\hat{\mu},\mu}^{\dagger}$. The shortcut notation for the plaquette variable is: $U_P(x, \mu, \nu) \equiv U_{x,\mu\nu}$, where $\mu\nu$ identifies the plane of the plaquette. In this way, the plaquette can be written as:

$$U_{x,\mu\nu} = U_{x,\mu} U_{x+a\hat{\mu},\nu} U_{x+a\hat{\nu},\mu}^{\dagger} U_{x,\nu}^{\dagger}.$$
 (1.33)

The gauge transformation on the lattice is associated with multiplication of the fermion and gluon fields by a site-dependent SU(3) matrix G(x). For the link matrices it can be written as:

$$U_{x,\mu} \to U'_{x,\mu} = G(x)U_{x,\mu}G(x+a\hat{\mu})^{\dagger}.$$
 (1.34)

This form of the gauge transformation implies that the trace of the plaquette (actually, the trace of any closed loop of link variables) is a gauge-invariant quantity:

$$U_{x,\mu\nu} \to U'_{x,\mu\nu} = G(x)U_{x,\mu}G(x+a\hat{\mu})^{\dagger}G(x+a\hat{\mu})U_{x+a\hat{\mu},\nu}G(x+a\hat{\mu}+a\hat{\nu})^{\dagger}$$

$$\times G(x+a\hat{\mu}+a\hat{\nu})U^{\dagger}_{x+a\hat{\nu},\mu}G(x+a\hat{\nu})^{\dagger}G(x+a\hat{\nu})U^{\dagger}_{x,\nu}G(x)^{\dagger} =$$

$$= G(x)U_{x,\mu}U_{x+a\hat{\mu},\nu}U^{\dagger}_{x+a\hat{\nu},\mu}U^{\dagger}_{x,\nu}G(x)^{\dagger}, \qquad (1.35)$$

$$\operatorname{Tr} U'_{x,\mu\nu} = \operatorname{Tr} G(x) U_{x,\mu} U_{x+a\hat{\mu},\nu} U^{\dagger}_{x+a\hat{\nu},\mu} U^{\dagger}_{x,\nu} G(x)^{\dagger} = (1.36)$$
$$= \operatorname{Tr} U_{x,\mu} U_{x+a\hat{\mu},\nu} U^{\dagger}_{x+a\hat{\nu},\mu} U^{\dagger}_{x,\nu} = \operatorname{Tr} U_{x,\mu\nu}.$$

We will consider the gauge transformation for the fermion fields in the next section.

In Appendix A, we show that the Wilson gauge action can be written as:

$$S_{gauge}[U] = \beta \frac{g^2 a^4}{6} \sum_{x} \sum_{\mu,\nu} \left\{ \frac{1}{4} F_{\mu\nu}(x)^2 + \mathcal{O}(a^2) \right\}.$$
 (1.37)

Comparing this expression with the continuum gauge action $\int d^4x \frac{1}{4} F_{\mu\nu}(x)^2$, we can immediately see that the continuum limit of the discretized action is the continuum gauge action if we set:

$$\beta = \frac{6}{g^2}.\tag{1.38}$$

The leading discretization effects are $\mathcal{O}(a^2)$, since the factor a^4 in front of the sum comes just from the discretization of the integral $\int d^4x \to a^4 \sum_x$.

In practical simulations, the Wilson gauge action is often replaced by an improved action, which helps to decrease the size of lattice discretization effects. Such actions have the same continuum limit, but this limit is approached faster. One of the first improved actions was derived by Weisz [23] and it is usually referred to as tree-level Symanzik improved gauge action. The form of this action is:

$$S_{\text{tlSym}}[U] = \frac{\beta}{3} \sum_{x} \left(b_0 \sum_{\substack{\mu,\nu=1\\1 \le \mu < \nu}} (1 - \operatorname{ReTr} U_{x,\mu\nu}) + b_1 \sum_{\substack{\mu,\nu=1\\\mu \neq \nu}} (1 - \operatorname{ReTr} U_{x,\mu\nu}) \right),$$
(1.39)

where b_0 , b_1 are parameters⁶, $U_{x,\mu\nu}$ is the (defined above) plaquette term and $U_{x,\mu\nu}^{\text{rect}}$ is the rectangle term:

$$U_{x,\mu\nu}^{\text{rect}} = U_{x,\mu} U_{x+a\hat{\mu},\mu} U_{x+2a\hat{\mu},\nu} U_{x+a\hat{\nu}+a\hat{\mu},\mu}^{\dagger} U_{x+a\hat{\nu},\mu}^{\dagger} U_{x,\nu}^{\dagger}.$$
 (1.40)

If $b_1 = 0$, this action becomes the Wilson action.

1.3 Discretizing fermions

1.3.1 Naive discretization

Let us start with a discretization of one-flavour continuum free fermion action in Euclidean space, given by:

$$S_{\text{quark}}^{\text{free}} = \int d^4x \, \bar{\psi}(x) D\psi(x), \qquad (1.41)$$

where $D = \gamma_{\mu}\partial_{\mu} + m$ is the Dirac operator and m is the quark mass. The discretization procedure is not unique and we show here one of the choices for the lattice derivative [25]:

$$\hat{\partial}_{\mu}\psi(x) = \frac{1}{2a} \left(\psi(x + a\hat{\mu}) - \psi(x - a\hat{\mu}) \right).$$
(1.42)

This can also be written as:

$$\hat{\partial}_{\mu}\psi(x) = \frac{1}{2a} \left(\psi(x + a\hat{\mu}) - \psi(x) + \psi(x) - \psi(x - a\hat{\mu}) \right) \equiv \frac{1}{2} \left(\nabla_{\mu} + \nabla^{*}_{\mu} \right) \psi(x),$$
(1.43)

⁶The computations relevant for further part of this work used gauge field configurations generated by the European Twisted Mass Collaboration (ETMC), who used this action in $N_f = 2$ simulations, with $b_1 = -1/12$ and $b_0 = 1 - 8b_1$ [24].

where we have defined the forward lattice derivative ∇_{μ} and the backward lattice derivative ∇^*_{μ} . We also discretize the space-time integral $(\int d^4x \rightarrow a^4 \sum_x)$, thus arriving at:

$$\hat{S}_{\text{quark}}^{\text{free}} = a^4 \sum_x \sum_\mu \bar{\psi}(x) (\gamma_\mu \hat{\partial}_\mu + m) \psi(x), \qquad (1.44)$$

where the hat denotes lattice quantities.

By Fourier-transforming the lattice Dirac operator (which is conventionally called the naive operator, since it corresponds to the simplest possible discretization) $\hat{D}_{\text{naive}} = \gamma_{\mu} \hat{\partial}_{\mu} + m$, one can obtain the expression for the Dirac operator in momentum space:

$$\dot{D}_{\text{naive}}(p) = i \mathring{p}_{\mu} \gamma_{\mu} + m \mathbb{1}, \qquad (1.45)$$

where we have defined:

$$\mathring{p}_{\mu} \equiv \frac{1}{a} \sin(ap_{\mu}) \tag{1.46}$$

for later convenience and 1 is the unit matrix in Dirac space.

The tree-level fermion propagator in momentum space is given by the inverse of the Dirac operator (1.45) and thus equals:

$$\hat{D}_{\text{naive}}^{-1}(p) = \frac{-i\dot{p}_{\mu}\gamma_{\mu} + m\mathbb{1}}{\sum_{\mu}\dot{p}_{\mu}^{2} + m^{2}}.$$
(1.47)

Let us consider the case of massless fermions. One can easily observe that this expression has the right continuum limit $-ip_{\mu}\gamma_{\mu}/p^2$. However, it also implies that the number of fermions is doubled for each space-time dimension, since the poles of the fermion propagator are located not only at zero momentum $(ap_{\mu} = (0, 0, 0, 0))$, which corresponds to the single fermion given by the continuum Dirac operator, but also whenever any momentum component equals π/a . Thus, in 4-dimensional space-time, we have $2^4 = 16$ fermions, of which 15 are unphysical and are called doublers. This is the so-called fermion doubling problem.

1.3.2 Wilson fermions

The first way to overcome the doubling problem consists in treating differently the physical pole and the unphysical ones and was introduced by Wilson [26], who suggested the following form of the lattice Dirac operator:

$$\hat{D}_{\text{Wilson}} = \frac{1}{2} \left(\gamma_{\mu} (\nabla^*_{\mu} + \nabla_{\mu}) - ar \nabla^*_{\mu} \nabla_{\mu} \right) + m, \qquad (1.48)$$

where r is the Wilson parameter. The second-derivative term is now called the Wilson term. In momentum space, this operator reads:

$$\hat{D}_{\text{Wilson}}(p) = i \mathring{p}_{\mu} \gamma_{\mu} + \frac{ar}{2} \widehat{p}_{\mu}^2 \mathbb{1} + m \mathbb{1}, \qquad (1.49)$$

where we have defined:

$$\hat{p}_{\mu} \equiv \frac{2}{a} \sin\left(\frac{ap_{\mu}}{2}\right) \tag{1.50}$$

and the tree-level fermion propagator is:

$$\hat{D}_{\text{Wilson}}^{-1}(p) = \frac{-i\mathring{p}_{\mu}\gamma_{\mu} + (\frac{ar}{2}\sum_{\mu}\hat{p}_{\mu}^{2} + m)\mathbb{1}}{\sum_{\mu}\mathring{p}_{\mu}^{2} + (\frac{ar}{2}\sum_{\mu}\hat{p}_{\mu}^{2} + m)^{2}}.$$
(1.51)

The physical pole at $ap_{\mu} = (0, 0, 0, 0)$ gets no contribution from the Wilson term, but the unphysical ones acquire an additional mass, which is proportional to a^{-1} and hence become infinitely heavy in the continuum limit and decouple.

However, the price one has to pay for removing the doublers is twofold. First, the Wilson term leads to an $\mathcal{O}(a)$ leading cut-off dependence in observables, which makes it, from the point of view of practical simulations, advantageous to introduce further terms to the action, e.g. a twisted mass term, which will be discussed later, or counterterms within the framework of the Symanzik improvement programme. The simplest way to obtain $\mathcal{O}(a)$ improvement (the absence of $\mathcal{O}(a)$ cut-off effects) is to add to the action a single term, called the Sheikholeslami-Wohlert (clover) term [27].

Second, the Wilson term, being a mass term, explicitly breaks chiral symmetry even in the chiral limit m = 0, i.e. even in this limit $\{\hat{D}_{\text{Wilson}}, \gamma_5\} \neq 0$. Moreover, it has been proven by Nielsen and Ninomiya [28] that it is not possible that a lattice Dirac operator \hat{D} fulfills at the same time the following conditions⁷:

- 1. locality i.e. the norm of the Dirac operator D decays exponentially, as a function of the distance between lattice points,
- 2. translational invariance i.e. the Fourier transform of the Dirac operator exists and equals $\hat{D}(p) = i\gamma_{\mu}p_{\mu} + \mathcal{O}(ap^2)$ for $p \ll \pi/a$,
- 3. no fermion doublers i.e. $\hat{D}(p)$ is invertible everywhere, except for $p_{\mu} = (0, 0, 0, 0),$

⁷Original formulation of the Nielsen-Ninomiya theorem is in fact different. Here we present an equivalent formulation (given e.g. in [29, 30]), which stresses the important properties from the point of view of lattice fermions.

4. chiral symmetry in the standard form of the anticommutation relation:

$$\{\hat{D}, \gamma_5\} = 0. \tag{1.52}$$

For many years, it seemed that it was not possible to have chiral fermions on the lattice without violating one of the other conditions. However, a great progress has been made on this topic when it was realized that (1.52) is not the only possible form of lattice chiral symmetry. The implications of this discovery will be discussed in the next section.

An important consequence of chiral symmetry breaking for the Wilson action is that the quark mass m requires additive renormalization. Hence, the massless case does not correspond to m = 0, but to $m = m_c$, where m_c is called the critical quark mass.

The quark mass is often expressed with the so-called hopping parameter κ , defined as:

$$\kappa = \frac{1}{8+2m}.\tag{1.53}$$

Now, we discuss how to add gauge fields to the Wilson fermion action. It is believed that in the interacting case the doubler modes also decouple. However, there is no rigorous proof of it.

Under gauge transformation, the fermion fields transform in the following way:

$$\psi(x) \to \psi'(x) = G(x)\psi(x), \qquad \overline{\psi}(x) \to \overline{\psi}'(x) = \overline{\psi}(x)G(x)^{\dagger}.$$
 (1.54)

For convenience, we remind here that the gauge fields transform as:

$$U_{x,\mu} \to U'_{x,\mu} = G(x)U_{x,\mu}G(x+a\hat{\mu})^{\dagger}.$$
 (1.55)

In this way, the fermion mass term is obviously gauge-invariant, but the derivative terms, e.g. $\bar{\psi}(x)\gamma_{\mu}\nabla_{\mu}\psi(x) = \bar{\psi}(x)\gamma_{\mu}(\psi(x+a\hat{\mu})-\psi(x))$ are not, since:

$$\bar{\psi}(x)\psi(x+a\hat{\mu}) \to \bar{\psi}(x)G^{\dagger}(x)G(x+a\hat{\mu})\psi(x+a\hat{\mu}).$$
(1.56)

However, introducing the covariant derivative:

$$\hat{D}_{\mu}\psi(x) = \frac{1}{2a} \left(U_{x,\mu}\psi(x+a\hat{\mu}) - U^{\dagger}_{x-a\hat{\mu},\mu}\psi(x-a\hat{\mu}) \right), \qquad (1.57)$$

one finds for the derivative term (1.56):

$$\bar{\psi}(x)U_{x,\mu}\psi(x+a\hat{\mu}) \to \bar{\psi}(x)G^{\dagger}(x)G(x)U_{x,\mu}G(x+a\hat{\mu})^{\dagger}G(x+a\hat{\mu})\psi(x+a\hat{\mu})$$
(1.58)

and hence the covariant derivative terms are gauge-invariant.

The gauge-invariant Wilson-Dirac operator can be written as:

$$\hat{D}_{\text{Wilson}}(m) = \frac{1}{2} \left(\gamma_{\mu} (\nabla^*_{\mu} + \nabla_{\mu}) - ar \nabla^*_{\mu} \nabla_{\mu} \right) + m, \qquad (1.59)$$

which is exactly the same form as in eq. (1.48), but now ∇_{μ} and ∇^{*}_{μ} are the forward and the backward covariant derivatives⁸, defined by:

$$\nabla_{\mu} = \frac{1}{a} \left(U_{x+a\hat{\mu},\mu} \psi(x+a\hat{\mu}) - \psi(x) \right), \qquad (1.60)$$

$$\nabla^*_{\mu} = \frac{1}{a} \left(\psi(x) - U^{\dagger}_{x-a\hat{\mu},\mu} \psi(x-a\hat{\mu}) \right).$$
(1.61)

1.3.3 Wilson twisted mass fermions

In the remainder of this section, we will discuss Wilson twisted mass fermions, which are relevant from the point of view of further considerations. Originally, they were introduced to deal with the problem of unphysically small eigenvalues (zero modes) of the Wilson-Dirac operator [31], which is another consequence of additive quark mass renormalization, which can bring the renormalized quark mass to zero. In the quenched approximation, the contribution of these modes is not balanced by the fermionic determinant and leads to large fluctuations, which affect ensemble averages in an uncontrolled way. The gauge field configurations which cause this problem are referred to as exceptional configurations. This is especially dangerous in the case of small quark masses and makes the approach towards the chiral limit practically impossible with Wilson fermions. In dynamical simulations with Wilson fermions the problem is suppressed by the fermionic determinant, but it can still cause technical problems, such as long autocorrelation times in certain observables, coming from accidental zero modes of the Wilson-Dirac operator. Moreover, it was realized that the twisted mass discretization can reduce the effects of explicit chiral symmetry breaking by the Wilson term by suppressing the mixing problem of operators belonging to different chiral representations. Finally, twisted mass action makes it possible to obtain automatic $\mathcal{O}(a)$ -improvement, by tuning just one parameter. This is an essential advantage of twisted mass fermions, since other improvement schemes make it necessary to compute improvement coefficients for different interpolating operators.

⁸We will use the same symbols ∇_{μ} and ∇^{*}_{μ} for the non-covariant and covariant derivatives and the meaning of these symbols will be determined from the context.

The twisted mass QCD lattice action [32] for two flavours of mass-degenerate quarks is given by:

$$\hat{S}_{\rm TM} = a^4 \sum_x \bar{\chi}(x) \hat{D}_{\rm TM} \chi(x),$$
 (1.62)

with:

$$\hat{D}_{\rm TM} = \hat{D}_{\rm Wilson}(m) + i\mu\gamma_5\tau_3, \qquad (1.63)$$

where μ is an additional mass parameter, called the twisted mass, τ_3 is the third Pauli matrix in flavour space and $\chi(x)$ is the quark field in the twisted basis.

The physical and twisted bases are related by an axial transformation:

$$\psi(x) \to \chi(x) = e^{i\omega\gamma_5\tau_3/2}\psi(x), \quad \bar{\psi}(x) \to \bar{\chi}(x) = \bar{\psi}(x)e^{i\omega\gamma_5\tau_3/2}, \quad (1.64)$$

where ω is called the twist angle. This transformation leaves the form of the action invariant, only transforming the mass parameters according to:

$$m \to m\cos(\omega) + \mu\sin(\omega),$$
 (1.65)

$$\mu \to -m\sin(\omega) + \mu\cos(\omega). \tag{1.66}$$

A special case of this transformation, referred to as maximal twist, is $\omega = \pi/2$, which corresponds to sending the bare quark mass m to 0 or, taking additive mass renormalization into account, to its critical value m_c . Conventionally, the value of the critical bare quark mass is expressed in terms of the parameter κ_c , given by eq. (1.53). This is the only parameter that needs to be tuned to obtain automatic $\mathcal{O}(a)$ -improvement. The tuning is usually done by employing one of two methods. First, one can just find the critical bare quark mass by looking for a quark mass value that gives a vanishing pion mass. Alternatively, one can also tune the so-called untwisted PCAC mass:

$$m_{PCAC} = \frac{\sum_{\vec{x}} \langle \partial_0 A_0^a(\vec{x}, t) P^a(0) \rangle}{2 \sum_{\vec{x}} \langle P^a(\vec{x}, t) P^a(0) \rangle}, \qquad a = 1, 2$$
(1.67)

to zero [24]. The latter method seems to work very well in practical simulations.

Thus, one can write the maximally twisted mass (MTM) QCD action as:

$$\hat{S}_{\rm MTM} = a^4 \sum_x \bar{\chi}(x) \hat{D}_{\rm MTM} \chi(x), \qquad (1.68)$$

with:

$$\hat{D}_{\rm MTM} = \hat{D}_{\rm Wilson}(m_c) + i\mu\gamma_5\tau_3.$$
(1.69)



Figure 1.1: Continuum limit scaling in fixed finite volume for $r_0 f_{PS}$ at fixed values of $r_0 m_{PS}$ (a) and for $(r_0 m_{PS})^2$ at fixed values of renormalized quark mass $r_0 \mu_R$ (b). In (b) data at $\beta = 4.2$ ($(a/r_0)^2 = 0.0144$) are not included, due to the missing value of the renormalization factor Z_P . Source: [33].

The special meaning of the maximally twisted case is that it guarantees an automatic $\mathcal{O}(a)$ -improvement, which was proven in [32]. This means that all terms of $\mathcal{O}(a)$ in the Symanzik expansion of parity even operators (which give e.g. the hadron masses) are absent. This observation makes the twisted mass formulation (at maximal twist) very useful from the point of view of practical simulations.

An example of $\mathcal{O}(a)$ -improvement is provided by ETMC simulations [33] and is depicted in Fig. 1.1. The left plot shows the continuum limit scaling of the pseudoscalar decay constant (in fixed volume) at fixed reference values of the pseudoscalar mass $r_0 m_{PS}$. Four lattice spacings are included, but the linear fit does not include the data at the largest lattice spacing. The right plot shows the scaling of the pseudoscalar mass (again in fixed volume) at fixed values of the renormalized quark mass $r_0\mu_R$. Here, the data for only three lattice spacings are presented (all of them included in the fit), since it was impossible to include the points at the finest lattice spacing $((a/r_0)^2 = 0.0144)$, due to the missing value of the renormalization factor of the pseudoscalar current Z_P . Both plots show that the leading cut-off effects are indeed $\mathcal{O}(a^2)$ and their overall magnitude is rather small.

However, one should mention here that the twisted mass term violates parity and the isospin symmetry. This effect e.g. makes the masses of the charged and neutral pions different from each other⁹ and in fact this mass

 $^{^{9}}$ In reality, these masses are, of course, different, but this is due to electromagnetic

difference is used to quantify the isospin violation by the twisted mass term. Both parity and isospin breaking are $\mathcal{O}(a^2)$ effects and hence they vanish in the continuum limit.

1.4 Chiral symmetry on the lattice

In this section we discuss the great breakthrough associated with the fact that it was realized that there is an alternative view on chiral symmetry on the lattice, i.e. that the Nielsen-Ninomiya theorem can be overcome in an elegant way.

1.4.1 Ginsparg-Wilson relation

In 1982 (i.e. only one year after establishing the Nielsen-Ninomiya theorem), Ginsparg and Wilson, basing on renormalization group transformations, showed [34] that a remnant of chiral symmetry is present on the lattice without the doubler modes, if the corresponding Dirac operator \hat{D} obeys an equation now called the Ginsparg-Wilson relation:

$$\gamma_5 \hat{D} + \hat{D}\gamma_5 = a\hat{D}\gamma_5 \hat{D}. \tag{1.70}$$

It is a modification of the anticommutation relation (1.52) and the term on the right-hand side vanishes in the continuum limit – hence, in this limit the standard chiral symmetry relation (1.52) is regained.

However, for many years it has not been realized that the Ginsparg-Wilson relation allows one to define chiral symmetry also on the lattice, i.e. at non-vanishing lattice spacing. It lasted until around 1997 before the Ginsparg-Wilson relation was "rediscovered". First, P. Hasenfratz realized that a kind of lattice fermions called the fixed point fermions satisfies this relation [35, 36] and shortly afterwards a similar observation was made by Neuberger regarding the overlap formalism [37, 38]. Moreover, Lüscher [29] found that the Ginsparg-Wilson relation leads to a non-standard realization of lattice chiral symmetry. The fermion action is invariant under the following chiral rotation:

$$\psi \to e^{i\theta\gamma_5\left(1-\frac{a\bar{D}}{2}\right)}\psi, \bar{\psi} \to \bar{\psi}e^{i\theta\gamma_5\left(1-\frac{a\bar{D}}{2}\right)}.$$
(1.71)

In the continuum limit this transformation is (1.26) with $u_i = 1$. To prove the invariance of the massless action with respect to the above transformation,

interactions and the explicit violation of isospin symmetry by different up and down quark masses. In Lattice QCD with mass-degenerate quarks the charged and neutral pion masses should be equal.

one has to use the Ginsparg-Wilson relation. Moreover, it is possible to define the left- and right-handed projectors of fermion fields [11] with a modified γ_5 -matrix $\hat{\gamma}_5 = \gamma_5(1 - a\hat{D})$:

$$\hat{\mathcal{P}}_{\pm} = \frac{1 \pm \hat{\gamma}_5}{2}.$$
 (1.72)

Thus defined projectors have the same properties as the standard continuum projectors and hence one can decompose the fermion part of the Lagrangian into left- and right-handed massless parts and a symmetry breaking mass term that mixes the left- and right-handed components. Taking the properties of the lattice projectors $\hat{\mathcal{P}}_{\pm}$ into account, one finds that the mass term is of the form $m\bar{\psi}\left(1-\frac{a\hat{D}}{2}\right)\psi$, which means that the massive Ginsparg-Wilson Dirac operator $\hat{D}(m)$ that corresponds to the massless operator \hat{D} reads:

$$\hat{D}(m) = \hat{D} + m\left(1 - \frac{a\hat{D}}{2}\right) = \left(1 - \frac{am}{2}\right)\hat{D} + m.$$
 (1.73)

Since the Ginsparg-Wilson relation is a non-standard realization of chiral symmetry, the conditions of the Nielsen-Ninomiya theorem do not apply and one can have chiral symmetry without the doublers, which was considered to be impossible for many years.

Moreover, it was also shown by Hasenfratz, Laliena, Niedermayer [39] and in a different way by Lüscher [29] that the Ginsparg-Wilson relation implies that the axial anomaly is correctly reproduced. The action is invariant under the transformation (1.71), but the fermionic measure $\mathcal{D}\bar{\psi}\mathcal{D}\psi$ is not – its Jacobian J is non-trivial: $J = \exp[-2i\theta \operatorname{Tr}(\gamma_5(1-a\hat{D}/2))]$ and it can also be expressed as $J = \exp[-2i\theta Q_{top}]$, where Q_{top} is the topological charge, to be discussed later. This issue was further elucidated by Fujikawa [40], who studied the continuum limit of this Jacobian.

Furthermore, a consequence of the Ginsparg-Wilson relation is that fermions are protected from additive mass renormalization and mixing between four-fermion operators in different chiral representations (Hasenfratz [36]) and there can be no $\mathcal{O}(a)$ lattice artefacts (Niedermayer [30]).

In the next section we discuss one of the solutions of the Ginsparg-Wilson equation, defining the so-called overlap operator.

1.4.2 Overlap fermions

As we have already stated, for many years it has not been realized that the Ginsparg-Wilson relation provides a useful (from the simulational viewpoint)

solution of the problem of lattice chiral symmetry, simply because no solutions of this equation have been known. In 1997, Neuberger [37, 38] found a particularly simple form of a lattice Dirac operator that obeys the Ginsparg-Wilson relation. It is now usually referred to as overlap fermions and the massless overlap Dirac operator is given by:

$$\hat{D}_{\rm ov}(0) = \frac{1}{a} \Big(1 - A (A^{\dagger} A)^{-1/2} \Big), \qquad (1.74)$$

where:

$$A = 1 + s - a\tilde{D}_{\text{Wilson}}(0) \tag{1.75}$$

and s is a parameter which satisfies |s| < 1 and can be used to optimize locality properties. Note that instead of $\hat{D}_{\text{Wilson}}(0)$, one could use in the kernel operator A any massless lattice Dirac operator that is local and has no doubler modes [30]. Moreover, if the operator used in A itself satisfies the Ginsparg-Wilson relation, it will be just reproduced by eq. (1.74), since then $A^{\dagger}A = 1$.

The massive operator is given, according to (1.73), by:

$$D_{ov}(m) = \left(1 + s - \frac{am}{2}\right) D_{ov}(0) + m, \qquad (1.76)$$

where m is the bare overlap quark mass.

After the overlap operator was proposed, it was essential to show that it is local. Else, this attitude would lead to causality violations and render it useless. The definition (1.74) includes the highly non-local term $(A^{\dagger}A)^{-1/2}$, which raises doubts about locality. Algebraically, strict locality (or ultralocality) would mean that the Dirac operator matrix element $\hat{D}(x, y)$ connecting sites x and y of the lattice is non-zero only if the distance between x and y is smaller than some specified small value and also that this matrix element depends on gauge links only in some small neighbourhood of sites x and y [41]. These properties are true for the Wilson-Dirac operator (hence, it is a sparse matrix), but the overlap Dirac operator has non-zero entries for all pairs of lattice sites and thus it is clear that it is not strictly local.

However, strict locality for a Dirac operator is not really needed. It is enough that the Dirac operator falls off exponentially, i.e. we have (suppressing the Dirac and color indices):

$$||\hat{D}(x,y)|| \le Ce^{-\rho||x-y||},\tag{1.77}$$

for some constants C and ρ , where $|| \cdot ||$ is the distance between sites x and y, e.g. the taxi-driver distance $||x - y|| = \sum_{\mu} |x_i - y_i|$. If such inequality holds, it means that the interaction range in physical units $1/\rho$ tends to 0

(the decay rate in lattice units $a\rho$ does not depend on the lattice spacing) as one approaches the continuum limit and in the continuum one has a local field theory, as desired [11].

A thorough analytical and numerical investigation of the locality of the overlap Dirac operator was performed by Hernandez, Jansen and Lüscher [41], who showed that this operator is local under very general conditions, i.e. for a wide range of bare coupling constants.

1.4.3 Other kinds of chiral fermions

Apart from overlap fermions, there a few kinds of lattice fermions that also preserve chiral symmetry. In this subsection, we shortly discuss a few of them.

1.4.3.1 Domain wall fermions

Closely related (mathematically equivalent) to overlap fermions are domain wall fermions, introduced by Kaplan [42] and Shamir [43] in 1992 and 1993, respectively. The general idea of this approach is to introduce an auxiliary (non-physical) fifth dimension and consider massive Dirac fermions with a space-dependent mass in the shape of a domain wall. Kaplan showed that such theory has a zero mode with definite chirality localized on the domain wall and from the point of view of the 4-dimensional theory this zero mode is a chiral fermion. The way that this formulation circumvents the Nielsen-Ninomiya theorem is that translational invariance in the 5-dimensional system is broken (by the space-dependent mass term), but it is still conserved in the 4-dimensional physical world [44]. If the fifth dimension is infinite, there does not exist a doubler mode. But in the case of a finite fifth dimension (which is of course always true in a lattice simulation), an extra zero mode of opposite chirality appears on a second domain wall. However, both zero modes have an exponentially small overlap and hence can not communicate if their separation is large enough. What is more, it was also shown that the anomaly structure is correct both in the infinite and finite fifth dimension case. A first investigation of these properties was performed by Jansen [45], shortly after the birth of the idea of domain wall fermions.

After the overlap formalism was invented, Neuberger also showed [46] that domain wall fermions with infinite fifth dimension are equivalent to overlap fermions. Therefore, at finite fifth dimension, they can be regarded as an approximation to overlap fermions.

In practical simulations, the domain wall formalism is now widely used in a dynamical setup (e.g. by the RBC/UKQCD Collaboration [47]) or in a mixed action approach (e.g. by the LHP Collaboration with improved staggered fermions in the sea sector [48]). However, the size of the fifth dimension is usually taken in the range 8-16, which means that the chiral symmetry is only approximate and this entails additive mass renormalization of the quark mass, i.e. a shift away from zero of the bare quark mass for which one has a vanishing pion mass [10]. The value of this shift is usually referred to as the residual mass.

The main advantage of domain wall fermions with respect to the Wilson fermions (and other non-chirally symmetric formulations) is that chiral symmetry breaking by the domain wall fermions is rather mild and is believed to be controllable. Their main disadvantage is that one needs to simulate a 5-dimensional theory, instead of a 4-dimensional one, and hence the computational cost is higher by a factor of the order of the size of the fifth dimension.

With respect to overlap fermions, an advantage is that this computational cost is still much smaller than the one for overlap, at the price, however, of not having exact chiral symmetry, but only an approximation to it.

1.4.3.2 Creutz fermions

A different approach to circumvent the Nielsen-Ninomiya theorem is to restrict oneself to the minimal number of doubler modes, i.e. to two modes of opposite chirality. This was pointed out in the 1980s by Karsten [49] and Wilczek [50]. Recently, this idea reemerged in the work of Creutz [51], who was motivated by the electronic structure of graphene (which is built of two-dimensional layers of graphite). The low-energy excitations in graphene are described by a two-dimensional Dirac equation for massless fermions and are hence chiral. Furthermore, chirality is achieved exactly in the way that involves the minimum number of fermion modes required by the Nielsen-Ninomiya theorem, i.e. they are minimally-doubled. Creutz showed how to generalize these properties to four dimensions. Creutz's idea was soon elaborated on by Borici [52], who derived a more general form of the action.

Creutz fermions exhibit an exact $N_{\rm f} = 2$ flavour continuum chiral symmetry, which implies also that the leading discretization errors are of $\mathcal{O}(a^2)^{10}$, and they are strictly local. These are very appealing properties, since they imply that one could simulate chiral fermions without the high computational cost of overlap fermions. However, Creutz fermions break a number of discrete symmetries, such as parity, charge conjugation and time reflection [53]. Therefore, to approach the continuum limit in the interacting case one

¹⁰An explicit test of this property will be discussed in Chapter 2.

would have to restore these symmetries by fine-tuning of several parameters in the Symanzik effective action and this would make the practical simulations with Creutz fermions very difficult. However, a preliminary quenched test was performed by Borici [54], who computed the pion mass and found a behaviour consistent with the predictions of chiral perturbation theory. This led him to a conclusion that Creutz fermions are still worth exploring in the future, despite the fact that they break important discrete symmetries. Also, the conclusion by Bedaque et al. [53] was that for certain values of the parameters, the minimally-doubled fermion actions may exhibit non-standard symmetries, that could eliminate relevant operators of the Symanzik effective theory and hence moderate the problem of discrete symmetries breaking.

The expressions for the Dirac operator for Creutz fermions (by which we will mean both fermions related to Creutz's original idea and Borici's generalization) will be discussed in Chapter 2, only in the context of a test of their continuum-limit scaling at tree-level of perturbation theory [55, 56].

1.4.4 Topology on the lattice

The QCD vacuum has a non-trivial topological structure, which has many important implications for hadron properties. For example, we have remarked in Section 1.1 that the mass of the flavour singlet η' meson is related to the topological fluctuations of the QCD vacuum. This is an inherently non-perturbative phenomenon and hence seems to be well-suited to be addressed by Lattice QCD calculations.

Let us start with the field-theoretical definition of the topological charge:

$$Q_{top} = \frac{1}{32\pi^2} \int d^4x \,\epsilon_{\mu\nu\rho\sigma} \operatorname{Tr}\left(F_{\mu\nu}(x), F_{\rho\sigma}(x)\right) \equiv \int d^4x \,q(x), \qquad (1.78)$$

where q(x) is called the topological charge density [57]. Gauge field configurations that have a non-zero and integer topological charge are e.g. superpositions of instantons [58] and anti-instantons, which are classical solutions of the Euclidean field equations.

The topological charge can be related to the number of chiral zero modes of the massless Dirac operator via the Atiyah-Singer index theorem [59]:

$$Q_{top} = Q_{index} \equiv N_{-} - N_{+}, \qquad (1.79)$$

where N_{\pm} denotes the number of zero modes in the positive/negative chirality sector and Q_{index} is called the index of the Dirac operator.

If one wants to compute the topological charge of a given gauge field configuration on the lattice, one can, in principle, use the discretized version of eq. (1.78). However, this can easily lead to non-integer values of the charge [60]. This can be overcome by applying smearing on gauge configurations, e.g. APE smearing [61], which moves the topological charge closer to integer values, but it can also destroy small topological objects and thus lead to incorrect values of the charge.

Such problems are avoided if one uses the index theorem and computes the topological charge as the index of the massless Dirac operator. For this to be possible, one has to employ a Dirac operator that can have chiral zero modes (at any value of the lattice spacing), i.e. eigenstates with zero eigenvalue, which have definite chirality (that is they are also eigenstates of γ_5 with eigenvalue ± 1). This means that the massless Dirac operator must obey (lattice) chiral symmetry, e.g. it can be the overlap Dirac operator, which will be used to compute topological charge in further part of this work.

Since the QCD path integral is symmetric with respect to the sign of the topological charge, we have $\langle Q_{top} \rangle = 0$. However, a non-trivial quantity that one can compute is related to the fluctuations of the topological charge and is called topological susceptibility. In the continuum, it is defined by:

$$\chi_{top} = \int d^4x \langle q(x)q(0)\rangle, \qquad (1.80)$$

which on the lattice becomes

$$\chi_{top} = \frac{\langle Q_{index}^2 \rangle}{V},\tag{1.81}$$

where V is the lattice volume.

It has been mentioned before that the topological susceptibility is related via the Witten-Veneziano formula (1.27) to the mass of the η' meson. Phenomenologically, this formula implies a value of $\chi_{top} \approx (180 \text{ MeV})^4$. It is worth to emphasize that this value agrees rather well with several quenched lattice computations, e.g. [62].

1.5 Observables in Lattice QCD

In this section, we show how one can extract hadron properties from Lattice QCD simulations, concentrating on the quantities of interest for further considerations.

Let us consider a general zero-momentum two-point correlation function of the form $C(t) \equiv \langle 0|O_i(t)\bar{O}_j(0)|0\rangle$, where $O_i(t)$ is some interpolating operator corresponding to the state with quantum numbers of the hadron we want to analyze. Since:

$$O_i(t) = e^{Ht} O_i e^{-Ht}, (1.82)$$

inserting a complete set of energy eigenstates into C(t) yields (we take i = j for simplicity):

$$\langle 0|O_i(t)\bar{O}_i(0)|0\rangle = \sum_n \frac{\langle 0|e^{Ht}O_ie^{-Ht}|n\rangle\langle n|O_i^{\dagger}|0\rangle}{2E_n} =$$
(1.83)
$$= \sum_n \frac{\langle 0|O_i|n\rangle\langle n|O_i^{\dagger}|0\rangle e^{-E_n t}}{2E_n} = \sum_n \frac{|\langle 0|O_i|n\rangle|^2 e^{-E_n t}}{2E_n},$$

where E_n is the energy of the state $n (1/2E_n)$ is a normalization factor for energy eigenstates).

One can immediately see that in the limit of large Euclidean time t, the above expression is dominated by the lowest energy state $|1\rangle$:

$$C(t) \xrightarrow{t \to \infty} \frac{|\langle 0|O_i|1\rangle|^2}{2E_1} e^{-E_1 t}, \qquad (1.84)$$

where E_1 is the energy of this state, i.e. the mass of the lightest particle. In this way, one can extract this mass by fitting (in some interval $t \in [t_{min}, t_{max}]$) the correlation function with an exponential function $A \exp(-m_1 t)$, where A, m_1 are fitting parameters, which provide estimates for the particle mass $E_1 = m_1$ and the matrix element $|\langle 0|O_i|1\rangle|^2 = 2Am_1$. To find the fit interval $[t_{min}, t_{max}]$, one usually computes the so-called effective mass:

$$m_{\rm eff}(t) \equiv \log\left(\frac{C(t)}{C(t+1)}\right)$$
 (1.85)

and plots it to find the plateau region, i.e. the region where the contribution of the excited states is negligible and the effective mass is stable, up to statistical fluctuations.

Since a lattice computation is usually performed with a finite lattice extent T in the temporal direction¹¹ with e.g. periodic boundary conditions in time, the large-time form of the correlation function is modified in the following way:

$$C(t) \xrightarrow{t \text{ large}} \frac{|\langle 0|O_i|1\rangle|^2}{2E_1} (e^{-E_1 t} + e^{-E_1(T-t)}) = \frac{|\langle 0|O_i|1\rangle|^2}{E_1} e^{-E_1 \frac{T}{2}} \cosh E_1 \left(t - \frac{T}{2}\right)$$
(1.86)

In such case, the effective mass at time t can be extracted by solving numerically the equation $C(t)/C(t+1) = \cosh E_1 \left(t - \frac{T}{2}\right)/\cosh E_1 \left(t + 1 - \frac{T}{2}\right)$.

¹¹However, it is sometimes possible to consider lattices with infinite time extent. An example will be given in the next chapter.
We now concentrate on meson correlators in the case of $N_f = 2$ degenerate quarks. The general form of an interpolating operator for mesons is:

$$O_i(\vec{x}, t) = \bar{\psi}(\vec{x}, t)\Gamma^i\psi(\vec{x}, t), \qquad (1.87)$$

where Γ denotes any Dirac matrix (an identity matrix, a gamma matrix or a combination of gamma matrices).

Explicitly introducing Dirac (μ, ν, ρ, σ) and colour (a, b) indices, the correlation function can be written as:

$$C(t) = \sum_{\vec{x}} \langle 0 | \bar{\psi}^{a}_{\mu}(\vec{x}, t) \Gamma^{i}_{\mu\nu} \psi^{a}_{\nu}(\vec{x}, t) \bar{\psi}^{b}_{\rho}(\vec{0}, 0) \Gamma^{j}_{\rho\sigma} \psi^{b}_{\sigma}(\vec{0}, 0) | 0 \rangle, \qquad (1.88)$$

where the sum over \vec{x} Fourier-transforms the correlation function to zero momentum. Contracting fermion fields pairwise into fermion propagators:

$$\langle 0|\psi^a_{\mu}(\vec{x},t)\bar{\psi}^b_{\nu}(0,0)|0\rangle = S^{ab}_{\mu\nu}(\vec{x},t;\vec{0},0), \qquad (1.89)$$

according to Wick's theorem, one finds that there are two possible contractions $(\psi^a_{\nu}(\vec{x},t) \leftrightarrow \bar{\psi}^a_{\mu}(\vec{x},t), \psi^b_{\sigma}(\vec{0},0) \leftrightarrow \bar{\psi}^b_{\rho}(\vec{0},0)$ and $\psi^a_{\nu}(\vec{x},t) \leftrightarrow \bar{\psi}^b_{\rho}(\vec{0},0), \psi^b_{\sigma}(\vec{0},0) \leftrightarrow \bar{\psi}^a_{\mu}(\vec{x},t))$, which lead to:

$$C(t) = \sum_{\vec{x}} \operatorname{Tr}(S(\vec{x}, t; \vec{x}, t) \Gamma^{i}) \operatorname{Tr}(S(\vec{0}, 0; \vec{0}, 0) \Gamma^{j}) + \sum_{\vec{x}} \operatorname{Tr}(S(\vec{x}, t; \vec{0}, 0) \Gamma^{i} S(\vec{0}, 0; \vec{x}, t) \Gamma^{j}), \qquad (1.90)$$

where the trace is over spin and colour.

The first term in the above expression can be represented by a disconnected diagram and contributes only to flavour singlet mesons. Later on, we will be interested only in flavour non-singlet mesons, i.e. ones that are represented by connected diagrams, corresponding to the second term in the above expression. Hence, we now drop the first term and use the γ_5 -hermiticity property of the propagator: $S(\vec{0}, 0; \vec{x}, t) = \gamma_5 S^{\dagger}(\vec{x}, t; \vec{0}, 0)\gamma_5$ to rewrite :

$$C(t) = -\sum_{\vec{x}} \operatorname{Tr}(S(\vec{x}, t; \vec{0}, 0) \Gamma^{i} \gamma_{5} S^{\dagger}(\vec{x}, t; \vec{0}, 0) \gamma_{5} \Gamma^{j}).$$
(1.91)

In this way, to evaluate this correlator it is enough to compute the propagator from a given source (located at the origin $(\vec{0}, 0)$ in the above formula) to all possible sinks (all lattice sites (\vec{x}, t)). Such propagator is called a point-to-all propagator. This can be done by solving the following matrix equation:

$$\hat{D}\psi_{\mu a} = \eta_{\mu a} \tag{1.92}$$

channel	J^{PC}	Γ
pseudoscalar	0^{-+}	$\gamma_5, \gamma_0 \gamma_5$
scalar	0^{++}	$\mathbb{1}, \gamma_0$
vector	1	$\gamma_i, \ \gamma_0 \gamma_i$
axial vector	1^{++}	$\gamma_i\gamma_5$
tensor	1^{+-}	$\gamma_i \gamma_j$

Table 1.1: Meson interpolating operators. J^{PC} classification denotes particle spin J, parity P and charge conjugation C [63].

12 times for each spin-colour combination μa , with a point source $\eta_{\mu a}$, i.e. a vector $(0...010...0)^T$, where the only non-zero number is placed in one of the first 12 entries, corresponding to 12 spin-colour components at lattice site (0, 0, 0, 0).

The solution of this equation:

$$\psi_{\mu a} = \hat{D}^{-1} \eta_{\mu a} \tag{1.93}$$

is the point-to-all quark propagator, denoted by $S(\vec{x}, t; \vec{0}, 0)$ in eq. (1.91), in which the spin-colour indices are suppressed.

Obviously, the Dirac equation (1.92) does not have to be solved with a point source located at the origin. Other choices of the source can be e.g. point sources with random location of the source or stochastic sources. The latter are of special relevance from the point of view of this work and will be discussed later.

Table 1.1 summarizes the most commonly used meson interpolating operators. The names of different channels come from the transformation properties of particles with respect to spin and parity. Here we have assumed that the Γ matrix at the source (denoted by Γ^{j} in eq. (1.91)) and at the sink (Γ_{i}) are the same. However, it is also possible to construct mesons with $\Gamma_{i} \neq \Gamma_{j}$, e.g. $\Gamma_{i} = \gamma_{5}$, $\Gamma_{j} = \gamma_{0}\gamma_{5}$, which belongs to the pseudoscalar channel and hence it can also be used to extract the mass of the pseudoscalar meson.

From the point of view of further considerations, the most important meson channel will be the pseudoscalar one. The PP correlation function $(\Gamma_i = \gamma_5 \equiv P, \Gamma_j = \gamma_5 \equiv P)$ is the simplest correlation function that can be constructed. Putting its gamma matrix structure in eq. (1.91), one obtains:

$$C_{PP}(t) = -\sum_{\vec{x}} \operatorname{Tr}(S(\vec{x}, t; \vec{0}, 0) S^{\dagger}(\vec{x}, t; \vec{0}, 0)).$$
(1.94)

According to eq. (1.83), one can extract the mass of the pseudoscalar meson (pion) m_{π} from the decay of the PP correlator and also the pion decay constant f_{π} from the matrix element $|\langle 0|P|\pi \rangle|$:

$$f_{\pi} = \frac{2m}{m_{\pi}^2} |\langle 0|P|\pi \rangle|, \qquad (1.95)$$

where m is the bare quark mass.

An equivalent definition of the pion decay constant reads:

$$f_{\pi} = \frac{Z_A}{m_{\pi}} |\langle 0|A_0|\pi\rangle|, \qquad (1.96)$$

where Z_A is the renormalization constant of the axial current and $|\langle 0|A_0|\pi\rangle|$ the matrix element of this current.

For the case of overlap fermions, the $\mathcal{O}(a)$ -improved interpolating operators for mesons are constructed in the following way [64]:

$$O_i^{\rm ov}(\vec{x},t) = \bar{\psi}(\vec{x},t)\Gamma^i\left(1 - \frac{a\hat{D}_{\rm ov}(0)}{2}\right)\psi(\vec{x},t) = \frac{1}{1 - \frac{am}{2}}\bar{\psi}(\vec{x},t)\Gamma^i\psi(\vec{x},t),$$
(1.97)

where the last equality holds for correlation functions at non-zero physical distance.

We also give here the expressions for baryon interpolating operators – for the proton p (uud), the neutron n (udd) and the deltas Δ^{++} (uuu), Δ^{+} (uud), Δ^{0} (udd), Δ^{-} (ddd) [65, 66], i.e. the octet and the decuplet baryons that contain only light quarks (up and down, no strange quarks).

$$J_p = \epsilon_{abc} \left(u_a^T C \gamma_5 d_b \right) u_c, \tag{1.98}$$

$$J_n = \epsilon_{abc} \left(d_a^T C \gamma_5 u_b \right) d_c, \tag{1.99}$$

$$J^{\mu}_{\Delta^{++}} = \epsilon_{abc} \left(u^T_a C \gamma^{\mu} u_b \right) u_c, \qquad (1.100)$$

$$J^{\mu}_{\Delta^{+}} = \frac{1}{\sqrt{3}} \epsilon_{abc} \left[2 \left(u^T_a C \gamma^{\mu} d_b \right) u_c + \left(u^T_a C \gamma^{\mu} u_b \right) d_c \right], \qquad (1.101)$$

$$J^{\mu}_{\Delta^0} = \frac{1}{\sqrt{3}} \epsilon_{abc} \left[2 \left(d^T_a C \gamma^{\mu} u_b \right) d_c + \left(d^T_a C \gamma^{\mu} d_b \right) u_c \right], \qquad (1.102)$$

$$J^{\mu}_{\Delta^{-}} = \epsilon_{abc} \left(d^{T}_{a} C \gamma^{\mu} d_{b} \right) d_{c}, \qquad (1.103)$$

where $C = \gamma_4 \gamma_2$ is the charge conjugation matrix.

The two-point correlation function for baryon B reads:

$$C_B(t) = \frac{1}{2} \text{Tr}(1 \pm \gamma_4) \sum_{\vec{x}} \langle J_B(\vec{x}, t) \bar{J}_B(\vec{0}, 0) \rangle, \qquad (1.104)$$

where $(1 \pm \gamma_4)/2$ is the parity projector. For example, the physical proton is described by the correlation function $C_p(t)$ with projection to positive parity and the negative parity projection corresponds to the baryon N^* , mentioned earlier in the context of spontaneous chiral symmetry breaking.

We will be interested in light baryon masses, which are evaluated in an analogous way as in the case of mesons, i.e. from the exponential fall-off of the corresponding correlation function. The effective masses are thus extracted numerically from the ratios of the correlation functions of the form (1.86) at two subsequent timeslices.

We finish by shortly discussing the degeneracies between the light baryons in the case of fermions that preserve isospin symmetry (e.g. overlap) and violate it (e.g. twisted mass). In the overlap case, the proton p and neutron n are degenerate, as well as all delta baryons. For the twisted mass case, the degeneracy is reduced, but still holds between p-n, $\Delta^{++} - \Delta^{-}$ and $\Delta^{+} - \Delta^{0}$, which is due to γ_{5} -hermiticity. Therefore, we will always refer to the proton and neutron as the nucleon N, but we will distinguish between Δ^{++} and Δ^{+} in the twisted mass case.

Chapter 2

Tree-level scaling test

In this chapter we will show the results of tree-level scaling tests of overlap, twisted mass and Creutz fermions and thus explicitly demonstrate the $\mathcal{O}(a)$ improvement in the observables [67, 55, 56]. We will consider three quantities – the pseudoscalar meson mass and decay constant and the pseudoscalar correlation function at a fixed physical distance. We will also analyze the case when the pseudoscalar correlation function is constructed with propagators corresponding to two different fermion discretizations.

2.1 Fermion propagators

The tree-level test of different kinds of lattice fermions consists in analytically evaluating the momentum-space fermion propagator and then using it to construct the relevant correlation function, from which the observables of interest can be extracted.

2.1.1 Overlap fermions

The starting point for the evaluation of the tree-level overlap fermion propagator is the free massless overlap Dirac operator in momentum space¹, which was given by Lüscher [29]:

$$a\hat{D}_{\rm ov}(p) = 1 - \left(1 - ia\gamma_{\mu}\mathring{p}_{\mu} - \frac{a^2}{2}\hat{p}^2\right) \left(1 + \frac{a^4}{2}\sum_{\mu<\nu}\hat{p}_{\mu}^2\hat{p}_{\nu}^2\right)^{-1/2}.$$
 (2.1)

The massive operator is, according to (1.73):

$$a\hat{D}_{\rm ov}(p,m) = \left(1 - \frac{am}{2}\right)a\hat{D}_{\rm ov}(p) + am, \qquad (2.2)$$

¹An explicit derivation of this operator is given in Appendix B.

where m is the bare overlap quark mass.

The expression for the quark propagator in momentum space $S_{ov}(p)$ can be found by computing the inverse of the above Dirac operator $a\hat{D}_{ov}(p,m)$:

$$S^{\rm ov}(p) = \frac{-i(1-\frac{ma}{2})F(p)^{-1/2}\mathring{p}_{\mu}\gamma_{\mu} + \mathcal{M}(p)\mathbb{1}}{(1-\frac{ma}{2})^2F(p)^{-1}\sum_{\mu}\mathring{p}_{\mu}^2 + \mathcal{M}(p)^2}$$
(2.3)

where $\mathbb{1}$ is the identity matrix in Dirac space and we have introduced the functions:

$$F(p) = 1 + \frac{a^4}{2} \sum_{\mu < \nu} \hat{p}_{\mu}^2 \hat{p}_{\nu}^2, \qquad (2.4)$$

$$\mathcal{M}(p) = \frac{1}{a} \left(1 + \frac{ma}{2} - \left(1 - \frac{ma}{2} \right) F(p)^{-1/2} \left(1 - \frac{a^2}{2} \sum_{\mu} \hat{p}_{\mu}^2 \right) \right).$$
(2.5)

The propagator has a matrix structure in Dirac space and for later convenience we write it here in terms of its components:

$$S^{\rm ov}(p) = S^{\rm ov}_{\mu}(p)\gamma_{\mu} + S^{\rm ov}_{0}(p)\mathbb{1}.$$
 (2.6)

2.1.2 Wilson twisted mass fermions

The twisted mass fermion propagator can be found as an inverse of the following Dirac operator in momentum space:

$$\hat{D}_{\rm tm}(p) = i \mathring{p}_{\mu} \gamma_{\mu} \mathbb{1}_{f} + \frac{ar}{2} \hat{p}_{\mu}^{2} \mathbb{1}_{f} + m \mathbb{1}_{f} + i \mu \gamma_{5} \tau_{3}, \qquad (2.7)$$

where the relevant notation has been introduced in Section 1.3.3 and we show here explicitly the matrix structure in flavour space. The first three terms have a trivial structure in flavour space ($\mathbb{1}_f$ is the identity matrix in this space), but the twisted mass term $i\mu\gamma_5\tau_3$ breaks the isospin symmetry between up and down quarks and hence it modifies the expression for the tree-level Wilson propagator in momentum space (1.51) in the following way:

$$\hat{S}_{\rm tm}(p) = \frac{-i\mathring{p}_{\mu}\gamma_{\mu}\mathbb{1}_{f} + (\frac{ar}{2}\sum_{\mu}\hat{p}_{\mu}^{2} + m)\mathbb{1}\mathbb{1}_{f} - i\mu\gamma_{5}\tau_{3}}{\sum_{\mu}\mathring{p}_{\mu}^{2} + (\frac{ar}{2}\sum_{\mu}\hat{p}_{\mu}^{2} + m)^{2} + \mu^{2}}.$$
(2.8)

The propagator has a matrix structure in Dirac and flavour space and we again write it here in terms of its components, explicitly distinguishing between up and down quark propagators:

$$S^{\text{tm,u}}(p) = S^{\text{tm}}_{\mu}(p)\gamma_{\mu} + S^{\text{tm}}_{5}(p)\gamma_{5} + S^{\text{tm}}_{0}(p)\mathbb{1}, \qquad (2.9)$$

$$S^{\text{tm,d}}(p) = S^{\text{tm}}_{\mu}(p)\gamma_{\mu} - S^{\text{tm}}_{5}(p)\gamma_{5} + S^{\text{tm}}_{0}(p)\mathbb{1}, \qquad (2.10)$$

where the propagators of the two flavours differ only in the sign of the γ_5 -matrix coefficient.

To obtain automatic $\mathcal{O}(a)$ -improvement (maximal twist), in the free theory it is enough to set the bare untwisted quark mass m to 0. Such variant of twisted mass fermions is usually referred to as maximally twisted mass (MTM) fermions.

2.1.3 Creutz fermions

It can be shown [55] that the momentum space tree-level Dirac operator for Creutz fermions can be written as:

$$D_{\text{Creutz}}(p) = i \sum_{\mu} \mathring{p}_{\mu} \, \bar{\gamma}_{\mu} - i \, \frac{a}{2} \sum_{\mu} \, \hat{p}_{\mu}^2 \, \bar{\Gamma}_{\mu} + m \, \mathbb{1}.$$
(2.11)

All notation used in this subsection is explained in Appendix B. This yields the following form of the fermion propagator:

$$S_{\text{Creutz}}(p) = \frac{-i \sum_{\mu} \left(\bar{s}_{\mu}(p) + \bar{c}_{\mu}(p) \right) \gamma_{\mu} + m \,\mathbb{1}}{\sum_{\mu} \left(\bar{s}_{\mu}(p) + \bar{c}_{\mu}(p) \right)^{2} + m^{2}}, \qquad (2.12)$$

where we have introduced auxiliary functions $\bar{s}_{\mu}(p)$ and $\bar{c}_{\mu}(p)$.

The tree-level Dirac operator for the variant suggested by Borici is:

$$D_{\text{Borici}}(p) = i \sum_{\mu} \mathring{p}_{\mu} \gamma_{\mu} - i \frac{a}{2} \sum_{\mu} \Gamma_{\mu} \hat{p}_{\mu}^{2} + m \,\mathbb{1}.$$
(2.13)

The corresponding propagator is:

$$S_{\text{Borici}}(p) = \frac{-i\sum_{\mu} G_{\mu}(p)\gamma_{\mu} + m_0 \,\mathbb{1}}{\sum_{\mu} G_{\mu}(p)^2 + m^2},\tag{2.14}$$

where we have again introduced an auxiliary function $G_{\mu}(p)$.

The matrix structure of both Creutz and Borici fermions is of the same form as in the case of overlap (2.6).

2.2 Observables

The tree-level test of different kinds of fermions will consist in computing three observables – the pseudoscalar correlation function at a fixed physical

distance, the pseudoscalar meson mass and decay constant. All of these quantities can be calculated from the pseudoscalar correlation function, given by eq. (1.94). Here we rewrite it for convenience, dropping the conventional minus sign:

$$C_{PP}(t) = \sum_{\vec{x}} \operatorname{Tr}(S(\vec{x}, t; \vec{0}, 0) \, S^{\dagger}(\vec{x}, t; \vec{0}, 0)).$$
(2.15)

The derivation of the final expression for the pseudoscalar correlation function in terms of momentum space propagator components $S_{\xi}(p)$, defined by decompositions of the form (2.6) or (2.9), can be found in Appendix B and gives:

$$C_{PP}(t) = \frac{N_c N_d}{N^3 N_4^2} \sum_{\vec{p}} \sum_{p_4, p_4'} \sum_{\xi=0}^{4 \text{ or } 5} S_{\xi}(\vec{p}, p_4) S_{\xi}^*(\vec{p}, p_4') e^{i(p_4 - p_4')t}, \qquad (2.16)$$

where N_d is the number of Dirac components (i.e. the dimension of spacetime) and N_c is the number of colours (in the free case the structure in colour space is trivial). The index ξ runs from 0 to 4 in the case of overlap and Creutz fermions or from 0 to 5 in the case of Wilson twisted mass fermions.

The above expression can be computed by explicitly evaluating the sum over discrete momenta. On the lattice, the possible values of momenta are (for periodic boundary conditions):

$$p_i = \frac{2\pi}{a} \frac{n_i}{N}, \qquad p_4 = \frac{2\pi}{a} \frac{n_4}{N_4},$$
 (2.17)

where $n_i = 0, 1, ..., N - 1, n_4 = 0, 1, ..., N_4 - 1$. The box length is in the spatial directions L = aN and in the temporal direction $L_4 = aN_4$.

At large enough times, the above correlation function has only the contribution from the lightest particle, i.e. it is of the form (1.84):

$$C_{PP}(t) \stackrel{t \to \infty}{=} \frac{|\langle 0|P|\pi \rangle|^2 e^{-m_{\pi}t}}{2m_{\pi}}, \qquad (2.18)$$

where we call the lightest pseudoscalar meson the pion and by m_{π} we denote its mass. However, since we are only considering here the tree-level quantities, the name "pion" does not correspond to the physical QCD pion, but it is only an abbreviation for the pseudoscalar meson.

The pion mass can be extracted from formula (1.85). In the free-field case it is practical to consider lattices with very large time extent² and hence t

 $^{^{2}}$ In the case of Wilson twisted mass fermions it is even possible to analytically go to infinite time extent [68, 69].

can be taken so large that no contribution from the excited states is present, up to machine precision. Therefore, one can obtain very precise values of the pion mass.

The pion decay constant can be extracted from expression (1.95), substituting the matrix element $\langle 0|P|\pi\rangle$ obtained from eq. (2.18). This yields:

$$f_{\pi} \stackrel{t \to \infty}{=} \frac{2m}{m_{\pi}^{3/2}} \sqrt{2C_{PP}(t)} e^{\frac{1}{2}m_{\pi}t}.$$
 (2.19)

The value of f_{π} does not depend on the timeslice t at which the above equation is evaluated, i.e. the product $\sqrt{2C_{PP}(t)}e^{\frac{1}{2}m_{\pi}t}$ is time-independent, provided that it is calculated in the plateau region.

2.3 Test setup

We would like to perform a fixed-volume, continuum limit scaling test of the three observables of interest – the pseudoscalar correlator, mass and decay constant. First, we have to define what is actually meant by fixed volume and continuum limit in the context of a free theory, which can not have assigned physically meaningful units.

By fixed volume, we will mean that the product of the box length in lattice units (N) and quark mass (m) Nm = const. Since N = L/a, simultaneously increasing the number of lattice sites and decreasing the quark mass in lattice units (such that Nm is held fixed) corresponds to decreasing the lattice spacing a. In this way, the continuum limit is equivalent to the infinite volume limit. However, this is special to the tree-level case – in full QCD these two limits are not equivalent.

For the test we will fix Nm (or $N\mu$ in the case of twisted mass fermions) to 0.5 and change N from 4 to 64. The temporal direction will have a much larger extent – in order not to have any contaminations from excited states we take $N_4 = 64N$ and extract observables at a fixed physical distance t = 4N. Thus, the largest considered lattice is $64^3 \times 4096$. The corresponding parameters for each lattice size are presented in Table 2.1.

2.4 Comparison of overlap, twisted mass and Creutz fermions

In this section, we present the results of a tree-level scaling test of different kinds of fermions:

N	N_4	$m ext{ or } \mu$	t = 4N
4	256	0.125000	16
8	512	0.062500	32
12	768	0.041667	48
16	1024	0.031250	64
20	1280	0.025000	80
24	1536	0.020833	96
28	1792	0.017857	112
32	2048	0.015625	128
36	2304	0.013889	144
40	2560	0.012500	160
44	2816	0.011364	176
48	3072	0.010417	192
52	3328	0.009615	208
56	3584	0.008929	224
64	4096	0.007813	256

Table 2.1: Simulation parameters for the tree-level scaling test.

- overlap fermions,
- Wilson twisted mass fermions at maximal twist (MTM),
- Creutz fermions with $C = 3/\sqrt{10}$,
- Creutz fermions with $C = 3/\sqrt{14}$,
- Borici fermions.

First, we consider the pion mass, which is depicted in Fig. 2.1. The points in the plot show the result extracted from the correlation function (2.16) and the corresponding lines are fits of the following formula:

$$Nm_{\pi} = a_m + b_m \frac{1}{N^2} + c_m \frac{1}{N^4}.$$
 (2.20)

In all cases, we find the expected behaviour – i.e. $\mathcal{O}(a^2)$ ($\mathcal{O}(1/N^2)$) scaling violations. It is worth to emphasize here again that in the case of overlap and Creutz fermions this results directly from chiral symmetry and in the case of twisted mass fermions from automatic $\mathcal{O}(a)$ -improvement, which is achieved only at maximal twist, i.e. for bare untwisted quark mass set to 0.



Figure 2.1: Continuum limit scaling of the pion mass for overlap, twisted mass and Creutz fermions.

fermion	a_m	b_m	c_m
MTM	1.0	-0.0104167	0.000296044
Overlap	1.0	0.0208333	0.000783869
Borici	1.0	-0.0494792	0.00564291
Creutz $C = 3/\sqrt{10}$	1.0	-0.0078125	-0.0101045
Creutz $C = 3/\sqrt{14}$	1.0	-0.0488282	0.00282578

Table 2.2: Fitting coefficients for the pion mass - eq. (2.20).

The continuum limit (the coefficient a_m) is the same for all kinds of fermions (and equal to the expected value $Nm_{\pi} = 2Nm$ (overlap, Creutz fermions) and $Nm_{\pi} = 2N\mu$ (twisted mass fermions)). This is a necessary condition that each fermion action has to fulfill – the continuum limit of all physical observables has to be the same. This is ensured if the continuum limit of the fermion propagator for the discretization of interest is equal to the



Figure 2.2: Continuum limit scaling of the pion decay constant for overlap, twisted mass and Creutz fermions.

continuum fermion propagator. In other words, various fermion discretizations differ in the way the lattice artefacts are introduced.

It is also interesting to compare the magnitude of $\mathcal{O}(1/N^2)$ discretization errors (coefficient b_m – Tab. 2.2) for this observable. They are the largest for Borici and Creutz ($C = 3/\sqrt{14}$) fermions, around twice smaller for overlap fermions, a further factor of two smaller for twisted mass fermions and the smallest for Creutz ($C = 3/\sqrt{10}$) fermions. Moreover, computations for different fixed values of Nm confirm that this behaviour is universal for a wide range of values of Nm.

Furthermore, the value of the coefficient c_m that characterizes the $\mathcal{O}(1/N^4)$ discretization errors is in general smaller than b_m , indicating that the corrections to the $\mathcal{O}(1/N^2)$ behaviour are small. However, there are some exceptions to this rule (e.g. the Creutz $C = 3/\sqrt{10}$ case), where c_m is slightly larger than b_m , but still rather small.

As the second observable, we consider the pion decay constant, shown in Fig. 2.2. The points in the plot show the result computed from eq. (2.19)

fermion	a_f	b_f	c_f
MTM	3.4641	0.0541266	-0.000811859
Overlap	3.4641	0.108253	0.00553143
Borici	3.4641	-0.0676584	-0.00527683
Creutz $C = 3/\sqrt{10}$	3.4641	0.293186	-0.0746106
Creutz $C = 3/\sqrt{14}$	3.4641	-0.00789431	-0.0379067

Table 2.3: Fitting coefficients for the pion decay constant – eq. (2.21).

and the corresponding lines are fits of the following formula:

$$Nf_{\pi} = a_f + b_f \frac{1}{N^2} + c_f \frac{1}{N^4}.$$
 (2.21)

In all cases, we observe again $\mathcal{O}(1/N^2)$ leading discretization errors. However, the coefficients b_f (Tab. 2.3) lead to different conclusions regarding the size of these effects for the kinds of fermions under analysis. The largest coefficient is observed for Creutz ($C = 3/\sqrt{10}$) fermions, which had the smallest discretization error in the pion mass (b_m). Accordingly, Creutz ($C = 3/\sqrt{14}$) fermions had the second largest coefficient b_m , but the coefficient b_f is the smallest among all discretizations.

Generalizing, this means that the size of discretization effects depends on the choice of the observable, i.e. that small $\mathcal{O}(a^2)$ effects in one observable do not mean that for other observables one can expect the same.

Table 2.4: Fitting coefficients for the pseudoscalar correlation function at a fixed physical distance t/N = 4 - eq. (2.22).

fermion	a_C	b_C	c_C
MTM	0.109894	0.00457891	-0.0000333779
Overlap	0.109894	0.00457891	0.000181293
Borici	0.109894	0.00114472	-0.0013941
Creutz $C = 3/\sqrt{10}$	0.109894	0.0194604	-0.00269918
Creutz $C = 3/\sqrt{14}$	0.109894	0.00486504	-0.00300215

This is confirmed by the result for the third observable – the correlation function at a fixed physical distance t = 4N, shown in Fig. 2.3. Again, the points in the plot correspond to the correlation function computed from eq.



Figure 2.3: Continuum limit scaling of the pseudoscalar correlation function at a fixed physical distance t/N = 4 for overlap, twisted mass and Creutz fermions.

(2.16) and the lines are fits of the following formula:

$$N^{3}C_{PP}(t=4N) = a_{C} + b_{C}\frac{1}{N^{2}} + c_{C}\frac{1}{N^{4}}.$$
(2.22)

The coefficient b_C is again the largest for Creutz $(C = 3/\sqrt{10})$ fermions and the smallest for Borici fermions. As a coincidence, b_C for overlap and twisted mass fermions is the same, which is not true for other values of Nm(for Nm < 0.5 the value for overlap is larger, for Nm > 0.5 it is smaller).

Other interesting quantities to compute are the mixed correlators. In the meson case they correspond to taking the two quarks discretized with different actions. This is relevant from the point of view of mixed action simulations in the interacting theory, where it is possible to build a meson from two valence quarks, two sea quarks or one valence and one sea quark. If one imposes a matching condition that the valence-valence pion and the sea-sea pion have the same mass, the mixed valence-sea pion in general has a different mass and the obtained mass difference quantifies unitarity violations



Figure 2.4: Continuum limit scaling of the pion mass for overlap-overlap, MTM-MTM and overlap-MTM quarks.

in the mixed action setup. It is, however, worth to emphasize that this effect is only a lattice artefact with no physical significance.

The way to construct the mixed pion at tree-level is to use two different propagators in formula (2.16) for the pseudoscalar correlation function. We will show an example of overlap-MTM mixed correlator, i.e. we will take one of the propagators to be the overlap fermion propagator and the other one to be the MTM fermion propagator. The results of the scaling test for such mixed case (with Nm = 0.5 and $N\mu = 0.5$) are shown in Figs. 2.4, 2.5 and 2.6.

The mixed pion mass, decay constant and correlator at a fixed physical distance all show leading $\mathcal{O}(a^2)$ cut-off effects. Furthermore, in all cases, the mixed meson line is situated exactly halfway between the overlap and MTM lines, which implies that the fitting coefficients b_m , b_f and b_C are always arithmetic averages of the corresponding coefficients for the overlap and the MTM case. The consequence of this is also that at tree-level it is not possible to observe a splitting between the mixed pion mass and the overlap/MTM pion masses, if the latter are matched. This results from the fact that at



Figure 2.5: Continuum limit scaling of the pion decay constant for overlapoverlap, MTM-MTM and overlap-MTM quarks.

tree-level there are no unitarity violations – their source is a different Dirac operator used to generate the gauge field configurations and a different one for the valence quarks and in the free case such situation does not occur.

To summarize, there are no definite conclusions from the tree-level test. It can not be deduced that one type of fermions exhibits the smallest or the largest discretization errors – this depends on the observable and of course in the interacting theory one should expect the same. A general conclusion from the test is that all fermions exhibit $\mathcal{O}(a^2)$ scaling violations. This again should hold in the interacting theory, but it has to be explicitly tested. The results of such test for overlap fermions will be presented in Chapter 4.

2.5 Matching twisted mass and overlap fermions

In this section, we will investigate the effects of matching of twisted mass and overlap fermions. The motivation for this test is the following. In Chapter 4, we will analyze a mixed action setup of overlap valence quarks and twisted



Figure 2.6: Continuum limit scaling of the pseudoscalar correlation function at a fixed physical distance t = 4N for overlap-overlap, MTM-MTM and overlap-MTM quarks.

mass sea quarks, i.e. gauge field configurations will be generated with the twisted mass action, but the propagators will be computed with overlap valence quarks (and also with twisted mass valence quarks for comparison). The reason for considering such setup will be discussed more thoroughly in Chapter 4 and is related to the computational cost of generating gauge field configurations with chirally symmetric actions. Therefore, it will be useful to investigate the effects that emerge in such setup also at tree-level.

In a mixed action approach, an important condition that has to be realized to minimize unitarity violations that necessarily arise in such formulation, is the matching condition between the quark masses. This can be done in a number of ways. We mention here two of them, postponing a full discussion until Chapter 4:

• matching of the pion mass – one finds a bare valence quark mass m^{val} , which leads to the same pion mass as the mass of a pion constructed from two sea quarks of mass m^{sea} : $m_{\pi}^{val-val} = m_{\pi}^{sea-sea}$,

• matching of renormalized quark masses: $m_{ren}^{val} = m_{ren}^{sea}$.

In the free case, there is no need of renormalization and hence the second condition is trivial. However, a general situation is that this matching can be done only up to $\mathcal{O}(a^2)$ effects. Hence, at tree-level we can investigate the effects of such mismatch between the quark masses.

Regarding the first condition, we will find the bare overlap quark mass that leads to the same pion mass as some specified MTM quark mass and test whether the two other observables – the pion decay constant and the pseudoscalar correlator at a fixed physical distance are also matched.

2.5.1 Unmatched quark masses

To investigate the effect of non-ideal matching between the quark masses, we impose the following setup. The MTM quark mass is fixed to $N\mu = 0.5$, but in the overlap quark mass we allow for an $\mathcal{O}(a^2)$ deviation from the twisted mass value, setting:

$$Nm = 0.5 - v/N^2. (2.23)$$

The mismatch parameter v will be varied from v = 0 to v = 4.

The results of the test are shown in Figs. 2.7 and 2.8. Both plots show that the leading $\mathcal{O}(1/N^2)$ cut-off effects can become very large if there is a substantial mismatch in quark masses (for large mismatch parameter v). Moreover, even the $\mathcal{O}(1/N^4)$ effects can become sizable, which can lead to a wrong continuum limit value in the pion mass and decay constant, if the fit includes too small lattices (i.e. all lattices from N = 4 to N = 64) – such fit corresponds to dashed lines on the plots. To get the correct continuum limit value, the fit has to be performed for large enough lattices. However, for the analyzed setup this becomes important only for v = 4 and even there it is enough to exclude the point N = 4 from the fit to obtain the right value in the continuum. If the quark masses are only slightly mismatched ($v \leq 2$), even a full ($N \in [4, 64]$) fit leads to the correct continuum limit. It is worth to emphasize that the effect that we observe at tree-level is rather small (the continuum limit is wrong by only ≈ 0.1 %), but it can be severely enhanced in the interacting theory.

A similar effect can occur if it is not possible to go to large enough lattices, i.e. if the fit can be performed e.g. only in the interval $N \in [16, 24]$. Once again, such effect can be of practical importance in the simulations of the interacting theory, where it might not be possible to go to very large lattices. However, for the setup analyzed here such effect is very small in comparison to the effect discussed above and hence it is not shown in a plot.



Figure 2.7: Continuum limit scaling of the pion mass at a fixed physical distance t/N = 4 for twisted mass and overlap fermions. The quark masses are matched up to $\mathcal{O}(1/N^2)$. The lower plot is a zoom of the upper one for large values of N.



Figure 2.8: Continuum limit scaling of the pion decay constant at a fixed physical distance t/N = 4 for twisted mass and overlap fermions. The quark masses are matched up to $\mathcal{O}(1/N^2)$. The lower plot is a zoom of the upper one for large values of N.



Figure 2.9: The matching of MTM and overlap quark masses.

2.5.2 Effects in the case of matched pion masses

In this subsection, we will investigate the other matching condition of matched pion masses. We will consider the case of N = 16 and fix the twisted quark mass to $N\mu = 0.5$.

Since the magnitude of $\mathcal{O}(a^2)$ effects is in general different for different fermion discretizations, the condition of equal pion masses $Nm_{\pi}^{\text{MTM}} = Nm_{\pi}^{\text{overlap}}$ does not have to correspond to equal quark masses $Nm = N\mu$. This is shown in Fig. 2.9, where the dependence of the (overlap) pion mass on the overlap quark mass Nm is depicted. The value of $Nm \approx 0.49994$ leads to the same pion mass as the value $N\mu = 0.5$ in the twisted mass case.

However, the matching of one observable does not mean that other observables have to be matched as well. This is a direct consequence of the fact that the discretization effects in different observables are in general different. Figs. 2.10 and 2.11 show that at the matching point $(Nm_{\pi}^{\text{MTM}} = Nm_{\pi}^{\text{overlap}})$, the pion decay constant and the pion correlation function at a fixed physical distance t = 4N are not matched. However, their difference is of $\mathcal{O}(a^2)$, which can be clearly observed in Figs. 2.12 and 2.13. Moreover, if the pion masses are matched, the quark mass is indeed matched only up to $\mathcal{O}(a^2)$ (Fig. 2.14).

This is a general situation that one can expect at the matching point in the



Figure 2.10: The mismatch between the MTM and overlap pion decay constants at the matching point $Nm_{\pi}^{\text{MTM}} = Nm_{\pi}^{\text{overlap}}$.



Figure 2.11: The mismatch between the MTM and overlap correlation functions (at a fixed physical distance) at the matching point $Nm_{\pi}^{\text{MTM}} = Nm_{\pi}^{\text{overlap}}$.



Figure 2.12: The difference between the MTM and overlap pion decay constants at the matching point $Nm_{\pi}^{\text{MTM}} = Nm_{\pi}^{\text{overlap}}$, as a function of $1/N^2$.

interacting theory. Regardless of the implemented matching condition, other observables can only be matched up to $\mathcal{O}(a^2)$ discretization effects. However, since all valid fermion discretizations must lead to the same continuum limit, the matching point differences in all observables that have a well-defined continuum limit must decrease when one moves towards this limit.

In Chapter 4, when we consider a mixed setup of overlap valence quarks and twisted mass sea quarks, we will use the same matching condition as in this subsection. Moreover, the matching of pion masses can never be exact in the interacting theory, since the relevant quantities are always extracted with some statistical error. Therefore, the matching is in general realized up to $\mathcal{O}(a^2)$ effects, as was the case in the previous subsection. Hence, at the matching point we have $\mathcal{O}(a^2)$ effects originating from non-ideal matching and additional $\mathcal{O}(a^2)$ effects in other observables computed at the matching point. Provided that the former are not too large (i.e. the counterpart of the mismatch parameter v is small enough), it should be possible to extract the right continuum limit for both discretizations. This will be explicitly tested in the interacting theory, where all the effects are obviously much more complex than in the case analyzed in this section.



Figure 2.13: The difference between the MTM and overlap correlation functions (at a fixed physical distance) at the matching point $Nm_{\pi}^{\text{MTM}} = Nm_{\pi}^{\text{overlap}}$, as a function of $1/N^2$.



Figure 2.14: The difference between the MTM and overlap quark mass at the matching point $Nm_{\pi}^{\text{MTM}} = Nm_{\pi}^{\text{overlap}}$, as a function of $1/N^2$.

Chapter 3

Algorithmic and technical details

3.1 Simulating QCD

In this section, we briefly outline the idea behind a Lattice QCD simulation (with any kind of fermions) and describe the most widely used algorithm of generating gauge field configurations – the Hybrid Monte Carlo algorithm.

3.1.1 General idea

As already stated in Section 1.1, computing any observable in a Lattice QCD simulation consists in approximately evaluating an integral of the form (1.16) by a Monte Carlo method. This is a high-dimensional integral over all possible gauge field and fermion field configurations. Fortunately, the dependence on the Grassmann-valued fermion fields can always be eliminated, leaving an integral over only the gauge fields, weighted by the Boltzmann factor $e^{-S_{eff}}$, where S_{eff} is some effective action dependent on the algorithm used. Moreover, for a majority of gauge field configurations the action is very large and hence their weight is negligibly small. Therefore, one should perform importance sampling, i.e. use an algorithm that effectively chooses configurations that have a high Boltzmann factor. Thus, having a large number (of the order of several thousand) of such configurations, one can compute the Monte Carlo average of an observable \mathcal{O} , which we will denote by $\overline{\mathcal{O}}$:

$$\bar{\mathcal{O}} = \frac{1}{N} \sum_{i=1}^{N} \mathcal{O}[U_i], \qquad (3.1)$$

where $\mathcal{O}[U_i]$ denotes the observable \mathcal{O} computed in a background gauge field U_i belonging to the Markov chain of generated configurations. If the simulation is performed correctly, in the limit $N \to \infty$ the Monte Carlo average $\bar{\mathcal{O}}$

will correspond to the actual ensemble average $\langle \mathcal{O} \rangle$. The conditions that have to be satisfied in order to obtain the correct average are measure preservation and detailed balance. The latter reads:

$$e^{-S[U]}P(U \to U') = e^{-S[U']}P(U' \to U),$$
(3.2)

where $P(U \to U')$ denotes the probability of transition from configuration U to U'.

Let us now consider the partition function (1.17). After integrating out the fermion fields, one obtains:

$$Z = \int DU \ e^{-S_{gauge}[U]} \prod_{i=1}^{N_f} \det(\hat{D}_i[U]), \qquad (3.3)$$

where $\det(\hat{D}_i[U])$ is the determinant of the Dirac operator matrix for fermion flavour *i*. Such form of the integrand implies that the probability distribution that has to be simulated depends on a highly non-local fermion determinant. The cost of calculating this determinant(s) is by far the highest cost in a Monte Carlo simulation. However, the first approximation to the partition function could be to neglect the fermion determinant, i.e. set it to a constant. Such approximation is called the quenched approximation and it physically consists in neglecting the fermion loops. As such, it is very crude. Still, for many years it was very much used in simulations, since the computational cost related to the determinant was just too high for the generation of computers then available.

However, the computational power has been increasing for many years and presently it is possible to perform fully dynamical simulations (i.e. with the determinant included¹), which is also due to many algorithmic improvements. In the next subsection we describe the algorithm of choice for most simulations with dynamical fermions – the Hybrid Monte Carlo algorithm.

3.1.2 Hybrid Monte Carlo

The Hybrid Monte Carlo (HMC) algorithm was originally introduced by Duane, Kennedy, Pendleton and Roweth [70]. It combines a molecular dynamics update of gauge fields with a Metropolis accept/reject step. Here we outline the basic steps that need to be performed in an HMC simulation [71].

Given the action to simulate S(U), first one constructs the Hamiltonian:

$$\mathcal{H}(\pi, U) = \frac{1}{2} \sum_{x,\mu} \pi^a_{x,\mu} \pi^a_{x,\mu} + S(U), \qquad (3.4)$$

¹The determinant is not computed explicitly – one usually represents it in an indirect way, e.g. by a set of pseudofermion fields, to be discussed later.

where $\pi^{a}_{x,\mu}$ is a component of a momentum field:

$$\pi_{x,\mu} = \pi^a_{x,\mu} t^a \tag{3.5}$$

conjugate to each lattice link $U_{x,\mu}$. In this way, the integral one wants to evaluate: $\int DU \mathcal{O}[U] \exp(-S(U))$ can be written in the equivalent form: $\int DUD\pi \mathcal{O}[U] \exp(-\mathcal{H}(\pi, U))$, since the additional integration over momentum fields π yields just a Gaussian integral and hence produces a constant factor.

Thus, one obtains a classical Hamiltonian system. The evolution of this system in a fictitious Monte Carlo time τ can be calculated from the Hamilton's equations:

$$\dot{\pi}_{x,\mu} = -F_{x,\mu},\tag{3.6}$$

$$U_{x,\mu} = \pi_{x,\mu} U_{x,\mu}, \tag{3.7}$$

where the dot denotes differentiation with respect to the fictitious time τ and the force $F_{x,\mu}$ is given by²:

$$F_{x,\mu} = \frac{\partial S(U)}{\partial U_{x,\mu}}.$$
(3.8)

Solving the above system of differential equations, one obtains a trajectory in phase space, i.e. the values of $U_{x,\mu}(\tau)$ and $\pi_{x,\mu}(\tau)$ for every value of τ .

The steps in the HMC algorithm are the following:

- 1. Randomly generate the initial $(\tau = 0)$ momentum field $\pi_{x,\mu}(0)$ according to the distribution $\exp(-\frac{1}{2}\sum_{x,\mu}\pi^a_{x,\mu}\pi^a_{x,\mu})$.
- 2. Numerically integrate (e.g. by the so-called leap-frog algorithm) Hamilton's differential equations (3.6)-(3.7) to obtain $U_{x,\mu}(\tau)$ and $\pi_{x,\mu}(\tau)$ from their initial values $U_{x,\mu}(0)$ and $\pi_{x,\mu}(0)$, respectively. By construction, such evolution preserves the value of the Hamiltonian up to a numerical integration error.
- 3. Accept the new configuration with probability:

$$P = \min\left(1, e^{-\Delta \mathcal{H}(\tau)}\right),\tag{3.9}$$

where $\Delta \mathcal{H}(\tau) = \mathcal{H}(\pi(\tau), U(\tau)) - \mathcal{H}(\pi(0), U(0))$ is in general non-zero, which is due only to the numerical integration error. If the configuration is rejected, then $U(\tau) = U(0)$, i.e. the initial configuration does not change.

 $^{^{2}}$ In (3.8) we use symbolic notation for a derivative of the action with respect to a link variable. The derivative with respect to an SU(3) element can be formally defined as $\frac{\partial S(\exp(\omega^a(x,\mu)t^a)U(x,\mu))}{\partial \omega^a(x,\mu)}\Big|$

 $[|]_{\omega^a(x,\mu)=0}$

4. Repeat steps 2-3 to obtain as many trajectories (gauge field configurations) as is desired. The initial values of the variables U and π for step 2 of trajectory N are the values of these variables at the end of step 3 of the preceding trajectory N-1, i.e.: $U^{\text{trajectory } N}(0) = U^{\text{trajectory } N-1}(\tau)$, $\pi^{\text{trajectory } N}(0) = \pi^{\text{trajectory } N-1}(\tau)$.

The above algorithm could in principle be used to simulate QCD with dynamical quarks. However, to make such simulations practical, one has to overcome the computational problem of effectively calculating the fermion determinant. This is usually done with the pseudo-fermion method, which consists in replacing the fermion fields by auxiliary bosonic fields³ and expressing the determinant as a Gaussian integral over these fields. The part of the force coming from the pseudo-fermion fields is the most intensive part of the simulation. Hence, dynamical simulations are by a large factor more computationally expensive than pure gauge simulations, where the pseudofermion field is not needed.

We have outlined here the general idea of the Hybrid Monte Carlo algorithm. However, in practice one can greatly reduce the computer resources that are needed by implementing the significant refinements of this algorithm that were proposed during the last ca. 10 years. Some of them are shortly discussed in Appendix C.

With these improvements, Lattice QCD is approaching the possibility of large-scale simulations with physical quark masses. Only around 10 years ago, it seemed that to reach the physical point one would need resources of the order of several PetaFlop-years to generate an ensemble of a few hundred independent dynamical gauge field configurations with typical parameters for the lattice spacing (≈ 0.08 fm) and physical box length (≈ 2.5 fm). This was illustrated by the famous "Berlin Wall" plot [72]. Around 2010 the computational cost seems to be some 3-4 orders of magnitude smaller with the aforementioned refinements [71]. Moreover, work on the algorithms is still in progress and hence further reduction of the cost is possible. Nevertheless, the computer resources needed to simulate QCD are still huge.

3.2 Computation of the overlap operator

We will now concentrate on technical details of simulations with overlap fermions as valence quarks.

³The auxiliary fields carry the same indices as the fermion fields, but they obey bosonic statistics. Hence, they are called pseudo-fermion fields.

The matrix $(A^{\dagger}A)^{-1/2}$ in the definition of the overlap operator is the source of many problems, including technical ones. It is a non-trivial task to compute this matrix in the first place and it is obviously needed to construct the overlap Dirac operator. The strategy that one usually follows is to construct an approximation of $(A^{\dagger}A)^{-1/2}$. There are several ways to do this, including polynomial approximations, Lanczos based methods and partial fraction expansion. An overview of these methods is provided e.g. in [73, 74]. Here we restrict ourselves to the description of the method relevant from the point of view of this work, i.e. the Chebyshev polynomial approximation method. The advantages of using this approximation are the well-controlled exponential fit accuracy and the possibility of having numerically very stable recursion relations, which allows for high degrees of the polynomial.

The operator $A^{\dagger}A$ depends on the gauge field configuration and therefore this approximation has to be performed separately for each configuration.

The Chebyshev polynomials $T_j(x)$ are solutions to the differential equation $(1-x^2)y''-xy'+j^2y=0$ for non-negative integer j and can be expressed recursively as: $T_0(x) = 1$, $T_1(x) = x$, $T_j(x) = 2xT_{j-1}(x) - T_{j-2}(x)$.

The Chebyshev polynomial approximation to the function $(A^{\dagger}A)^{-1/2}$ is a polynomial $P_n(A^{\dagger}A)$ of degree n [11]:

$$\frac{1}{\sqrt{A^{\dagger}A}} \approx P_n(A^{\dagger}A) = \sum_{j=0}^n c_j T_j(X), \qquad (3.10)$$

where:

$$X = \frac{2A^{\dagger}A - (\lambda_{min} + \lambda_{max})\mathbb{1}}{\lambda_{max} - \lambda_{min}},$$
(3.11)

 λ_{min} and λ_{max} are the smallest and largest eigenvalue of $A^{\dagger}A$, respectively, and the coefficients c_i are calculated from the formula:

$$c_j = \frac{\pi}{n} \sum_{k=1}^n f(x_k) T_j(x_k), \qquad (3.12)$$

where:

$$f(x_k) = \left(\frac{1}{2}(\lambda_{\min} + \lambda_{\max}) + \frac{x_k}{2}(\lambda_{\max} - \lambda_{\min})\right)^{-1/2}$$
(3.13)

and

$$x_k = \cos\left(\left(k - \frac{1}{2}\right)\frac{\pi}{n}\right). \tag{3.14}$$

Any eigenvalue $\lambda \in [\lambda_{min}, \lambda_{max}]$ of the matrix $A^{\dagger}A$ satisfies the following condition:

$$\frac{1}{\sqrt{\lambda}} - P_n(\lambda) = \mathcal{O}(e^{-2(n+1)\sqrt{\lambda_{min}/\lambda_{max}}}).$$
(3.15)

This means that the approximation error decreases exponentially fast with increasing polynomial degree and depends on the condition number of the matrix $A^{\dagger}A$, i.e. on the ratio $\lambda_{max}/\lambda_{min}$. In other words, to achieve the desired precision, one has to choose a polynomial degree which is proportional to the condition number of $A^{\dagger}A$. Since the eigenvalues of the Wilson operator can go arbitrarily low, the necessary degree of polynomial can easily become prohibitively high. Therefore, one usually supplements the Chebyshev approximation method with eigenvalue deflation for the operator $A^{\dagger}A$. This will be discussed in the next section.

In practical simulations, one usually wants to ensure that the Ginsparg-Wilson relation (for massless overlap Dirac operator) is satisfied with a very high precision – usually machine precision. To ensure this, the following condition should be satisfied [76]:

$$||R - A^{\dagger}A(P_n(A^{\dagger}A))^2 R||^2 / ||R||^2 < \xi, \qquad (3.16)$$

where R is a random vector and ξ has to be a very small number, typically set to 10^{-16} to achieve a compromise between good quality of approximation and its cost⁴.

3.3 Reducing the condition number of $A^{\dagger}A$

We now discuss the possibilities of reducing the condition number of the operator $A^{\dagger}A$.

3.3.1 Eigenvalue deflation

The eigenvalues of $A^{\dagger}A$ are bounded from above and hence the ones that can be responsible for large condition numbers are the lowest eigenvalues. This is illustrated in Fig. 3.1, which shows the cases of:

• fixed lattice spacing $a \approx 0.079$ fm, variable physical size of the lattice (upper plots),

⁴Such level of precision corresponds to "double" precision in the C programming language. Increasing precision is still possible with specialized libraries, e.g. GNU Multiple Precision Arithmetic Library, but it would lead to a significant increase in computational cost.



Figure 3.1: 5 lowest eigenvalues and the highest eigenvalue for various gauge field ensembles. The lattice spacing is $a \approx 0.079$ fm ($\beta = 3.9$) for upper plots, $a \approx 0.063$ fm ($\beta = 4.05$) for bottom left and $a \approx 0.051$ fm ($\beta = 4.2$) for bottom right plot.

• (approximately) fixed physical size of the lattice with box length $L \approx 1.3$ fm, variable lattice spacing (upper left and bottom plots).

The former shows that increasing the volume at a fixed lattice spacing increases the probability of having very low eigenvalues – hence the condition number of $A^{\dagger}A$ increases with the volume. Decreasing the lattice spacing (going from $\beta = 3.9$ towards $\beta = 4.2$) causes the spectrum of the lowest eigenvalues to move up (eigenvalues in lattice units tend to become higher), which results from the fact that the gauge field configurations become smoother. Therefore, the condition number of $A^{\dagger}A$ decreases with decreasing lattice spacing.

As can be seen on the plots, the eigenvalues of $A^{\dagger}A$ can go very low and hence the condition numbers of $A^{\dagger}A$ can be very large, thus leading to very high degrees of Chebyshev polynomials (necessary to satisfy the Ginsparg-Wilson relation up to desired precision), which can typically reach 1000-2000 or even more, depending on the gauge field configuration under analysis and in general on the parameters (e.g. lattice volume, lattice spacing).

Since large condition numbers are caused by the lowest eigenvalues, it is profitable to compute a certain number N_{ev} (out of the total number N_{total}) of eigenmodes of $A^{\dagger}A$ and split $(A^{\dagger}A)^{-1/2}$ into two parts:

$$\frac{1}{\sqrt{A^{\dagger}A}} = \sum_{i}^{N_{total}} \frac{1}{\sqrt{\lambda_i}} |\lambda_i\rangle \langle\lambda_i| = \sum_{i}^{N_{ev}} \frac{1}{\sqrt{\lambda_i}} |\lambda_i\rangle \langle\lambda_i| + \frac{1}{\sqrt{\tilde{A}^{\dagger}\tilde{A}}}$$
(3.17)

where λ_i are the eigenvalues of $A^{\dagger}A$, $|\lambda_i\rangle$ the corresponding eigenvectors and $(\tilde{A}^{\dagger}\tilde{A})^{-1/2}$ is the part of the full operator that has the N_{ev} lowest modes projected out.

In this way, the Chebyshev approximation (3.10) is applied just to the part $(\tilde{A}^{\dagger}\tilde{A})^{-1/2}$, which has a reduced condition number, since the lowest modes have been projected out.

The resulting degree of Chebyshev polynomial, after the deflation procedure, is of order 200-400 for optimally chosen N_{ev} . The word "optimal" in this context refers to the fact that the procedure of eigenmodes computation is computer-time intensive and hence such number N_{ev} has to chosen that the additional computer-time cost of calculating the eigenmodes is balanced by the profit of having lower Chebyshev polynomial degree, e.g. for the inversion of the Dirac operator. The number of eigenmodes N_{ev} that should be projected out has to be found experimentally, but in general it grows with increasing lattice volume, as a consequence of the behaviour observed in the numerical test presented above.

3.3.2 HYP smearing of gauge fields

Eigenvalue deflation is not the only way to lower the condition number of the matrix $A^{\dagger}A$ and thus the degree of Chebyshev polynomial. A useful technique that can be applied before the computation of the lowest modes of $A^{\dagger}A$ is to perform HYP smearing on the gauge fields. This link fattening method was introduced by A. Hasenfratz and F. Knechtli [77] and allows to eliminate short-distance fluctuations of the gauge fields and thus decrease the probability of having very low eigenvalues of $A^{\dagger}A$. In this way, one iteration of HYP smearing helps to achieve a smaller condition number of $A^{\dagger}A$ and thus decrease the degree of Chebyshev polynomial. In comparison with other link fattening methods (e.g. APE smearing [61]), HYP smearing is believed to preserve better the short-distance quantities, because it mixes links from hypercubes attached only to the original link. Thus, it should not affect the physical properties of gauge field configurations and the physical observables calculated from HYP-smeared configurations. Finally, the degree of Chebyshev polynomial that one usually reaches by a combination of one iteration of HYP smearing and eigenvalue deflation is of order 100-200 for the optimal choice of the number of deflated eigenvalues N_{ev} . This is a considerable improvement with respect to the first number quoted for the polynomial degree – 1000-2000, which is typical without eigenvalue deflation and HYP smearing. Therefore, the reduction is by a factor of around 10, a factor of ≈ 2 brought in by HYP smearing and a factor of ≈ 5 by eigenvalue deflation.

Obviously, the fact that one needs to work with the Chebyshev polynomial approximation (or any other) still increases the computational cost of using overlap fermions by a large factor – typically of order 30-120 with respect to e.g. twisted mass fermions [75], even after the condition number reduction techniques have been used. Moreover, this number tends to increase when one decreases the pion mass. This speed factor is now considered to be one of the main drawbacks of overlap fermions and it motivates e.g. the mixed action approach, in which overlap fermions are used only in the valence sector, whereas to generate gauge field configurations a cheaper fermion discretization is used. The hope of this approach is that while avoiding the most expensive part of a simulation, which is the generation of gauge fields, one can still profit from the exact chiral symmetry that overlap fermions provide. The mixed action approach will be discussed further in Chapter 4.

3.4 Inverting the Dirac operator

After constructing the overlap Dirac operator, to calculate most observables, such as hadronic correlation functions, it is necessary to compute the quark propagator. To obtain complete information about quark propagation from each possible source site to every other sink site, it would be necessary to compute the inverse of the Dirac operator matrix. This is clearly a formidable task for typical lattice sizes – even storing such matrix in computer memory would be very difficult. Fortunately, the complete propagator that corresponds to a given gauge field configuration is not needed from the practical point of view, since the information about quark propagation from some site x to site y is very much correlated with the information about propagation between some other site x' and y.

Therefore, the strategy that is usually followed consists in solving the matrix equation:

$$\hat{D}(m)\psi = \eta, \tag{3.18}$$

where ψ is called the propagator, m is the bare quark mass and η is the source – a vector whose choice will be commented on below.

3.4.1 Stochastic sources

An important aspect of solving eq. (3.18) is the choice of the source η . The simplest possible choice is the point source, which means that the vector η is chosen to be 1 at one space-time point x_{src} , spin μ_{src} and color c_{src} and 0 otherwise:

$$\eta(x)_{\mu c} = \delta_{x, x_{src}} \delta_{\mu, \mu_{src}} \delta_{c, c_{src}}.$$
(3.19)

The propagator $\psi_{\mu c}$ is called the point-to-all propagator, since it corresponds to one column of the full inverse Dirac operator matrix and hence to quark propagation from one point x_{src} (with spin-color indices μ_{src} and c_{src}) to all other lattice points (with all possible spin-color indices). In this way, to obtain a propagator suitable for computation of hadronic correlation functions of interest in this work, it is necessary to solve eq. (3.18) 12 times – once for each combination of spin and color components of the source μ_{src} and c_{src} .

However, for mesonic correlators it is possible and advisable to use the information provided in gauge field configurations more fully by using timeslice stochastic sources. Let us consider the following choice of the source:

$$\eta(x)_{\mu c} = \left[\frac{\pm 1 \pm i}{\sqrt{2}}\right]_{x \in T_{src}} \delta_{\mu,\mu_{src}} \delta_{c,c_{src}}, \qquad (3.20)$$

where the symbol $[\cdot]_{x\in T_{src}}$ means that the source vector is non-zero for all lattice sites on a given timeslice T_{src} and the \pm signs in the expression in parentheses are chosen stochastically and independently for all x. The remaining Kronecker deltas imply that the only non-zero entries are for a specified spin μ_{src} and colour component c_{src} . Since the stochastic numbers are of the form $(\pm 1 \pm i)/\sqrt{2}$, we will refer to these sources as $\mathcal{Z}(2)$ stochastic sources (formally, they should be called the $\mathcal{Z}(2) \times \mathcal{Z}(2)$ stochastic sources, since here complex numbers are involved). In the context of Lattice QCD, the $\mathcal{Z}(2)$ stochastic noise was first proposed by Dong and Liu [78]. The motivation to use this kind of noise is that it produces a minimum variance of inverted matrix elements due to stochastic estimation.

The propagator element obtained from sample r of a stochastic source is:

$$\psi_i^r = \hat{D}_{ij}^{-1} \eta_j^r, \tag{3.21}$$

where the indices i, j encompass lattice site, spin and colour.

Hence, the full propagator matrix element estimate is: $\hat{D}_{ij}^{-1} = (\eta_j^r)^* \psi_i^r$. This estimate differs from the actual matrix element by stochastic noise, which is in general rather large – the noise-to-signal ratio for the timeslice stochastic source is expected to be of the order of $\sqrt{V_{src}}/\sqrt{R}$, where V_{src} is the volume of the source, i.e. the number of non-vanishing entries in the source, and R is the number of noise samples. Clearly, to get a useful signal the number of noise samples would have to be very large [24].

However, it is possible to reduce the noise-to-signal ratio considerably by employing the so-called one-end trick, introduced in [79]. Let us consider the product:

$$(\psi_i^r)^* \psi_j^r = \left(\hat{D}_{ik}^{-1} \eta_k^r\right)^* \hat{D}_{jl}^{-1} \eta_l^r = \left(\hat{D}_{ik}^{-1}\right)^* \hat{D}_{jk}^{-1} + \text{noise.}$$
(3.22)

This is a stochastic estimate of the product of quark propagators from the source to lattice sites *i* and *j*. Contracting now with δ_{ij} ("one end") allows to determine two-point mesonic correlators. The noise-to-signal ratio in this case is of the order of $\sqrt{V_{src}^2}/\sqrt{R}V_{src} = 1/\sqrt{R}$, where the factor $\sqrt{V_{src}^2}$ is the standard deviation associated with the noise and the signal is of the order of V_{src} itself (the other factor of V_{src}). Hence, even one sample per gauge configuration (R = 1) should be sufficient to extract the signal.

Moreover, to allow for any Dirac structure of the mesonic correlators, one can consider "linked" sources of the form:

$$\eta(x)_{\mu c} = \left[\frac{\pm 1 \pm i}{\sqrt{2}}\right]_{c; x \in T_{src}} \delta_{\mu, \mu_{src}}, \qquad (3.23)$$

where the Z_2 numbers are chosen independently for all lattice sites and all colours on a given timeslice T_{src} and for a specified spin component μ_{src} , but the noise is common to all spin components. For this reason, such sources are also called spin-diluted sources. In such case, one has 4 sources for each gauge configuration (one per spin component) and therefore eq. (3.18) has to be solved 4 times per configuration.

It is also possible to consider fully linked sources, i.e. spin and colourdiluted:

$$\eta(x)_{\mu c} = \left[\frac{\pm 1 \pm i}{\sqrt{2}}\right]_{\mu; \, c; \, x \in T_{src}}.$$
(3.24)

In this case, the stochastic numbers are chosen independently for all lattice sites on a given timeslice, all colours and all spins. Therefore, one has one source for each gauge configuration and only one inversion is needed. However, this method can only be used for some types of mesonic correlators, i.e. ones that have the γ_5 matrix at the source.

Another choice that has to be made when using stochastic sources is the way of selecting the timeslice for each gauge configuration. The two strategies that can be followed is to move the source timeslice cyclically through the lattice or to choose it randomly. Earlier studies [24] have shown that the latter method seems to work better (it leads to shorter autocorrelation times) and in this work we stay with this choice.

To improve the signal, when working with stochastic sources of the form (3.23), we will use two samples of stochastic noise per configuration and for one sample for each configuration we will apply Jacobi smearing with fuzzed gauge links. This method helps to reduce excited-state contamination in the mesonic correlators and thus also helps to obtain a better signal [24]. In practice, the addition of smeared stochastic sources allows to obtain four kinds of correlation functions: local-local (LL), local-fuzzed (LF), fuzzed-local (FL) and fuzzed-fuzzed (FF), depending on the propagator used in the construction of each correlation function. Averaging the local-fuzzed and fuzzed-local correlators, one can obtain three estimates of every correlation function at each timeslice and therefore e.g. three estimates of the effective pion mass at each timeslice (LL, FF and the average of LF and FL, which we will denote again by LF).

The general advantage of using stochastic sources with respect to point sources is the reduction of statistical error on mesonic quantities like the pion mass and decay constant, especially for small quark masses.

3.4.2 The SUMR solver

Equation (3.18), which has to be solved to find the quark propagator, is a matrix equation involving a matrix of a very large dimension, of the order of several million by several million. This means that solving this equation is the most intensive part of the computation of correlation functions of interest in this project. Therefore, it is essential to do it in an effective way. Specifically, this means that an appropriate solver has to be chosen.

The efficiency of different solvers for overlap and twisted mass fermions was investigated by Chiarappa et al. [75]. It was found that for the case of (quenched) overlap and small volume $(12^4 \text{ and } 16^4)$, the most effective solvers are the chiral conjugate gradient algorithm and the SUMR solver. Since the former algorithm can only be used for exact overlap operator, the polynomial approximation that we use would lead to some corrections that would have to be explicitly calculated. Therefore, the latter algorithm seems to be better suited for this project.

The SUMR (Shifted Unitary Minimal Residual) algorithm was introduced in [80] and first analyzed in the context of Lattice QCD in [81], where it was also shown that it is theoretically superior to certain variants of the Conjugate Gradient and the Minimal Residual algorithms.

To improve the performance of the SUMR algorithm, we have also used adaptive precision. This means that the Chebyshev polynomial degree is adapted to the accuracy that is actually needed in the present iteration step. From the practical point of view, when the solver is heading towards the
requested precision, the accuracy of approximation (the polynomial degree) can be substantially decreased. For example, if the degree of Chebyshev polynomial at the start of inversion is typically (for our parameters) of order 100-200, the final iterations can be performed with the polynomial degree down to 20-40 with adaptive precision. This saves a factor of around 2 in inversion time.

Since we are interested in the dependence of various observables on the bare overlap quark mass, it is also crucial that the inversion does not have to be performed separately for each quark mass. It was first shown by Frommer et al. [82] that for some kinds of solver algorithms it is possible to obtain the solution for an arbitrary quark mass at the cost of one inversion for only the smallest quark mass. Therefore, the dependence of the observables on the quark mass can be computed with very little additional cost, since the SUMR algorithm has the necessary multiple mass capability – the mass shift enters the algorithm only through scalar coefficients in the solution vector [75].

To finalize this chapter, we comment on computer codes that were used in this project. The gauge field configurations were generated by the ETM Collaboration using the tmLQCD package of Jansen and Urbach [83]. Stochastic sources were generated and the mesonic correlation functions were computed using the Contraction Code of Urbach and Wagner [84], while the baryonic correlators were calculated with the contraction code of Drach. Inversions with the overlap operator were performed using the GWC code, written by several contributors to the papers [64, 75]. The modifications of this code by the author of this thesis included:

- implementation of HYP smearing,
- input/output routines for reading in stochastic sources and writing propagators to allow the use of the Contraction Code,
- modification of the Contraction Code routines to generate fully linked stochastic sources and to perform contractions of propagators inverted on these sources,
- implementation of subtraction procedures for zero modes (discussed in Chapter 4).

Chapter 4

Investigations of the continuum limit scaling properties of the mixed action setup

4.1 Mixed action approach

Overlap fermions have many appealing properties. However, their main disadvantage is that their use is very time-consuming and needs $\mathcal{O}(100)$ times larger computer resources with respect to e.g. twisted mass fermions. This makes dynamical simulations with overlap fermions a big challenge. Such simulations are performed [85], but in comparison with other kinds of lattice actions it is still not possible to reach very fine lattice spacings and very large lattices. Dynamical overlap fermions simulations also lead to algorithmic difficulties, the foremost being the discontinuity in the operator $1/\sqrt{A^{\dagger}A}$, which implies that the overlap Dirac operator changes discontinuously when its index changes (i.e. when the number of chiral zero modes of the Dirac operator changes in a simulation) [86]. This problem can be overcome, e.g. by using the reflection/refraction algorithm [87], but this procedure is very costly and hence still too demanding for the present generation of supercomputers. Another way to overcome the discontinuity problem is to modify the action in such a way that the topological charge can not change [88]. However, this leads to an additional finite volume effect which has to be taken into account.

The above discussion shows that while clearly the importance of dynamical overlap simulations will increase in the future, it is still desirable to investigate alternative approaches that make it possible to take advantage of good chiral properties of overlap fermions and at the same time avoid the immense computational cost of dynamical overlap simulations. One such approach is provided by the mixed action setup.

The mixed action approach consists in choosing a different discretization for sea and valence fermions. This means that the gauge field configurations are generated with a relatively cheap fermionic action, such as the Wilson twisted mass action and the overlap operator is only used to invert the Dirac operator, i.e. to construct propagators, and then to compute the correlation functions.

The mixed action simulations have been performed for the following setups:

- clover sea quarks and overlap valence quarks [89, 90, 91],
- Wilson twisted mass sea quarks and overlap valence quarks [92, 93, 94],
- improved staggered sea quarks,
 - overlap valence quarks [95, 96, 97],
 - domain wall valence quarks e.g. [98, 99, 100, 101, 102, 103, 104, 105, 48].

As can be deduced from the above summary, the most widely used mixed action setup employs domain wall valence quarks and improved staggered sea quarks. This results from the relative abundance of gauge field configurations generated with the improved staggered lattice action and from the relative cheapness of domain wall fermions, as compared with overlap fermions, however at the price of sacrificing exact chiral symmetry with respect to the latter.

The use of overlap valence quarks has been relatively rare and for Wilson twisted mass sea quarks only an exploratory study has been performed. The current project is the continuation of the analysis performed in [92, 93] and its first results have been reported in [94]. It is also well-motivated from the point of view of the availability of twisted mass sea gauge configurations, generated by the European Twisted Mass Collaboration (ETMC) [106, 24].

However, before reporting the project results, let us shortly discuss the validity of the mixed action approach in general. Let us consider the expression for a mesonic correlation function:

$$C_{ij}(x,y) = \frac{1}{Z} \int DU \, e^{-S_{\text{gauge}}[U]} \left(\det \left(\hat{D}_{sea}(m_{sea}) \right) \right)^2$$

$$\times \operatorname{Tr} \left[\left(\hat{D}_{val}(m_{val,1}) \right)^{-1}(y,x) \Gamma_i \left(\hat{D}_{val}(m_{val,2}) \right)^{-1}(x,y) \Gamma_j \right].$$

$$(4.1)$$

In $N_f = 2$ simulations, one can have the following situations:

- $\hat{D}_{sea} = \hat{D}_{val}, m_{sea} = m_{val,1} = m_{val,2}$ unitary setup,
- $\hat{D}_{sea} = \hat{D}_{val}, m_{sea} \neq m_{val,1} = m_{val,2}$ or $m_{sea} = m_{val,1} \neq m_{val,2} partially quenched (PQ) setup,$
- $\hat{D}_{sea} \neq \hat{D}_{val}$ mixed action setup.

Since all valid lattice Dirac operators differ only by discretization effects, i.e. terms proportional to some power of the lattice spacing, they have the same continuum limit. This has been explicitly shown in Chapter 2 for selected discretizations at tree-level. Therefore, it is clear from eq. (4.1) that even taking different lattice Dirac operators for sea and valence quarks (the mixed action setup) must lead to the same continuum limit as the unitary setup, provided that the sea quarks and the valence quarks masses are properly matched such that a fixed physical situation is realized in the approach to the continuum limit. In the unitary setup, this obviously holds if the bare quark masses are equal. However, in the mixed case the equality of bare quark masses does not have to be the proper matching condition, i.e. one leading to the same continuum limit as the unitary case. This is due to the fact that the renormalization constants of the quark masses do not have to be the same for different discretizations. Hence, a proper matching condition is to take equal renormalized quark masses. However, this is not always straightforward, since the computation of renormalization constants can't always be performed with sufficient precision. Therefore, alternative matching conditions can be considered – one can match some hadronic observable that can be computed precisely.

The choice that we will follow is to match the pion mass. This amounts to finding a bare valence quark mass $m_{val,1} = m_{val,2} \equiv m_q$, which leads to the same pion mass as the mass of a pion constructed from two sea quarks of mass m_{sea} : $m_{\pi}^{val-val} = m_{\pi}^{sea-sea}$. We also expect (and again it has been shown in the free case) that at the matching point other physical observables, such as the pion decay constant, are also matched, but only up to $\mathcal{O}(a^2)$, since discretization effects are in general different in different observables.

However, even if we expect that the continuum limit of a mixed action theory is the same as of unitary QCD, such theory is still non-unitary and this can lead to various effects observed at non-zero lattice spacing. A pronounced effect of this kind regards the scalar correlation function. It was first shown in quenched QCD by Bardeen et al. [107, 108] that the scalar correlator can obtain an unphysical negative contribution from one kind of diagrams. This is especially important for low quark masses and it is attributed to the $\eta' - \pi$ intermediate state. Such effect also appears in partially quenched QCD and Prelovsek et al. derived an expression for this contribution [109] within the framework of Partially Quenched Chiral Perturbation Theory. Golterman, Izubuchi and Shamir [110] adapted this result to the case of mixed actions. At large time t, the dominant contribution to the scalar correlation function is:

$$C(t) \to \frac{B_0^2}{2L^3} \left[\frac{e^{-2M_{VS}t}}{M_{VS}^2} \frac{N_f}{2} - \frac{e^{-2M_{VV}t}}{M_{VV}^4} \left(\frac{M_{VV}^2 + M_{SS}^2}{N_f} + RM_{VV}t \right) \right], \quad (4.2)$$

where B_0 is a low-energy constant, L – the physical length of the box, $M_{VV} \equiv m_{\pi}^{val-val}$, $M_{SS} \equiv m_{\pi}^{sea-sea}$, $M_{VS} \equiv m_{\pi}^{val-sea}$ (at leading order $M_{VS}^2 = (M_{VV}^2 + M_{SS}^2)/2$),

$$R = (M_{SS}^2 - M_{VV}^2)/N_f + a^2(\gamma_{VV} + \gamma_{SS} - 2\gamma_{VS})$$
(4.3)

is the residue from the double pole, which arises only in the case of a partially quenched or a mixed action setup. γ_{VV} , γ_{SS} and γ_{VS} are additional lowenergy constants, which are all equal in the case of a partially quenched setup – hence in such case the second term in the residue from the double pole vanishes. If we consider the case of matched pion masses, the formula (4.2) reduces (in the $N_f = 2$ case) to:

$$C(t) \to -\frac{B_0^2}{2L^3} \frac{e^{-2M_{VV}t}}{M_{VV}^3} \left(\gamma_{VV} + \gamma_{SS} - 2\gamma_{VS}\right) a^2 t.$$
(4.4)

Thus, in the mixed action case the residue R does not vanish even if we match the pion masses and even in this case it should be possible to observe a potentially negative contribution (its sign depends on the signs of γ low-energy constants) to the scalar correlator at large time, as an indication of a unitarity violation caused by the different discretization of sea and valence quarks. This effect was further investigated by Furchner [111], who derived finite volume corrections to the considered effect.

However, it is important to emphasize here that the unitarity violation is a discretization effect and thus it vanishes in the continuum limit. Moreover, even at finite lattice spacing, the χPT formulas allow to control the unitarity violation and hence the effect can be taken into account and analyzed.

4.2 Scaling test – light sea quark mass

In this section, we will show the results of a continuum limit scaling test of the pion decay constant, employing overlap valence quarks and maximally twisted mass sea quarks with a light mass, corresponding in infinite volume to a pion mass of around 300 MeV.

4.2.1 Simulation parameters

A continuum limit scaling test in the interacting theory consists in computing a certain observable at a few values of the lattice spacing, but in a fixed volume and in fixed physical situation, and extrapolating the result to a = 0. The range of lattice spacings and volumes covered by the available $N_f = 2$ ETMC configurations is broad. There are four lattice spacings – between $a \approx 0.05$ fm (which corresponds to $\beta = 4.2$) and $a \approx 0.1$ fm ($\beta = 3.8$) and a range of physical extents of the box L covering the interval between 1.3 and 2.7 fm. In order to minimize the effect of finite volume, in simulations with twisted mass valence quarks one usually works with $L \geq 2$ fm. However, such volume is very computer-time demanding in the case of overlap valence quarks and practically out-of-reach for the physical extent L reaching 2.4 fm, since it would require dealing with lattices of $48^3 \times 96$ at the finest lattice spacing. Therefore, this scaling test will be performed with the smallest volume available, corresponding to the physical size of the box of $L \approx 1.3$ fm. In order to estimate the size of the finite volume effects, we will also perform an analysis for larger volumes, but only for the coarsest lattice spacing, corresponding to $\beta = 3.9$.

There are three available lattice spacings at the physical lattice extent of 1.3 fm, corresponding to the light sea quark mass that leads to a pion mass of around 300 MeV. The simulation parameters are^{1} :

- $16^3 \times 32$, $a \approx 0.079$ fm ($\beta = 3.9$, $r_0/a = 5.25(2)$), $a\mu = 0.004$, 544 configurations,
- $20^3 \times 40$, $a \approx 0.063$ fm ($\beta = 4.05$, $r_0/a = 6.61(2)$), $a\mu = 0.003$, 300 configurations,
- $24^3 \times 48$, $a \approx 0.051$ fm ($\beta = 4.2$, $r_0/a = 8.33(5)$), $a\mu = 0.002$, 400 configurations.

We have chosen only a subset of available thermalized gauge field configurations in each ensemble, in order to minimize the effect of autocorrelations. For inversions with the overlap Dirac operator, we have chosen every 10th Monte Carlo trajectory (at $\beta = 3.9, 4.2$) or every 20th trajectory (at $\beta = 4.05$). The number of configurations for each ensemble was chosen to roughly match the accuracy of the twisted mass data, i.e. achieve a similar statistical error on the pion mass and decay constant as in the unitary setup. This requires roughly the same number of configurations in both cases.

¹The values of the lattice spacing and the hadronic length scale r_0/a are taken from [33].

As discussed in the previous chapter, we have applied one iteration of HYP smearing to the gauge field configurations.

4.2.2 Locality

Before concentrating on the scaling test, we investigate the issue of locality of the overlap Dirac operator for our setup [112]. In this way, we will be able to choose the optimal value of the parameter s which enters the definition of this operator (equations (1.75) and (1.76)).

First, we analyze the dependence of the maximal norm of the overlap Dirac operator $||\hat{D}_{ov}||_{max}$ on the taxi-driver distance ||x||, defined in Section 1.4.2. The norm of the overlap operator is defined as the row-sum norm:

$$||\hat{D}_{ov}(x,y)|| = \max_{1 \le \mu \le 4} \sum_{\nu=1}^{4} |\hat{D}(x,y)_{\mu\nu}|$$
(4.5)

and, since the operator norm may differ for the same taxi-driver distance due to different paths that can be followed, we define the maximal norm for the taxi driver distance d as:

$$||\hat{D}_{ov}||_{max}(d) = \max_{||x-y||=d} ||\hat{D}_{ov}(x-y,0)||.$$
(4.6)

The decay rate ρ of the maximal norm is defined by the formula:

$$||\hat{D}_{ov}||_{max}(d) = Ce^{-\rho d},$$
(4.7)

where ρ and C can be extracted from a fit.

Fig. 4.1 shows in logarithmic scale the taxi-driver distance dependence of the maximal norm of the overlap operator for different values of the parameter s. For all values of s we observe an exponential decay of the norm and the maximal decay rate is observed for s = 0 (for this value a linear fit is shown). This is further illustrated in Fig. 4.2, which shows that the decay rate ρ is indeed maximal in the vicinity of s = 0. We also show here the result for gauge field configurations without HYP smearing. In this case, the maximal decay rate ρ is obtained for s = 0.4 and is slightly smaller than the decay rate corresponding to s = 0 in the HYP-smeared case². Hence, for further simulations it is optimal from the point of view of locality to set s = 0.

The overlap operator decay rate in lattice units $a\rho$ should not depend on lattice spacing. This means that the values of $1/\rho$ extracted from plots

²A similar value of ρ is obtained also for s close to -1. However, negative values of s mean that a non-physical phase may be entered [113].



Figure 4.1: Maximal norm of the overlap operator in logarithmic scale. The linear fit corresponds to the value of s which yields the maximal decay rate. Parameters: $\beta = 3.9$, L/a = 16.



Figure 4.2: The dependence of the overlap Dirac operator norm decay rate ρ on the parameter s for gauge field configurations with and without HYP smearing. Parameters: $\beta = 3.9$, L/a = 16.



Figure 4.3: The continuum limit scaling of the overlap operator decay rate.



Figure 4.4: The continuum limit scaling of the ratio of the pion mass (at the matching mass) and the overlap operator decay rate.

like Fig. 4.1 should have a linear dependence on the lattice spacing and in the continuum limit $1/\rho$ should vanish. Fig. 4.3 shows that this is the case for our setup – the lattice spacing dependence is linear and the value extrapolated to the continuum limit is consistent with zero.

Fig. 4.4 shows the ratio of m_{π}/ρ . At finite lattice spacing the condition $m_{\pi} < \rho$ must hold [30] in order that the interaction can be considered local



Figure 4.5: Effective pion mass plateau for the ensemble $16^3 \times 32$, $a \approx 0.079$ fm ($\beta = 3.9$), $a\mu = 0.004$. The bare valence quark mass is $am_q = 0.04$. For each timeslice 3 values of the pion mass are computed, corresponding to different kinds of smearing of the sources (described in Section 3.4.1). The horizontal band corresponds to a simultaneous fit of the LL, LF and FF pseudoscalar correlation functions, which yields a value 0.2884(17).

from the point of view of the considered particle. For the pion at the matching mass, the ratio m_{π}/ρ is well below 1 and thus locality is guaranteed. The continuum limit value of m_{π}/ρ is consistent with zero, which is due to the fact that m_{π} has a non-zero value in the continuum, while $1/\rho$ vanishes for a = 0.

All these tests show that for the analyzed setup there should be no problems with the locality of the overlap Dirac operator [112]. This operator decays exponentially and we have maximized its decay rate by choosing a suitable value of the parameter s, i.e. s = 0.0 in the case of HYP-smeared gauge field configurations.

4.2.3 Matching the pion mass

As discussed in Section 4.1, a mixed action setup will lead to the same continuum limit as the unitary setup, provided that the quark masses are properly matched. Here we show the results of the matching procedure, with the



Figure 4.6: Matching the pion mass for three values of the lattice spacing, corresponding to $\beta = 3.9$, 4.05 and 4.2. The horizontal bands are unitary MTM (maximally twisted mass) values and the curves show the bare quark mass dependence of the overlap pion mass.

matching criterion of equal sea-sea and valence-valence pion masses. Employing a multi-mass solver, it was possible to obtain the dependence of the pion mass on the bare overlap quark mass. A typical effective mass plateau in the extraction of the pion mass from the pseudoscalar correlation function is shown in Fig. 4.5. The different points that correspond to each timeslice are related to different kinds of smearing of the sources used to compute the propagators (as explained in Section 3.4.1) and hence three estimates of the



Figure 4.7: The dependence of the pion decay constant on the bare overlap quark mass. The dashed lines correspond to the matching quark masses $a\hat{m}$.

pion mass are obtained for each timeslice.

The matching plots in Fig. 4.6 show the pion mass in the unitary setup (horizontal bands) and in the mixed setup. The intersection point of the two lines defines the matching mass $a\hat{m}$ for each ensemble. However, since the error bands are non-negligible, the matching mass is not determined precisely, but also with a statistical error. The values that we find are:

- $\beta = 3.9 a\hat{m} = 0.007(1),$
- $\beta = 4.05 a\hat{m} = 0.005(1),$
- $\beta = 4.2 a\hat{m} = 0.002(1).$

4.2.4 Pion decay constant – scaling test

In addition to the pion mass, we have also computed the pion decay constant from eq. (1.95). The dependence of this quantity on the bare overlap quark



Figure 4.8: Continuum limit scaling of the overlap pion decay constant at the matching mass and two other reference values of $r_0 m_{\pi}$.

mass is depicted in Fig. 4.7. The horizontal bands in this plot again correspond to the unitary setup and the curves above to the mixed action setup. The dashed vertical lines show the location of the matching bare overlap quark mass $a\hat{m}$.

In Chapter 2 we have performed a tree-level continuum limit scaling test for the pion decay constant and we have shown that the leading discretization effects are $\mathcal{O}(a^2)$. Now, we would like to perform a similar test in the interacting case. The matching between the physical volumes of the lattices $(L \approx 1.3 \text{ fm})$ is imposed by the choice of the ensembles and here we also have to fix the quark mass to allow for a comparison of the decay constants at three distinct lattice spacings. This can be done e.g. by fixing r_0m_{π} . We will take three values of $r_0m_{\pi} \approx 1.5$, $r_0m_{\pi} \approx 1.0$ and $r_0m_{\pi} \approx 0.85$, which corresponds roughly to the matching mass \hat{m} (as can be seen from the matching plot 4.6, the MTM (sea-sea) pion masses are approximately matched for the three ensembles under investigation).

The results of the test are shown in Fig. 4.8. For all investigated values of $r_0 m_{\pi}$, we observe good scaling with $\mathcal{O}(a^2)$ leading cut-off dependence, as expected from previous considerations and confirmed at the tree-level.

However, we would still like to check whether the continuum limit of the pion decay constant computed with overlap valence fermions is consistent



Figure 4.9: Continuum limit scaling of the MTM pion decay constant at the matching mass.

with the one computed in the unitary setup, i.e. with maximally twisted mass valence quarks. This would provide an explicit test of universality of fermion discretizations. The continuum limit value that has to be compared is the one obtained for the matching mass.

Fig. 4.9 shows a continuum limit scaling of $r_0 f_{\pi}$ in the unitary setup. As in the case of overlap valence quarks, the MTM pion decay constant shows a leading $\mathcal{O}(a^2)$ cut-off dependence. However, the continuum limit is different than the one obtained from the extrapolation of overlap data. This is in strong contrast with our earlier expectation that both discretizations should lead to the same continuum value. To illustrate this result more clearly, we plot in Fig. 4.10 the difference $r_0(f_{\pi}^{overlap} - f_{\pi}^{MTM})$. This confirms that the discrepancy between the overlap and MTM pion decay constant decreases much too slowly as the continuum limit is approached.

This is a very surprising and unexpected outcome. Fig. 4.10 suggests that using one of the Dirac operators leads to a wrong continuum limit, which is in contradiction to the widely accepted knowledge that both constitute valid lattice Dirac operators. The observed discrepancy is therefore a mystery at this stage and it has been a major part of the present thesis to resolve this mystery and find an explanation for the behaviour depicted in Fig. 4.10.

The qualitative difference of the twisted mass and overlap discretizations



Figure 4.10: Continuum limit scaling of the difference of the overlap and MTM pion decay constant at the matching mass.

is that the latter exactly preserves chiral symmetry. Therefore, it is natural to look in the direction of this difference. Namely, we will investigate the role of chiral zero modes of the overlap Dirac operator.

4.3 Chiral zero modes and their contribution to mesonic correlators

4.3.1 Chiral zero modes

There is a clear difference in the eigenvalue spectra of chiral and non-chiral massless lattice Dirac operators. In the case of the former, it is possible that eigenmodes $\phi(x)$ with zero eigenvalue appear at any value of the lattice spacing a. Moreover, such zero modes have a definite chirality, i.e. they are eigenmodes of γ_5 :

$$\gamma_5 \phi(x) = \pm \phi(x) \tag{4.8}$$

with eigenvalue ± 1 . If the eigenvalue equals +1, we call such eigenmode a zero mode in the positive chirality sector (or a right-handed zero mode) and for eigenvalue -1 we speak of a zero mode in the negative chirality sector

(or a left-handed zero mode). In Section 1.4.4 we have discussed the relation between the zero modes and topological properties of gauge fields.

Non-chiral lattice Dirac operators can also develop zero modes, but this can only happen at sufficiently small values of the lattice spacing. The values that are presently reached in simulations are far too large to have exact zero modes of non-chiral Dirac operators – from the practical point of view we can therefore assume that in our mixed action setup with overlap valence quarks and twisted mass sea quarks the valence Dirac operator admits zero modes and the sea Dirac operator does not. Hence, in a finite volume situation the zero modes of the valence Dirac operator lead to a contribution that is not compensated by the fermionic determinant and can affect certain correlation functions and hence some observables. It was shown by Blum et al. [114] that the contribution of the zero modes (e.g to mesonic correlators) is proportional to $1/\sqrt{V}$, where V is the lattice volume, and therefore it is a finite volume artefact.

It is interesting to speculate about the role of zero modes in an unitary overlap simulation³. In such case, the contribution of the zero modes would be suppressed by the (overlap) fermionic determinant. In other words, an effect of the zero modes that we want to investigate in the mixed action setup or the analogous effect in the quenched approximation [119] results from the fact that the contribution of the zero modes is not properly suppressed by the fermionic determinant, since it is a determinant that originates from a non-chirally symmetric action (the MTM case) or there is no determinant at all (i.e. it is set to a constant in the quenched approximation). Moreover, it can be hypothesized that very close to the continuum limit, zero modes of the MTM Dirac operator would also appear and the contribution of the zero modes in the valence sector would be suppressed by the MTM fermionic determinant. In this way, it would lead to a lowered continuum limit of the overlap pion decay constant in the PP case with respect to the one extracted from the linear extrapolation in a^2 and under the assumption of universality a limit more consistent with the unitary MTM value. However, such hypothesis is not testable in lattice calculations, since probably a simulation with a very small lattice spacing would have to be performed. Nevertheless, the pion decay constant continuum limit scaling test in the unitary overlap setup would be interesting from this point of view and should confirm that the continuum limit of both unitary overlap and unitary MTM is the same, even when one looks at the PP correlator in the former case, as we have done in the previous section.

³For unitary overlap simulations appropriate algorithms need to be used, which take the zero modes into account, e.g. the Polynomial HMC (PHMC) algorithm [115, 116, 117, 118].

4.3.2 The contribution of the zero modes to mesonic correlators

We now proceed to show how the contribution of the zero modes can be calculated and subtracted from the observables. In this way, we will be able to compute the overlap pion decay constant without the contribution of the zero modes and then perform the continuum limit scaling test of Section 4.2 again and check whether the finite volume effect of the zero modes is responsible for the difference in the continuum value.

Let us consider the spectral decomposition of the propagator S(x, y):

$$S(x,y) = \sum_{i} \frac{\phi_i(x)\phi_i^{\dagger}(y)}{\lambda_i + m_q},$$
(4.9)

where λ_i are the eigenvalues of the massless Dirac operator \hat{D} , i.e.:

$$\hat{D}\phi_i(x) = \lambda_i \phi_i(x), \qquad (4.10)$$

and m_q is the bare quark mass.

Inserting this decomposition into the expression for the mesonic correlation function (1.91), we obtain:

$$C(t) = \sum_{\vec{x}} \sum_{i,j} \frac{\text{Tr}(\phi_i(\vec{x},t)\phi_i^{\dagger}(\vec{0},0) \Gamma^1 \gamma_5 \phi_j(\vec{0},0)\phi_j^{\dagger}(\vec{x},t) \gamma_5 \Gamma^2)}{(\lambda_i + m_q)(\lambda_j + m_q)}.$$
 (4.11)

Let us now isolate the contribution of the zero modes:

$$C(t) = C_{00}(t) + 2C_{0N}(t) + C_{NN}(t), \qquad (4.12)$$

where $C_{00}(t)$ is the part of the sum that contains only the zero modes ($\lambda_i = 0$, $\lambda_j = 0$), $2C_{0N}(t) = C_{0N}(t) + C_{N0}(t)$ contains the mixed terms that couple the zero modes and non-zero modes ($\lambda_i = 0, \lambda_j \neq 0$ or $\lambda_i \neq 0, \lambda_j = 0$) and $C_{NN}(t)$ is the contribution of the non-zero modes ($\lambda_i \neq 0, \lambda_j \neq 0$). We find:

$$C_{00}(t) = \sum_{\vec{x}} \sum_{\lambda_i=0} \sum_{\lambda_j=0} \frac{\text{Tr}(\phi_i(\vec{x},t)\phi_i^{\dagger}(\vec{0},0)\,\Gamma^1\gamma_5\,\phi_j(\vec{0},0)\phi_j^{\dagger}(\vec{x},t)\,\gamma_5\Gamma^2)}{m_q^2},\quad(4.13)$$

$$C_{0N}(t) = \sum_{\vec{x}} \sum_{\lambda_i=0} \sum_{\lambda_j\neq 0} \frac{\text{Tr}(\phi_i(\vec{x}, t)\phi_i^{\dagger}(\vec{0}, 0) \Gamma^1 \gamma_5 \phi_j(\vec{0}, 0)\phi_j^{\dagger}(\vec{x}, t) \gamma_5 \Gamma^2)}{m_q(\lambda_j + m_q)}, \quad (4.14)$$

$$C_{NN}(t) = \sum_{\vec{x}} \sum_{\lambda_i \neq 0} \sum_{\lambda_j \neq 0} \frac{\text{Tr}(\phi_i(\vec{x}, t)\phi_i^{\dagger}(\vec{0}, 0) \Gamma^1 \gamma_5 \phi_j(\vec{0}, 0)\phi_j^{\dagger}(\vec{x}, t) \gamma_5 \Gamma^2)}{(\lambda_i + m_q)(\lambda_j + m_q)}.$$
 (4.15)

Let us now consider the contributions of the zero modes $C_{00}(t)$, $C_{0N}(t)$ to the pseudoscalar ($\Gamma^1 = \Gamma^2 = \gamma_5$) and scalar ($\Gamma^1 = \Gamma^2 = \mathbb{1}$) correlation functions. In both cases we obtain the same result:

$$C_{00}^{PP,SS}(t) = \sum_{\vec{x}} \sum_{\lambda_i=0} \sum_{\lambda_j=0} \frac{\text{Tr}(\phi_i(\vec{x},t)\phi_i^{\dagger}(\vec{0},0)\phi_j(\vec{0},0)\phi_j^{\dagger}(\vec{x},t))}{m_q^2}, \qquad (4.16)$$

$$C_{0N}^{PP,SS}(t) = \sum_{\vec{x}} \sum_{\lambda_i=0} \sum_{\lambda_j \neq 0} \frac{\text{Tr}(\phi_i(\vec{x},t)\phi_i^{\dagger}(\vec{0},0)\phi_j(\vec{0},0)\phi_j^{\dagger}(\vec{x},t))}{m_q(\lambda_j + m_q)}, \qquad (4.17)$$

where in the scalar case we have used eq. (4.8). The terms that contain the zero modes contribution are proportional to $1/m_q^2$ and $1/m_q$ and hence diverge in the chiral limit $m_q = 0$. Since in our simulation setup the sea quark mass is rather light, at the matching mass also the valence quark mass is light and therefore the zero modes contribution can be important.

However, since the zero mode contribution to the pseudoscalar $(C_{PP}(t))$ and scalar $(C_{SS}(t))$ correlation functions is equal, it is possible to exactly cancel this contribution by taking the difference of these two correlators. This was first suggested by Blum et al. [114]. We define:

$$C_{PP-SS}(t) = C_{PP}(t) - C_{SS}(t).$$
(4.18)

This is a valid correlation function with a proper transfer matrix decomposition. Therefore, it should be possible to extract the pion mass and decay constant from this correlation function. $C_{PP-SS}(t)$ is contaminated by the scalar excitation. However, since the lightest scalar meson is much heavier than the lightest pseudoscalar meson, if we look at large enough time, the contribution of the scalar states should be absent and we can indeed extract the pion observables of interest.

In a mixed action setup there is an additional complication. The scalar correlator is particularly vulnerable to the double pole contribution, which has already been discussed in Section 4.1. The residue from this double pole does not vanish even in the case of matched pion masses. Hence, by considering the correlation function $C_{PP-SS}(t)$ we exchange the contribution of the zero modes for a unitarity violation related to the mixed action setup. However, this is an effect of $\mathcal{O}(a^2)$, which can be considered to be an extra discretization effect, in addition to the standard $\mathcal{O}(a^2)$ scaling violations present in all observables. Therefore, such unitarity violations vanish in the continuum and they should not affect the extrapolation of the pion decay constant (computed from $C_{PP-SS}(t)$) to the continuum.

The effect of the zero modes on the pion mass can be observed in Fig. 4.11, which shows the bare overlap quark mass dependence of the pion mass



Figure 4.11: The comparison of the quark mass dependence of the pion mass extracted from PP and PP-SS correlators for $\beta = 3.9$ ensemble.

extracted from the pseudoscalar (PP) correlator and the PP-SS correlator $C_{PP-SS}(t)$. As expected from considerations in this section, the effect is the most pronounced for small quark masses, while for larger masses the pion mass extracted from both correlators is the same (up to statistical error). The pion mass extrapolated to the chiral limit $(m_q = 0)$ is zero, when the effects of the zero modes have been subtracted. This is in accordance with the leadingorder prediction of Partially Quenched Chiral Perturbation Theory – $m_{\pi}^2 \propto$ m_q [120, 121]. Also, the shape of the quark mass dependence of the pion mass agrees with this prediction – in this range of masses the curvature implied by the next-to-leading order prediction is only slightly visible and, especially, there is no evidence for chiral logarithms $\propto m_q \log m_q$. An extrapolation to the chiral limit in the PP case yields a non-zero value. The observed shape could be mistaken for a chiral logarithm relevant for small quark masses, but it is entirely due to the chiral zero modes, i.e. it is a finite-volume effect. The plot also shows that the zero modes have a significant effect with respect to the matching mass, which moves towards larger values of the bare quark mass.



Figure 4.12: The comparison of the quark mass dependence of the pion decay constant extracted from PP and PP-SS correlators for $\beta = 3.9$ ensemble.

We also show the influence of the zero modes on the quark mass dependence of the pion decay constant (Fig. 4.12). As for the pion mass, the effect is significant for small quark masses and the PP-SS curve lies below the PP one. This effect brings the decay constant towards the twisted mass value. However, since the matching mass increases, the effect at the matching mass is rather small (for $\beta = 3.9$) and hence an investigation of the continuum limit scaling is needed to check whether the zero modes are enough to explain the difference between the continuum limit values of the pion decay constant. This will be performed in the following section.

4.3.3 Comparison of correlation functions

To illustrate the effects of subtracting the zero modes in two different ways, we plot in Fig. 4.13 the following correlation functions: PP, SS and PP-SS. We also plot the PP and PP-SS correlation functions for one chosen gauge field configuration. Ensemble parameters are: $\beta = 3.9$, L/a = 16, $a\mu = 0.004$, $am_q = 0.004$, i.e. we choose the lightest available valence quark



Figure 4.13: Ensemble averages for the following correlation functions: pseudoscalar (PP), scalar (SS), the difference of PP and SS (PP-SS). The inset shows the PP and PP-SS correlation functions on a single configuration. Parameters: $\beta = 3.9$, L/a = 16, $a\mu = 0.004$, $am_q = 0.004$.

mass to have the biggest contribution of the zero modes.

Let us summarize the conclusions from this plot.

• The PP-SS correlator has a smaller slope (with respect to the PP correlator) in the plateau region – thus it corresponds to a smaller pion mass. This was already observed in Fig. 4.11 (the valence quark mass in Fig. 4.13 corresponds to the leftmost pair of points in Fig. 4.11).



Figure 4.14: Ensemble averages for the following correlation functions: pseudoscalar (PP), scalar (SS), the difference of PP and SS (PP-SS). Parameters: $\beta = 3.9$, L/a = 16, $a\mu = 0.004$, $am_q = 0.04$ (much larger valence quark mass than in Fig. 4.13).

From Fig. 4.11, one can also conclude that the effect of the change of slope in the plateau region is smaller for larger valence quark masses. This is in accordance with our previous considerations – the leading quark-mass dependence of the zero-mode contribution to the PP and SS correlators is $\mathcal{O}(1/m_q^2)$.

- The matrix element of the PP-SS correlator $|\langle 0|P|\pi\rangle|_{PP-SS}$ is largely reduced with respect to the PP correlator matrix element $|\langle 0|P|\pi\rangle|$. However, this leads to a relatively small decrease in the pion decay constant (observed in Fig. 4.12), since the decrease in this matrix element is almost compensated for by a decrease in m_{π}^2 , which comes in the denominator of eq. (1.95).
- The effect of the zero modes on a single configuration consists in pro-

ducing an unphysical peak at the timeslice (t = 12 in Fig. 4.13) that corresponds to the location of the zero mode. This peak is removed in the PP-SS correlator.

We also consider (Fig. 4.14) the case of a heavier valence quark mass $am_q = 0.04$ (the remaining parameters are the same). The plot shows only the large-time behaviour of the correlation functions.

- The SS correlator is consistent with zero. For $t \in [10, 16]$, there is no contribution from the scalar excitation, as the scalar meson is too heavy. Since the scalar correlator is zero, also the contribution of the zero modes is negligible and hence the PP and PP-SS correlation functions lead to the same result.
- For this value of quark mass, one also expects a negligible contribution from the double pole to the scalar correlator eq. (4.2) implies that for large M_{VV} this contribution is very small.
- Hence, the pion mass and decay constant extracted at this mass from the PP/PP-SS correlator do not seem to be contaminated by either the contribution of the zero modes or unitarity violations.

The analysis of this subsection implies that, as expected, the role of the zero modes decreases as the quark mass is increased. In the next section we will use the PP-SS correlation function to perform an analysis of the behaviour of the pion decay constant with the zero modes contribution removed. In particular, we would like to check its continuum limit – if the zero modes are indeed responsible for the mismatch of continuum limits observed in Fig. 4.10, their removal should lead to the same continuum limit of the pion decay constant as the one of the unitary approach.

4.4 The role of the zero modes – small volume, light sea quark mass

We would now like to perform a continuum limit scaling test of the pion decay constant extracted from the PP-SS correlator $C_{PP-SS}(t)$. We will proceed in the same manner as before, i.e. we start by finding the matching mass for each ensemble. The results of the matching procedure are shown in Fig. 4.15 and the bare overlap quark masses that lead to the same pion mass as in the unitary setup are the following:

• $\beta = 3.9 - a\hat{m} = 0.011(1),$



Figure 4.15: Matching the pion mass (extracted from the PP-SS correlator) for three values of the lattice spacing, corresponding to $\beta = 3.9$, 4.05 and 4.2.

- $\beta = 4.05 a\hat{m} = 0.006(1),$
- $\beta = 4.2 a\hat{m} = 0.004(1).$

In comparison with the PP case, the matching masses are shifted towards larger values. This is a result of the fact that they were artificially lowered due to the zero mode contribution.

As already discussed, the pion decay constant curve extracted from the PP-SS correlation function lies below the one extracted in the PP case. At the



Figure 4.16: The dependence of the pion decay constant on the bare overlap quark mass. The dashed lines correspond to the matching quark masses $a\hat{m}$ (from PP-SS correlator). The solid vertical lines (left of the dashed lines) show the difference of $f_{\pi}^{overlap}$ and f_{π}^{MTM} (at the matching mass) extracted from the PP correlator.

same time, however, the matching masses are shifted towards larger values, which corresponds to an increase in the pion decay constant. The interplay of these two effects determines the difference between the overlap $f_{\pi}^{overlap}$ and the MTM pion decay constant f_{π}^{MTM} at the matching mass. One can explicitly compare these differences for different ensembles by looking at Fig. 4.16, which shows the quark mass dependence of the pion decay constant extracted from the PP-SS correlator. The dashed vertical lines show the analyzed difference in the PP-SS case, while the solid vertical lines (left of the dashed lines) show the corresponding matching point difference in the PP case (the length of the solid lines is exactly the same as the length of the vertical lines in Fig. 4.7). Crucially, this difference is the most significant for the $\beta = 4.2$ ensemble and hence it implies a large shift in the difference $f_{\pi}^{overlap} - f_{\pi}^{MTM}$ extrapolated to the continuum limit.



Figure 4.17: Continuum limit scaling of the overlap pion decay constant (extracted from the PP-SS correlator) at the matching mass and two other reference values of $r_0 m_{\pi}$.

Fig. 4.17 shows the continuum limit scaling of the pion decay constant. We again take three reference values of $r_0m_{\pi} \approx 1.5$, $r_0m_{\pi} \approx 1.0$ and the one that corresponds to the matching criterion $r_0m_{\pi} \approx 0.85$. As before, for all analyzed values of r_0m_{π} , we observe good scaling with $\mathcal{O}(a^2)$ leading discretization effects. A comparison to the PP case (Fig. 4.8) indicates that the extrapolated continuum limit value is mostly affected for small r_0m_{π} and there is almost no effect for the largest r_0m_{π} . Also, in all cases the point that is most affected is the one that corresponds to the smallest lattice spacing and the one at $\beta = 3.9$ practically does not move.

Clearly, such behaviour results from the interplay of various effects – intrinsic $\mathcal{O}(a^2)$, unitarity violating $\mathcal{O}(a^2)$ and the zero mode effects. We can not disentangle all of these effects, but a possible qualitative explanation for the observed behaviour can be provided by a working hypothesis that the method of extracting the pion observables from the PP-SS correlation function exactly cancels the contribution of the zero modes, but at the same time introduces the $\mathcal{O}(a^2)$ unitarity violation related to the double pole contribution to the scalar correlator. In this way, the effect of the zero modes may be basically equal for all lattice spacings (as expected for a finite volume effect), but the unitarity violation effect causes that the pion decay constant



Figure 4.18: Continuum limit scaling of the difference of the overlap (from the PP-SS correlator) and MTM pion decay constant at the matching mass.

increases by an $\mathcal{O}(a^2)$ term. Hence, one might expect that at even larger lattice spacing, the pion decay constant extracted from the PP-SS correlator at the matching mass would be even larger than the one from the PP correlator, since then the unitarity violation effect could be larger than the finite-volume contribution of the zero modes.

The essential question is whether the continuum limit of the pion decay constant extracted from the PP-SS correlation function agrees with the MTM continuum limit. Fig. 4.18 shows the differences $r_0(f_{\pi}^{overlap} - f_{\pi}^{MTM})$ for the investigated lattice spacings and the value extrapolated to a = 0 is consistent with zero.

Hence, we can conclude that the continuum limit of the pion decay constant computed for two different discretizations of valence quarks is the same, provided that one takes into account the role of the chiral zero modes of the overlap operator, i.e. they have to be subtracted from the overlap data in order to compare the continuum limits.

4.5 The role of the zero modes – finite volume effects analysis

4.5.1 Simulation parameters

In order to check the finite volume effects in the current setup, we have investigated two additional ensembles at the coarsest lattice spacing $a \approx$ 0.079 fm, corresponding to $\beta = 3.9$ and with the same sea quark mass value $a\mu = 0.004$. The parameters are (including the ensemble at the smallest volume):

- $16^3 \times 32$, $L \approx 1.3$ fm, 544 configurations,
- $20^3 \times 40$, $L \approx 1.7$ fm, 239 configurations,
- $24^3 \times 48$, $L \approx 2.0$ fm, 435 configurations.

In order to minimize the effect of autocorrelations, for propagator computations we have chosen every 10th Monte Carlo trajectory (for L/a = 16, 24) or every 20th trajectory (for L/a = 20). In addition, for the L/a = 24ensemble, we have used the fully linked sources, described in Section 3.4.1. Thus, only 1 inversion per gauge field configuration is required to construct the pseudoscalar correlation function. However, in this way it is not possible to calculate the scalar correlator and hence extract the pion decay constant from the PP-SS correlator.

4.5.2 Matching the pion mass – PP correlator

Finite volume effects in the quark mass dependence of the pion mass can be seen in Fig. 4.19. The finite-volume effect corresponding to a change in the linear extent of the lattice from 1.3 to 1.7 fm is significant and approximately equal for the overlap and the MTM case, whereas the effect of going from 1.7 to 2.0 fm is very small in both cases. The only exception to this observation can be discerned for the lightest valence quark masses, where the decrease related to the change in volume is noticeable. This is especially meaningful if the extrapolation to the chiral limit is performed. For L/a = 20 it clearly gives a non-zero value, which means that the effects of the zero modes are still very important. In turn, for L/a = 24, the chirally extrapolated value of m_{π} is much closer to zero, signalling that the importance of the zero modes effect decreases. However, m_{π} at $m_q = 0$ is still non-zero and therefore one should expect that the contribution of the zero modes is still non-negligible.

Fig. 4.19 also shows the matching mass values for each volume:



Figure 4.19: Matching the pion mass for 3 different volumes at a fixed lattice spacing $a \approx 0.079$ fm.

- $L/a = 16 a\hat{m} = 0.007(1),$
- $L/a = 20 a\hat{m} = 0.007(1),$
- $L/a = 24 a\hat{m} = 0.008(1)$.

For all volumes, the matching mass is approximately the same, which is due to the fact that the finite volume effects (in the pion mass) of overlap and MTM fermions are very similar.

4.5.3 Pion decay constant – PP correlator

Fig. 4.20 shows the quark mass dependence of the pion decay constant for three investigated volumes, together with the values in the unitary MTM setup. The difference in f_{π} at the matching point decreases as the volume is increased, which is in accordance with the expectation based on the fact that the zero modes contribution is a finite volume effect. However, the discrepancy between the overlap and MTM values for $L \approx 2$ fm is still rather



Figure 4.20: The quark mass dependence of the pion decay constant for 3 different volumes at a fixed lattice spacing $a \approx 0.079$ fm.

large (of order $15 \pm 5\%$) and one can suspect that the zero modes still play a non-negligible (although much reduced) role.

This is further illustrated in Fig. 4.21, which shows the difference in f_{π} as a function of the lattice size L/a. One can estimate from this plot that at L/a = 32 it would be of the order of a few percent, thus signalling that the contribution of the zero modes is negligible for practical reasons. This analysis is performed at a non-zero lattice spacing and hence it can not be expected that the difference in f_{π} goes to zero even in infinite volume – at the matching point one expects an $\mathcal{O}(a^2)$ difference due to different discretization effects from different sea and valence quarks actions. However, a test at L/a = 32, which corresponds to $L \approx 2.6$ fm is beyond the scope of this work, since it would require a very computer-time intensive computation.



Figure 4.21: The relative difference between the overlap and MTM pion decay constant at the matching point.

4.6 The role of the zero modes – small volume, heavier sea quark mass

4.6.1 Motivation and simulation setup

We now investigate the effects of the zero modes for a heavier sea quark mass. The motivation for this test is provided by Fig. 4.22. The solid curve shows the pion mass dependence of the pion decay constant for the mixed action setup of overlap valence quarks and MTM sea quarks (the $\beta = 4.05$, L/a = 20 ensemble). The corresponding unitary point ($a\mu = 0.003$) is situated below the curve and the vertical distance from this point to the overlap curve measures the discrepancy between the overlap and MTM pion decay constants at the matching mass.

The other unitary point corresponds to a heavier sea quark mass ($a\mu = 0.006$) and this point lies very close to the overlap curve. Since the dependence of the valence-valence pion mass and decay constant on the sea quark mass is much smaller than the dependence on the valence quark mass⁴, we

 $^{^4{\}rm This}$ can be estimated from the formulas of Partially Quenched Chiral Perturbation Theory [120, 121].



Figure 4.22: The pion mass dependence of the pion decay constant for overlap valence quarks on MTM sea. Also shown are two unitary points (MTM valence quarks on MTM sea), differing only by the sea quark mass. Parameters: $\beta = 4.05$, L/a = 20.

can expect that the overlap curve for a heavier quark mass will not move substantially from its position for $a\mu = 0.003$, thus implying that the difference between the pion decay constant at the matching mass will be much smaller than the one observed for $a\mu = 0.003$.

An explicit computation of the overlap dependence for $a\mu = 0.006$ will also provide a further check of the hypothesis that the zero modes are responsible for the mismatch in the continuum limit values between the mixed and the unitary approach. Since the matching mass will be heavier, the contribution of the zero modes will be much smaller. Thus, we can expect a smaller mismatch in the continuum limit. Furthermore, we can again check whether the procedure of cancelling the zero modes contribution by taking the PP-SS correlation function will lead to a consistency between the mixed and unitary continuum limit values of the pion decay constant. For this, we will also use ensembles at $\beta = 3.9$ and $\beta = 4.2$ with a heavier quark mass which leads to approximately the same sea-sea pion mass as $a\mu = 0.006$ in the case of the $\beta = 4.05$ ensemble.

Simulation parameters are:

- $16^3 \times 32$, $a \approx 0.079$ fm ($\beta = 3.9$, $r_0/a = 5.25(2)$), $a\mu = 0.0074$, 260 configurations,
- $20^3 \times 48$, $a \approx 0.063$ fm ($\beta = 4.05$, $r_0/a = 6.61(2)$), $a\mu = 0.006$, 299 configurations,
- $24^3 \times 48$, $a \approx 0.051$ fm ($\beta = 4.2$, $r_0/a = 8.33(5)$), $a\mu = 0.005$, 137 configurations.

In order to minimize the effect of autocorrelations, we have chosen every 16th Monte Carlo trajectory (at $\beta = 3.9, 4.2$) or every 20th trajectory (at $\beta = 4.05$) for inversions with the overlap Dirac operator.

4.6.2 Pion decay constant – scaling test

To perform the pion decay constant continuum limit scaling test, we first have to find the matching quark masses for each ensemble. For this, we have found the quark mass dependence of the pion mass. The pion mass has been extracted from the PP correlator – hence we expect that it might be contaminated by zero modes effects. It is interesting to compare the quark mass dependence of the pion mass for the cases of the light sea quark mass and the heavier one. Superimposing the heavier sea quark mass curves on the corresponding ones for light sea quark mass, one finds that they are consistent within statistical error (hence, we don't show this plot for the heavier sea quark mass case), i.e. that at most a mild dependence of the valence-valence pion mass on the sea quark mass can be observed. This is in agreement with the predictions of Partially Quenched Chiral Perturbation Theory, i.e. this dependence should be very small.

However, since the sea-sea pion mass changes substantially when the sea quark mass value is increased (it is $r_0m_{\pi} \approx 1$ for all cases), there is a substantial change of the matching mass values:

- $\beta = 3.9 a\hat{m} = 0.015(1),$
- $\beta = 4.05 a\hat{m} = 0.011(1),$
- $\beta = 4.2 a\hat{m} = 0.009(1).$

We now proceed to analyze the quark mass dependence of the pion decay constant. Again, the curves corresponding to both values of the sea quark mass for each ensemble are very close to each other. The sea-sea pion decay constant values are for practical reasons equal for all ensembles and considerably higher than in the case of light sea quark mass. This implies that the differences at the matching point are much smaller than in the latter case.



Figure 4.23: Continuum limit scaling of the overlap pion decay constant at the matching mass – light and heavier sea quark mass.

In Fig. 4.23, we show the results of the continuum limit scaling test for the matching mass, contrasting the cut-off effects in the case of the two sea quark masses. Also in the case of the heavier sea quark mass, the leading discretization effects are $\mathcal{O}(a^2)^{-5}$. Moreover, they are smaller in the case of the heavier sea quark mass, i.e. the slope of the lattice spacing dependence is smaller in this case.

The corresponding scaling plot for the MTM case (only heavier sea quark mass) is shown in Fig. 4.24. Since we work at maximal twist, the leading cut-off effects are also $\mathcal{O}(a^2)$. However, the slope of the fitted line is negative in this case, as opposed to a positive slope in the case of the light sea quark mass.

To assess the role of the zero modes for heavier sea quark mass, a similar analysis has also been performed using the PP-SS correlator to extract the pion mass and decay constant. Here we just quote the values of the matching mass for this case:

- $\beta = 3.9 a\hat{m} = 0.0165(15),$
- $\beta = 4.05 a\hat{m} = 0.012(1),$

⁵We have also checked that for other reference values of $r_0 m_{\pi}$ the leading cut-off effects are also $\mathcal{O}(a^2)$.



Figure 4.24: Continuum limit scaling of the MTM pion decay constant at the matching mass. The case of the heavier sea quark mass.



Figure 4.25: Continuum limit scaling of the difference of the overlap and MTM pion decay constant at the matching mass. The case of the heavier sea quark mass, PP and PP-SS correlators.
• $\beta = 4.2 - a\hat{m} = 0.0095(15).$

At these values of the matching masses, the pion decay constant has been calculated. Again, the scaling test shows that the leading discretization effects are $\mathcal{O}(a^2)$.

The essential issue is now to compare the continuum limits of the overlap and MTM discretization, with the overlap data from both the PP and the PP-SS correlator. In Fig. 4.25 we plot the difference $r_0(f_{\pi}^{overlap} - f_{\pi}^{MTM})$ between overlap (PP) vs. MTM and overlap (PP-SS) vs. MTM (slightly shifted to the right for better presentation). The difference $r_0(f_{\pi}^{overlap} - f_{\pi}^{MTM})$ is consistent with zero in both cases. However, the subtraction of the scalar correlator still affects the pion observables, which is especially visible at the coarsest lattice spacing. This allows us to conclude that the role of the zero modes at the matching mass corresponding to the heavier sea quark mass is very much reduced with respect to the light quark mass. It is, nevertheless, still nonnegligible at this sea quark mass and this volume.

4.7 The role of the zero modes – conclusion

In this section, we gather the most relevant conclusions regarding the role of the zero modes.

We have investigated the role of the zero modes in three contexts:

- fixed volume corresponding to linear lattice extent of $L \approx 1.3$ fm, fixed pion mass, corresponding in infinite volume to $m_{\pi} \approx 300$ MeV, 3 lattice spacings -0.051, 0.063, 0.079 fm,
- fixed lattice spacing $a \approx 0.079$ fm (fixed $\beta = 3.9$), fixed pion mass $m_{\pi} \approx 300$ MeV, 3 volumes with L ranging from 1.3 to 2.0 fm,
- fixed volume corresponding to linear lattice extent of $L \approx 1.3$ fm, fixed pion mass, corresponding in infinite volume to $m_{\pi} \approx 450$ MeV, 3 lattice spacings -0.051, 0.063, 0.079 fm.

The first and third setup allowed us to test the continuum limit scaling of the pion decay constant and assess the influence of the quark mass on the contribution of the zero modes. The second setup enabled us to estimate the volume dependence of the zero modes effects. Clearly, the role of the zero modes is non-negligible in all of the investigated cases. We have shown that it is considerably reduced at $L \approx 2.0$ fm and sea quark masses corresponding to $m_{\pi} \approx 300$ MeV and at $L \approx 1.3$ fm and sea quark masses giving $m_{\pi} \approx 450$ MeV. The analysis of finite volume effects allowed us to conclude that in the



Figure 4.26: The safe, hazardous and non-safe regions of parameters in physical units (linear extent of the lattice vs. pion mass) in mixed action simulations with overlap valence and MTM sea quarks. The "safe" region corresponds to parameters for which the effects of chiral zero modes of the overlap operator are negligible.

case of $m_{\pi} \approx 300$ MeV, one can expect that a linear lattice extent of $L \approx 2.6$ fm would be needed to ensure that the zero modes effects can be neglected. At the higher pion mass of $m_{\pi} \approx 450$ MeV, the corresponding "safe" lattice volume can be estimated to be around $L \approx 2.0$ fm.

These conclusions are summarized in Fig. 4.26, which shows our estimates of the parameters that are needed to ensure that one is safe against the contribution of zero modes. As their role decreases when the sea quark mass is increased, the linear lattice extent that is needed to simulate in the *safe* region also decreases with increasing matching pion mass. We have also distinguished a region where the zero modes effects are reduced, although they are still non-negligible (the *hazardous* region). If the lattice linear extent is too small with respect to the pion mass, the simulation results may be strongly contaminated by unsuppressed contribution from the zero modes (the *non-safe* region). In this region, one has to be very careful when interpreting the results of simulations – certain observables may be largely affected and a wrong continuum limit may be reached. We have to emphasize here that the boundaries of the regions are not sharp – the effects of the zero modes are clearly observable-dependent. However, the plot may serve as a hint on the parameter values (lattice size and matching pion mass) that are needed to avoid the non-physical contributions from the zero modes.

4.8 Explicit subtraction of zero modes

In addition to subtracting the zero modes contribution by constructing the PP-SS correlator, it is also possible to explicitly compute the zero modes of the overlap Dirac operator and subtract them from the propagators. We will use this procedure to cross-check the conclusion about the role of the zero modes. However, we will also show that this procedure is dangerous and hence its results have to be interpreted with caution.

4.8.1 Subtraction procedure

The starting point for this analysis is again the spectral decomposition of the propagator (4.9). The full propagator is obtained from a standard inversion. In addition, we can construct the propagator coming only from the zero modes:

$$S^{0}(x,y) = \sum_{\lambda_{i}=0} \frac{\phi_{i}(x)\phi_{i}^{\dagger}(y)}{\lambda_{i}+m_{q}},$$
(4.19)

where the sum runs only over the zero eigenvalues. Then, we can subtract S^0 from the full propagator, thus arriving at the propagator coming only from the non-zero modes:

$$S^{N}(x,y) = S(x,y) - S^{0}(x,y).$$
(4.20)

The drawback of this method is that the calculation of the zero modes of the overlap operator is computer-time intensive. We have chosen the following method for this computation [122]. We construct the operators:

$$\hat{D}_{\pm} = P_{\pm} \hat{D}_{ov}(0) P_{\pm}, \tag{4.21}$$

where $P_{\pm} \equiv (1\pm\gamma_5)/2$. It can be shown that the spectrum of both \hat{D}_+ and $\hat{D}_$ is exactly the same for the non-chiral (non-zero) modes, but the chiral zero modes in the positive (negative) chirality sector occur only in the spectrum of \hat{D}_+ (\hat{D}_-). Clearly, the zero modes of the operators \hat{D}_{\pm} are also zero modes of the massless Dirac operator $\hat{D}_{ov}(0)$, due to the Ginsparg-Wilson relation.

In practical computations, we therefore compute a certain number of eigenvalues of both \hat{D}_+ and \hat{D}_- and thus we can identify the zero eigenvalues and their corresponding eigenvectors.

Hence, we can compute the propagator coming only from the zero modes. Since the full propagators in our setup are spinors of the form $\Psi = \hat{D}_{ov}^{-1}(m_q)\eta$, where η are stochastic sources, we have to take it into account by using the following formula:

$$\Psi^{0} = \sum_{\lambda_{i}=0} \frac{1}{m_{q}} \phi_{i}^{\alpha} \phi_{i}^{\dagger} \eta.$$
(4.22)

Then, we obtain the propagators from non-zero modes by taking the difference $\Psi - \Psi^0$ and from this object all relevant correlation functions can be constructed. At the level of correlators, only the part $C_{NN}(t)$ is thus calculated (eq. (4.15)), i.e. subtraction of the zero modes at the level of propagators removes the diagonal contributions $C_{00}(t)$ and the mixed contributions $C_{0N}(t)$, $C_{N0}(t)$ of the zero modes.

In Appendix D we present the results of a free-field test of routines used to subtract the zero modes at the level of propagators, which confirms that the subtraction procedure is performed in the correct way.

4.8.2 Effects of explicit zero modes subtraction

An effect of the subtraction procedure on the pion mass and decay constant (with respect to the PP case) can be observed in Figs. 4.27 and 4.28. For comparison, also the curves corresponding to the PP-SS case are plotted.

The pion mass extracted from the PP-SS correlator and the PP correlator with subtracted zero modes (PP subtr.) agree for small quark masses, while the behaviour of the pion decay constant is very different. At the level of correlation functions, this results from the fact that the PP subtr. correlator has a very similar slope to the one of the PP-SS correlator, but its matrix element is significantly lower.

For larger quark masses (larger than $r_0m_q \approx 0.08$), the pion masses extracted from the PP-SS and the PP subtr. correlators are not consistent with each other – the PP subtr. curve changes slope and deviates the more from the PP-SS curve the larger the quark mass. This is in apparent contradiction with the expectation that explicit subtraction of zero modes removes the contribution of these modes, since at larger quark mass values this contribution tends to zero and the PP subtr. curve should converge to the PP (and PP-SS) curve. Such behaviour of the pion mass from the PP subtr. correlator provides a warning about the explicit subtraction method. It was observed before in quenched studies with the fixed point Dirac operator, which is another variant of a chirally improved lattice Dirac operator. The studies by Hauswirth [123] and Gattringer et al. [124] obtained a similar picture – the pion mass at small quark mass is approximately the same from the PP-SS



Figure 4.27: The comparison of the quark mass dependence of the pion mass extracted from PP, PP-SS and PP with explicitly subtracted zero modes (PP subtr.) correlators for $\beta = 3.9$ ensemble.



Figure 4.28: The comparison of the quark mass dependence of the pion decay constant extracted from PP, PP-SS and PP with explicitly subtracted zero modes (PP subtr.) correlators for $\beta = 3.9$ ensemble.



Figure 4.29: Effective mass plateaus for PP subtr. correlation functions. Parameters: $\beta = 3.9$, L/a = 16, $a\mu = 0.004$. Upper plot: $am_q = 0.011$. Lower plot: $am_q = 0.04$.

and the PP subtr. correlator, while at larger quark masses the PP subtr. correlation function leads to much smaller pion masses than ones obtained from the PP and PP-SS correlators (which tend to agree at quark masses for which the effects of zero modes are negligible).

This conclusion is further confirmed by Fig. 4.29, which shows the effective pion mass plateaus from the PP subtr. correlator, for two quark masses – the matching mass (upper plot) and a significantly heavier mass (lower plot). The plateau observed for the matching mass looks rather normal, which means that the shape of the correlation function is the one expected from the spectral decomposition (1.83). However, for the heavier quark mass, there is no plateau (this plot can be compared to Fig. 4.5, which shows the same quark mass, but the effective mass is extracted from the (unsubtracted) PP correlator). This implies that the PP subtr. correlation function might not be a sum of exponential functions, but rather a sum of power functions. This results from the fact that explicit subtraction of zero modes is a non-local procedure, i.e. it can modify the simulated theory in a non-local way, thus leading to unphysical effects in the correlation functions, which causes that the spectral decomposition (1.83) is not valid. It also implies that the pion mass values obtained from the PP subtr. correlator are not meaningful at high values of the quark mass. However, since there is no fundamental reason why different quark masses should lead to qualitatively different behaviour of the correlation functions, we can not be sure that even at a relatively small quark mass (such as the matching mass) the subtraction procedure is valid.

The above discussion leads to a conclusion that explicit subtraction of zero modes is a dangerous hand-made procedure, which may lead to uncontrollable unphysical effects in the extracted observables. However, since we have observed the consistency between the pion masses from the PP-SS and PP subtr. correlators (for relatively small quark masses), we may assume here as a working hypothesis that at the matching mass the explicit subtraction procedure is valid, i.e. that the unphysical effects of subtraction are small. This is justified by the fact that the effective mass plateau for the matching mass does not show the pathology observed at the larger quark mass.

To conclude this subsection, we show in Fig. 4.30 the scalar correlation function with explicitly subtracted zero modes (SS subtr.) for two values of the valence quark mass – the lightest considered mass and the matching mass. The plot shows that the dominant contribution to the full SS correlator comes from the zero modes (the SS subtr. curve for $am_q = 0.004$ should be compared to the full SS curve at the same quark mass – Fig. 4.13). Moreover, after the zero modes are subtracted, the scalar correlator is negative, which may be attributed to the unitarity violation effect discussed in Section 4.1. We have also hypothesized in Section 4.4 that this effect influences the pion decay constant extracted from the PP-SS correlator. This would also explain the difference in f_{π} extracted from the PP-SS and PP subtr. correlators – the latter does not have the enhanced unitarity violation effect from the scalar correlator. This effect will be investigated further in the next chapter.

In the next subsection we will use the PP subtr. correlation function to extract the pion decay constant and perform its continuum limit scaling test.



Figure 4.30: The SS subtr. correlation function (SS with explicitly subtracted zero modes). Parameters: $\beta = 3.9$, L/a = 16, $a\mu = 0.004$, 2 valence quark masses: $am_q = 0.004$, $am_q = 0.011$ (matching mass).

The results will not be contaminated by the zero modes contribution, but we again emphasize that they have to be interpreted with caution, due to the fact that the subtraction procedure is not clean from the field-theoretical point of view.

4.8.3 Pion decay constant – scaling test – PP subtr. correlator

We again begin by finding the matching mass for each ensemble. The results of the matching procedure are shown in Fig. 4.31 and the bare overlap quark masses that lead to the same pion mass as in the unitary setup are:

- $\beta = 3.9 a\hat{m} = 0.0115(15),$
- $\beta = 4.05 a\hat{m} = 0.0065(15),$
- $\beta = 4.2 a\hat{m} = 0.0055(15).$

These matching masses are consistent with the ones obtained from the PP-SS correlation function, confirming again the conclusion that these methods give consistent results for small quark masses.



Figure 4.31: Matching the pion mass (extracted from the PP subtr. correlator) for three values of the lattice spacing, corresponding to $\beta = 3.9$, 4.05 and 4.2.

The curves that show the quark mass dependence of the pion decay constant extracted from the PP correlator with explicitly subtracted zero modes (PP subtr.) lie well below the corresponding curves for the PP and the PP-SS case (Fig. 4.32). This effect has already been discussed in the previous subsection. In comparison with the PP case, the values of the pion decay constant at the matching mass are very much reduced, which is shown in the plots by vertical lines – the dashed ones correspond to the difference in the pion decay constant in the PP subtr. case and the solid ones to the PP case.



Figure 4.32: The dependence of the pion decay constant on the bare overlap quark mass. The dashed lines correspond to the matching quark masses $a\hat{m}$ (from PP subtr. correlator). The solid vertical lines (left of the dashed lines) show the difference of $f_{\pi}^{overlap}$ and f_{π}^{MTM} (at the matching mass) extracted from the PP correlator.

Again, the influence of zero modes cancellation is relatively the largest for $\beta = 4.2$.

Fig. 4.33 shows the continuum limit scaling of the pion decay constant for three reference values of $r_0m_{\pi} \approx 1.3$ (here we take the highest value available for the $\beta = 3.9$ ensemble), $r_0m_{\pi} \approx 1.0$ and the one that corresponds to the matching criterion $r_0m_{\pi} \approx 0.85$. As in the previous cases of the PP and the PP-SS correlation functions, we observe good scaling behaviour for all analyzed values of r_0m_{π} , with $\mathcal{O}(a^2)$ leading cut-off effects.

Moreover, the continuum limit of the pion decay constant extracted from the PP subtr. correlation function agrees with the MTM continuum limit, which is shown in Fig. 4.34. Therefore, both methods of subtracting the zero modes lead to a consistent continuum limit value, which is the one of the unitary approach. This is a strong hint that the zero modes are indeed responsible for the observed behaviour of the pion decay constant extracted



Figure 4.33: Continuum limit scaling of the overlap pion decay constant (extracted from the PP subtr. correlator) at the matching mass and two other reference values of $r_0 m_{\pi}$.

from the PP correlator, i.e. for the wrong continuum limit value of this observable.

However, we have to emphasize again that the results of the explicit zero modes subtraction procedure have to be treated with caution. The consistency between both methods is a hint that the pathological effects of the hand-made subtraction procedure are not very large at the matching mass, but this method of cancelling the zero modes contribution is not recommended, since there is no systematic way to control the potential non-physical effects.

A clearly safer procedure to remove the contribution of the zero modes is the one with the PP-SS correlation function. This method does not suffer from the aforementioned effects, since no modification at the level of propagators is made. In this way, both the PP and SS correlation functions have the proper spectral decomposition and, as we have shown, the contribution of the zero modes is exactly cancelled in the correlator difference. The price to pay, however, is that the scalar correlator may introduce enhanced unitarity violations coming from the double pole contribution specific to non-unitary approaches (quenched, partially quenched and mixed action theories). On the other hand, such effects are $\mathcal{O}(a^2)$ lattice artefacts and hence should



Figure 4.34: Continuum limit scaling of the difference of the overlap (from the PP subtr. correlator) and MTM pion decay constant at the matching mass.

not affect extrapolations to the continuum limit. This effect will be further analyzed in the next chapter.

Chapter 5

Various further results

In the previous chapter we have performed an analysis of the continuum limit scaling of the pion decay constant. We have discussed the role of the zero modes in a mixed action setup of chirally-symmetric valence quarks and non-chirally-symmetric sea quarks. To cancel the non-physical contribution of the zero modes we have used the PP-SS correlation function and we have hypothesized that while this correlator correctly removes the zero modes contribution, it also introduces enhanced unitarity violations. In this chapter we will analyze this effect. We will also present some additional results regarding the continuum limit scaling of baryon (nucleon and delta) masses, as well as some topological aspects.

5.1 Unitarity violations

In this section we attempt at an analysis of the unitarity violation described in Section 4.1. We begin by illustrating this effect more clearly, taking as an example the behaviour of the pion decay constant at one lattice spacing $a \approx 0.079$ fm. Finite volume effects in f_{π} extracted from the PP correlator were analyzed in Section 4.5. We now show the outcome of the analogous analysis for the PP-SS correlation function.

5.1.1 Motivation

We have remarked earlier that the computation of propagators for the L/a = 24 ensemble was done with fully linked stochastic sources, which means that there was only 1 inversion per gauge field configuration and thus it was not possible to compute the scalar correlator for this volume. However, at the earlier stage of this project this ensemble was partly analyzed using point



Figure 5.1: Matching the pion mass (from the PP-SS correlator) for 3 different volumes at a fixed lattice spacing $a \approx 0.079$ fm.

sources (with 54 independent gauge field configurations and 12 inversions per configuration) [93] and in this part of the work we use the correlation functions computed at that stage, including the scalar correlation function. This enables us to perform the finite volume effects test also for the PP-SS correlator.

Fig. 5.1 shows the quark mass dependence of the pion mass extracted from the PP-SS correlator. With this method of computing the pion mass, the linear extrapolation of m_{π}^2 to the chiral limit gives a value consistent with zero for all three volumes, thus indicating that the contribution of the zero modes has been cancelled.

The matching mass values are for each volume:

- $L/a = 16 a\hat{m} = 0.011(1),$
- $L/a = 20 a\hat{m} = 0.009(1),$
- $L/a = 24 a\hat{m} = 0.008(1)$.



Figure 5.2: The dependence of the pion decay constant on the bare overlap quark mass. The dashed lines correspond to the matching quark masses $a\hat{m}$ (from the PP-SS correlator). The solid vertical lines (left of the dashed lines) show the difference of $f_{\pi}^{overlap}$ and f_{π}^{MTM} (at the matching mass) extracted from the PP correlator.

With these values, we can compare the pion decay constant at the matching mass from the PP and the PP-SS correlator.

The comparison of the pion decay constant at the matching mass is shown in Fig. 5.2. The subtraction of the zero modes by means of taking the PP-SS correlation function has very little effect for all volumes. However, in the previous chapter, we have shown that the effect of the zero modes is present in the pion decay constant and since we observe no effect on this observable when taking the PP-SS correlator values, we can conclude that there must be two competing effects emerging when taking the difference of PP and SS correlation functions:

- 1. removal of the zero mode contribution (finite volume effect) decreases the value of f_{π} ,
- 2. contamination by the unitarity violation ($\mathcal{O}(a^2)$ effect) increases the

value of f_{π} .

Our analysis suggests that these two effects roughly compensate each other at $\beta = 3.9$, while the zero modes removal effect dominates the unitarity violation effect at $\beta = 4.05$ and $\beta = 4.2$. We will now proceed to explicitly investigate the unitarity violation effect.

5.1.2 Small volume analysis

For convenience, we rewrite here the formula for the scalar correlation function at the matching mass:

$$C_{SS}(t) \xrightarrow{t \to \infty} -\frac{B_0^2}{2L^3} \frac{e^{-2M_{VV}t}}{M_{VV}^3} \left(\gamma_{VV} + \gamma_{SS} - 2\gamma_{VS}\right) a^2 t.$$
(5.1)

The low-energy constants $\gamma_{VV} = \gamma_{VS} = 0$, due to exact chiral symmetry in the valence sector [110], but γ_{SS} is non-vanishing, since the sea Dirac operator is not chirally-symmetric.

Formula (5.1) implies that the scalar correlation function for the matching quark mass can become negative at large times (provided that $\gamma_{SS} > 0$). However, the shape of this correlator is basically the one observed in Fig. 4.13, which shows the $\beta = 3.9$ case at a quark mass below the matching mass. Clearly, this correlation function does not become negative, since it has a large positive contribution from the zero modes and the unitarity violation effect is obscured.

In order to analyze the effect predicted by eq. (5.1), we would have to remove the zero mode contribution from the scalar correlator or work at large enough volume and quark mass so that this contribution would be negligible. The latter requires a very computer-time intensive computation and is hence beyond the scope of the current project. However, such analysis is planned for the future and would provide the cleanest way of testing the prediction of eq. (5.1).

In the current project, we therefore have to restrict ourselves to the former method, i.e. to remove the zero mode contribution from the SS correlator. This is possible by following the procedure of explicit subtraction of zero modes at the level of propagators. As we have shown in the previous chapter, this is a dangerous procedure with hard to control systematic effects. Therefore, the results of this analysis have to be interpreted with caution and treated as an outlook on this kind of analysis, which will be later performed in a clean setup of large volume and large enough quark mass, so that the zero mode effects will be negligible. An alternative approach could consist in using only configurations in the trivial topological sector, which are not contaminated by zero modes effects. However, the number of available configurations in this sector is too small to allow for meaningful fits of eq. (5.1).

Fig. 4.30 shows that after the zero mode contribution is removed, the scalar correlator at the matching mass becomes negative indeed. We have also checked that the SS correlator on topologically trivial configurations is negative at large time (the error bands are too large to perform fits of eq. (5.1), however, the conclusion about the sign of the correlator is unambiguous), which confirms that the unitarity effect is really present in our mixed action setup.

Our strategy is the following. We use three small-volume ensembles whose parameters are given in Section 4.2.1 and explicitly subtract the zero modes at the level of propagators, as described in Section 4.8.1. In this way, we obtain for each ensemble the SS subtr. correlator at the matching mass. Then, we fit eq. (5.1) to the lattice data.

Specifically, we write this equation as:

$$C_{SS}(t) \stackrel{t \to \infty}{=} -\gamma t \, e^{-2M_{VV}t}. \tag{5.2}$$

where we have defined a parameter γ :

$$\gamma \equiv \frac{B_0^2 \gamma_{SS}}{2(M_{VV}L)^3} a^2 \equiv \tilde{\gamma} a^2.$$
(5.3)

Since the temporal extent of the lattice is finite and equals T for each ensemble (with periodic boundary conditions in time), the fitting formula that we use reads:

$$C_{SS}(t) \stackrel{t \text{ large}}{=} -\gamma \left(t \, e^{-2M_{VV}t} + (T-t) \, e^{-2M_{VV}(T-t)} \right). \tag{5.4}$$

The parameters that we fit are γ and the pion mass M_{VV} . The definition of the parameter γ implies that γ should have a quadratic dependence on the lattice spacing, since B_0 and γ_{SS} are low-energy constants and $M_{VV}L$ is approximately the same for each ensemble.

The fit for the ensemble at the coarsest lattice spacing ($\beta = 3.9$) is shown in Fig. 5.3. The fitting interval is $t \in [9, 23]$ and in this interval the fit represents a very good description of lattice data. Qualitatively similar behaviour is observed also in the $\beta = 4.05$ and $\beta = 4.2$ cases.

One of the fitting parameters is the pion mass M_{VV} . Its values extracted from the fits can be compared with values of the matching pion mass (known precisely from the maximally twisted mass PP correlator). This provides a consistency check for the fits. In all cases the fitted values of M_{VV} are around



Figure 5.3: The SS subtr. correlation function at the matching mass. The solid line represents the fit of eq. (5.4).

2 standard deviations below the matching pion mass. This is a reasonable agreement, taking into account the unknown systematic effect related to the subtraction procedure.

The fitting parameter γ has a few sources of uncertainties, related to:

- 1. statistical errors in $C_{SS}(t)$ (error bars in Fig. 5.3),
- 2. the choice of the fitting interval to estimate it we have performed several fits with different fitting intervals,
- 3. errors of the matching procedure to estimate it we have performed fits not only for the matching quark masses, but also for quark masses differing in lattice units by ± 0.001 (which corresponds to the error in the matching mass),
- 4. the fact that the product $M_{VV}L$ is not exactly matched for all ensembles,
- 5. unknown values of the renormalization constant Z_S of the scalar current we assume that Z_S is equal for all ensembles,
- 6. an unknown systematic error introduced by the zero modes subtraction procedure.



Figure 5.4: Continuum limit scaling of the fitting parameter γ , defined by eq. (5.3).

Fig. 5.4 shows the fitted values of γ . The errors on each value include sources 1-4 from the above list of uncertainties. The error related to the unknown value of Z_S should be rather small compared to the overall size of the error from sources 1-4. We have not tried to estimate the error related to the zero modes subtraction procedure.

We observe good scaling of the parameter γ with leading $\mathcal{O}(a^2)$ cut-off dependence. The value of this parameter extrapolated to the continuum is consistent with zero. This result is in very good agreement with the hypothesis that the scalar correlator is influenced by the unitarity violation effect predicted and analyzed in [107, 108, 109, 110]. It also provides an explanation for the behaviour described in the previous subsection, i.e. the seemingly inconsistent with the hypothesis about the role of the zero modes lack of effect of subtracting the SS correlator at $\beta = 3.9$. The unitarity violations analysis suggests that there are indeed two competing effects in the PP-SS correlator – the zero mode contribution is removed, but the correlator is contaminated by a unitarity violation originating from an enhanced double pole contribution. These two effects are roughly balanced at $\beta = 3.9$, but at $\beta = 4.05$ and $\beta = 4.2$, the finite volume effect of the zero modes cancellation dominates over the $\mathcal{O}(a^2)$ unitarity violation effect, which is smaller at these lattice spacings. This interplay of effects also explains the difference between the pion decay constant extracted from the PP-SS and the PP subtr. correlator, since the latter does not have the double pole contribution of the SS correlator. However, it has to be remembered that this analysis has been performed with the unphysical zero modes subtraction procedure and it may suffer from unpredictable effects. Therefore, this analysis has to be treated with caution. It provides a plausible explanation of the observed effects. However, in order to quantitatively analyze the effect of unitarity violations in the scalar correlator and reliably extract the low-energy constant γ_{SS} , a simulation with large enough volume and quark mass would have to be performed in order to have a negligible contribution from the zero modes to the full scalar correlator (without explicit subtraction procedure). In addition, eq. (5.1) was derived for an infinite volume and hence it would be very advantageous to have large volume data for the SS correlation function in order to use the fitting ansatz of this formula in an appropriate way.

5.2 Light baryon masses

In this section, we show the results of a calculation of light baryon masses in the case of overlap valence and MTM sea quarks, as well as in the unitary setup [112]. Particularly, we would like to compare the overlap and MTM values at the matching mass and check whether they have the same continuum limit.

The calculation of baryon correlation functions with stochastic sources yields an unfavourable noise-to-signal ratio [125]. Therefore, we repeated the propagator computation using Gaussian smeared point sources, where the smearing helps significantly to suppress excited state contributions [65, 66].

We again used the small-volume, light-quark ensembles with parameters given in Section 4.2.1. We report simulation results at two lattice spacings, corresponding to $\beta = 3.9$ (426 configurations) and $\beta = 4.2$ (around 370 configurations). The simulations at $\beta = 4.05$ are on-going.

The example of effective nucleon mass plateaus in the case of $\beta = 4.2$ is shown in Fig. 5.5. The quality of the plateau is the best at the largest quark mass, but also at overlap quark masses corresponding to the neighbourhood of the matching mass it is reasonable and allows for the extraction of the nucleon mass.

The (overlap) quark mass dependence of the nucleon and delta mass is shown in Fig. 5.6 ($\beta = 3.9$) and Fig. 5.7 ($\beta = 4.2$). We also show the unitary values (horizontal bands) – the lower one corresponds to the nucleon and the upper one to the deltas. In the MTM case, the baryons Δ^{++} and Δ^{+} are



Figure 5.5: The effective nucleon mass plateaus for 3 values of the overlap quark mass. Parameters: $\beta = 4.2$, L/a = 24, $a\mu = 0.002$.

non-degenerate due to isospin symmetry breaking. However, this is an $\mathcal{O}(a^2)$ effect and at the lattice spacings we are working at this effect is consistent with zero. To be precise, at $\beta = 3.9$ we have: $am_{\Delta^{++}} = 0.739(17)$, $am_{\Delta^{++}} = 0.764(19)$ and at $\beta = 4.2$ we obtain: $am_{\Delta^{++}} = 0.512(9)$, $am_{\Delta^{++}} = 0.512(10)$. Hence, on the plots we only show the values for Δ^{++} .

However, we are mostly interested in the comparison of the nucleon and delta masses at the matching mass. Clearly, at both lattice spacings the nucleon and delta masses in the overlap case are consistent with the MTM unitary values. This is further illustrated in Fig. 5.8, which implies that also the continuum limits of both masses are consistent with each other. Since we only have the results for two lattice spacings, we do not quote any number for the continuum limit values.

We conclude that the role of the zero modes for this kind of observables – the light baryon masses – is significantly smaller than in the case of the pion decay constant. We can not exclude that the values that we have extracted are still contaminated by the zero modes effects, but they are not large enough to show at the current level of precision and with only two lattice spacings.



Figure 5.6: The quark mass dependence of the nucleon and delta mass. Parameters: $\beta = 3.9$, L/a = 16, $a\mu = 0.004$.



Figure 5.7: The quark mass dependence of the nucleon and delta mass. Parameters: $\beta = 4.2$, L/a = 24, $a\mu = 0.002$.



Figure 5.8: Continuum limit scaling of the MTM and overlap light baryon masses (nucleon, delta). The overlap masses are computed at the matching mass. The MTM vales are slightly shifted to the left and the overlap ones to the right, for clearer presentation.

In particular, even if the baryon masses are not considerably affected by the zero modes, the matrix elements of the baryonic correlation functions still might change significantly, as is anticipated in [124]. Therefore, this issue will be investigated further in the future [112]. In particular, the role of the zero modes can be assessed by using different interpolating operators for baryonic correlation functions, since different operators couple in a different way to zero modes [124]. Moreover, the explicit subtraction procedure may be followed and the overlap of the sources and the zero modes may be computed.

However, the present analysis already allows us to conclude that the magnitude of the zero modes effects in different observables may be different and that some observables may be much more vulnerable to the zero modes contribution (e.g. f_{π}) than some other (e.g. the baryon masses).

5.3 Topological charge and susceptibility

In this section, we report the results of investigation of some topological issues related to gauge field configurations that we have used. For some of them, we have computed the zero modes, which allows us to calculate their topological



Figure 5.9: Monte Carlo history of the index of the overlap operator for different ensembles. The vertical axis scale is the same for all plots.

charge as the difference of the numbers of zero modes in the negative and positive chirality sectors (eq. (1.79)), i.e. the index of the overlap Dirac operator. In practice, zero modes on a given configuration occur only in one chirality sector or, in other words, the probability of having zero modes in both sectors for the same configuration is zero [122].

Fig. 5.9 shows the Monte Carlo histories of the index of the overlap operator for four different ensembles of configurations: $\beta = 3.9$, L/a = 16, $a\mu = 0.004$; $\beta = 3.9$, L/a = 16, $a\mu = 0.0074$; $\beta = 4.05$, L/a = 20, $a\mu = 0.003$; $\beta = 4.2$, L/a = 24, $a\mu = 0.002$; all of them corresponding to linear lattice extent of $L \approx 1.3$ fm. The plots indicate that the autocorrelations in Monte Carlo time are rather not large and different topological sectors are sampled. The vertical scale on each of the plots is the same and hence it is noticeable that topological charge fluctuations are the largest for $\beta = 3.9$ and considerably smaller and comparable to each other for $\beta = 4.05$ and $\beta = 4.2$.

The histograms of the index are shown in Fig. 5.10. To allow for comparison, the number of configurations which corresponds to the given index N(index) has been normalized by the total number of configurations for each



Figure 5.10: Histograms of the index of the overlap operator for different ensembles. Also shown are Gaussian fits of the distributions. The axes scales are the same for all plots.

ensemble N(total) and the axes are plotted in the same scale. We also show fits to the Gaussian probability distribution:

$$p(Q) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{Q^2}{2\sigma^2}},$$
 (5.5)

where Q is the index and σ is the only fitting coefficient, i.e. we enforce the mean of the distribution to be 0, since the probability distribution should be symmetric with respect to configurations with negative and positive topological charge.

The plots lead to the conclusion that the probability distributions of the index Q are approximately Gaussian. However, the quality of the fits is rather poor – the most frequent value of the index is in two cases at $Q \neq 0$ and in general the symmetry with respect to Q = 0 is not very good. This results from the fact that the total number of configurations for each ensemble is too small and an order of magnitude increase in statistics would be needed to obtain a reliable distribution.



Figure 5.11: Topological susceptibility for 4 ensembles of gauge field configurations. The $m_{\pi} \approx 450$ MeV ensemble is slightly shifted to the right for better visibility.

The fluctuations of the topological charge determine the value of topological susceptibility χ_{top} for each ensemble. This quantity can be computed from eq. (1.81), i.e. as the mean value of the topological charge squared, normalized by the volume. Alternatively, it can also be determined from the Gaussian fit (5.5) as the variance σ^2 , again normalized by the volume. Even though the probability distributions are rather far away from Gaussian, the statistical errors of $\langle Q^2 \rangle$ and of σ^2 are large and we have checked that both methods lead to consistent results. In Fig. 5.11 we plot the results of the former method for three light-quark ensembles with sea quark masses corresponding to the pion mass of around 300 MeV and one ensemble at the heavier pion mass of approximately 450 MeV. However, since the statistical errors are large, a meaningful extrapolation to the continuum limit is not possible – one would clearly need more statistics. The same holds true with regard to the sea quark mass dependence of the topological susceptibility the expected increase of χ_{top} for larger quark mass is observed, but it is not statistically significant.

Therefore, the topological aspects also need to be investigated further in the future – a considerable increase in precision is needed to draw meaningful physical conclusions.

Conclusions and prospects

Chiral symmetry is of utmost importance for low-energy properties of QCD. Therefore, when discretizing QCD on a 4-dimensional space-time grid to address non-perturbative phenomena, retaining chiral symmetry in this lattice version of QCD (LQCD) is an essential element. Hence, chirally-symmetric fermion discretizations are needed to fully explore the low energy regime of QCD. A very appealing kind of chiral fermions are the overlap fermions. However, their use in dynamical Lattice QCD simulations is still a challenge, since they are very demanding from the computational point of view.

Chiral properties of fermions are especially important in the valence sector. At the same time, the most expensive part of a simulation is the generation of gauge field configurations. Hence, a possible way to overcome the cost problem of dynamical overlap simulations, which at the same time keeps their good chiral properties, is to follow a mixed action approach where gauge field configurations are generated using a computationally cheaper fermion discretization and the overlap operator is used only in the valence sector.

The main aim of this thesis was to investigate a particular mixed action setup of overlap valence and maximally twisted mass (MTM) sea quarks. In this way, we could profit from a wide set of gauge field configurations generated by the European Twisted Mass Collaboration (ETMC).

In particular, we wanted to perform a continuum limit scaling test of overlap fermions, a study that has not been done before. However, to perform such investigation with a typical linear lattice extent of 2 fm very large computer resources would be required, even if the overlap operator was used only in the valence sector. Therefore, we decided to employ a small volume with $L \approx 1.3$ fm. Such volume is sufficient to test the continuum limit scaling behaviour. We decided to take the pion decay constant as our main physical observable to study the lattice artefacts of the overlap discretization. Using a suitable matching condition of overlap and twisted mass fermions, for which we have taken the pion mass, and assuming universality, the same continuum limit value for f_{π} should be reached with both kinds of lattice fermions. We explicitly checked in the free theory that this expectation is fulfilled. We

clearly observed the $\mathcal{O}(a^2)$ leading cut-off dependence and demonstrated that f_{π} agrees in the continuum limit.

However, when moving to the interacting case, we encountered a puzzle in that the continuum limits of the two lattice fermions used came out to be inconsistent with each other. It is one of the main results of this thesis that the solution of this puzzle could be identified as the exact chiral zero modes of the overlap Dirac operator. Being chiral, this operator admits zero modes at any value of the lattice spacing. This is in contrast to the non-chiral twisted mass Dirac operator which does not admit such chiral zero modes, at least not at our current values of the lattice spacing. In order to demonstrate that the chiral zero modes are indeed the cause of the mismatch of f_{π} in the continuum limit, we used the fact that the zero modes couple in an identical way to the pseudoscalar and scalar correlation functions. Hence, in the difference of these correlation functions (the socalled PP-SS correlator), the zero modes contribution is exactly cancelled. Performing now a continuum limit scaling test of the pion decay constant as computed from the overlap PP-SS correlator, which is not affected by the zero modes, we obtained indeed consistent continuum limit values for f_{π} computed from the two fermion discretizations.

We also cross-checked this result by explicitly subtracting the zero modes at the level of overlap propagators. This further confirmed the picture that the chiral zero modes need to be treated specially, at least in the small finite volume used here. However, the modification of propagators by explicit subtraction of a part of eigenmodes of the Dirac operator is a field-theoretically not well defined procedure and may lead to uncontrollable systematic uncertainties. Therefore, we interpret our findings when subtracting the zero modes explicitly only as a plausibility check, which however points in the right direction.

The use of the PP-SS correlator is, in contrast, safe from the fieldtheoretical point of view. However, it leads to another difficulty. The subtraction of the zero modes from the scalar correlator introduces significant $\mathcal{O}(a^2)$ effects related to the enhanced double pole contribution to the scalar correlation function, as suggested by results from chiral perturbation theory. This effect results from the fact that the sea and valence quarks are discretized in a different way and thus unitarity is violated at any non-zero value of the lattice spacing. Although being a discretization effect it vanishes in the continuum limit, it may render the approach to this limit difficult.

Therefore, the conceptually cleanest way to tackle the zero mode problem is to avoid the region of parameters where the zero modes contribution is significant. To find this region, we analyzed the dependence of the zero mode effects on the lattice volume and the sea quark mass. In this way, we determined three regimes of parameters: one that is "safe" against the zero modes contribution, a "hazardous" and a "non-safe" regime. We consider the identification of these regions to be the most important result of this work. It allows to provide parameter values for future simulations where problems with the zero modes will be completely absent. The situation is best illustrated in Fig. 4.26. Let us give two explicit examples of the values of pion masses and lattice sizes for safe simulations:

- at $m_{\pi} \approx 300$ MeV, the "safe" linear lattice extent is $L \approx 2.6$ fm,
- at $m_{\pi} \approx 450$ MeV, the "safe" linear lattice extent is down to $L \approx 2.0$ fm.

Clearly, the identification of safe simulation regions for valence overlap fermions is not only important for extensions of the present work, but also for other collaborations worldwide who are using overlap fermions in the valence sector.

Let us finish by giving some directions for further work. We group these in two areas. The first are possible physics targets with the "safe" simulation parameters. With our knowledge of these parameters, we plan to:

- compute observables for which good chiral properties of valence fermions are essential e.g. the kaon bag parameter B_K , or the decay $K \to \pi\pi$;
- investigate questions that are related to topology, i.e. the computation of topological susceptibility and the determination of the singlet meson mass η' ;
- analyze in the mixed action setup unitarity violations in the scalar correlator and in mixed correlation functions (with one valence and one sea quark) this needs a setup with negligible zero modes contribution to isolate this effect;
- confront the simulation results with (Mixed Action) Partially Quenched Chiral Perturbation Theory formulas to extract the corresponding low energy constants;
- perform a continuum limit scaling test of the pion decay constant (and other observables) at larger volume in order to check for the size of quadratic lattice spacing dependence.

Moreover, it would also be interesting to further investigate the role of the zero modes to reach a better understanding. To this end, we plan to:

- test alternative matching conditions, different from the matching of the pion mass. In particular, we plan to compute the necessary renormalization constants in order to use the matching condition of equal renormalized quark masses;
- investigate the role of the zero modes in baryonic observables;
- perform an analysis of topological aspects by explicitly computing the zero modes.

Summarizing, we believe that the results of this work provide an essential and so far missing basis for future large scale simulations using mixed actions. In particular, for our setup of overlap valence and maximally twisted mass sea quarks we have determined simulation parameters for safe simulations on a quantitative level. Thus, respecting the limits on the parameters determined here and performing simulations on large enough lattice volume at a given pion mass, it will be possible to profit from the good chiral properties of overlap fermions and obtain precise physical results for quantities that would be hard to address with non chirally-symmetric versions of lattice fermions.

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Appendix A

Wilson gauge action

We show here that the expression for the Wilson gauge action has the right QCD continuum limit. We will use the Baker-Campbell-Hausdorff formula:

$$e^{aA}e^{aB} = e^{aA+aB+\frac{a^2}{2}[A,B]+\mathcal{O}(a^3)},$$
 (A.1)

generalized to:

$$e^{aA}e^{aB}e^{aC}e^{aD} = e^{a(A+B+C+D)+\frac{a^2}{2}([A,B]+[A,C]+[A,D]+[B,C]+[B,D]+[C,D])+\mathcal{O}(a^3)},$$
(A.2)

setting: $A = igA_{\mu}(x), B = igA_{\nu}(x+a\hat{\mu}), C = igA_{\mu}(x+a\hat{\nu}) \text{ and } D = igA_{\nu}(x)$. Now, inserting (1.30) in (1.33) and using (A.2), we obtain:

$$U_{x,\mu\nu} = \exp\left[iga(A_{\mu}(x) + A_{\nu}(x + a\hat{\mu}) - A_{\mu}(x + a\hat{\nu}) - A_{\nu}(x)) + -\frac{g^{2}a^{2}}{2}\left([A_{\mu}(x), A_{\nu}(x + a\hat{\mu})] - [A_{\mu}(x), A_{\mu}(x + a\hat{\nu})] + -[A_{\mu}(x), A_{\nu}(x)] - [A_{\nu}(x + a\hat{\mu}), A_{\mu}(x + a\hat{\nu})] + -[A_{\nu}(x + a\hat{\mu}), A_{\nu}(x)] + [A_{\mu}(x + a\hat{\nu}), A_{\nu}(x)]\right) + + \mathcal{O}(a^{3})\right].$$
(A.3)

We Taylor-expand terms like:

$$A_{\mu}(x+a\hat{\nu}) \approx A_{\mu}(x) + a\partial_{\nu}A_{\mu}(x) \tag{A.4}$$

to order a and this implies:

$$U_{x,\mu\nu} = \exp\left[iga(a\partial_{\mu}A_{\nu}(x) - a\partial_{\nu}A_{\mu}(x)) + -\frac{g^{2}a^{2}}{2}\left([A_{\mu}(x), A_{\nu}(x)] - [A_{\mu}(x), A_{\mu}(x)] - [A_{\mu}(x), A_{\nu}(x)] - [A_{\nu}(x), A_{\mu}(x)] - [A_{\nu}(x), A_{\nu}(x)] + [A_{\mu}(x), A_{\nu}(x)]\right) + O(a^{3})\right] =$$

$$= \exp\left[iga^{2}\left(\partial_{\mu}A_{\nu}(x) - \partial_{\nu}A_{\mu}(x) + ig[A_{\mu}(x), A_{\nu}(x)]\right) + O(a^{3})\right].$$
(A.5)

From (1.8) and (1.6), the commutator of the gauge fields can be rearranged as:

$$[A_{\mu}(x), A_{\nu}(x)] = A^{b}_{\mu}(x)A^{d}_{\nu}(x)[t_{b}, t_{d}] = if^{bdc}A^{b}_{\mu}(x)A^{d}_{\nu}(x)t_{c}, \qquad (A.6)$$

finally yielding (neglecting $\mathcal{O}(a^3)$ terms):

$$U_{x,\mu\nu} = \exp\left[iga^{2}\left(\partial_{\mu}A_{\nu}(x) - \partial_{\nu}A_{\mu}(x) - gf^{bdc}A^{b}_{\mu}(x)A^{d}_{\nu}(x)t_{c}\right)\right] = \\ = \exp\left[iga^{2}F_{\mu\nu}\right].$$
(A.7)
(A.8)

Expanding to $\mathcal{O}(a^4)$, we obtain for the Wilson action (1.31):

$$S_{gauge}[U] = \beta \sum_{x} \sum_{1 \le \mu < \nu \le 4} \left\{ \frac{g^2 a^4}{6} \operatorname{Tr} F_{\mu\nu}(x)^2 + \mathcal{O}(a^6) \right\}, \qquad (A.9)$$

since $\mathcal{O}(a^2)$ terms are purely imaginary. Finally, we use $\sum_x \sum_{1 \le \mu < \nu \le 4} = \frac{1}{2} \sum_x \sum_{\mu,\nu}$ and the fact that $\operatorname{Tr}(t_a t_b) = \frac{1}{2} \delta_{ab}$ to obtain:

$$S_{gauge}[U] = \beta \frac{g^2 a^4}{6} \sum_{x} \sum_{\mu,\nu} \left\{ \frac{1}{4} F_{\mu\nu}(x)^2 + \mathcal{O}(a^2) \right\}.$$
 (A.10)

Appendix B

Tree-level scaling test

B.1 Overlap fermions

We show here explicitly the computation of the overlap Dirac operator in momentum space, which was given by Lüscher [29]. We begin with the derivation of the kernel operator – the massless Wilson-Dirac operator in momentum space. In position space, this operator is given by:

$$\hat{D}_{\text{Wilson}} = \frac{1}{2} \left(\gamma_{\mu} (\nabla^*_{\mu} + \nabla_{\mu}) - ar \nabla^*_{\mu} \nabla_{\mu} \right), \qquad (B.1)$$

where we use the notation introduced in Chapter 1. The Euclidean action can be written as:

$$S = \sum_{x,y} \bar{\psi}(x) K_{xy} \psi(y), \qquad (B.2)$$

with:

$$K_{xy} = \frac{1}{2} \sum_{\mu} \left(\gamma_{\mu} \left(\delta_{x+\hat{\mu},y} - \delta_{x-\hat{\mu},y} \right) - r \left(\delta_{x+\hat{\mu},y} + \delta_{x-\hat{\mu},y} - 2\delta_{x,y} \right) \right).$$
(B.3)

Using the integral representation of the Kronecker delta:

$$\delta_{x,y} = \int_{-\pi}^{\pi} \frac{d^4 p}{(2\pi)^4} e^{ip(x-y)a},$$
(B.4)

we obtain:

$$K_{xy} = \int_{-\pi}^{\pi} \frac{d^4 p}{(2\pi)^4} e^{ip(x-y)a} \left[\sum_{\mu} \left(\frac{1}{2} \gamma_{\mu} \left(e^{ip\mu a} - e^{-ip\mu a} \right) + \left(B.5 \right) - \frac{r}{2} \left(e^{ip\mu a} + e^{-ip\mu a} - 2 \right) \right) \right].$$
(B.5)

Substituting now the identities:

$$e^{ip\hat{\mu}a} - e^{-ip\hat{\mu}a} = 2i\sin ap_{\mu},\tag{B.6}$$

$$e^{ip\hat{\mu}a} + e^{-ip\hat{\mu}a} - 2 = 2(\cos ap_{\mu} - 1) = -4\sin^2\frac{ap_{\mu}}{2},$$
 (B.7)

we obtain:

$$K_{nm} = \int_{-\pi}^{\pi} \frac{d^4 p}{(2\pi)^4} e^{ip(n-m)a} \left[\sum_{\mu} \left(i\gamma_{\mu} \sin ap_{\mu} + 2r \sin^2 \frac{ap_{\mu}}{2} \right) \right].$$
(B.8)

The expression in brackets is the Fourier transform of K_{mn} , i.e. the Wilson-Dirac operator in momentum space $\hat{D}_{Wilson}(p)$. Hence, adding explicitly the identity matrix in Dirac space, we have:

$$\hat{D}_{\text{Wilson}}(p) = i\gamma_{\mu}\mathring{p}_{\mu} + \frac{ar}{2}\hat{p}^{2}\mathbb{1}, \qquad (B.9)$$

which is expression (1.49) for the Wilson-Dirac operator at m = 0 or expression (1.45) for the naive Dirac operator, if the Wilson parameter r = 0. One can also notice that the inverse of this formula immediately gives expressions for the fermion propagator (1.47) in the naive case and (1.51) in the Wilson case.

We now set the Wilson parameter r = 1 and then the definition of the operator A for overlap fermions (1.75) (with s = 0) yields:

$$A = 1 - aD_W(p) = 1 - ia\gamma_\mu \mathring{p}_\mu - \frac{a^2}{2}\widehat{p}^2.$$
 (B.10)

Since the massless overlap Dirac operator is given by:

$$\hat{D}_{\rm ov}(0) = \frac{1}{a} \Big(1 - A (A^{\dagger} A)^{-1/2} \Big), \tag{B.11}$$

we have to calculate $A^{\dagger}A$:

$$A^{\dagger}A = \left(1 - \frac{a^2}{2}\hat{p}^2\right)^2 + a^2 \sum_{\mu,\nu} \gamma_{\mu}\gamma_{\nu}\dot{p}_{\mu}\dot{p}_{\nu}.$$
 (B.12)

Using now the following rearrangements:

$$\left(1 - \frac{a^2}{2}\hat{p}^2\right)^2 = 1 - a^2\hat{p}^2 + \frac{a^4}{4}\sum_{\mu,\nu}\hat{p}_{\mu}^2\hat{p}_{\nu}^2, \qquad (B.13)$$
$$a^{2} \sum_{\mu,\nu} \gamma_{\mu} \gamma_{\nu} \mathring{p}_{\mu} \mathring{p}_{\nu} = a^{2} \sum_{\mu} \left(\mathring{p}_{\mu} \right)^{2}, \qquad (B.14)$$

$$(\mathring{p}_{\mu})^{2} = \frac{1}{a^{2}}\sin^{2}ap_{\mu} = \frac{4}{a^{2}}\sin^{2}\frac{ap_{\mu}}{2}\left(1 - \sin^{2}\frac{ap_{\mu}}{2}\right) = \hat{p}_{\mu}^{2}\left(1 - \frac{a^{2}}{4}\hat{p}_{\mu}^{2}\right).$$
 (B.15)

in (B.12), we obtain:

$$A^{\dagger}A = 1 - a^{2}\hat{p}^{2} + \frac{a^{4}}{4}\sum_{\mu,\nu}\hat{p}_{\mu}^{2}\hat{p}_{\nu}^{2} + a^{2}\hat{p}^{2} - \frac{a^{4}}{4}\sum_{\mu}\hat{p}_{\mu}^{4}.$$
 (B.16)

We can reduce:

$$\frac{a^4}{4} \sum_{\mu,\nu} \hat{p}^2_{\mu} \hat{p}^2_{\nu} - \frac{a^4}{4} \sum_{\mu} \hat{p}^4_{\mu} = \frac{a^4}{2} \sum_{\mu < \nu} \hat{p}^2_{\mu} \hat{p}^2_{\nu}.$$
 (B.17)

In the end, we obtain for the operator $A^{\dagger}A$:

$$A^{\dagger}A = 1 + \frac{a^4}{2} \sum_{\mu < \nu} \hat{p}_{\mu}^2 \hat{p}_{\nu}^2.$$
 (B.18)

The final form of the tree-level overlap Dirac operator in momentum space is:

$$a\hat{D}_{\rm ov}(p) = 1 - \left(1 - ia\gamma_{\mu}\mathring{p}_{\mu} - \frac{a^2}{2}\hat{p}^2\right) \left(1 + \frac{a^4}{2}\sum_{\mu<\nu}\hat{p}_{\mu}^2\hat{p}_{\nu}^2\right)^{-1/2}.$$
 (B.19)

B.2 Creutz fermions

One can show [55] that the free Dirac operator for Creutz fermions can be written in momentum space as:

$$D_{\text{Creutz}}(p) = i \sum_{\mu} \mathring{p}_{\mu} \, \bar{\gamma}_{\mu} - i \, \frac{a}{2} \sum_{\mu} \, \hat{p}_{\mu}^2 \, \bar{\Gamma}_{\mu} + m \, \mathbb{1}, \qquad (B.20)$$

where $\bar{\gamma}_{\mu}$, $\bar{\Gamma}_{\mu}$ are defined as:

$$\bar{\gamma}_{\mu} \equiv \bar{a}^T \gamma_{\mu} , \ \bar{\Gamma}_{\mu} \equiv \bar{\alpha} \bar{\gamma}_{\mu} = \bar{\alpha} \bar{a}^T \gamma_{\mu}, \ \bar{\alpha} \equiv \bar{a}^{-1} \bar{b}$$
 (B.21)

with:

$$\bar{a} = \frac{1}{R} \begin{pmatrix} 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ -\frac{3S}{C} & -\frac{3S}{C} & -\frac{3S}{C} & -\frac{3S}{C} \end{pmatrix}$$

$$\bar{b} = \frac{1}{R} \frac{S}{C} \begin{pmatrix} 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ \frac{3C}{S} & \frac{3C}{S} & \frac{3C}{S} & \frac{3C}{S} \end{pmatrix},$$

where the constants C, R and S are parameters chosen appropriately to ensure the correct continuum limit of the fermion propagator. One can show that these values are: $C = 3/\sqrt{10}$, R = 2 and $S = \pm 1/\sqrt{10}$ or $C = 3/\sqrt{14}$, $R = 2\sqrt{2}$ and $S = \pm \sqrt{5/14}$.

This fermion propagator is:

$$S_{\text{Creutz}}(p) = \frac{-i \sum_{\mu} \left(\bar{s}_{\mu}(p) + \bar{c}_{\mu}(p) \right) \gamma_{\mu} + m \,\mathbb{1}}{\sum_{\mu} \left(\bar{s}_{\mu}(p) + \bar{c}_{\mu}(p) \right)^{2} + m^{2}},\tag{B.22}$$

where:

$$\bar{s}_k(p) = \frac{1}{R} s_k(p) , \ \bar{s}_4(p) = \frac{3S}{RC} s_4(p)$$
 (B.23)

$$\bar{c}_k(p) = \frac{S}{RC} c_k(p) , \ \bar{c}_4(p) = \frac{3}{R} c_4(p)$$
 (B.24)

with the functions s and c given by

$$s_1(p) = [\mathring{p}_1 + \mathring{p}_2 - \mathring{p}_3 - \mathring{p}_4], \qquad (B.25)$$

$$s_2(p) = [\mathring{p}_1 - \mathring{p}_2 - \mathring{p}_3 + \mathring{p}_4], \qquad (B.26)$$

$$s_{3}(p) = [\check{p}_{1} - \check{p}_{2} + \check{p}_{3} - \check{p}_{4}], \qquad (B.27)$$

$$s_{4}(p) = [\check{p}_{1} - \check{p}_{2} + \check{p}_{3} - \check{p}_{4}], \qquad (B.28)$$

$$s_4(p) = [-\dot{p}_1 - \dot{p}_2 - \dot{p}_3 - \dot{p}_4], \qquad (B.28)$$

$$c_1(p) = -\frac{\alpha}{2} \left[\hat{p}_1^2 + \hat{p}_2^2 - \hat{p}_3^2 - \hat{p}_4^2 \right], \qquad (B.29)$$

$$c_2(p) = -\frac{a}{2} \left[\hat{p}_1^2 - \hat{p}_2^2 - \hat{p}_3^2 + \hat{p}_4^2 \right], \qquad (B.30)$$

$$c_3(p) = -\frac{a}{2} \left[\hat{p}_1^2 - \hat{p}_2^2 + \hat{p}_3^2 - \hat{p}_4^2 \right], \qquad (B.31)$$

$$c_4(p) = -\frac{a}{2} \left[\hat{p}_1^2 + \hat{p}_2^2 + \hat{p}_3^2 + \hat{p}_4^2 \right].$$
 (B.32)

The free Dirac operator for the modification suggested by Borici is:

$$D_{\text{Borici}}(p) = i \sum_{\mu} \mathring{p}_{\mu} \gamma_{\mu} - i \frac{a}{2} \sum_{\mu} \Gamma_{\mu} \hat{p}_{\mu}^{2} + m \,\mathbb{1}, \qquad (B.33)$$

where $\Gamma_{\mu} = \sum_{\nu} \alpha_{\mu\nu} \gamma_{\nu}$, with:

The corresponding propagator is:

$$S_{\text{Borici}}(p) = \frac{-i\sum_{\mu} G_{\mu}(p)\gamma_{\mu} + m_0 \,\mathbb{1}}{\sum_{\mu} G_{\mu}(p)^2 + m^2},\tag{B.35}$$

where:

$$G_1(p) = \mathring{p}_1 - \frac{a}{4} \left[\hat{p}_1^2 + \hat{p}_2^2 - \hat{p}_3^2 - \hat{p}_4^2 \right], \qquad (B.36)$$

$$G_2(p) = \mathring{p}_2 - \frac{a}{4} \left[-\hat{p}_1^2 + \hat{p}_2^2 - \hat{p}_3^2 - \hat{p}_4^2 \right], \qquad (B.37)$$

$$G_3(p) = \mathring{p}_3 - \frac{a}{4} \left[-\hat{p}_1^2 - \hat{p}_2^2 + \hat{p}_3^2 - \hat{p}_4^2 \right], \qquad (B.38)$$

$$G_4(p) = \mathring{p}_4 - \frac{a}{4} \left[-\hat{p}_1^2 - \hat{p}_2^2 - \hat{p}_3^2 + \hat{p}_4^2 \right].$$
(B.39)

B.3 Correlation functions

The starting point for the derivation of the expression for the pseudoscalar correlation function as a sum over momenta is eq. (2.15):

$$C_{PP}(t) = \sum_{\vec{x}} \operatorname{Tr}(S(\vec{x}, t; \vec{0}, 0) \, S^{\dagger}(\vec{x}, t; \vec{0}, 0)). \tag{B.40}$$

We introduce the Fourier transform of the position space propagator:

$$S(\vec{x},t;\vec{0},0) = \frac{1}{N^3 N_4} \sum_{\vec{p},p_4} S(\vec{p},p_4) e^{i\vec{p}\cdot\vec{x}} e^{ip_4 t}, \qquad (B.41)$$

where N and N_4 are the number of lattice sites in the spatial and temporal directions, respectively. This yields:

$$C_{PP}(t) = \frac{1}{N^6 N_4^2} \sum_{\vec{x}} \sum_{\vec{p}, p_4} \sum_{\vec{p}', p_4'} \operatorname{Tr}(S(\vec{p}, p_4) S^{\dagger}(\vec{p}', p_4')) e^{i\vec{p}\cdot\vec{x}} e^{ip_4 t} e^{-i\vec{p}'\cdot\vec{x}} e^{-ip_4' t}.$$
(B.42)

Using the following expression for the Dirac-delta function:

$$\delta(\vec{p} - \vec{p}') = \frac{1}{N^3} \sum_{\vec{x}} e^{i(\vec{p} - \vec{p}') \cdot \vec{x}},$$
(B.43)

we obtain:

$$C_{PP}(t) = \frac{1}{N^3 N_4^2} \sum_{\vec{p}} \sum_{p_4, p_4'} \operatorname{Tr}(S(\vec{p}, p_4) \, S^{\dagger}(\vec{p}, p_4')) e^{i(p_4 - p_4')t}.$$
 (B.44)

Now, we insert the matrix decomposition of the momentum space propagator:

$$S(p) = \sum_{\xi=0}^{4 \text{ or } 5} S_{\xi}(p) \gamma_{\xi}, \qquad (B.45)$$

where $\gamma_0 \equiv 1$ and the index ξ runs from 0 to 4 in the case of overlap and Creutz fermions or from 0 to 5 in the case of Wilson twisted mass fermions. Hence, we obtain:

$$C_{PP}(t) = \frac{N_c N_d}{N^3 N_4^2} \sum_{\vec{p}} \sum_{p_4, p_4'} \sum_{\xi=0}^{4 \text{ or } 5} S_{\xi}(\vec{p}, p_4) S_{\xi}^*(\vec{p}, p_4') e^{i(p_4 - p_4')t}, \qquad (B.46)$$

where $N_d = \text{Tr}(1)$ is the number of Dirac components (i.e. the dimension of space-time) and $N_c = \text{Tr}(1_c)$ is the number of colours (in the free case the structure in colour space is trivial).

Appendix C

Improvements of the HMC algorithm

The gauge field configurations that we have used for this project were generated with the twisted mass Lattice QCD program suite (tmLQCD) of Jansen and Urbach [83]. A detailed description of all the technical details is given in this reference. Here we shortly discuss a few improvements of the HMC algorithm that are relevant from the point of view of this thesis.

For some lattice Dirac operators (e.g. Wilson twisted mass), it is possible to decompose the Dirac matrix into subspaces of even and odd lattice sites, thus reducing the dimension of the problem. Such technique is called evenodd preconditioning [126].

Another approach is to use more than one set of pseudo-fermion fields, i.e. split the fermion determinant into two (or more) parts. One of the widely used methods of this kind is called the Hasenbusch trick (or mass preconditioning) [127, 128] and consists in utilizing the identity (example for the $N_f = 2$ case with degenerate quark masses μ):

$$|\det(\hat{D})|^2 = \det(\hat{D}\hat{D}^{\dagger} + \mu^2) \det\left(\frac{\hat{D}\hat{D}^{\dagger}}{\hat{D}\hat{D}^{\dagger} + \mu^2}\right).$$
 (C.1)

Such decomposition splits the contribution of the low-frequency and highfrequency modes of $\hat{D}\hat{D}^{\dagger}$ and thus reduces the condition number of the problem. It also allows for integration of different parts of the action on different time scales, such that the most expensive part can be simulated on the coarsest time scale. A general version of an HMC algorithm incorporating even-odd preconditioning, mass preconditioning and multiple time scale integration was presented by Urbach, Jansen, Shindler and Wenger [129]. It was also shown by numerical investigation that such version of the algorithm indeed produces a considerable improvement, especially when approaching the small quark mass limit. This version of the algorithm is the base of the tmLQCD suite in its part that was relevant for the generation of gauge field configurations used in this project.

Another important improvement of the HMC algorithm comes under the name of Polynomial HMC (PHMC). It was introduced and analyzed in [115, 116, 117, 118]. This version of the algorithm can be applied to simulate non-degenerate quarks. It is used e.g. in the tmLQCD suite in simulations including the strange and charm quark.

The number of other improvements of the HMC algorithm is very large and is still increasing. To finalize this appendix we just mention a few more. For their description we refer to original papers. A wide and important class of improvements concern integration schemes and come under the name of multiple time-scale integration. The generalization of the leap-frog scheme to multiple time scales was originally proposed by Sexton and Weingarten [130]. Another approach is the so-called second order minimal norm (2MN) integrator [131, 132]. A variant of the HMC algorithm called Rational HMC (RHMC) was discussed in [133, 134, 135, 136]. Domain-decomposed HMC was introduced in a series of papers by Lüscher [137, 138, 139] and later augmented by low-mode deflation [140].

Appendix D

Tree-level test of zero modes subtraction

In this appendix, we show the results of a free-field test of routines used to subtract the zero modes (we will refer to them as "subtraction routines") at the level of propagators. The test is performed on a small lattice of $4^3 \times 8$, with quark mass set to am = 0.2. We perform the subtraction in three ways for the pseudoscalar (PP) and scalar (SS) correlation function, using:

- formula (2.16) for the PP correlator and an analogous formula for SS ("analytical formula"),
- GWC code with subtraction routines for point sources,
- GWC code with subtraction routines for stochastic sources.

Using notation of Section 4.3, we write the mesonic correlation function as:

$$C(t) = C_{00}(t) + 2C_{0N}(t) + C_{NN}(t), \qquad (D.1)$$

where the first two terms involve the zero modes. Computing correlation functions from the full propagator (with all modes) leads to C(t), while if the zero modes are subtracted at the level of propagators, only the part $C_{NN}(t)$ is obtained by performing contractions, i.e. subtraction of zero modes cancels both the diagonal contribution $C_{00}(t)$ and the mixed one $C_{0N}(t)$.

D.1 Analytical formula

We remind here the formula for the pseudoscalar correlator (2.16) and generalize it to include the scalar case:

$$C(t) = \frac{N_c N_d}{N^3 N_4^2} \sum_{\vec{p}} \sum_{p_4, p_4'} \sum_{\xi=0}^4 s(\xi) S_{\xi}(\vec{p}, p_4) S_{\xi}^*(\vec{p}, p_4')) e^{i(p_4 - p_4')t},$$
(D.2)

where we obtain the pseudoscalar correlator by choosing: $s(\xi) = 1$ for all ξ and the scalar correlator if we take $s(\xi) = -1$ for $\xi = 0$ and $s(\xi) = 1$ for $\xi = 1, 2, 3, 4$.

To isolate the contribution of the zero-modes, we have to calculate the diagonal part $C_{00}(t)$ and the mixed part $C_{0N}(t)$:

$$C_{00}(t) = \frac{12}{N^3 N_4^2} \sum_{\xi=0}^4 s(\xi) S_{\xi}(\vec{0}, 0) S_{\xi}^*(\vec{0}, 0), \qquad (D.3)$$

i.e. $p_1 = p_2 = p_3 = p_4 = p'_4 = 0$ and the sum runs only over ξ and:

$$C_{0N}(t) = \frac{12}{N^3 N_4^2} \sum_{p'_4 \neq 0} \sum_{\xi=0}^4 e^{-ip'_4 t} s(\xi) S_{\xi}(\vec{0}, 0) S_{\xi}^*(\vec{0}, p'_4), \qquad (D.4)$$

i.e. $p_1 = p_2 = p_3 = p_4 = 0$ and the sum runs over ξ and also over p'_4 (the latter corresponds to non-zero modes in the mixed term).

The contribution of the zero modes is $C_{00}(t) + 2C_{0N}(t)$ and it is for the PP and the SS case:

- t C_PP(t)
- $0\ 0.19336502258508669882530739$
- 1 0.06854269349589653392840205
- 2 0.05598313737623755725891783
- 3 0.04864480650410332729371987
- 4 0.04623120266243796461225202
- 5 0.04864480650410329953814426
- 6 0.05598313737623752950334222
- 7 0.06854269349589661719512890
- t C_SS(t)
- 0 -0.19336502258508669882530739
- 1 -0.06854269349589653392840205
- 2 0.05598313737623755725891783

- 3 -0.04864480650410332729371987
- $4 \ -0.04623120266243796461225202$
- 5 0.04864480650410329953814426
- 6 -0.05598313737623755725891783
- 7 0.06854269349589661719512890

As we have shown analytically in Section 4.3, the contribution of the zero modes is the same in both the pseudoscalar and the scalar correlator, up to a sign, which is a matter of convention. With such convention, the contribution of the zero modes exactly cancels in the sum $C_{PP+SS} = C_{PP} + C_{SS}$.

We also show the part $C_{NN}(t)$ of the PP and SS correlators, i.e. the part with zero modes subtracted:

```
t C_PP(t)
0 3.20704955982560369065481609
1 0.05387552324984687390774241
2 0.01185159451402884034365570
3 0.00436850362097932626292973
4 0.00257470328781685825481063
5 0.00436850362097952055195904
6 0.01185159451402885422144351
7 0.05387552324984717921907418
t C_SS(t)
0 -2.89984667245719363037892435
1 0.05349572434485626304390138
2 0.00979860668208997614980760
3 0.00023495453740399879771772
4 -0.00240740901956542491246793
5 0.00023495453740363103634081
6 0.00979860668209000390538321
7 0.05349572434485556221561708
```

We will use these numbers to compare with the subtraction routines.

D.2 GWC code – point sources

For the test of subtraction routines, the first step was to explicitly compute the zero modes. The number of zero modes in the free-field case is equal to $N_c N_d$, i.e. there are 12 zero modes in our case of interest, 6 in the positive and 6 in the negative chirality sector. The test of the subtraction routines consisted in performing the following steps:

- 1. Read in all zero modes.
- 2. Compute the propagator Ψ^0 coming only from the zero modes, using formula 4.22, i.e. taking into account the source. This source has to be exactly the same as the one used for full inversion (with all modes).
- 3. Compute (or read in, if computed before) the full propagator Ψ (with all modes) with the same point source as in the previous step.
- 4. Construct the non-zero modes propagator $\Psi^N = \Psi \Psi^0$.
- 5. Use the GWC contraction code to compute the PP and SS correlation functions from Ψ^N . This gives the part $C_{NN}(t)$ of these correlators.

The result for the correlation functions with no contribution from the zero modes is:

```
C_PP(t)
t
  +3.2070498264e+00
0
1
  +5.3875529993e-02
2
  +1.1851597433e-02
  +4.3685038347e-03
3
4
  +2.5747032913e-03
5
  +4.3685038347e-03
6
  +1.1851597433e-02
   +5.3875529993e-02
7
t
  C_SS(t)
0
  -2.8998469255e+00
1
   +5.3495732753e-02
2
  +9.7986124350e-03
  +2.3495604466e-04
3
4
  -2.4074086241e-03
5
  +2.3495604466e-04
6
  +9.7986124350e-03
7
   +5.3495732753e-02
```

These numbers are exactly the same as ones obtained with the analytical formula in the previous section.

D.3 GWC code – stochastic sources

We follow an analogous procedure in the case of stochastic sources:

- 1. Read in all zero modes.
- 2. Read in sample r of stochastic source.
- 3. Compute the propagator Ψ_r^0 coming only from the zero modes, using formula 4.22 with sample r of the source
- 4. Compute (or read in, if computed before) the full propagator Ψ_r (with all modes) with the same sample of the source r.
- 5. Construct the non-zero modes propagator $\Psi_r^N = \Psi_r \Psi_r^0$.
- 6. Use the "light" contraction code to compute the PP and SS correlation functions from Ψ_r^N .

Such procedure is then repeated N_r times for different samples of stochastic noise. Each sample of the source leads to a correlation function $C_{NN}(t)$. We have used $N_r = 600$ samples and finally averaged the correlation functions to obtain:

```
t C_PP(t)
               dC_PP(t)
0 3.207395e+00 6.036502e-04
1 5.341456e-02 4.634707e-04
2 1.163657e-02 2.135815e-04
3 4.276079e-03 9.325929e-05
4 2.518227e-03 5.732913e-05
5 4.276079e-03 9.325929e-05
6 1.163657e-02 2.135815e-04
7 5.341456e-02 4.634707e-04
t C_SS(t)
               dC_SS(t)
0 2.899527e+00 3.025145e-04
1 -5.303857e-02 4.597752e-04
2 -9.629567e-03 1.669140e-04
3 -2.358282e-04 3.102437e-06
4 2.351388e-03 5.740869e-05
5 -2.358282e-04 3.102437e-06
6 -9.629567e-03 1.669140e-04
7 -5.303857e-02 4.597752e-04
```

The third column is the standard deviation. Comparing these numbers with the ones from the analytical formula and from the GWC code with point sources, we conclude that all results are consistent, up to the statistical error for the case of stochastic sources. The "light" contraction code uses a different sign convention for the scalar correlator and hence the sign of $C_{SS}(t)$ is always opposite to the one from the GWC contraction code and the analytical formula. Hence, with the "light" contraction code the contribution of the zero modes is exactly cancelled in the difference $C_{PP} - C_{SS}$. Therefore, for computations in the interacting case we always use $C_{PP} - C_{SS}$.

Bibliography

- [1] Wilson K.G. (1974), Confinement of Quarks, Phys.Rev. D10, 2445.
- [2] Creutz M. (1980), Monte Carlo study of quantized SU(2) theory, Phys. Rev. D21, 2308.
- [3] Peskin M.E., Schroeder D.V. (1995), An Introduction to Quantum Field Theory, Addison-Wesley Publishing Group.
- [4] Pokorski S. (2000), Gauge Field Theories, Cambridge University Press, Cambridge.
- [5] Feynman R.P. (1948), Space-time approach to non-relativistic quantum mechanics, Rev.Mod.Phys. 20, 367.
- [6] Aoyama T., Hayakawa M., Kinoshita T., Nio M. (2008), Revised value of the eighth-order QED contribution to the anomalous magnetic moment of the electron, Phys.Rev. D77, 053012; 0712.2607 (hep-ph).
- [7] Osterwalder K., Schrader R. (1973), Axioms for Euclidean Green's functions, Comm.Math.Phys. 31, 83.
- [8] Osterwalder K., Schrader R. (1975), Axioms for Euclidean Green's functions 2, Comm.Math.Phys. 42, 281.
- [9] Lüscher M. (1977), Construction of a selfadjoint, strictly positive transfer matrix for euclidean lattice gauge theories, Comm.Math.Phys 54, 283.
- [10] DeGrand T., DeTar C. (2006), Lattice Methods for Quantum Chromodynamics, World Scientific, Singapore.
- [11] Gattringer C., Lang C.B. (2010), Quantum Chromodynamics on the Lattice. An Introductory Presentation, Springer-Verlag, Berlin Heidelberg.

- [12] Witten E. (1979), Current algebra theorems for the U(1) Goldstone boson, Nucl.Phys. B156, 269.
- [13] Veneziano G. (1979), U(1) without instantons, Nucl. Phys. B159, 213.
- [14] Gasser J., Leutwyler H. (1984), Chiral perturbation theory to one loop, Ann. Phys. 158, 142.
- [15] Gasser J., Leutwyler H. (1985), Chiral perturbation theory: Expansions in the mass of the strange quark, Nucl. Phys. B250, 465.
- [16] Greiner W., Schramm S., Stein E. (2002), Quantum Chromodynamics, Springer-Verlag, Berlin Heidelberg.
- [17] Jido D., Nemoto Y., Oka A., Hosaka A. (2000), Chiral Symmetry for Positive and Negative Parity Nucleons, Nucl.Phys. A671, 471; hepph/9805306.
- [18] Gell-Mann M., Oakes R.J., Renner B. (1968), Behavior of Current Divergences under $SU_3 \times SU_3$, Phys. Rev. 175, 2195.
- [19] Fuchs N.H., Sazdjian H., Stern J. (1991), How to probe the scale of $\langle \bar{q}q \rangle$ in chiral perturbation theory, Phys.Lett. B269, 183.
- [20] Stern J., Sazdjian H., Fuchs N.H. (1993), What $\pi \pi$ Scattering Tells Us About Chiral Perturbation Theory, Phys.Rev. D47, 3814; hep-ph/9301244.
- [21] DeTar C. (2008), Recent Progress in Lattice QCD Thermodynamics, PoS LATTICE2008, 001; 0811.2429 (hep-lat).
- [22] Montvay I., Münster G. (1997), Quantum Fields on a Lattice, Cambridge University Press, Cambridge.
- [23] Weisz P. (1983), Continuum limit improved lattice action for pure Yang-Mills theory (I), Nucl.Phys. B212, 1.
- [24] Boucaud P. et al. (2008), Dynamical Twisted Mass Fermions with Light Quarks: Simulation and Analysis Details, Comput.Phys.Commun. 179, 695; 0803.0224 (hep-lat).
- [25] Rothe H.J. (2005), Lattice Gauge Theories. An Introduction, 3rd edition, World Scientific, Singapore.

- [26] Wilson K.G. (1975), Quarks and strings on a lattice, in: New Phenomena In Subnuclear Physics. Part A. Proceedings of the First Half of the 1975 International School of Subnuclear Physics, Erice, Sicily, July 11 August 1, 1975, ed. A. Zichichi, Plenum Press, New York, 1977, p. 69.
- [27] Sheiholeslami B., Wohlert R. (1985), Improved continuum limit lattice action for QCD with Wilson fermions, Nucl.Phys. B259, 572.
- [28] Nielsen N.B., Ninomiya M. (1981), Phys.Lett. B105, 211.
- [29] Lüscher M. (1998), Exact chiral symmetry on the lattice and the Ginsparg-Wilson relation, Phys. Lett. B428, 342; arXiv: heplat/9802011.
- [30] Niedermayer F. (1999), Exact chiral symmetry, topological charge and related topics, Nucl. Phys. B (Proc. Suppl.) 73, 105; arXiv:heplat/9810026.
- [31] Frezzotti R., Grassi P.A., Sint S., Weisz P. (2001), Lattice QCD with a chirally twisted mass term, JHEP 0108, 058; hep-lat/0101001.
- [32] Frezzotti R., Rossi G.C. (2004), Chirally improving Wilson fermions I. O(a) improvement, JHEP 0408, 007; hep-lat/0306014.
- [33] Baron R. et al. (2009), Light Meson Physics from Maximally Twisted Mass Lattice QCD, 0911.5061 (hep-lat).
- [34] Ginsparg P., Wilson K. (1982), A remnant of chiral symmetry on the lattice, Phys.Rev. D25, 2649.
- [35] Hasenfratz P. (1998), Prospects for perfect actions, Nucl.Phys.Proc.Suppl. 63, 53; hep-lat/9709110.
- [36] Hasenfratz P. (1998), Lattice QCD without tuning, mixing and current renormalization, Nucl.Phys. B525, 401; hep-lat/9802007.
- [37] Neuberger H. (1998), Exactly massless quarks on the lattice, Phys. Lett. B 417, 141; hep-lat/9707022.
- [38] Neuberger H. (1998), More about exactly massless quarks on the lattice, Phys. Lett. B 427, 353; hep-lat/9801031.
- [39] Hasenfratz P., Laliena V., Niedermayer F. (1998), The index theorem in QCD with a finite cut-off, Phys.Lett. B427, 125; hep-lat/9801021.

- [40] Fujikawa K. (1999), A continuum limit of the chiral Jacobian in lattice gauge theory, Nucl.Phys. B546, 480; hep-th/9811235.
- [41] Hernandez P., Jansen K., Lüscher M. (1999), Locality properties of Neuberger's lattice Dirac operator, Nucl.Phys. B552, 363; heplat/9808010.
- [42] Kaplan D.B. (1992), A Method for simulating chiral fermions on the lattice, Phys.Lett. B288, 342; hep-lat/9206013.
- [43] Shamir Y. (1993), Chiral Fermions from Lattice Boundaries, Nucl.Phys. B406, 90; hep-lat/9303005.
- [44] Jansen K. (1996), Domain Wall Fermions and Chiral Gauge Theories, Phys.Rept. 273, 1-54; hep-lat/9410018.
- [45] Jansen K. (1992), Chiral fermions and anomalies on a finite lattice, Phys.Lett. B288, 348.
- [46] Neuberger H. (1998), Vector like gauge theories with almost massless fermions on the lattice, Phys.Rev. D57, 5417; hep-lat/9710089.
- [47] Allton C. et al. (2007), 2+1 flavor domain wall QCD on a $(2 \text{ fm})^3$ lattice: light meson spectroscopy with $L_s = 16$, Phys.Rev. D76, 014504; heplat/0701013.
- [48] Walker-Loud A. et al. (2009), Light hadron spectroscopy using domain wall valence quarks on an Asqtad sea, Phys.Rev. D79, 054502; 0806.4549 (hep-lat).
- [49] Karsten L.H. (1981), Lattice fermions in euclidean space-time, Phys.Lett. B104, 315.
- [50] Wilczek F. (1987), Lattice Fermions, Phys.Rev.Lett. 59, 2397.
- [51] Creutz M. (2008), Four-dimensional graphene and chiral fermions, JHEP 0804, 017; 0712.1201 (hep-lat).
- [52] Borici A. (2008), Creutz Fermions on an Orthogonal Lattice, Phys.Rev. D78, 074504; 0712.4401 (hep-lat).
- [53] Bedaque P.F., Buchoff M.I., Tiburzi B.C., Walker-Loud A. (2008), Broken Symmetries from Minimally Doubled Fermions, Phys.Lett. B662, 449; 0801.3361 (hep-lat).

- [54] Borici A. (2008), Minimally Doubled Fermion Revival, PoS LAT-TICE2008, 231; 0812.0092 (hep-lat).
- [55] Cichy K., Gonzalez Lopez J., Jansen K., Kujawa A., Shindler A. (2008), Twisted Mass, Overlap and Creutz Fermions: Cut-off Effects at Treelevel of Perturbation Theory, Nucl.Phys. B800, 94; 0802.3637 (hep-lat).
- [56] Cichy K., Gonzalez Lopez J., Kujawa A. (2008), A comparison of the cut-off effects for Twisted Mass, Overlap and Creutz fermions at treelevel of Perturbation Theory, Acta Phys.Pol. B39, 3463; 0811.0572 (hep-lat).
- [57] Smit J. (2002), Introduction to Quantum Fields on a Lattice, Cambridge University Press, Cambridge.
- [58] Belavin A.A., Polyakov A.M., Schwartz A.S., Tyupkin Yu.S. (1975), Pseudoparticle solutions of the Yang-Mills equations, Phys.Lett. B59, 85.
- [59] Atiyah M., Singer I. (1963), The index of elliptic operators on compact manifolds, Bull. Amer. Math. Soc. 69, 422.
- [60] Bruckmann F., Gruber F., Jansen K., Marinkovic M., Urbach C., Wagner M. (2009), Comparing topological charge definitions using topology fixing actions, 0905.2849 (hep-lat).
- [61] Albanese M. et al. (1987), Glueball masses and string tension in lattice QCD, Phys.Lett. B192, 163.
- [62] Del Debbio L., Giusti L., Pica C. (2005), Topological susceptibility in the SU(3) gauge theory, Phys.Rev.Lett. 94, 032003; hep-th/0407052.
- [63] Gupta R. (1998), Introduction to Lattice QCD, Lectures given at the LXVIII Les Houches Summer School "Probing the Standard Model of Particle Interactions", July 28-Sept 5, 1997.
- [64] Bietenholz W. et al. (2004), Going chiral: overlap versus twisted mass fermions, JHEP 0412, 044; hep-lat/0411001.
- [65] Alexandrou C. et al. (2008), Light baryon masses with dynamical twisted mass fermions, Phys.Rev. D78, 014509; 0803.3190 (hep-lat).
- [66] Alexandrou C. et al. (2009), The low-lying baryon spectrum with two dynamical twisted mass fermions, Phys.Rev. D80, 114503; 0910.2419 (hep-lat).

- [67] Cichy K., Gonzalez Lopez J., Jansen K., Kujawa A., Shindler A. (2007), Cutoff effects for Wilson twisted mass fermions at tree-level of perturbation theory, PoSLAT2007, 098; 0710.2036 (hep-lat).
- [68] Carpenter D.B., Baillie C.F. (1985), Free fermion propagators and lattice finite-size effects, Nucl.Phys. B260, 103.
- [69] Gonzalez Lopez J. (2007), Cut-off effects and continuum limit at tree-level of perturbation theory for Wilson twisted mass fermions at maximal twist, Ph.D. thesis preparation report, Humboldt University, Berlin.
- [70] Duane S., Kennedy A.D., Pendleton B.J., Roweth D. (1987), Hybrid Monte Carlo, Phys.Lett. B195, 216.
- [71] Lüscher M. (2010), Computational Strategies in Lattice QCD, Lectures given at the Summer School on "Modern perspectives in lattice QCD", Les Houches, August 3-28, 2009; 1002.4232 (hep-lat).
- [72] Ukawa A. (2002), Computational cost of full QCD simulations experienced by CP-PACS and JLQCD Collaborations, Nucl. Phys. B (Proc.Supp.) 106, 195.
- [73] Van den Eshof J. et al. (2002), Numerical Methods for the QCD Overlap Operator: I. Sign-Function and Error Bounds, Comput.Phys.Commun. 146, 203; hep-lat/0202025.
- [74] Frommer A., Lippert T., Medeke B., Schilling K. (eds.), Numerical Challenges in Lattice Quantum Chromodynamics, Lecture Notes in Computational Science and Engineering 15, Heidelberg 2000.
- [75] Chiarappa T. et al. (2006), Iterative methods for overlap and twisted mass fermions, hep-lat/0609023.
- [76] Hernandez P., Jansen K., Lellouch L. (1999), Finite-size scaling of the quark condensate in quenched lattice QCD, Phys.Lett. B469, 198; heplat/9907022.
- [77] Hasenfratz A., Knechtli F. (2001), Flavor Symmetry and the Static Potential with Hypercubic Blocking, Phys.Rev. D64, 034504; heplat/0103029.
- [78] Dong S.J., Liu K.F. (1994), Stochastic Estimation with Z_2 Noise, Phys.Lett. B328, 130; hep-lat/9308015.

- [79] Foster M., Michael C. (1999), Phys.Rev. D59, 074503; hep-lat/9810021.
- [80] Jagels C.F., Reichel L. (1994), A fast minimal residual algorithm for shifted unitary matrices, Numer. Linear Algebra Appl. 1(6), 555.
- [81] Arnold G. et al. (2003), Numerical Methods for the QCD Overlap Operator: II. Optimal Krylov Subspace Methods, hep-lat/0311025.
- [82] Frommer A., Güsken S., Lippert T., Nöckel B., Schilling K. (1995), Many Masses on One Stroke: Economic Computation of Quark Propagators, Int.J.Mod.Phys. C6, 627; hep-lat/9504020.
- [83] Jansen K., Urbach C. (2009), tmLQCD: a program suite to simulate Wilson Twisted mass Lattice QCD, 0905.3331 (hep-lat).
- [84] Wagner M. (2008), Contraction Code Documentation, unpublished.
- [85] Aoki S. et al. (2008), Two-flavor QCD simulation with exact chiral symmetry, Phys.Rev. D78, 014508; 0803.3197 (hep-lat).
- [86] Schaefer S. (2006), Algorithms for dynamical overlap fermions, PoSLAT2006, 020; hep-lat/0609063.
- [87] Fodor Z., Katz S.D., Szabo K.K. (2004), Dynamical overlap fermions, results with hybrid Monte-Carlo algorithm, JHEP 0408, 003l heplat/0311010.
- [88] Fukaya H. et al. (2006), Lattice gauge action suppressing near-zero modes of H_W , Phys.Rev. D74, 094505; hep-lat/0607020.
- [89] Dürr S. et al. (2007), Mixed action simulations: approaching physical quark masses, PoSLAT2007, 113; 0710.4866 (hep-lat).
- [90] Dürr S. et al. (2007), Chiral behavior of pseudo-Goldstone boson masses and decay constants in 2+1 flavor QCD, PoSLAT2007, 115; 0710.4769 (hep-lat).
- [91] Bernardoni F. et al. (2009), Mixed action computations on fine dynamical lattices, 0911.3756 (hep-lat).
- [92] Bär O., Jansen K., Schaefer S., Scorzato L., Shindler A. (2006), Overlap fermions on a twisted mass sea, PoSLAT2006, 199; hep-lat/0609039.
- [93] Garron N., Scorzato L. (2007), Results from overlap valence quarks on a twisted mass sea, PoSLAT2007, 083; 0710.1582 (hep-lat).

- [94] Cichy K., Herdoiza G., Jansen K. (2009), Continuum-Limit Scaling of Overlap Fermions As Valence Quarks, Acta Phys.Pol.B Proc.Suppl. 2, 497; 0910.0816 (hep-lat).
- [95] Bowler K.C. et al. (2004), Exploratory spectrum calculations using overlap valence quarks on a staggered sea, hep-lat/0408043.
- [96] Bowler K.C. et al. (2005), Lattice QCD with mixed actions, JHEP 0508, 003; hep-lat/0411005.
- [97] Hasenfratz A., Hoffmann R. (2006), Mixed Action Simulations on Staggered Background; Interpretation and Result for the 2-flavor QCD Chiral Condensate, Phys.Rev. D74, 114509; hep-lat/0609067.
- [98] Renner D.B. et al. (2005), Hadronic physics with domain-wall valence and improved staggered sea quarks, Nucl.Phys.Proc.Suppl. 140, 255; hep-lat/0409130.
- [99] Edwards R.G. et al. (2006), The nucleon axial charge in full lattice QCD, Phys.Rev.Lett. 96, 052001; hep-lat/0510062.
- [100] Beane S.R., Bedaque P.F., Orginos K., Savage M.J. (2006), $I = 2\pi\pi$ Scattering from Fully-Dynamical Mixed-Action Lattice QCD, Phys.Rev. D73, 054503; hep-lat/0506013.
- [101] Alexandrou C., Leontiou T., Negele J.W., Tsapalis A. (2007), The axial N to Delta transition form factors from Lattice QCD, Phys.Rev.Lett. 98, 052003; hep-lat/0607030.
- [102] Beane S.R. et al. (2007), Hyperon-Nucleon Scattering from Fully-Dynamical Lattice QCD, Nucl.Phys.A794, 62; hep-lat/0612026.
- [103] Beane S.R. et al. (2008), Precise Determination of the $I = 2 \pi \pi$ Scattering Length from Mixed-Action Lattice QCD, Phys.Rev. D77, 014505; 0706.3026 (hep-lat).
- [104] Hägler P. et al. (2008), Nucleon Generalized Parton Distributions from Full Lattice QCD, Phys.Rev. D77, 094502; 0705.4295 (hep-lat).
- [105] Alexandrou C. et al. (2008), The nucleon to Delta electromagnetic transition form factors in lattice QCD, Phys.Rev.D77, 085012; 0710.4621 (hep-lat).
- [106] Boucaud P. et al. (2007), Dynamical Twisted Mass Fermions with Light Quarks, Phys.Lett. B650, 304; hep-lat/0701012.

- [107] Bardeen W., Duncan A., Eichten E., Isgur N., Thacker H. (2001), Chiral Loops and Ghost States in the Quenched Scalar Propagator, Phys.Rev. D65, 014509; hep-lat/0106008.
- [108] Bardeen W., Eichten E., Thacker H. (2004), Chiral Lagrangian Parameters for Scalar and Pseudoscalar Mesons, Phys.Rev. D69, 054502; hep-lat/0307023.
- [109] Prelovsek S., Dawson C., Izubuchi T., Orginos K., Soni A. (2004), Scalar meson in dynamical and partially quenched two-flavor QCD: lattice results and chiral loops, Phys.Rev.D70, 094503; hep-lat/0407037.
- [110] Golterman M., Izubuchi T., Shamir Y. (2005), The role of the double pole in lattice QCD with mixed actions, Phys.Rev. D71, 114508; heplat/0504013.
- [111] Furchner A. (2010), Unitarity violation in mixed action QCD, Diploma Thesis, Humboldt Universität zu Berlin.
- [112] Cichy K., Drach V., Garcia Ramos E., Herdoiza G., Jansen K. (2010), in preparation.
- [113] Jansen K., Schmaltz M. (1992), Critical Momenta of Lattice Chiral Fermions, Phys.Lett. B296, 374; hep-lat/9209002.
- [114] Blum T. et al. (2004), Quenched Lattice QCD with Domain Wall Fermions and the Chiral Limit, Phys.Rev. D69, 074502; heplat/0007038.
- [115] de Forcrand P., Takaishi T. (1997), Fast Fermion Monte Carlo, Nucl.Phys.Proc.Suppl. 53, 968; hep-lat/9608093.
- [116] Frezzotti R., Jansen K. (1997), A Polynomial Hybrid Monte Carlo Algorithm, Phys.Lett. B402, 328; hep-lat/9702016.
- [117] Frezzotti R., Jansen K. (1999), The PHMC algorithm for simulations of dynamical fermions: I – description and properties, Nucl.Phys. B555, 395; hep-lat/9808011.
- [118] Frezzotti R., Jansen K. (1999), The PHMC algorithm for simulations of dynamical fermions: II - Performance analysis, Nucl.Phys. B555, 432; hep-lat/9808038.

- [119] Giusti L., Hoelbling C., Rebbi C. (2001), Light Quark Masses with Overlap Fermions in Quenched QCD, Phys.Rev. D64, 114508; Erratum Phys.Rev. D65, 079903; hep-lat/0108007.
- [120] Sharpe S.R. (1997), Enhanced chiral logarithms in partially quenched QCD, Phys.Rev. D56, 7052; Erratum Phys.Rev. D62, 099901; heplat/9707018.
- [121] Golterman M., Leung K.C. (1998), Applications of Partially Quenched Chiral Perturbation Theory, Phys.Rev. D57, 5703; hep-lat/9711033.
- [122] Giusti L., Hoelbling C., Lüscher M., Wittig H. (2003), Numerical techniques for lattice QCD in the ϵ -regime, Comput.Phys.Commun. 153, 31; hep-lat/0212012.
- [123] Hauswirth S. (2002), Light hadron spectroscopy in quenched lattice QCD with chiral Fixed-Point fermions, University of Bern; heplat/0204015.
- [124] Gattringer C. et al. (2004), Quenched spectroscopy with fixed-point and chirally improved fermions, Nucl.Phys. B677, 3; hep-lat/0307013.
- [125] Capitani S. (2009), Mesonic and baryonic correlation functions at fine lattice spacings, PoS LAT2009, 095; 0910.5578 (hep-lat).
- [126] DeGrand T., Rossi P. (1990), Conditioning techniques for dynamical fermions, Comp.Phys.Comm. 60, 211.
- [127] Hasenbusch M. (2001), Speeding up the Hybrid-Monte-Carlo algorithm for dynamical fermions, Phys.Lett. B519, 177; hep-lat/0107019.
- [128] Hasenbusch M., Jansen K. (2003), Speeding up Lattice QCD simulations with clover-improved Wilson Fermions, Nucl.Phys. B659, 299; hep-lat/0211042.
- [129] Urbach C., Jansen K., Shindler A., Wenger U. (2006), HMC algorithm with multiple time scale integration and mass preconditioning, Comput.Phys.Commun. 174, 87; hep-lat/0506011.
- [130] Sexton J.C., Weingarten D.H. (1992), Hamiltonian evolution for the hybrid Monte Carlo algorithm, Nucl. Phys. B380, 665.
- [131] Omelyan I.P., Mryglod I.M., Folk R. (2003), Symplectic analytically integrable decomposition algorithms: classification, derivation, and application to molecular dynamics, quantum and celestial mechanics simulations, Comp.Phys.Comm. 151, 272.

- [132] Takaishi T., de Forcrand P. (2006), Testing and tuning symplectic integrators for Hybrid Monte Carlo algorithm in lattice QCD, Phys.Rev. E73, 036706; hep-lat/0505020.
- [133] Horvath I., Kennedy A.D., Sint S. (1999), A New Exact Method for Dynamical Fermion Computations with Non-Local Actions, Nucl.Phys.Proc.Suppl. 73, 834; hep-lat/9809092.
- [134] Clark M.A., Kennedy A.D. (2003), The RHMC Algorithm for 2 Flavours of Dynamical Staggered Fermions, hep-lat/0309084.
- [135] Clark M.A. (2006), The Rational Hybrid Monte Carlo Algorithm, PoSLAT2006, 004; hep-lat/0610048.
- [136] Clark M.A., Kennedy A.D. (2007), Accelerating Dynamical Fermion Computations using the Rational Hybrid Monte Carlo (RHMC) Algorithm with Multiple Pseudofermion Fields, Phys.Rev.Lett. 98, 051601; hep-lat/0608015.
- [137] Lüscher M. (2003), Lattice QCD and the Schwarz alternating procedure, JHEP 0305, 052; hep-lat/0304007.
- [138] Lüscher M. (2004), Solution of the Dirac equation in lattice QCD using a domain decomposition method, Comp.Phys.Comm. 156, 209; heplat/0310048.
- [139] Lüscher M. (2005), Schwarz-preconditioned HMC algorithm for twoflavour lattice QCD, Comp.Phys.Comm. 165, 199; hep-lat/0409106.
- [140] Lüscher M. (2007), Deflation acceleration of lattice QCD simulations, JHEP 0712, 011; 0710.5417 (hep-lat).

List of Tables

1.1	Meson interpolating operators. J^{PC} classification denotes par-	
	ticle spin J , parity P and charge conjugation C [63]	38
2.1	Simulation parameters for the tree-level scaling test	46
2.2	Fitting coefficients for the pion mass $-$ eq. (2.20)	47
2.3	Fitting coefficients for the pion decay constant – eq. (2.21) .	49
2.4	Fitting coefficients for the pseudoscalar correlation function at	
	a fixed physical distance $t/N = 4 - eq. (2.22)$	49

List of Figures

1.1	Continuum limit scaling in fixed finite volume for $r_0 f_{PS}$ at fixed values of $r_0 m_{PS}$ (a) and for $(r_0 m_{PS})^2$ at fixed values of renormalized quark mass $r_0 \mu_R$ (b). In (b) data at $\beta = 4.2$ $((a/r_0)^2 = 0.0144)$ are not included, due to the missing value of the renormalization factor Z_P . Source: [33]	28
2.1	Continuum limit scaling of the pion mass for overlap, twisted	17
2.2	Continuum limit scaling of the pion decay constant for overlap, twisted mass and Creutz fermions	41
2.3	Continuum limit scaling of the pseudoscalar correlation func- tion at a fixed physical distance $t/N = 4$ for overlap, twisted	40
	mass and Creutz fermions	50
2.4	Continuum limit scaling of the pion mass for overlap-overlap, MTM-MTM and overlap-MTM quarks	51
2.5	Continuum limit scaling of the pion decay constant for overlap- overlap, MTM-MTM and overlap-MTM guarks.	52
2.6	Continuum limit scaling of the pseudoscalar correlation func- tion at a fixed physical distance $t = 4N$ for overlap-overlap,	
	MTM-MTM and overlap-MTM quarks	53
2.7	Continuum limit scaling of the pion mass at a fixed physical distance $t/N = 4$ for twisted mass and overlap fermions. The quark masses are matched up to $O(1/N^2)$. The lower plot is	
	a zoom of the upper one for large values of N	55
2.8	Continuum limit scaling of the pion decay constant at a fixed physical distance $t/N = 4$ for twisted mass and overlap fermions. The quark masses are matched up to $\mathcal{O}(1/N^2)$. The lower plot	
	is a zoom of the upper one for large values of N	56
2.9	The matching of MTM and overlap quark masses	57
2.10	The mismatch between the MTM and overlap pion decay con-	F 0
	stants at the matching point $N m_{\pi}^{\text{MIM}} = N m_{\pi}^{\text{overlap}}$	58

2.11	The mismatch between the MTM and overlap correlation func-	
	tions (at a fixed physical distance) at the matching point	
	$Nm_{\pi}^{\text{MTM}} = Nm_{\pi}^{\text{overlap}}$	58
2.12	The difference between the MTM and overlap pion decay con-	
	stants at the matching point $Nm_{\pi}^{\text{MTM}} = Nm_{\pi}^{\text{overlap}}$, as a func-	
	tion of $1/N^2$.	59
2.13	The difference between the MTM and overlap correlation func-	
	tions (at a fixed physical distance) at the matching point	
	$Nm_{\pi}^{\text{MTM}} = Nm_{\pi}^{\text{overlap}}$, as a function of $1/N^2$	60
2.14	The difference between the MTM and overlap quark mass at	
	the matching point $Nm_{\pi}^{\text{MTM}} = Nm_{\pi}^{\text{overlap}}$, as a function of $1/N^2$.	60
01	Flowert simples and the bightest simples for maine	
3.1	5 lowest eigenvalues and the highest eigenvalue for various	
	gauge field ensembles. The lattice spacing is $u \approx 0.079$ fm	
	$(\beta = 5.9)$ for upper plots, $a \approx 0.005$ fm $(\beta = 4.05)$ for bottom	67
	There and $u \approx 0.051$ hill $(p = 4.2)$ for bottom right plot	07
4.1	Maximal norm of the overlap operator in logarithmic scale.	
	The linear fit corresponds to the value of s which yields the	
	maximal decay rate. Parameters: $\beta = 3.9$, $L/a = 16$.	81
4.2	The dependence of the overlap Dirac operator norm decay rate	
	ρ on the parameter s for gauge field configurations with and	
	without HYP smearing. Parameters: $\beta = 3.9$, $L/a = 16.$	81
4.3	The continuum limit scaling of the overlap operator decay rate.	82
4.4	The continuum limit scaling of the ratio of the pion mass (at	
	the matching mass) and the overlap operator decay rate.	82
4.5	Effective pion mass plateau for the ensemble $16^3 \times 32$, $a \approx$	
	0.079 fm ($\beta = 3.9$), $a\mu = 0.004$. The bare valence quark mass	
	is $am_a = 0.04$. For each timeslice 3 values of the pion mass	
	are computed, corresponding to different kinds of smearing	
	of the sources (described in Section 3.4.1). The horizontal	
	band corresponds to a simultaneous fit of the LL, LF and	
	FF pseudoscalar correlation functions, which yields a value	
	0.2884(17)	83
4.6	Matching the pion mass for three values of the lattice spacing,	
	corresponding to $\beta = 3.9, 4.05$ and 4.2. The horizontal bands	
	are unitary MTM (maximally twisted mass) values and the	
	curves show the bare quark mass dependence of the overlap	
	pion mass.	84

4.7	The dependence of the pion decay constant on the bare overlap	
	quark mass. The dashed lines correspond to the matching	
	quark masses $a\hat{m}$.	85
4.8	Continuum limit scaling of the overlap pion decay constant at	
	the matching mass and two other reference values of $r_0 m_{\pi}$.	86
4.9	Continuum limit scaling of the MTM pion decay constant at	
	the matching mass.	87
4.10	Continuum limit scaling of the difference of the overlap and	
	MTM pion decay constant at the matching mass.	88
4.11	The comparison of the quark mass dependence of the pion	00
	mass extracted from PP and PP-SS correlators for $\beta = 3.9$	
	ensemble.	92
4.12	The comparison of the quark mass dependence of the pion	0 -
	decay constant extracted from PP and PP-SS correlators for	
	$\beta = 3.9$ ensemble.	93
4.13	Ensemble averages for the following correlation functions: pseu-	
	doscalar (PP), scalar (SS), the difference of PP and SS (PP-	
	SS). The inset shows the PP and PP-SS correlation functions	
	on a single configuration. Parameters: $\beta = 3.9$, $L/a = 16$,	
	$a\mu = 0.004, am_a = 0.004$	94
4.14	Ensemble averages for the following correlation functions: pseu-	
	doscalar (PP), scalar (SS), the difference of PP and SS (PP-	
	SS). Parameters: $\beta = 3.9, L/a = 16, a\mu = 0.004, am_a = 0.04$	
	(much larger valence quark mass than in Fig. 4.13).	95
4.15	Matching the pion mass (extracted from the PP-SS correlator)	
	for three values of the lattice spacing, corresponding to $\beta =$	
	3.9, 4.05 and 4.2.	97
4.16	The dependence of the pion decay constant on the bare overlap	
	quark mass. The dashed lines correspond to the matching	
	quark masses $a\hat{m}$ (from PP-SS correlator). The solid vertical	
	lines (left of the dashed lines) show the difference of $f_{\pi}^{overlap}$	
	and f_{π}^{MTM} (at the matching mass) extracted from the PP	
	correlator.	98
4.17	Continuum limit scaling of the overlap pion decay constant	
	(extracted from the PP-SS correlator) at the matching mass	
	and two other reference values of $r_0 m_{\pi}$	99
4.18	Continuum limit scaling of the difference of the overlap (from	
	the PP-SS correlator) and MTM pion decay constant at the	
	matching mass.	100
4.19	Matching the pion mass for 3 different volumes at a fixed lat-	
	tice spacing $a \approx 0.079$ fm.	102

4.20	The quark mass dependence of the pion decay constant for 3
	different volumes at a fixed lattice spacing $a \approx 0.079$ fm 103
4.21	The relative difference between the overlap and MTM pion
	decay constant at the matching point
4.22	The pion mass dependence of the pion decay constant for over-
	lap valence quarks on MTM sea. Also shown are two unitary
	points (MTM valence quarks on MTM sea), differing only by
	the sea quark mass. Parameters: $\beta = 4.05$, $L/a = 20$ 105
4.23	Continuum limit scaling of the overlap pion decay constant at
	the matching mass – light and heavier sea quark mass 107
4.24	Continuum limit scaling of the MTM pion decay constant at
	the matching mass. The case of the heavier sea quark mass. $% \left[108\right] =1000$. 108
4.25	Continuum limit scaling of the difference of the overlap and
	MTM pion decay constant at the matching mass. The case of
	the heavier sea quark mass, PP and PP-SS correlators 108
4.26	The safe, hazardous and non-safe regions of parameters in
	physical units (linear extent of the lattice vs. pion mass)
	in mixed action simulations with overlap valence and MTM
	sea quarks. The "safe" region corresponds to parameters for
	which the effects of chiral zero modes of the overlap operator
	are negligible
4.27	The comparison of the quark mass dependence of the pion
	mass extracted from PP, PP-SS and PP with explicitly sub-
	tracted zero modes (PP subtr.) correlators for $\beta = 3.9$ ensemble.113
4.28	The comparison of the quark mass dependence of the pion de-
	cay constant extracted from PP, PP-SS and PP with explicitly
	subtracted zero modes (PP subtr.) correlators for $\beta = 3.9$ en-
	semble
4.29	Effective mass plateaus for PP subtr. correlation functions.
	Parameters: $\beta = 3.9$, $L/a = 16$, $a\mu = 0.004$. Upper plot:
	$am_q = 0.011$. Lower plot: $am_q = 0.04$
4.30	The SS subtr. correlation function (SS with explicitly sub-
	tracted zero modes). Parameters: $\beta = 3.9, L/a = 16, a\mu =$
	$0.004, 2$ valence quark masses: $am_q = 0.004, am_q = 0.011$
	(matching mass)
4.31	Matching the pion mass (extracted from the PP subtr. corre-
	lator) for three values of the lattice spacing, corresponding to
	$\beta=3.9,4.05$ and $4.2.$

4.32	The dependence of the pion decay constant on the bare over- lap quark mass. The dashed lines correspond to the match- ing quark masses $a\hat{m}$ (from PP subtr. correlator). The solid vertical lines (left of the dashed lines) show the difference of	
4.33	$f_{\pi}^{overlap}$ and f_{π}^{MTM} (at the matching mass) extracted from the PP correlator.	118
	(extracted from the PP subtr. correlator) at the matching mass and two other reference values of r_0m_{π} .	119
4.34	Continuum limit scaling of the difference of the overlap (from the PP subtr. correlator) and MTM pion decay constant at	
	the matching mass.	120
5.1	Matching the pion mass (from the PP-SS correlator) for 3 different volumes at a fixed lattice spacing $a \approx 0.079$ fm	122
5.2	The dependence of the pion decay constant on the bare over- lap quark mass. The dashed lines correspond to the match- ing quark masses $a\hat{m}$ (from the PP-SS correlator). The solid vertical lines (left of the dashed lines) show the difference of $f^{overlap}$ and f^{MTM} (at the matching mass) extracted from the	
	PP correlator	123
5.3	The SS subtr. correlation function at the matching mass. The solid line represents the fit of eq. (5.4) .	126
5.4	Continuum limit scaling of the fitting parameter γ , defined by eq. (5.3)	127
5.5	The effective nucleon mass plateaus for 3 values of the overlap guark mass. Parameters: $\beta = 4.2$, $L/a = 24$, $au = 0.002$	1.90
5.6	The quark mass dependence of the nucleon and delta mass.	129
	Parameters: $\beta = 3.9, L/a = 16, a\mu = 0.004.$	130
5.7	The quark mass dependence of the nucleon and delta mass. Parameters: $\beta = 4.2$, $L/a = 24$, $a\mu = 0.002$.	130
5.8	Continuum limit scaling of the MTM and overlap light baryon	
	masses (nucleon, delta). The overlap masses are computed at	
	the matching mass. The MTM vales are slightly shifted to the	101
5.0	Monte Carle history of the index of the overlap operator for	131
0.9	different ensembles. The vertical axis scale is the same for all	
	normality of the vertical axis scale is the same for all plots	132
5.10	Histograms of the index of the overlap operator for different ensembles. Also shown are Gaussian fits of the distributions.	102
	The axes scales are the same for all plots	133

5.11	Topological	susceptib	oility fo	or 4 er	nsemb	les of	f gaug	je fie	eld co	on-	
	figurations.	The m_{π}	≈ 450	MeV	enser	nble i	is slig	htly	shift	ted	
	to the right	for bette	r visibi	lity.							134