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Some properties of meson excited states from lattice QCD

Ekaterina V. Mastropas

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Some Properties Of Meson Excited States From Lattice QCD

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The work presented here is devoted to the calculations of the decay constants of the pion and its excited states. All calculations were carried out in the framework of lattice quantum chromodynamics, a well-established formalism of strong interactions enabling the \textit{ab initio} solution of the theory. After a short introduction and review of the fundamental approaches and methods commonly used in lattice QCD, I provide a detail description of the numerical simulations which were performed at three values of the pion mass between 400 and 700 MeV, using an anisotropic clover fermion action with three flavors of quarks. The results obtained indicate that the decay constant of the first excitation, and more notably of the second, is suppressed with respect to that of the ground-state pion, but that the suppression shows little dependence on the quark mass. The second part of this thesis is focused on applications of the methods of perturbation theory to lattice QCD. Here, I give some motivation, and describe the main techniques of perturbative calculations on the lattice, emphasizing its distinctions from the continuum counterpart. I then employ the same anisotropic clover action that was used in numerical study for derivation of lattice Feynman rules which might be used for the calculations of the renormalization parameters helping to connect bare lattice results with real physics.
TABLE OF CONTENTS

Acknowledgments ......................................................................................................................... v
Dedication .......................................................................................................................................... vi
List of Tables ................................................................................................................................ vii
List of Figures .................................................................................................................................viii

CHAPTER

1 Introduction: from QCD to lattice gauge theories ................................................................. 2
   1.1 Theory of strong interactions: puzzles and solutions. ......................................................... 2
   1.2 Need for non-perturbative approach ............................................................................... 7
   1.3 Outline ............................................................................................................................... 8

2 Lattice formulation of QCD ....................................................................................................... 11
   2.1 Lattice discretization ....................................................................................................... 12
      2.1.1 Lattice spacing ...................................................................................................... 12
      2.1.2 Euclidean correlation function ............................................................................... 13
      2.1.3 Path integral approach ......................................................................................... 14
      2.1.4 Discretization errors ............................................................................................ 17
   2.2 Lattice regularization: a recipe ......................................................................................... 18
   2.3 Lattice QCD ....................................................................................................................... 19
      2.3.1 Quarks on the lattice ............................................................................................ 20
      2.3.2 Doubling problem and Wilson’s fermion action ...................................................... 23
      2.3.3 Gluons on the lattice ............................................................................................ 26
   2.4 Numerical simulations for lattice QCD ............................................................................... 30
2.4.1 Importance sampling ................................................................. 30
2.4.2 Numerical methods for fermions ............................................... 32

2.5 Data analysis for lattice calculations ................................................. 33
2.5.1 Statistical uncertainties ............................................................... 34
2.5.2 Sources of systematic uncertainties ............................................. 36

3 Hadron spectroscopy on the lattice ......................................................... 39
3.1 Hadron spectroscopy: general approach and difficulties with excited states 40

3.2 Details of calculations ................................................................. 42
3.2.1 Improved anisotropic lattice action with stout-smeared link variables ................................................................. 42
3.2.2 Symanzik improvement program and the "clover" term .................. 43
3.2.3 Tadpole improvement ................................................................. 47
3.2.4 Stout smearing ................................................................................. 49
3.2.5 Some technicalities ......................................................................... 52

3.3 Meson spectroscopy on the lattice: methods .................................... 53
3.3.1 Variational method ......................................................................... 53
3.3.2 Interpolating operator basis ............................................................ 55
3.3.3 Distillation ......................................................................................... 57
3.3.4 "Ideal" operators ............................................................................. 59

4 Pion decay constants ........................................................................... 61
4.1 Pseudoscalar leptonic decay constants ............................................ 61
4.1.1 Calculation of pion decay constant ................................................ 63
4.1.2 Axial-vector Current ........................................................................ 66
4.2 Results ............................................................................................... 68
4.2.1 Mass spectrum ............................................................................. 68
4.2.2 Decay constants .......................................................... 68
4.2.3 Discussion ................................................................. 75
4.2.4 Leptonic decay constants: some concluding remarks and future challenges. .......................................................... 79

5 Lattice Perturbation Theory ............................................. 81
  5.1 Lattice perturbation theory: why? .............................. 82
  5.2 Renormalization in LQCD ........................................... 84
  5.3 Feynman rules on the lattice: general approach .......... 86
  5.4 Details of calculation .................................................. 87
    5.4.1 An anisotropic lattice action ................................. 87
    5.4.2 Fourier transforms on the lattice ......................... 88
    5.4.3 Quark propagator ............................................... 89
    5.4.4 Quark-quark-gluon vertex .................................. 93
    5.4.5 Gluon propagator ............................................... 95

6 Conclusion and Outlook ................................................. 99

APPENDIX A
APPENDIX B
APPENDIX C
  A.1 Natural units, notation, and Euclidean space ............ 102
  A.2 $SU(N)$ algebra generators ................................. 103

B.1 Axial-vector current improvement ............................. 105

C.1 Fourier transformations on the lattice ....................... 110
C.2 Some standard definitions: derivatives and field strength 111

iii
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I would like to dedicate this thesis to my family - my husband Zak Brown and son Luka for being my best friends, for understanding and for always being there for me. Also, to my mom Zinaida Mastropas for her care and continuous support and, finally, to my cousin Petr Mostrapass who has always encouraged me and helped to turn my ideas into reality. Without them, this dissertation would not have been possible.
LIST OF TABLES

3.1 Lattice extents ($N_s$ and $N_t$), the bare masses of light quark $a_t m_l$ and strange quark $a_t m_s$, the pion mass $a_t m_\pi$, the Sommer scale $r_0$, and the number $N_{\text{cfg}}$ of gauge-field configurations. On each configuration, solution vectors are computed from $N_{\text{vecs}} = 64$ distillation vectors [1], located on a single time slice. ................................................. 52

3.2 Gamma matrix naming scheme. ............................................................ 56

3.3 Continuum spins subduced into lattice irreps $\Lambda$ (the numbers in parentheses are the dimensions of the irreps). ............................................. 56

4.1 The first line for each ensemble lists the masses of the pion and its first three excitations in lattice units ($a_t m_\pi$) obtained from the variational method. The second line lists the pion masses in lattice units obtained from a two-exponential fit to the correlator $C_{A_4, N(t)}$ using the optimal interpolating operator from the variational method at the source, and the unimproved axial-vector current at the sink. In the third line the pion masses in physical units (MeV) obtained from the variational method are presented. ........... 69

4.2 The unrenormalized values of $a_t f_{\pi N}$ for the ground state and first three excitations. For each ensemble, the first line are the values computed using the unimproved axial-vector current, while the second and third lines employ the improved axial-vector current of Eqn. (4.21) with the derivative of the pseudoscalar current computed using the corresponding energy of the state, and a finite time difference, respectively. .......................................... 72

4.3 Naming scheme of the $A_1^{-+}$ basis operators obtained from the variational method $f_{\pi N}$. ................................................................. 79
LIST OF FIGURES

2.1 Path connecting the space-time points \((x_i, t_i)\) and \((x_f, t_f)\) contributing to the integral (2.4). ............................................. 15

2.2 Lattice discretization. Quarks (maroon dots) are placed on the lattice sites, and gluon fields reside on the links between the lattice sites (green lines). 21

2.3 The plaquette \(U_{\mu\nu}(x)\) (Eqn.(2.44)). ..................................................... 28

3.1 Graphical representation of the “clover” term corresponding to the sum of plaquettes in Eqn. 3.14. .............................................................. 46

3.2 The expansion (up to the first order in \(\rho_{\mu\nu}\)) of the “stout” link variable \(U^{(1)}\) in terms of paths of the original links. This Figure is borrowed from Ref. [2]. 51

4.1 The data for \(a_t f_{\pi N}\) in units of the temporal lattice spacing from Eqn. (4.17), for the ensemble at \(m_\pi = 702\) MeV; the line corresponds to the value of \(a_t f_{\pi N}\) obtained from a three-parameter fit to the data as discussed in the text. The optimal operators are obtained from the variational method with \(t_0 = 7\) and the eigenvectors determined at \(t_{\text{ref}} = 15\). ........................................... 70

4.2 The unrenormalized pion decay constants \(a_t f_{\pi N}\) on each of our ensembles obtained using the unimproved axial-vector current. ......................... 71

4.3 The unrenormalized pion decay constants \(a_t f_{\pi N}\) on each of our ensembles obtained using the improved axial-vector current. ......................... 73

4.4 Lattice values for the ratio of the “improved” decay constants for the first excited \(f_{\pi_1}\) and ground-state \(f_{\pi_0}\) pion as a function of the pion mass squared. The green points represent unimproved values, while data in red color correspond to the ratios of improved decay constants. We present linear (upper) and constant (bottom) fits in \(m_\pi^2\) to the ratio of decay constants. ........... 74
4.5 Ratios of the excited-state decay constants $f_{\pi N}$ to the ground-state decay constant $f_{\pi 0}$ for the first three pion excitations ($N = 1, 2, 3$), using the unimproved current. .............................................................. 75

4.6 Ratios of the excited-state decay constants $f_{\pi N}$ to the ground-state decay constant $f_{\pi 0}$ for the first 3 pion excitations ($N = 1, 2, 3$), using the improved current. .............................................................. 76

4.7 The histogram shows the overlap of the operators of the variational basis to the five lowest-lying states in the spectrum, for the data corresponding to a pion mass of 391 MeV, as described in Refs. [3, 4]. The yellow bar denotes the overlap onto an operator derived from a $J = 4$ continuum construction; we associate the fourth excitation with a state of spin 4, and do not discuss further. Grey bars denote overlaps onto “hybrid” operators, as discussed in the text. .............................................................. 78
SOME PROPERTIES OF MESON EXCITED STATES FROM LATTICE QCD
CHAPTER 1

Introduction: from QCD to lattice gauge theories

1.1 Theory of strong interactions: puzzles and solutions.

Prior to the immersion into the particular technical details of my research, I would like to take a brief detour and follow a short but thrilling history of the development of the beautiful theory of strong interactions. Its characteristic features and unsolved puzzles served as a great inspiration and prerequisite for the foundation of lattice quantum chromodynamics, which is the subject of this thesis.

Even though all the main components of the theory of strong interactions - such as quantum field theory, internal symmetries, and gauge interactions - were developed in the 1930’s, they were not enough for the construction of the fully solvable theory. The world of strong interaction physics was still an unexplored mystery; only the collaborative input from both theorists and experimentalists led to a fuller understanding.
The historical formation of the theory of strong interactions can be divided into three ten-year periods. First, the basics of non-abelian gauge theories were formulated in 1950's, when Yang and Mills published results on their research [5]. Ten years later, at the beginning of the 1960's, it was found that all known hadrons can be classified according to the representations of the SU(3) group: they can be grouped into the corresponding octets and decuplets. But the particles belonging to the fundamental representations of this group (triplets and anti-triplets) were not observed in experiment. This problem led Gell-Mann [6] and Zweig [7] to postulate that physical hadrons are not fundamental, but consist of unobserved particles which were called quarks. It was predicted that these basic building blocks of hadronic matter come in six different types, or "flavors" (up (u), down (d), strange (s), charmed (c), bottom (b), and top (t)), and they carry fractional electric charge (+2/3e for u, c, and t quarks, and −1/3e for the d, s, and b quarks). Baryons, which are grouped in octets and decuplets, were proposed to consist of three quarks, while mesons (grouped in octets) represent bound states of quark and anti-quark. But quarks were not associated then in any way with the mathematical methods of non-Abelian theories which seemed to be purely formal at a time. Even as the constituent quark model for hadrons was created, the nature of the forces binding together these constituents inside hadrons remained completely unknown.

This model did not have enough recognition among scientists until 1969, when the results from SLAC experiments on deep inelastic electron-proton scattering (DIS) became known [8]. These data were interpreted by J. Bjorken [9] and R. Feynman [10] in terms of so-called partons: it turned out that the total DIS cross section of virtual photons on nucleons has the same behavior as the cross section of the scattering of a virtual photon on a charged point-like particle. It soon become clear that these partons probed by electrons through virtual photon exchange should have the same quantum numbers as quarks. However, certain technical difficulties arose: the Δ++ resonance in the framework of the constituent
quark model was interpreted as made of three quarks with the same spin orientation, which was forbidden by Pauli's principle. Fortunately, this problem was solved shortly thereafter, when it was proposed by Gell-Mann and others that each flavor of quark have different values of a new internal quantum number called color [11, 12]. Pauli's principle was not violated anymore, since the wave function for the baryons could now be written in the antisymmetric form $\epsilon^{ikl}q^iq^kq^l$, where $i, k, l = 1, 2, 3$ are color indices. It was natural to suggest that quarks interact with each other through the exchange of photon-like bosons, which were called gluons. In 1971, the possibility of measuring the total fraction of the proton momentum carried by quarks was proposed [13], and subsequent experiments demonstrated that this fraction was about a half of the total proton momentum. This fact served as the first indirect indication of the existence of the gluons.

In 1973, D. Gross and F. Wilczek [14] and H. Politzer [15] demonstrated the asymptotic freedom of non-Abelian theories - the property of renormalization that drives the coupling constant of a field theory to smaller (larger) values at shorter (larger) distances [16]. It was also pointed out that non-Abelian gauge theory could describe the dynamics of strong interactions, and this proposal came to be known as quantum chromodynamics (QCD). According to this theory, the colored gluons are able to couple to themselves, and the belief is that these self couplings explain why quarks, interacting weakly at small distances and large energies, appear to be strongly connected to each other as the space between them, and the coupling strength, increases, and cannot fly out of the hadron. Such an argument could also serve as a justification for the fact that free quarks have never been seen in nature, and why only color neutral hadrons are observed. This new, unexpected feature of strong interactions pointed that the basic degrees of freedom cannot be observed in the particle spectrum, was called confinement [17].

The effect of confinement was not the only discrepancy between the observed world and
the phenomenological models such as the constituent quark model, etc. If this new theory is to describe reality, then the up and down quarks must have very small masses. But then the equations within this model possess some additional symmetries, which allow separate transformations among the right-handed and the left-handed quarks. In reality, there is no such chiral symmetry among the observed strongly interacting particles; they do not come in opposite-parity pairs. Therefore, chiral symmetry must be spontaneously broken [18]. Moreover, even though QCD was considered in those days as the only candidate theory of the strong interactions, it was lacking the direct proof of the existence of gluons. Eventually, J. Ellis, G. Ross and M. Gaillard predicted and calculated the experimental expectation for the direct search for the gluon through production via bremsstrahlung in electron-positron annihilation $e^+e^- \rightarrow q\bar{q}g$ [19], and the first observation of a three-jet event being detected came in June 1979 at DESY. Similar events were observed by the TASSO collaboration, and in the August of 1979 the public announcement of the gluon discovery was made at Fermilab [20]; QCD became the established theory of strong interactions.

The fundamental fields which are included in the QCD Lagrangian are those of quarks and gluons, and this Lagrangian represents, in principal, a complete description of the strong interactions. Of course, in practice it leads to equations that are notoriously hard to solve, but an impressive feature of QCD is that it is conceptually a simple theory whose structure is determined entirely by symmetry principles with just a few adjustable parameters. There are some limits in which we can neglect quarks masses (for instance, while considering the structure of ordinary matter, we can neglect masses of heavy quarks since they only play a tiny role in this sector). Due to the mechanism of dimensional transmutation QCD generates its own scale ($\Lambda_{QCD}$) such that the hadron masses are in principle calculable in terms of $\Lambda_{QCD}$. This allow us to obtain a better understanding of proton mass generation: it appears that its mass is mostly due to the binding energy of the quarks and gluons.
inside the proton. Thus, quantum chromodynamics allows us to build up an abundance of physical consequences from a very few input elements, and to describe nature reliably. The reliability of theoretical predictions has already been tested in a set of experiments relating elegantly simple QCD concepts to the observed world around us, and more experiments are on the way. The perturbative properties of QCD can be observed in electron-positron annihilation, where photons (and sufficiently high energy Z bosons) decay often into quark-antiquark pairs which, in turn, fragment into a multi-particle jets. Quarks and gluons, confined permanently due to the QCD interaction, are able to show parts of their identity at high energies via particle jets. Another classic QCD experiment - deep inelastic lepton-nucleon scattering, which was already mentioned above - showed Bjorken-scaling violations at SLAC in the late sixties, and its excellent agreement with the theoretical predictions for this violation allow us to proclaim a spectacular success of the theory [16]. Since these first tests, significant progress in understanding the internal structure of the nucleus has been achieved. Modern DIS experiments present us with the possibility to test the theory under extreme circumstances (with much higher values of the momentum transfer $Q^2$ than were accessible before). Nowadays, some of the most interesting research sectors are experimental efforts in the energy region of $Q^2$ of order 10000 GeV$^2$, where perturbative and non-perturbative aspects of QCD are related closely to each other, and where non-perturbative phenomena can be approached from the perturbative side. In the process of evolving the measured parton densities from the scale $Q$ to a different one, QCD evolution equations plays an essential part.

Overall, after many decades of extraordinary research, QCD has grown up from a set of diverse ideas into an actual quantum field theory of the strong interactions and, together with two other concomitant theories describing the weak and electromagnetic interactions, has became part of the Standard Model of modern physics. The dramatic success of the QCD represents itself a crucial step forward toward better understanding of our universe,
even though a long list of unresolved questions remains.

1.2 Need for non-perturbative approach

Quantum chromodynamics has been proved to be very successful in predicting phenomena involving large momentum transfer. Due to the property of asymptotic freedom, the coupling constant $\alpha_s$ in this regime is small, and perturbation theory serves as a reliable tool. However, at small momenta, due to the increase in $\alpha_s$, perturbation theory is no longer applicable, and a different approach is needed. Its mathematical apparatus should allow to find solutions to problems such as the calculation of fundamental constants of QCD, the mass spectrum, the study of bound state dynamics, and others. Non-perturbative methods are also required if one wants to understand the mechanism of confinement, and determine whether QCD actually accounts for this phenomenon. Such an approach was initially lacking, and for some time all QCD predictions were restricted to the perturbative regime.

This situation changed radically in 1974, when Kenneth Wilson [21] formulated the basic ideas of lattice quantum chromodynamics (LQCD), and thereby opened the possibility for the study of non-perturbative phenomena using numerical methods. His discovery provided the scientific community with a powerful computational tool that can be used for calculating the hadronic spectrum and the matrix elements of any operator within these hadronic states from first principles. Later, in 1980, following ideas proposed by Wilson, M. Creutz [22] performed the first numerical calculations of physical quantities in non-Abelian gauge theory. A vast array of results, obtained in the following twenty years, initiated the beginning of a tremendous lattice QCD era and made significant contribution into the modern understanding of non-perturbative properties of strong interactions, even
though, due to the absence of adequate computing powers and the limited effectiveness of the employed algorithms, the majority of these computations was performed in the so-called *quenched* approximation, where the contribution of virtual quark pairs is not taken into account.

Since Wilson's seminal work, the lattice regularization of QCD has become one of the basic methods for non-perturbative studies in field theory. The answers to the broad range of questions: does QCD account for the confinement and for the observed hadron spectrum? in which way do strong interactions reveal themselves in weak decays? does QCD account for the spontaneous breakdown of chiral symmetry? etc. require a non-perturbative treatment of strong interactions, and the lattice formulation provides the only *ab initio* framework.

1.3 Outline

The following thesis is devoted to the techniques and applications developed within the field of lattice QCD. The organization of the rest of the text is as follows. Chapter 2 serves as an introduction to the basic methods and approaches for gauge field theory on the lattice. Starting with lattice discretization and the path integral approach, I will present the main definitions and formulae that will be used throughout this thesis. I will also note some technical problems of lattice formulations and introduce possible ways to avoid them. In the last two sections of this chapter, I will describe briefly the main ideas of numerical simulations for lattice QCD, and mention the usual sources of uncertainties that arise at the computational stage.

Chapter 3 presents the discussion of the field of hadron spectroscopy on the lattice. After introducing briefly the general approach for calculating masses of hadrons, I will con-
centrate on the difficulties one encounters while dealing with excited states on the lattice. Using the example of the particular improved anisotropic lattice action, that was exploited for all the calculations within this project, I describe the Symanzik and tadpole improvement programs, as well as some smearing techniques. The last section of chapter 3 will be devoted entirely to the methods of meson spectroscopy. I give details about the variational method, "distillation", and interpolating operators basis that were used in numerical part of my work.

Chapter 4 represents the core of this text since it provides the results of the calculations of the pion decay constants for the excited states. Here, after providing a motivation for this study and discussing the current states of the field, I describe the calculational method that was used to extract decay constants from lattice calculations, and introduce some novel results that were obtained for the decay constants of pion excitations. This chapter concludes with a discussion of the results obtained, and with their comparison to similar calculations.

In chapter 5, I firstly motivate the need for perturbative QCD calculations, and present the general idea of renormalization in lattice QCD. Then, after introducing some standard definitions, such as Fourier transforms on the lattice, I describe the common method for the derivation of Feynman rules on the lattice, emphasizing the complexity of this process in comparison with continuum perturbation theory. Eventually, the last section of this chapter presents the most technical part of this text, where the detailed derivation of the Feynman rules is given for the improved anisotropic lattice action used for the numerical calculations within this research.

Finally, conclusions are given in chapter 6, while the basic definitions and notational conventions common for lattice QCD are summarized in Appendix A. Appendix B presents a detailed derivation of the formula for axial-vector current improvement that was used for the calculation of pion decay constants in chapter 4. All formulae relevant for perturbation
theory on the lattice, together with explicit expressions obtained during the derivation of lattice Feynman rules for the improved anisotropic action, are given in Appendix C.
CHAPTER 2

Lattice formulation of QCD

It might seem that lattice regularization of gauge field theories implements the old theorists dream: from continuum space-time one can switch over to the discrete lattice with some finite spacing between sites, and then integrate the functional defined on this lattice. Unfortunately, the real situation is much more complicated, since the treatment of the corresponding integrals is only possible with help of numerical methods. This, probably, can explain the absence of new LQCD results in the decade immediately following the publication of Wilson’s pioneering work in 1974. But the development and improvement of specific numerical methods, as well as the manufacture of more and more powerful computers, led eventually to some drastic advances in this segment of research. Let me introduce in the following section the basic ideas of lattice approach, and discuss some techniques developed in LQCD throughout the time of its existence.
2.1 Lattice discretization

According to ideas developed by K. Wilson in 1974, the lattice formulation of QCD allows to perform non-perturbative calculations by numerical evaluation of the path integral that defines the theory. His approach is Euclidean, since the actual calculations are done in discretized Euclidean space-time, due to the practical reasons which will be explained later in this text. It is worth to mention that in 1975 Kogut and Susskind [23] suggested an alternative lattice approach in which time is treated as a continuum variable, and only space is discretized. But, so far, Wilson’s formulation is still the most powerful and popular, especially since the principal numerical method - the Monte Carlo simulations - was formulated in the Euclidean approach [24]. Let us look at the lattice concepts in detail.

2.1.1 Lattice spacing

As already pointed out, in lattice QCD continuous four-dimensional space-time is discretized. The most common discretization among researchers are hypercubic lattices, which have equal lattice spacing $a$ in all directions, even though, as we shall see later, these spacings do not necessarily have to be equal in all directions. Similar to other regularization procedures with a momentum cut-off, the lattice spacing $a$ in LQCD is an important variable playing the role of the ultraviolet regulator. A length scale, associated with this momentum cut-off, establishes a certain limit above which phenomenological contributions are unphysical. In lattice field theory, space and time are defined only at discrete lattice points and, since $e^{\frac{2\pi i x \mu}{a}} = 1$ for all points $x$, the Fourier transforms of functions in momentum space are periodic with periodicity $\frac{2\pi}{a}$, establishing therefore a momentum cut-off of $\frac{\pi}{a}$. Because the spacing $a$ is only introduced into this formalism as a regulator, no physical quantity should depend on it, and in order to reach a continuum limit of the
theory $a$ has to be sent to zero. Obviously, when one attempts to reach this limit, the momentum cut-off $\frac{\pi}{a}$ goes to infinity, and for obtaining final results for physical quantities the application of a renormalization procedure is necessary.

### 2.1.2 Euclidean correlation function

On the lattice, one of the most frequently calculated quantities that is of particular interest is the so-called Euclidean correlation function. For two operators (say, creation and annihilation operators $\hat{O}_1$ and $\hat{O}_2$) it is defined through

$$\langle O_2(t)O_1(0) \rangle_T = \frac{1}{Z_T} \left[ e^{-(T-t)\hat{H}} \hat{O}_2 e^{-t\hat{H}} \hat{O}_1 \right]. \quad (2.1)$$

Here $Z_T$ is the normalization factor which is given by

$$Z_T = tr \left[ e^{-T\hat{H}} \right]; \quad (2.2)$$

the operator $\hat{H}$ is the Hamiltonian of the system; the parameters $T$ and $t$ denote Euclidean time distances of propagation ($T$ is a formal maximal distance, which will eventually be taken to infinity).

This correlation function (2.1) can be expressed as a sum over eigenstates of the Hamiltonian operator, labeled by $n$. The terms in the sum contain matrix elements of the operators $\hat{O}_i$ taken between vacuum $|0\rangle$ and the physical states $|n\rangle$. These matrix elements are weighted with exponentials containing the energy eigenvalues $E_n$ of the system:

$$\lim_{T \to \infty} \langle O_2(t)O_1(0) \rangle_T = \sum_n \langle 0 | \hat{O}_2 | n \rangle \langle n | \hat{O}_1 | 0 \rangle e^{-tE_n}. \quad (2.3)$$
Euclidean correlation functions, once they are presented in such a form, allow to extract matrix elements of the operators and the energy spectrum of the theory.

### 2.1.3 Path integral approach

In lattice QCD calculations, the Feynman path integral approach serves as a basic tool for quantizing fields on the space-time grid. Here I will describe briefly the essence of the path integral formalism, and show how Euclidean correlation functions can be interpreted using this approach on the lattice.

To introduce the basic idea of path integration, one can use a simple example from quantum mechanics, where the evolution of a position eigenstate $|x_i\rangle$ from some initial time $t_i$ to some final time $t_f$ can be studied through the path integral representation:

$$
\langle x_f, t_f|x_i, t_i \rangle \equiv \langle x_f|e^{-H(t_f-t_i)}|x_i \rangle = \int \mathcal{D}x(t)e^{-S[x]}.
$$

(2.4)

To obtain this form, the original time interval $[t_i, t_f]$ is first divided into a number of infinitesimal segments (see Figure 2.1). Then, all possible paths $x(t)$ are approximated by straight-line segments, and each one of them is weighted with factor $e^{-S[x]}$. Eventually, all these exponentials are summed over all paths, which is done by integrating over all possible coordinates at intermediate times. Therefore, in the above example, $\int \mathcal{D}x(t)$ represents a summation over all possible particle paths $x(t)$ starting at $x_i$ at time $t = t_i$ and ending at $x_f$ at time $t = t_f$, and $S[x]$ is the classical action evaluated for each path $x(t)$:

$$
S[x] = \int_{t_i}^{t_f} dt L(x, \dot{x}).
$$

(2.5)
FIG. 2.1: Path connecting the space-time points \((x_i, t_i)\) and \((x_f, t_f)\) contributing to the integral (2.4).
Once the path-integral treatment is applied to the Euclidean correlation function introduced in previous section, expression (2.1) can be rewritten in the form

\[ \langle O_2(t)O_1(0) \rangle_T = \frac{1}{Z_T} \int \mathcal{D}[\phi] e^{-S_E[\phi]} O_2[\phi] O_1[\phi], \]  

(2.6)

with

\[ Z_T = \int \mathcal{D}[\phi] e^{-S_E[\phi]}. \]  

(2.7)

Here, the integration \( \int \mathcal{D}[\phi] \) denotes a functional integration, which is, in general, a product of an infinite number of ordinary integrals. In other words, analogously to \( \int \mathcal{D}[x(t)] \) in the quantum mechanical system, \( \int \mathcal{D}[\phi] \) represents a product measure of integration measures \( d\phi(n) \) for the classical field variables at all points \( n \) of the four-dimensional lattice \( \Lambda \) \( (\mathcal{D}[\phi] = \prod_{n \in \Lambda} d\phi(n)) \).

Now it is a good time to step aside and clarify the name “Euclidean” that has been used extensively throughout this chapter. As one might notice, there are no \( i \)'s in the above formulae. This is because instead of real time \( \tau \) we choose to work with imaginary, or Euclidean time \( t \), which can be obtained by applying the special field theory procedure called Wick rotation \( t \to i\tau \). After this change, the relative sign between time and space components of the metric vanishes, and it becomes the Euclidean metric \( \delta_{\mu \nu} \), instead of the Minkowski \( g_{\mu \nu} \); more information concerning Minkowski vs. Euclidean metrics is provided in Appendix A. In Euclidean space, the time evolution operator \( e^{-i\hat{H}\tau} \) becomes the operator \( e^{-i\hat{H}(-it)} = e^{-\hat{H}t} \). Therefore this change of time coordinate simplifies the numerical implementation significantly, since the corresponding Euclidean path integrals become real, and their integrands do not oscillate strongly in sign. Thus we can use the method of “importance sampling”, which I will introduce later in this chapter.
2.1.4 Discretization errors

For the numerical evaluation of the Euclidean correlation functions using a path integral, it is important to find an efficient way of representing an arbitrary particle path \( x(t) \), where \( t_i \leq t \leq t_f \), in a computer. In principle, the function \( x(t) \) can be infinitely complex and, therefore, impossible to deal with. To simplify calculations, on the lattice path \( x(t) \) is usually approximated by specifying it only at the sites on a discretized time axis:

\[
t_k = t_j + ka, \quad k = 0, 1 \ldots N.
\] (2.8)

After such an approximation, \( x(t) \) is described by a vector of numbers - a so called “configuration”:

\[
x = \{x(t_0), x(t_1), \ldots x(t_N)\},
\] (2.9)

and the integral over all paths in this approximation becomes an ordinary integral over all possible values of the \( x(t_k) \)'s. Therefore, introduction of the lattice spacing \( a \) converts the Feynman path integral into an ordinary integral of very large dimensionality.

Another issue that one has to take into account is that the spatial and temporal derivatives in the Hamiltonian operator also needed to be discretized in order to perform numerical calculations. Using the Taylor series expansion of the field operators \( \phi(x) \)

\[
\phi(x \pm a) = \phi(x) \pm a\phi'(x) + a^2\frac{\phi''(x)}{2} \pm a^3\frac{\phi'''(x)}{6} \ldots,
\] (2.10)

it is easy to see that, for a small lattice spacing \( a \), the derivative may be approximated as forward differences

\[
\phi'(x) = \frac{1}{a} [\phi(x + a) - \phi(x)] + \mathcal{O}(a),
\] (2.11)
or using central differences:

\[
\phi'(x) = \frac{1}{2a} [\phi(x + a) - \phi(x - a)] + O(a^2).
\]

(2.12)

From here one can see that, due to the smaller discretization errors, it is more advantageous to use the central difference formula.

### 2.2 Lattice regularization: a recipe

Here I would like to summarize briefly an elegant prescription for the numerical implementation of the path integral approach on the lattice. Usually, it is done through the utilization of the following steps:

- A Wick rotation \( t \rightarrow i\tau \) to Euclidean space is performed in order to obtain better behaved integrals so that one can employ the importance sampling algorithm.

- Continuum space-time is discretized by replacing it with a four dimensional Euclidean lattice with lattice spacing \( a \). The degrees of freedom are classical field variables \( \phi \) living on the lattice.

- A suitable Euclidean action functional \( S_E[\phi] \) is defined and discretized on the lattice in such way that in the limit \( a \rightarrow 0 \) it provides the Euclidean continuum action.

- The Euclidean quantum expectation values of operators - so called "lattice values" - are constructed as an average over field configurations, using a measure \( e^{-S_E[\phi]} \):

\[
\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}[\phi] \mathcal{O}[\phi] e^{-S_E[\phi]}}{\int \mathcal{D}[\phi] e^{-S_E[\phi]}}.
\]

(2.13)
The construction of a suitable discretized lattice action, and subsequent recovery of the continuum limit are the two most crucial steps in this procedure, and the following sections will be devoted to the discussion of these issues.

## 2.3 Lattice QCD

In the continuum, the Euclidean space-time QCD action looks like

$$S_{QCD} = \frac{1}{4} \int d^4x F_{\mu\nu}^a F^{a\mu\nu} + \sum_{f=1}^{N_f} \int d^4x \bar{\psi}_f(x) (\gamma_\mu D_\mu + M_f) \psi_f(x). \quad (2.14)$$

Here $\psi_f$ and $\bar{\psi}_f$ are quark fields of flavor $f$, $M_f$ is the mass of the quark with flavor $f$, and $N_f$ is the number of flavors.

$$D_\mu = \partial_\mu + igA_\mu(x) \quad (2.15)$$

is the covariant derivative, and

$$F_{\mu\nu}^a = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a + igf^{abc} A_\mu^b A_\nu^c \quad (2.16)$$

is the field strength tensor (here $f^{abc}$ are the structure constants of SU(3) group). The Euclidean gamma matrices $\gamma_\mu$ satisfy

$$\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}. \quad (2.17)$$

Let us see now how this continuum action transforms on the lattice.
2.3.1 Quarks on the lattice

I consider here the case of a four-dimensional isotropic \((a_s = a_t = a)\) Euclidean \(L^3T\) lattice. The spatial volume of the lattice is \(V = L_1 L_2 L_3\) (here \(L_j\) are spacial extensions), and there are \(L_4 = T\) Euclidean time slices, so the total number of lattice points is \(VT = L_1 L_2 L_3 T\). For simplicity, one usually works with a symmetric cubic grid, where \(L_1 = L_2 = L_3 = L\). The Euclidean space-time positions \(x = (x_1, x_2, x_3, x_4)\) (with the Euclidean time being the fourth coordinate: \(x_4 \equiv t\)) are restricted to lie on the sites of the lattice, i.e. \(x = a(n_1, n_2, n_3, n_4)\), with \(n_j\) being integers, and chosen in the intervals \(0 \leq x_\mu \leq L_\mu - 1\) (\(\mu = 1, 2, 3, 4\)).

The quark and antiquark fields are placed on the lattice sites (see Figure 2.2), and a quark or antiquark state can be specified by a set of numbers \(|n, f, c, \sigma\rangle\). Here \(n\) is a lattice vector with integer components that gives the location of a site on the lattice \((x_\mu = a n_\mu\), \(f\) is the flavor index mentioned previously, \(c\) is the color index, and \(\sigma\) is a Dirac spinor index.

Multiple quark states may be formed by putting more than one quark on the lattice, and the number of quarks that can exist on a single lattice site is limited only by the Pauli principle. The Dirac operators \(\bar{\psi}_{n,f,c,\sigma}\) and \(\psi_{n,f,c,\sigma}\) that create and destroy quarks are like those of a continuum theory, except they act on the lattice sites only. In the following discussion, for simplicity, I will omit the indices and use matrix/vector notation instead.

In the continuum, the action \(S_F\) for a free fermion is given by (see (2.14), if we set \(A_\mu = 0\):

\[
S_F^0[\psi, \bar{\psi}] = \int d^4x \bar{\psi}(x) (\gamma_\mu \partial_\mu + m) \psi(x). \tag{2.18}
\]

For the lattice transcription of this action, we need to discretize the integral and the partial derivative. The naive discretization is implemented by replacing the partial derivative with
FIG. 2.2: Lattice discretization. Quarks (maroon dots) are placed on the lattice sites, and gluon fields reside on the links between the lattice sites (green lines).

the symmetric first order approximation from a Taylor series expansion (see (2.12)),

$$\partial_\mu \psi(x) \rightarrow \frac{1}{2a} [\psi(n + \hat{\mu}) - \psi(n - \hat{\mu})],$$

(2.19)

were we have used \(n\) for the lattice positions of the quarks, instead of the actual physical space-time point \(x = an\). Also, the four dimensional integral needs to be replaced by a sum over all lattice sites:

$$\int dx^4 \rightarrow a^4 \sum_{n \in \Lambda},$$

(2.20)

where \(\Lambda\) is the four dimensional lattice:

$$\Lambda = \{n = (n_1, n_2, n_3, n_4)\}, \quad n_\mu = 0, 1, \ldots, L - 1.$$  

(2.21)
After these substitutions, the lattice version of the free fermion action takes the following form:

$$S^0_F[\psi, \bar{\psi}] = a^4 \sum_{n \in \Lambda} \bar{\psi}(n) \left( \sum_{\mu=1}^{4} \frac{1}{2a} \gamma_\mu [\psi(n + \hat{\mu}) - \psi(n - \hat{\mu})] + m\psi(n) \right). \tag{2.22}$$

We require the invariance of the action with respect to a local gauge transformation $V(n)$, where $V(n)$ is an SU(3) matrix. The quark fields are subject to this transformation:

$$\psi(n) \rightarrow V(n) \psi(n), \quad \bar{\psi}(n) \rightarrow \bar{\psi}(n)V(n)^\dagger. \tag{2.23}$$

The mass term of the fermion action (2.22) is invariant under transformation (2.23), but this is not the case for the discretized derivative terms. However, the introduction of gauge fields $U_\mu(n)$ as elements of the gauge group SU(3), transforming according to

$$U_\mu(n) \rightarrow V(n) U_\mu(n) V(n)^\dagger, \tag{2.24}$$

makes a combination $\bar{\psi}(n) U_\mu(n) \psi(n + \hat{\mu})$ gauge invariant. The next section will be devoted to the detailed discussion of these so-called link variables $U_\mu(n)$, but for now we state that their introduction allows us to obtain the gauge invariant naive lattice action for fermions:

$$S^0_F[\psi, \bar{\psi}, U] = a^4 \sum_{n \in \Lambda} \bar{\psi}(n) \left( \sum_{\mu=1}^{4} \frac{1}{2a} \gamma_\mu [U_\mu(n)\psi(n + \hat{\mu}) - U_{-\mu}(n)\psi(n - \hat{\mu})] + m\psi(n) \right). \tag{2.25}$$

In this expression we used the fact that since the link variables are oriented, one can also define link variables that point in the negative $\mu$ direction:

$$U_{-\mu}(n) \equiv U_\mu(n - \hat{\mu})^\dagger. \tag{2.26}$$
2.3.2 Doubling problem and Wilson’s fermion action

The action (2.25) suffers from a severe problem: it describes \(2^d\) equivalent fermion fields in the continuum limit in \(d\) dimensions. This situation can be illustrated as follows [25]. The naive fermion action (2.25) can be written in the form that includes the lattice Dirac operator \(D(n|m)\):

\[
S_F^0[\psi, \bar{\psi}, U] = a^4 \sum_{n, m \in \Lambda} \bar{\psi}(n) D(n|m) \psi(m),
\]

(2.27)

where

\[
D(n|m) = \sum_{\mu=1}^{4} \frac{1}{2a} \gamma_{\mu} [U_{\mu}(n) \delta_{n+\mu, m} - U_{-\mu}(n) \delta_{n-\mu, m}] + m \delta_{n, m}.
\]

(2.28)

For trivial gauge fields \(U_{\mu}(n) = 1\), the corresponding lattice Dirac operator for free lattice fermions has a form

\[
D(n|m) = \sum_{\mu=1}^{4} \frac{1}{2a} \gamma_{\mu} [\delta_{n+\mu, m} - \delta_{n-\mu, m}] + m \delta_{n, m}.
\]

(2.29)

In momentum space, this operator becomes

\[
\hat{D}(p|q) = \frac{1}{|\Lambda|} \sum_{n, m \in \Lambda} e^{-ip \cdot na} D(n|m) e^{iq \cdot ma} =
\]

\[
= \frac{1}{|\Lambda|} \sum_{n, m \in \Lambda} e^{-ip \cdot na} \left( \sum_{\mu=1}^{4} \frac{1}{2a} \gamma_{\mu} [\delta_{n+\mu, m} - \delta_{n-\mu, m}] + m \delta_{n, m} \right) e^{iq \cdot ma} =
\]

\[
= \frac{1}{|\Lambda|} \sum_{n \in \Lambda} e^{-i(p-q) \cdot na} \left( \sum_{\mu=1}^{4} \frac{1}{2a} \gamma_{\mu} [e^{iqa} - e^{-iqa}] + m 1 \right) =
\]

\[
= \frac{1}{|\Lambda|} \sum_{n \in \Lambda} e^{-i(p-q) \cdot na} \hat{D}(p) = \delta(p - q) \hat{D}(p),
\]

(2.30)
where $\tilde{D}(p)$ is the Fourier transform of the lattice Dirac operator,

$$\tilde{D}(p) = \frac{i}{a} \sum_{\mu=1}^{4} \gamma_{\mu} \sin(p_{\mu}a) + m1,$$

(2.31)

and at the last step of derivation the following identity has been used [25]:

$$\frac{1}{|\Lambda|} \sum_{n \in \Lambda} e^{-i(p-q)na} = \delta_{p_1,q_1} \delta_{p_2,q_2} \delta_{p_3,q_3} \delta_{p_4?q_4} = \delta(p-q).$$

(2.32)

The inverse of the lattice Dirac operator $D^{-1}(n|m)$ - the quark propagator - is given as

$$D^{-1}(n|m) = \frac{1}{|\Lambda|} \sum_{p \in \Lambda} \tilde{D}(p)^{-1} e^{ip(n-m)a},$$

(2.33)

where

$$\tilde{D}(p)^{-1} = \frac{ia^{-1} \sum_{\mu} \gamma_{\mu} \sin(p_{\mu}a) + m1}{a^{-2} \sum_{\mu} \sin(p_{\mu}a)^2 + m^2}.$$ 

(2.34)

One can see that in the naive continuum limit $a \to 0$ the fermion propagator in the momentum space (at $m = 0$) behaves as

$$\tilde{D}(p)^{-1}|_{m=0,a \to 0} \to -\frac{i}{p^2} \sum_{\mu} \gamma_{\mu} p_{\mu},$$

(2.35)

i.e. it has a single pole at $p = (0, 0, 0, 0)$. But on the lattice, where $-\frac{\pi}{a} < p_{\mu} \leq \frac{\pi}{a}$, this propagator has additional unphysical poles whenever momentum components $p_{\mu}$ are 0 or $\frac{\pi}{a}$. In other words, there are 16 poles while only one of them is physical. These unwanted modes are called *doublers*, and they must be eliminated so as to define a theory with the correct number of the quark degrees of freedom. Historically, there were two commonly used methods for treating this problem, even though neither of them is completely satisfactory. The first method, *Kogut-Susskind fermions* (also known as *staggered fermions*)
[26], accepts the doubling but only preserves the residue of chiral symmetry. The second method - so-called Wilson fermions [21] - utilizes the most simple way of avoiding unwanted doublers by including an additional term $\tilde{D}(p)_{\text{Wilson}}$, so that modified momentum space Dirac operator looks like

$$
\tilde{D}(p) = \tilde{D}(p)_{\text{naive}} + \tilde{D}(p)_{\text{Wilson}} = \frac{i}{a} \sum_{\mu=1}^{4} \gamma_{\mu} \sin(p_{\mu} a) + \frac{1}{a} \sum_{\mu+1}^{4} (1 - \cos(p_{\mu} a)) + m \mathbb{1}. \tag{2.36}
$$

In position space, the Wilson term, which is proportional to the negative Laplace operator, has the form

$$
S_{F}^{\text{Wilson}} = -\frac{r}{2a} \sum_{n \in \Lambda} \sum_{\mu=1}^{4} \bar{\psi}(n) \left[ \psi(m + \hat{\mu}) + \psi(m - \hat{\mu}) - 2\psi(m) \right] \delta_{n,m}
= r \bar{\psi}(n) D_{\text{Wilson}}(n|m) \psi(m), \tag{2.37}
$$

where $r$ is called the Wilson parameter, and the popular choice is $r = 1$. In the continuum limit, the total Wilson fermion action $S_{F}^{W} = S_{F}^{0} + S_{F}^{\text{Wilson}}$ behaves as

$$
S_{F}^{W} \rightarrow \int \bar{\psi}(x) \left( \gamma_{\mu} D_{\mu} + m_{F} \right) \psi(x) \, d^{4}x + O(a), \tag{2.38}
$$

i.e. it converges to the continuum limit more slowly than the gauge action through the $O(a)$ discretization uncertainty. This imperfection is usually ameliorated in various improved fermion actions (see next chapter). The appearance of the extra doubler fermions in the naive discretization of the fermion action (2.25) is inevitable and related to the deeper theoretical problem of formulating chirally symmetric fermions on the lattice. This is encapsulated by the Nielsen-Ninomiya no-go theorem [27]: it is impossible to define a chirally invariant, local, translation invariant, real bilinear fermion action on the lattice without producing unphysical fermion degeneracy - something must be sacrificed. The
Wilson term (2.37) violates chiral symmetry, but the chiral breaking is proportional to the lattice spacing so it disappears in the continuum limit. It also introduces discretization errors linear in $a$, while the naive fermion action has smaller discretization error of order $\mathcal{O}(a^2)$. In spite of these shortcomings, Wilson fermions and their improved versions are extensively studied because of their simplicity. A commonly used variant that eliminates the $\mathcal{O}(a)$ discretization error is the $\mathcal{O}(a)$-improved Wilson (or so-called clover) fermions, and I will talk about this approach in the next chapter in more detail.

2.3.3 Gluons on the lattice

In the continuum, the gluon fields, mediating interactions between quarks, are described by a vector potential $A^c_\mu(x)$. It is convenient to work with this vector potential multiplied by the gauge group generator so that the eight types of gluons are written in terms of the Hermitian matrix:

$$A_\mu(x) \equiv \sum_{c=1}^{8} A^c_\mu(x) \cdot \frac{\lambda_c}{2}, \quad (2.39)$$

where $\lambda_a$ are eight generators of the SU(3) group, normalized to $Tr \lambda_a \lambda_b = 2\delta_{ab}$.

On the lattice, the gauge fields reside on the links between the lattice sites (see Figure 2.2), and transport color information between them. Naturally associated with the link joining neighboring sites $n$ and $n+\hat{\mu}$, the lattice gluon field corresponds in the continuum to a Wilson line connecting these two points,

$$U = \mathcal{P} e^{i \int_{z}^{z+\hat{\mu}} A_{\mu}^{cont}(x)dx_\mu}. \quad (2.40)$$

This is the so called gauge transporter, where $\mathcal{P}$ indicates a path-ordered exponential integral of the continuum gauge field $A_\mu$ along some path connecting two points. We can
associate with each link a discrete version of this path-ordered product, and the lattice
gauge transporter corresponding to (2.40) for the lattice gauge fields $A_\mu(n)$ on the link
between lattice sites $n$ and $n + \hat{\mu}$ is defined as

$$U_\mu(n) \equiv U(n, n + \hat{\mu}) = e^{iga_\mu(n + \frac{\hat{\mu}}{2})}, \quad (2.41)$$

with the average field $A_\mu$ defined at the midpoint of the link, which will be important
later for the general economy of calculations. These gauge degrees of freedom, called link
variables and represented by an SU(3) matrices $U_\mu(x)$, were already introduced briefly
in the previous section, where I also pointed out their gauge transformation properties
(2.24). It is also worth to mention that since the link variables have orientation, one can
also define the link variable pointed in the negative $\mu$ direction:

$$U_{-\mu}(n) \equiv U_\mu(n - \hat{\mu})^\dagger = e^{-iga_\mu(n - \frac{\hat{\mu}}{2})}. \quad (2.42)$$

The action for any lattice gauge theory can be obtained from the corresponding action
of the continuum theory by the substitution of the derivatives, included into this action,
with finite differences, and by using summation over lattice sites instead of integration.
However, in the presence of interactions such a method would break local gauge invariance.
This is why in lattice QCD one uses a formulation where gauge fields correspond not to
the lattice sites, but to the links connecting these sites. Apart from gauge invariance, the
lattice action should also produce the correct naive continuum limit at $a \rightarrow 0$, at which
point lattice action should turn into the continuum one.

Taking these points into account, it can be demonstrated that there are two types of gauge
invariant objects that one can construct on the lattice:

- a string consisting of a path-ordered product of links (with end points $n$ and $m$) capped
by a fermion and an anti-fermion. The simple example is

\[ Tr \bar{\psi}(n)U_\mu(n)U_\nu(n + \hat{\mu}) \ldots U_\rho(m - \hat{\rho})\psi(m), \]  

(2.43)

with the trace over color indices;

- a closed Wilson loop \( W_C = Tr U_C(n, n) \) (here \( C \) indicates the closed path). The simplest example is a rectangle of four sites and four links (plaquette) - the shortest, nontrivial closed loop (see Figure 2.3):

\[ U_{\mu\nu}(n) \equiv W_{\mu\nu}^{1\times1} = Re Tr \left( U_\mu(n)U_\nu(n + \hat{\mu})U_\mu^1(n + \hat{\nu})U_\nu^1(n) \right). \]  

(2.44)

For SU(N \geq 3) group, the trace of any Wilson loop in the fundamental representation is complex, with the two possible path-orderings giving complex conjugate values. Thus, taking the trace in the expression (2.44) insures gauge invariance, and taking its real part
is equivalent to averaging the loop and its charge conjugate.

The simplest possible gauge action, usually called the \textit{Wilson gauge action}, is given by the product of gauge links around elementary plaquettes:

\[
S_G = \frac{2}{g^2} \sum_{n \in \Lambda} \sum_{\mu < \nu} \text{Re} \text{Tr} \left( 1 - U_{\mu\nu}(n) \right). \tag{2.45}
\]

Substituting in here the expansion for link variable (2.41),

\[
U_{\mu}(n) \equiv U(n, n + \hat{\mu}) = e^{i g A_{\mu}(n + \frac{\hat{\mu}}{2})} = 1 + i g A_{\mu}(n + \frac{\hat{\mu}}{2}) + \frac{1}{2} \left( i g A_{\mu}(n + \frac{\hat{\mu}}{2}) \right)^2 + \ldots, \tag{2.46}
\]

it is easy to see that in the limit \( a \to 0 \) the action (2.45) gives the continuum gauge action (compare to (2.14)):

\[
S_G \to \int d^4 x \frac{1}{4} F_{\mu\nu} F_{\mu\nu} + \mathcal{O}(a^2). \tag{2.47}
\]

The correction, which in this case is quadratic in lattice spacing \( a \), might be reduced to \( \mathcal{O}(a^4) \) by addition of new terms of higher dimension with more complex structure. Such modified actions are used nowadays in majority of lattice calculations, and in the next Chapter I will discuss some possible improvements for the Wilson action using the example of the particular lattice action I did my research with.

From the complete lattice action for QCD (in the simple case of Wilson fermions), which is given as the sum of a fermion action with Wilson term and a gauge action, any correlation function of the fermionic and link variables can be computed. In the next section, I will introduce briefly some basic numerical methods and approaches that are used for numerical calculations of the non-perturbative observables within the framework of lattice QCD.
2.4 Numerical simulations for lattice QCD

2.4.1 Importance sampling

The biggest problem that always arises at the stage of the numerical implementation of lattice QCD is the necessity to perform a tremendously large number of integrations while calculating the expectation values of the physical observables \( \mathcal{O} \)

\[
\langle \mathcal{O} \rangle = \frac{1}{Z} \int [DU] \mathcal{O}[U] e^{-S[U]},
\]

(2.48)

where a general functional integral for the partition function for a bosonic field \( U(x) \) has the form

\[
Z = \int [DU] e^{-S(U)}.
\]

(2.49)

Here \([DU]\) assumes an integration over the values of the field on each lattice site \( n \), i.e. \([DU] = \prod_n dU_n\); it is clear that some statistical methods must be used for evaluation of these ensemble averages, whose expressions (2.48) involve multiple integrations. Fortunately, it was realized that only a small fraction of the possible link configurations makes a significant contribution to the integral (2.48), and soon an efficient way of computing the observables was found. The corresponding technique, called Monte Carlo importance sampling, consists of generating a sequence of random gauge field configurations \( \{U\}_i \) \((i = 1, \ldots N\), where \( N \) is the number of samples\) with a probability distribution given by a Boltzmann factor \( e^{-S[U]} \), which is real in Euclidean space. Then, if the generated sequence is itself a representative set of configurations, the expectation value of the observable \( \langle \mathcal{O} \rangle \) is replaced by the average of this observable over the sample set of gauge field configurations \( \{U\}_i \):

\[
\langle \mathcal{O} \rangle \approx \frac{1}{N} \sum_{i=1}^{N} \mathcal{O}(\{U\}_i),
\]

(2.50)
where $\mathcal{O}(\{U\}_i)$ represents the observable $\mathcal{O}$ calculated on the configuration $\{U\}_i$.

There are various systematic procedures available to do this exist, but two specific Monte Carlo schemes are in common use: the Metropolis algorithm [28] and the heat bath method [29]. Briefly, the procedures within both of these methods begin with some initial field configuration $\{U\}$, after which a new configuration $\{U'\}$ is generated through a sequence of prescribed random updates of the link variable $U_\mu$. In the case when the conditions of the particular algorithm are satisfied, the old configuration $\{U\}$ is replaced by the new one; otherwise the old configuration is kept. In the Metropolis algorithm, this procedure is repeated successively for each link in the lattice, and a sweep (or iteration) of the lattice is completed after all links are sampled. Eventually, after sufficient iterations, the algorithm brings the lattice to approximate “thermal distribution” (which is the name for limiting probability distribution, in analogy with statistical mechanics). Then the expectation value of the observable is evaluated after the distribution reaches the equilibrium distribution.

Within the heat-bath algorithm, which is an alternative to the Metropolis procedure, each lattice link is placed successively into a contact with a “heat bath reservoir” (the computer) which selects a new link variable stochastically with a probability distribution given by a Boltzmann factor. This method usually brings a lattice to equilibrium in fewer iteration steps than the Metropolis algorithm, but the computations within each iteration usually take longer. The majority of lattice calculations nowadays uses so-called Hybrid Monte Carlo method combining the Metropolis algorithm with another class of updating method - molecular dynamics, which uses classical dynamics and the ergodic hypothesis to obtain the desired statistical distribution [30, 31].
2.4.2 Numerical methods for fermions

The inclusion of dynamical fermions in lattice gauge calculations represents a tremendous technical problem for the numerical implementation of the lattice Monte Carlo algorithms. An expectation value of an observable is represented in this case by

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}[\tilde{\psi}] \mathcal{D}[\psi] \mathcal{O}(\tilde{\psi}, \psi, U) e^{-S[\tilde{\psi}, \psi, U]},$$

(2.51)

with

$$Z = \int \mathcal{D}[\tilde{\psi}] \mathcal{D}[\psi] e^{-S[\tilde{\psi}, \psi, U]}.$$

(2.52)

The total lattice action $S[\tilde{\psi}, \psi, U]$, which includes the Wilson fermion action, can be represented schematically in the form

$$S[\tilde{\psi}, \psi, U] = S_G[U] + S_F[\tilde{\psi}, \psi, U] = S_G[U] + \sum \tilde{\psi}(1 - \kappa M)\psi,$$

(2.53)

where under the sum over quark flavors, $\kappa$ is the so-called hopping parameter corresponding to the inverse of quark mass, and the hopping matrix $M$ depends on the gauge fields and plays the role of a covariant derivative of the continuum theory. The fermion fields $\tilde{\psi}$ and $\psi$, being elements of a Grassmann algebra, cannot be represented on computers and therefore must be first integrated out. This procedure leads to a fermion determinant in the Euclidean partition function $Z$:

$$Z = \int \mathcal{D}[U] \text{Det}(1 - \kappa M)^{N_f} e^{-S_G}.$$

(2.54)

The computation of this determinant of the typically million-dimensional hopping matrix, which represents the effects of virtual quark loops, increases enormously the required computational time; its direct computation is practically impossible, and a great deal of
effort has been invested in developing efficient algorithms and special “tricks”. It is inherently non-local, reflecting the need to satisfy exchange symmetry for the quark fields. At first, the absence of sufficiently powerful computers led to the utilization of the mentioned already quenched approximation, where $\text{Det}(1 - \kappa M)$ is set to unity. Even though the computational simplicity of this approach is a major advantage, it ignores the effects of virtual quarks-antiquarks excitations on the lattice. That is why in last decades persistent attempts at the full inclusion of the fermion determinant have been made, and they led eventually to several proposed methods of dealing with fermions on the lattice without the quenched approximation. Many results have been obtained for two mass-degenerate light quarks ($N_f = 2$), which corresponds to the inclusion of $u$ and $d$ quarks. The studies with a third additional quark, which corresponds to the $s$ quark ($N_f = 3$ or $N_f = 2 + 1$), are also extensive in modern LQCD, with mass $m_s$ much bigger than $m_u, d$.

### 2.5 Data analysis for lattice calculations

All results obtained in numerical lattice QCD simulations have both statistical and systematic uncertainties. The statistical uncertainty, which decreases as $1/\sqrt{N}$, arises through the use of Monte Carlo importance sampling during the evaluation of path integrals, and in order for a certain LQCD-produced result for some physical quantity to serve as a useful prediction for experiment or phenomenology, the final outcome of a lattice QCD calculation is presented as the average value of this observable with an estimate for the corresponding statistical error [25]. A number of different systematic uncertainties, which I will list later in this section, also always exists in lattice calculations, even though their sizes depend on the particular physical quantity and on the parameters of the lattices used in the study.
2.5.1 Statistical uncertainties

The use of the Monte Carlo simulation algorithm, which produces a new configuration in the chain by evolving the previous one, leads to the fact that observables are correlated, i.e. we cannot assume safely that successive measurements of some observable $O_i$ are statistically independent. These autocorrelations lead to systematic uncertainties of order $\mathcal{O}(e^{-\tau_{\text{exp}}/\tau})$, where $\tau_{\text{exp}}$ is so-called autocorrelation time, and $\tau$ is the computer time between subsequent measurements. The final results for physical observables in lattice calculations are obtained usually by performing fit analyses. These procedures are based on the expectation that the correlation function is described by some model function $f(t_i, \alpha_a)$ which is parametrized by a set of coefficients $\alpha_s$ - for example, the masses and amplitudes. The estimated values of these parameters, and the statistical uncertainty on these estimates are determined usually from the data by adjusting them in a conventional least-$\chi^2$ fit.

If we assume that we generated $N$ independent configurations, and then averaged the correlator at a set of distances $t_i$ on each of these configurations (we denote the result for the $k$'th configuration as $R_{ik}$), then the average over a sample of configurations at distance $t_i$ can be written as

$$\bar{R}_i = \frac{1}{N} \sum_k R_{ik}. \quad (2.55)$$

The covariance matrix for these averaged quantities $\bar{R}_i$ is defined as

$$C_{ij} = \frac{1}{N(N-1)} \sum_{k=1}^{N} (R_{ik} - \bar{R}_i) (R_{jk} - \bar{R}_j) ; \quad (2.56)$$

the square roots of its diagonal elements are the standard errors on the $\bar{R}_i$, while the off diagonal elements contain the information about the correlations among the different $\bar{R}_i$. After repeating our simulation many times, we would get a distribution of results whose
probability distribution is given by

\[ P(\bar{R}) = \exp\left[ -\frac{1}{2} (\bar{R}_i - f(t_i, \alpha_a)) C_{ij}^{-1} (\bar{R}_j - f(t_j, \alpha_a)) \right], \]  

(2.57)

assuming that the theory correctly describes the data. After this, we need to adjust the parameters in a model function \( f(t_i, \alpha_a) \) to obtain the best fit to the sample average \( \bar{R}_i \). Even though there is no unique definition of best fit, the most commonly used method is to find parameters maximizing the probability \( P(\bar{R}) \), or minimizing the exponent [32]. Twice this exponent is called \( \chi^2 \):

\[ \chi^2 = (\bar{R}_i - f(t_i, \alpha_a)) C_{ij}^{-1} (\bar{R}_j - f(t_j, \alpha_a)) . \]  

(2.58)

In order to find the inverse of this correlation matrix \([C^{-1}]_{ij}\), which can be a tricky problem if it contains nearly singular eigenvalues, the method of single value decomposition (SVD) serves as a possible solution. The analysis within this method starts with a spectral decomposition of the \( C_{ij} \), and the inverse of the correlation matrix is approximated then by a restricted sum over the modes. After construction of \( C^{-1} \) is done, the data are fitted, and the statistical error of the fit result is calculated, usually using the jackknife or bootstrap methods.

Within the jackknife [33] resampling technique, the \( n \)-th entry \((n = 1, \ldots, N)\) is removed from the original set of \( N \) values, and the full statistical analysis is performed on the reduced sample obtained this way. The process is then repeated, removing each entry in turn, and the best fit results for the parameters \( \alpha_a \) are recorded. As well as jackknife, the statistical bootstrap resamples the original set of \( N \) data points. The difference is that bootstrap analyzes \( N_{\text{boot}} \) data sets, each one of them being obtained by random Monte Carlo sampling of the original set of \( N \) points, while jackknife considers \( N \) new data.
sets, each of them containing all the original data points except for one. Both the reduced jackknife samples and randomly chosen bootstrap samples are large enough for performing a fitting, therefore, these methods are used broadly for determining the uncertainties of the fitted quantities without the need for additional data.

2.5.2 Sources of systematic uncertainties

In this section, I will give a short description of the most common sources of systematic uncertainties in lattice QCD, whose actual evaluation is quite involved.

**Continuum limit.** In order to obtain actual physical results, the continuum limit as $a \to 0$ of the evaluated lattice quantities has to be calculated. In practice, this is done by performing the calculations at few different values of lattice spacing $a$ (typical values for $a$ lay in the range $0.05 - 0.15$ fm), and after that results are extrapolated to $a = 0$.

**Finite volume effects.** Numerical simulations on the lattice, which itself represents a finite space-time box, lead to the fact that calculated physical quantities differ from their infinite volume values. For the spectroscopy studies, one usually uses $N^3 \times N_t$ lattices which are much larger in temporal direction in comparison with the spatial directions. Neglecting the finite time extent, the leading finite size effects are due to the spatial volume. The estimation of the finite volume errors is usually done by repeating the simulations on two or more different volumes, keeping other parameters fixed, and the leading exponential correction to the mass is of order $O(e^{-L_{max}})$ [25]. The typical lattice sizes $L_s = aN$ these days are about $3 - 4$ fm and, according to PDG [34], the finite size effects are negligible for $m_{\pi}L_s > 4$; most large-scale simulations use lattices satisfying this condition.
Extrapolation to physical quark mass (chiral extrapolation). The dynamical LQCD simulations with physical masses of up and down quarks are quite difficult and expensive, therefore the calculations are performed usually for several values of light quark masses $m_u$ and $m_d$ lying at the rather large quark mass region between $0.1 m_s$ and $m_s$ (with the mass $m_s$ of the strange quark equal approximately to its physical value). After that, the result is extrapolated to the physical value of the mass of light quarks, with the help of the chiral perturbation theory (ChiPT). However, a fit of the result according to the prediction of ChPT is highly nontrivial, and large systematic errors are usually produced.

Number of dynamical flavors and heavy quarks. The results in the case of quenched or $N_f = 2$ simulations obviously suffer from the errors from the number of dynamical flavors. From the other side, calculations involving heavy quarks, such as the charm $c$ and the bottom $b$ quarks, cannot be performed the same way as they are done for light quarks, and special techniques are required since the condition $m_q a << 1$ does not hold in their case. The solution is in the use of two specially developed approaches: heavy quark effective theory (HQET) and non-relativistic QCD (NRQCD). Their central idea is focused on the removing the dominant scale (the mass $m_q$ of the heavy quark), and on the study of the effective action, which is the $\frac{1}{m_q}$ expansion of the initial action.

Overall, numerical lattice calculations represent a sequence of the following steps. Firstly, gauge configurations are generated with the use of the Hybrid Monte Carlo algorithm. During the second step, the quark propagators (i.e., $M^{-1}$) are calculated on each configuration. After that, hadron correlation functions are computed, and the physical values - such as masses, matrix elements, etc. - are obtained from them. Eventually, measured quantities are analyzed. The next chapter of my thesis will be devoted to the description of possible ways of improving lattice actions and measuring physical observ-
ables on the lattice. I will apply the lattice approach to the study of hadronic spectrum and its excitations, as well as to calculation of some of its properties.
CHAPTER 3

Hadron spectroscopy on the lattice

The calculation of the hadron spectrum represents the most basic prediction of lattice QCD. Once the input parameters $m_u, m_d, m_s, m_c$ and $m_b$ are fixed, a whole variety of light, heavy-light and heavy-heavy hadron masses can be predicted from lattice simulations. The comparison of these numerical results with the experimentally measured masses, most of which are known to a high precision, is an important check of non-perturbative QCD, and over the last two decades, lattice QCD hadron spectroscopy calculations of the lowest lying states have reached impressive agreement with experimental data.

The theoretical research presented within this thesis is devoted to the study of the spectrum of hadronic excitations, with its main focus on computation of some properties of the excited states. In particular, I performed calculations of the leptonic decay properties of the pion - the lightest system with simple quark-antiquark structure - and its excitations. Needless to say, obtaining precise information about excited hadrons on the lattice poses numerous challenges. The main source of difficulties in these studies is caused by the faster decay of their Euclidean correlation functions in comparison with those of the ground state, which leads to the worsening of the signal-to-noise ratio. There are also some additional
complications which arise at the stage of constructing hadronic operators, where one seeks to balance the computational cost with the level of overlap achieved by a set of operators. Despite all these obstacles, the latest development in advanced computational lattice QCD techniques makes it possible to produce precise quantitative predictions that can confront both existing and forthcoming experiments. Experiments include those at the 12 GeV upgrade of the Continuous Electron Beam Accelerator Facility (CEBAF) at Jefferson Lab [35], with its new meson spectroscopy program in the mass range up to 3.5 GeV. The expectation is that new data produced in such experiments, combined with recent lattice QCD results aimed at extracting the spectrum of excited states for both mesons and baryons [4, 3, 36, 37, 38], will represent a unique opportunity for the study of the nature of confinement mechanism, and for identifying the role of gluonic degrees of freedom in the spectrum.

3.1 Hadron spectroscopy: general approach and difficulties with excited states

It is a well-established procedure to evaluate numerically the Euclidean correlation function of some interpolators $O_i$ and $O_j$ on the lattice, and then express it using its spectral decomposition form:

$$C_{ij}(t, 0) = \langle O_i(t)O_j^\dagger(0) \rangle = \sum_n \frac{1}{2E_n} \langle 0|O_i(0)|n\rangle \langle n|O_j^\dagger(0)|0\rangle e^{-E_n t},$$

(3.1)

where the sum runs over all eigenstates $|n\rangle$ of the QCD Hamiltonian. Such a representation of $C_{ij}$ enables one to extract the mass of the particular hadron. To do this, the same interpolator $O_N$ with the quantum numbers of a particle of interest is used for both $O_i$ and $O_j$, and the matrix element $\langle n|\hat{O}_N^\dagger|0\rangle$ is non-vanishing only for those terms, where $|n\rangle$
is the state of the hadron, or one of its excitations [39].

Then the energy of the lowest-lying hadron can be extracted from the exponential decay:

$$\langle O_N(t)O^\dagger_N(0) \rangle = Ae^{-tE_0} (1 + O(e^{-t\Delta E})) ,$$

(3.2)

where $A$ is a constant, $E_0$ is the energy of the ground state, and $\Delta E$ is the energy difference to the first excited state. Therefore, in general, the procedure for a hadron spectroscopy calculation consists of identifying a hadron operator $O_N$ that correspond to the particle one wants to analyze, and of the subsequent analysis of the Euclidean correlator of corresponding hadron interpolators located at two separate time slices.

The spectral decomposition form of the Euclidean correlator Eqn.(3.1), which allows to extract energies and physical matrix elements, is also suitable for the exploration of excited states, since it is represented as a sum of exponentials including contributions of higher excitations. However, such a form reveals the source of difficulties arising in the studies of hadronic excitations: one can see that the contributions of the excited states are suppressed exponentially, and the extraction of these subleading exponentials is a hard problem. As we climb up the spectrum, the signal-to-noise ratio tends to worsen with increasing $t$ (correlation functions decrease rapidly while statistical noise does not), and obtaining signals from the higher excitations becomes more and more problematic.

One of the approaches to this problem is to use anisotropic lattices with a finer temporal than spatial discretization. Such lattices make it possible to examine the behavior of the Euclidean correlation functions at small temporal separations, while the calculations are performed at a manageable computational cost. In the next two sections, I will explain the main technicalities of the calculations that were done within this research project. First, I will describe the particular improved anisotropic lattice action, and, after that, I will introduce some basic ideas and techniques that were applied to the current study of the
meson excitations on the lattice.

3.2 Details of calculations

For this project, the dynamical anisotropic lattices generated by the Hadron Spectrum collaboration were used. Here I will outline briefly the basic formulae for the fermion and gauge actions, as well as the main characteristics of the lattices; the detailed description of the corresponding lattice actions can be found in references [40, 41]. In the following subsections, I will provide further explanation, so that the terms used in the description of this action will have significance for a reader.

3.2.1 Improved anisotropic lattice action with stout-smeared link variables

The calculations were done on the $N_f = 2 \oplus 1$ anisotropic lattices, with two mass-degenerate light quarks of mass $m_l$ and a strange quark of mass $m_s$. These lattices employ improved gluon and "clover" fermion actions, with stout smearing restricted to spatial directions only. The fermion action is of the following form:

$$S_F^\xi[U, \bar{\psi}, \psi] = \sum_x \bar{\psi}(x) \frac{1}{\tilde{u}_t\tilde{m}_0 + \tilde{W}_t + \frac{1}{\gamma_f} \sum_s \tilde{W}_s} - \frac{1}{2} \left[ \frac{1}{2} \left( \frac{\gamma_g}{\gamma_f} + \frac{1}{\xi} \right) \frac{1}{\tilde{u}_t\tilde{u}_s^2} \sum_s \sigma_{ts} \tilde{F}_{ts} + \frac{1}{\gamma_f} \frac{1}{\tilde{u}_s^2} \sum_{s<s'} \sigma_{ss'} \tilde{F}_{ss'} \right] \psi(x). \tag{33}$$

Here $\tilde{u}_s$ and $\tilde{u}_t$ are the spatial and temporal tadpole factors, dividing the spatial and temporal gauge links, respectively; $\gamma_g$ and $\gamma_f$ are the bare gauge and fermion anisotropies.
which were introduced for convenience of parametrization and defined as

\[ \gamma_g = \xi_0, \quad \gamma_f = \frac{\xi_0}{\nu}. \]  

(3.4)

Here parameter \( \xi_0 \) is the bare anisotropy, which equals the true (or "renormalized") anisotropy \( \xi = \frac{a_s}{a_t} \) only at the classical level [42]; the bare anisotropy \( \xi_0 \) is tuned at each \( \beta = \frac{2N_c}{g^2} \) to keep \( \xi \) the same; \( \nu \) is the ratio of bare gauge to the bare fermion anisotropy.

The dimensionless variables \( \hat{m}_0, \hat{W}_\mu \) and \( \hat{F}_{\mu\nu} \) can be written as:

\[ \hat{m}_0 = m_0 a_t, \quad \hat{F}_{\mu\nu} = a_\mu a_\nu F_{\mu\nu} = \frac{1}{4} I m \mathcal{P}_{\mu\nu}(x), \quad \hat{W}_\mu = a_\mu^2 \nabla_\mu - \frac{1}{2} \gamma_\mu a_\mu \Delta_\mu, \]

where \( \nabla_\mu \) and \( \Delta_\mu \) are the standard covariant first- and second-order lattice derivatives, and \( \mathcal{P} \) is the plaquette. Finally, \( \sigma_{\mu\nu} \) are Dirac matrices \( (\sigma_{\mu\nu} = \frac{i}{2} [\gamma_\mu, \gamma_\nu]) \).

The gauge action used is similar to that one utilized in the glueball study [43]. It incorporates \( O(a^2) \) Symanzik and tadpole improved action and has the following form:

\[ S_G^\xi[U] = \frac{\beta}{N_c \gamma_g} \left\{ \sum_{x,s,s'} \left[ \frac{5}{3u_s^4} \mathcal{P}_{ss'} - \frac{1}{12u_s^6} \mathcal{R}_{ss'} \right] + \sum_{x,s} \left[ \frac{4}{3u_s^6} u_t^2 \mathcal{P}_{ss'lt} - \frac{1}{12u_s^6} u_t^2 \mathcal{R}_{ss'lt} \right] \right\}, \]

(3.5)

where \( \mathcal{R} \) is the \( 2 \times 1 \) rectangular Wilson loop.

### 3.2.2 Symanzik improvement program and the "clover" term

The initial stage of lattice calculations involves the discretization of derivative terms that contribute to the continuum QCD action. Such discretization always gives rise to some effects that are usually of \( O(a) \) through Wilson term for fermions, and of \( O(a^2) \) for gauge fields. Since numerical simulations are always performed at finite \( a \), one always has to deal with discretization errors. The technique for the systematic reduction of
discretization errors, which represents an elegant way of approaching this problem, is known as “improvement” of the lattice action. It is based on the fact that any chosen discretization of the derivative is not unique, and, in principle, it is possible to add some combination of extra terms to the lattice actions that have different discretization but lead to the same continuum limit.

There have been a number of methods proposed to improve lattice actions; the basic idea of the most popular among them can be explained using the simple example with two different types of discretization ($\Delta_1$ and $\Delta_2$) for the derivative operator. Starting with the following definitions:

$$\Delta_1 f = \frac{f(x + a) - f(x - a)}{2a}$$

and

$$\Delta_2 f = \frac{f(x + 2a) - f(x - 2a)}{4a},$$

one can show, using the Taylor series expansion, that

$$\Delta_1 f = f'(x) + \frac{a^2}{6} f''(x)$$

and

$$\Delta_2 f = f'(x) + \frac{2a^2}{3} f''(x).$$

Therefore the contribution of the $O(a^2)$ terms can be cancelled with the combination $\frac{4}{3} \Delta_1 f - \frac{1}{3} \Delta_2 f$, so that only term of the $O(a^4)$ remains.

A generalization and systematic implementation of these ideas for lattice QCD form the so-called Symanzik improvement program. Its main difficulty is in the determination of the coefficients $c_i$ that would reduce eventually the discretization errors. In the above example, these constants $c_1 = \frac{4}{3}$ and $c_2 = -\frac{1}{3}$ were obtained from simple algebra, but in the case of quantum chromodynamics their determination is much more involved.
In lattice QCD calculations, by “improvement” one implies the improvement of Euclidean correlation function

\[
\langle O_1(x)O_2(y) \rangle = \frac{1}{Z} \int \mathcal{D}[U] \mathcal{D}[\bar{\psi}, \psi] e^{-S[U, \bar{\psi}, \psi]} O_1[U, \bar{\psi}, \psi; x]O_2(y)[U, \bar{\psi}, \psi; y],
\]  

(3.10)

which assumes the improvement of both the action \( S \) and the operators \( O_1 \) and \( O_2 \) to the same order. However, for the calculation of the spectrum only action needs to be improved.

The improvement of the action usually starts with the identification of a continuum expression for the correction terms. These should be ordered according to their dimension and have the symmetries of the QCD action. The effective action can be written in the form

\[
S_{\text{eff}} = \int d^4x \left( L^{(0)}(x) + aL^{(1)}(x) + a^2L^{(2)}(x) + \ldots \right).
\]  

(3.11)

Here \( L^{(0)} \) is the usual QCD Lagrangian, and terms \( L^{(k)} \) \( (k \geq 1) \) are additional correction terms built from products of quark and gluon fields such that they have dimensions \( 4+k \).

Compared to \( L^{(0)} \), these terms contain additional derivatives or powers of the quark mass \( m \).

Requiring the symmetries of the lattice action, one can show that the leading correction term \( L^{(1)}(x) \) can be written as a linear combination of a few dimension five operators. This list of operators may be reduced using the field equations, and it turns out that for \( O(a) \) improvement of Wilson action it is sufficient to add just one term \( \bar{\psi}(x)\sigma_{\mu\nu}F_{\mu\nu}(x)\psi(x) \) such that the improved action can be rewritten as

\[
S_I = S_{\text{Wilson}} + c_{SW}a^5 \sum_{n \in \Lambda} \sum_{\mu < \nu} \frac{1}{2} \bar{\psi}(n)\sigma_{\mu\nu}F_{\mu\nu}(n)\psi(n).
\]  

(3.12)
Here $c_{SW}$ is the so-called Sheikoleslami-Wohlert coefficient [44]. $\hat{F}_{\mu\nu}$ is the lattice form of the field strength tensor

$$\hat{F}_{\mu\nu} = -\frac{i}{8a} (Q_{\mu\nu}(n) - Q_{\nu\mu}(n)), \quad (3.13)$$

with $Q_{\mu\nu}(n)$ being the sum of plaquettes $U_{\mu,\nu}(n)$ in the $\mu - \nu$ plane:

$$Q_{\mu\nu}(n) \equiv U_{\mu,\nu}(n) + U_{\nu,\mu}(n) + U_{\mu,\nu}(n) + U_{\nu,\mu}(n). \quad (3.14)$$

Due to its form, the additional improvement term in the LQCD action is also called the clover term (see Figure 3.1).

The improvement of the interpolators is done usually in a similar way: one writes down the continuum expressions for the correction terms. These terms are organized with respect to their dimension and are identified by requiring that they have the symmetries of the unimproved operator $O_i$. For example, the $O(a)$ improvement of the isovector axial current $A_{a\mu}^a$:

$$A_{\mu}^a = \frac{1}{2} \bar{\psi}(n) \gamma_{\mu} \gamma_5 \tau^a \psi(n), \quad (3.15)$$
(where \( \tau^a \) \( a = 1, 2, 3 \) are Pauli matrices acting in \( N_f = 2 \) flavor space), after employing steps similar to those described above for the improvement of the lattice action, can be written as

\[
(A_I)^a_{\mu}(n) = A^a_{\mu}(n) + c_A a \delta_{\mu} P^a(n). \tag{3.16}
\]

Here \( \delta_{\mu} \) is the symmetric difference operator,

\[
\delta_{\mu} f(n) = \frac{1}{2a} [f(n + \mu) - f(n - \mu)], \tag{3.17}
\]

and \( P^a(n) = \frac{1}{2} \bar{\psi}(n) \gamma_5 \tau^a \psi(n) \) is the pseudoscalar density.

The determination of the coefficients \( c_{SW} \) and \( c_A \) can be done using perturbation theory, but for many important LQCD applications one works in a regime where the coupling \( g \) is not small and the results provided by perturbation theory are not so useful. The non-perturbative determination of these coefficients is performed usually with help of chiral symmetry of QCD, in particular, axial Ward identity (AWI). This identity demonstrates that after renormalization, the lattice interpolators approach the continuum partially conserved axial current relation (PCAC), and the corrections in PCAC may be used to determine \( c_{SW} \) and \( c_A \).

### 3.2.3 Tadpole improvement

Even for lattice QCD, perturbation theory is often essential, and chapter 5 of my thesis will be devoted entirely to the detailed description of the methods of lattice perturbation theory, as well as to some derivations that were performed within this study using perturbation theory. Let me say for now that lattice QCD Feynman diagram rules can be derived using the same approach as in the continuum, but applied to the lattice Lagrangian. The perturbative calculations in LQCD are performed by the expanding the
link variable as

\[ U_\mu(x) = e^{iagA_\mu(x)} \rightarrow 1 + iagA_\mu(x) - \frac{a^2g^2}{2} A_\mu^2(x) + \ldots, \quad (3.18) \]

and such representation gives rise to local quark-gluon vertices with different numbers of gluons. The two-gluon term \( \frac{a^2g^2}{2} A_\mu^2(x) \) in this expansion produces so-called *tadpole* diagrams, which are lattice artifacts, i.e. the corresponding interaction vertices are zero in the naive continuum limit. These gluon tadpoles lead to large numerical results in comparison to other diagrams and, therefore, to large corrections in lattice perturbation theory. In 1993, Lepage and Mackenzie [45], in order to make the lattice perturbation theory expansions closer to the continuum ones, proposed a tadpole re-summation method, called *tadpole improvement*, which became a useful tool for getting rid of corresponding lattice artifacts. The authors realized that the tadpole diagrams are in fact only suppressed by powers of \( g^2 \), but not \( a \), due to the ultraviolet divergences generated by the tadpole loops. The solution is to split the lattice fields into ultra-violet (UV) and infra-red (IR) parts, to parametrize the UV part with a rescaled "tadpole" factor \( u_0 \) containing the high-energy part of the link variable, and then to integrate the UV part out:

\[ U_\mu(x) = e^{iga[A_\mu^{IR}(x) + A_\mu^{UV}(x)]} = u_0 e^{igaA_\mu^{IR}(x)} = u_0 \tilde{U}_\mu(x). \quad (3.19) \]

Under such rescaling, when each of the link variables \( U_\mu(x) \) is replaced with \( u_0 \tilde{U}_\mu(x) \), the effective coupling constant becomes \( \tilde{g}_0^2 = \frac{g_0^2}{u_0^4} \), and perturbative expansions are done in terms of \( \tilde{g}_0^2 \). The tadpole factor \( u_0 \) depends on the parameters of the theory and can be measured in the simulation. There are two common definitions for \( u_0 \) - one of them uses
the expectation value of the plaquette:

\[ u_0 = \left( \frac{1}{N_c} \langle Tr \mathcal{P}_{\mu\nu} \rangle \right)^{1/4}, \tag{3.20} \]

and another uses the mean value of the link in Landau gauge:

\[ u_0 = \langle \frac{1}{N_c} Tr U_{\mu}(x) \rangle. \tag{3.21} \]

Within this approach, once the lattice action and operators are properly rescaled, the large tadpole contributions can be reabsorbed, and the expansion coefficients in the results of perturbative lattice expressions are in general much smaller. It is possible to use tadpole improvement on Symanzik-improved actions, as done in the case of calculations presented here. In this situation, its clover coefficients are rescaled with appropriate powers of tadpole factor \( u_0 \):

\[ \tilde{c}_{SW} = u_0^3 c_{SW}. \tag{3.22} \]

### 3.2.4 Stout smearing

The violent short distance fluctuations of the gauge fields are typical for gauge theories, but the correlation signal can be improved considerably by a special procedure called *smearing*. As already mentioned in chapter 2, while constructing the lattice action, one introduces a gauge link to make the derivative included in Dirac term gauge invariant:

\[ \bar{\psi}(x)\psi(x + \hat{\mu}) \rightarrow \bar{\psi}(x)U_{\mu}(x)\psi(x + \hat{\mu}). \tag{3.23} \]

In this simple case the gauge link is introduced along the shortest path between two lattice sites. But, as an alternative approach, one can take non-direct path between two lattice
sites, where the link variable is replaced by local averages over short paths connecting the link’s endpoints - corresponding links are called “fat”, or smeared links. All such smoothing algorithms represent average products of links along certain paths connecting the two endpoints of an original link. It has been shown that smoothing of gauge configurations, similar to the tadpole improvement program, suppresses tadpoles dramatically. Also, lattice actions with fat links have much smaller chiral symmetry violations in comparison to those with ordinary links. But, with all its advantages, smearing comes at a price - it washes out short-range information about the system. There are many different variations of smearing techniques in existence, the most common are so-called APE [46], AsqTad [47, 48], HYP [49], and stout smearing [2].

In our action, in order to smooth the short-distance fluctuations in the clover fermion action, we use three-dimensional stout-smeared links. Following the analytic algorithm of smearing link variables, which is presented in [2], at each step \( n \) the links \( U^{(n)}(x) \) are mapped into links \( U^{(n+1)}(x) \):

\[
U^{(n+1)}(x) = e^{\i Q^{(n)}(x)} U^{(n)}(x),
\]

where \( Q^{(n)}(x) \) is traceless Hermitian matrix constructed from staples

\[
Q^{(n)}(x) = \frac{i}{2} \left( \Omega^{(n)}(x) - \Omega_{\mu}(x) \right) - \frac{i}{2N} \text{Tr} \left( \Omega^{(n)}_{\mu}(x) - \Omega_{\mu}(x) \right),
\]

\[
\Omega_{\mu}(x) = C_{\mu}(x) U^{(n)}_{\mu}(x),
\]

\[
(3.24)
\]

\[
(3.25)
\]

\[
(3.26)
\]
and $C_\mu(x)$ defined as the weighted sum of the perpendicular staples beginning at lattice site $x$ and ending at neighboring site $x + \hat{\mu}$, and $U^\mu_+(x)$:

$$C_\mu(x) = \sum_{\mu \neq \nu} \rho_{\mu\nu} \left( U_\nu(x) U_\mu(x + \hat{\nu}) U^\mu_+(x + \hat{\mu}) + U^\nu_+(x - \hat{\nu}) U_\nu(x - \hat{\nu} + \hat{\mu}) \right),$$  

(3.27)

with $\rho_{\mu\nu}$ being staples weights.

After iterating this step $n_\rho$ times (twice in our case), the final “stout link” $\tilde{U}$ is produced (see Figure 3.2):

$$U \rightarrow U^{(1)} \rightarrow U^{(2)} \rightarrow \ldots \rightarrow U^{(n_\rho)} \equiv \tilde{U}. \quad (3.28)$$

We use the choice of staple weights,

$$\rho_{ij} = \rho,$$

$$\rho_{4\mu} = \rho_{\mu4} = 0,$$  

(3.29)

so only the spatial links are smeared. Our smearing parameters are $\rho = 0.22$ and $n_\rho = 2$.

The advantage of the stout smearing algorithm is that the new smeared link $\tilde{U}_\mu(x)$ is differentiable with respect to the original link variables, and this is highly beneficial for the use of Hybrid Monte Carlo method when applied to dynamical fermion simulations.

FIG. 3.2: The expansion (up to the first order in $\rho_{\mu\nu}$) of the “stout” link variable $U^{(1)}$ in terms of paths of the original links. This Figure is borrowed from Ref. [2].
3.2.5 Some technicalities

The grid spacings of the lattices used in the simulations for this research project are $a_s$ in the spatial directions and $a_t$ in the temporal direction. The physical volumes of these lattices are $L_s^3 \times L_t$ (here $L_s = N_s a_s$ and $L_t = N_t a_t$). We employed the volume of $N_s^3 \times N_t = 16^3 \times 128$, which corresponds to the spatial extents of $\sim 1.9$ fm. The parameters described above correspond to a spatial lattice spacing of $a_s \simeq 0.123$ fm. The temporal lattice spacing is $a_t \sim 0.03$ fm, which corresponds to a temporal scale $a_t^{-1} \sim 5.6$ GeV. The renormalized anisotropy parameter $\xi$, the ratio of the spatial and temporal lattice spacings, is the following:

$$\xi = \frac{a_s}{a_t} \simeq 3.5.$$ (3.30)

The calculations were performed at three different values of the light quark masses, corresponding to pion masses of 391, 524 and 702 MeV. The heaviest case, the 702 MeV pion mass, corresponds to the $SU(3)$ flavor-symmetric point; here the light up and down quarks have the same masses as that of the strange quark. The parameters of the lattices used are summarized in Table 3.1. The mass of the $\Omega$-baryon, which is used to set the scale, was determined within an estimated uncertainty of 2% in Ref. [50] on the same ensembles; to facilitate comparison with other calculations, we also provide the value of the Sommer parameter $r_0$ on each ensemble.

<table>
<thead>
<tr>
<th>$N_s$</th>
<th>$N_t$</th>
<th>$a_t m_l$</th>
<th>$a_t m_s$</th>
<th>$a_t m_\pi$</th>
<th>$r_0/a_s$</th>
<th>$N_{cfg}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>128</td>
<td>-0.0743</td>
<td>-0.0743</td>
<td>0.1483(2)</td>
<td>3.21(1)</td>
<td>535</td>
</tr>
<tr>
<td>16</td>
<td>128</td>
<td>-0.0808</td>
<td>-0.0743</td>
<td>0.0996(6)</td>
<td>3.51(1)</td>
<td>470</td>
</tr>
<tr>
<td>16</td>
<td>128</td>
<td>-0.0840</td>
<td>-0.0743</td>
<td>0.0691(6)</td>
<td>3.65(1)</td>
<td>480</td>
</tr>
</tbody>
</table>

TABLE 3.1: Lattice extents ($N_s$ and $N_t$), the bare masses of light quark $a_t m_l$ and strange quark $a_t m_s$, the pion mass $a_t m_\pi$, the Sommer scale $r_0$, and the number $N_{cfg}$ of gauge-field configurations. On each configuration, solution vectors are computed from $N_{vecs} = 64$ distillation vectors [1], located on a single time slice.
3.3 Meson spectroscopy on the lattice: methods

3.3.1 Variational method

To extract the spectrum of the excited states from the subleading exponentials, I have used the variational method [51, 52, 53] which makes it possible to obtain more information from the system by analyzing a whole matrix of correlators, instead of using only a single one of the possible correlators. A detailed description of the Hadron Spectrum Collaboration implementation of this technique can be found in [3], and I will explain its basic ideas here.

The mass spectrum is extracted from the $k \times k$ matrix of correlators:

$$C_{ij}(t) = \langle 0 | \mathcal{O}_i(t) \mathcal{O}^\dagger_j(0) | 0 \rangle = \begin{pmatrix}
\langle \mathcal{O}_1(t) \mathcal{O}_{1}^\dagger(0) \rangle & \langle \mathcal{O}_1(t) \mathcal{O}_{2}^\dagger(0) \rangle & \cdots \\
\langle \mathcal{O}_2(t) \mathcal{O}_{1}^\dagger(0) \rangle & \langle \mathcal{O}_2(t) \mathcal{O}_{2}^\dagger(0) \rangle & \cdots \\
\vdots & \vdots & \ddots \\
\langle \mathcal{O}_k(t) \mathcal{O}_{1}^\dagger(0) \rangle & \langle \mathcal{O}_k(t) \mathcal{O}_{2}^\dagger(0) \rangle & \langle \mathcal{O}_k(t) \mathcal{O}_{k}^\dagger(0) \rangle
\end{pmatrix}, \tag{3.31}
$$

where each of interpolators $\mathcal{O}_i$ has the quantum numbers of the channel we are interested in.

The variational approach involves solution of the generalized eigenvalue problem (GEVP)

$$C(t)v_N(t, t_0) = \lambda_N(t, t_0)C(t_0)v_N(t, t_0), \quad t > t_0. \tag{3.32}$$

Eigenvalues in this equation are normalized to unity at $t = t_0$: $\lambda_N(t_0) = 1$, and at sufficiently large $t > t_0$, they behave like

$$\lambda_N(t, t_0) \to e^{-F_N(t-t_0)} ,$$
where $E_N$ is the energy of the $N^{th}$ state. As one can see, the GEVP involves two time separations, $t_0$ and $t$, where $t > t_0$. However, it was shown in [53] that, even if it is challenging numerically, a large $t_0$ is more important than a large $t$ to keep systematic uncertainties small (more details on the sensitivity of extracted spectrum to the value of $t_0$ can be found in [3]).

Using the notion of the overlap factors, which are the vacuum-state matrix elements $Z_i^a$

$$Z_i^N = \langle N|\mathcal{O}_i^a|0\rangle,$$  \hspace{1cm} (3.33)

the spectral decomposition of the two-point correlator can be rewritten in the following way:

$$C_{ij}(t) = \sum_N \frac{\langle 0|\mathcal{O}_i|N\rangle \langle N|\mathcal{O}_j^a|0\rangle}{2m_N} e^{-m_N t} = \sum_N \frac{Z_i^N \ast Z_j^N}{2m_N} e^{-m_N t}.$$  \hspace{1cm} (3.34)

Identifying the energy of the $N^{th}$ state with its mass, the overlap factors $Z_i^N$ of the spectral representation are straightforwardly related to the eigenvectors through

$$Z_i^N = \sqrt{2m_N} e^{m_N t_0/2} \nu_j^{(N)\ast} C_{ji}(t_0).$$  \hspace{1cm} (3.35)

Extraction of the masses for different states is implemented through fitting the dependence of eigenvalues $\lambda^{(N)}$, also called "principal correlators", on $t - t_0$; the form of the fit allows for the second exponential:

$$\lambda^{(N)}(t) = (1 - A_N) e^{-m_N(t-t_0)} + A_N e^{-m'_N(t-t_0)},$$  \hspace{1cm} (3.36)

with the fit parameters $m_N$, $m'_N$ and $A_N$.

For the variational analysis in particular calculations within this project, I have used "reconfit.svd" code created by Hadron Spectrum collaboration; the previous version is
available within the adat suite [54].

3.3.2 Interpolating operator basis

The efficacy of the variational method, which employs a finite basis of operators for each set of quantum numbers in the spectrum, relies on an operator basis $\mathcal{O}_i$ that faithfully spans the low-lying spectrum. But how one can construct, in a cost-efficient way, these “good” hadron interpolators that would generate states from the vacuum with large overlap with the physical states under consideration?

One of the possibilities is to use different Dirac structures to obtain different interpolators with the same quantum numbers. This method, whilst an important ingredient, is not enough for analyzing the tower of excitations, since it usually gives rise to only two or three different hadron interpolators. A brief overview of different ways of constructing a basis of hadron interpolators, such as implementing non-trivial spatial wave functions on the lattice, can be found in [39]. In this work, the derivative-based operator construction, described in detail in Refs. [4] and [3], has been used. Within this method, gauge-covariant spatial derivatives are combined with a gamma matrix within a fermion bilinear. Thus each operator is constructed from elements of the general form:

$$\bar{\psi} \Gamma \vec{D}_i \vec{D}_j \ldots \psi,$$

where $\vec{D} \equiv \vec{D} - \vec{D}$ is a lattice discretization of gauge-covariant derivatives, and $\Gamma$ is one of the sixteen Dirac matrices (the naming scheme for $\Gamma$, used by Hadron Collaboration, is presented in Table 3.2). Then an operator of definite $J$ and $M$ is formed, which we denote by

$$\mathcal{O}^{J,M} = \left(\Gamma \times D_{j_D}^{[N_\parallel]}\right)^J,$$
TABLE 3.2: Gamma matrix naming scheme.

<table>
<thead>
<tr>
<th>$\Gamma$</th>
<th>$\gamma_5$</th>
<th>$\gamma_0\gamma_5$</th>
<th>$\gamma_0$</th>
<th>$\gamma_i$</th>
<th>$\gamma_0\gamma_i$</th>
<th>$\gamma_5\gamma_i$</th>
<th>$\gamma_0\gamma_5\gamma_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_0$</td>
<td>$\pi$</td>
<td>$\pi_2$</td>
<td>$b_0$</td>
<td>$\rho$</td>
<td>$\rho_2$</td>
<td>$a_1$</td>
<td>$b_1$</td>
</tr>
</tbody>
</table>

according to the notation introduced in [3], where each operator with desired quantum numbers contains a gamma matrix $\Gamma$ and $N$ derivatives coupled to spin $J_D$, overall coupled to spin $J$:

$$\mathcal{O}^{J,M} = \left( \Gamma \times D_{J_D}^{[N]} \right)^J.$$  (3.39)

It is worth noting that both charge conjugation, for neutral particles, and parity are good symmetries on the lattice, but the full three-dimensional rotational symmetry of the continuum is reduced to the symmetry group of a cube. In the case of integer spin, there are only five lattice irreducible representations, irreps, labelled by $\Lambda$ with row $\lambda$, instead of infinite number of irreducible representations labelled by spin $J$ in the continuum. These lattice irreps $\Lambda$ are listed in Table 3.3. In this study I was interested in mesons of spin 0, lying in the $A_1$ irrep; this irrep also contains continuum states of spin 4 and higher. The subduction from the continuum operators $\mathcal{O}^{J,M}$ of Eqn. (3.38) onto the lattice irreps

TABLE 3.3: Continuum spins subduced into lattice irreps $\Lambda$ (the numbers in parentheses are the dimensions of the irreps).

<table>
<thead>
<tr>
<th>$J$</th>
<th>$\Lambda$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$A_1(1)$</td>
</tr>
<tr>
<td>1</td>
<td>$T_1(3)$</td>
</tr>
<tr>
<td>2</td>
<td>$T_2(3) \oplus E(2)$</td>
</tr>
<tr>
<td>3</td>
<td>$T_1(3) \oplus T_2(3) \oplus A_2(1)$</td>
</tr>
<tr>
<td>4</td>
<td>$A_1(1) \oplus T_1(3) \oplus T_2(3) \oplus E(2)$</td>
</tr>
</tbody>
</table>
denoted by $\Lambda$ and row $\lambda$ is performed through the projection formula (see [4, 3])

\[
\mathcal{O}_{\Lambda,\lambda}^{[j]} = \sum_{M} S_{J,M}^{\Lambda,\lambda} \mathcal{O}_{J,M}^{[j]},
\]

where $S_{J,M}^{\Lambda,\lambda}$ are the subduction coefficients. For each irrep, I have used all possible continuum operators with up to three derivatives, yielding a basis of 12 operators. After that, the variational procedure, described above, was applied to the obtained correlator matrix $C_{ij}^{\Lambda}$, in order to extract the spectrum of hadronic excitations.

An important observation is that for the "single-particle" operators used here, there is a remarkable manifestation of continuum rotational symmetry at the hadronic scale, that is the subduced operators of Eqn. (3.47) retain a memory of their continuum antecedents [4, 3]. One of the operators arises from a continuum operator of spin 4. Several operators, in particular those of the form $(\Gamma \times D_{j=1}^{[2]})^{J=0}$, correspond to the coupling of a chromo-magnetic gluon field to the quark and antiquark; these operators are used as signatures for "hybrid" states with manifest gluonic content.

### 3.3.3 Distillation

Physically relevant signals in correlation functions fall exponentially and are dominated by statistical fluctuations at increasing times. Therefore, it is essential to use operators with strong overlaps onto the low-lying states, and whose overlaps to the high-energy modes are suppressed. If the interpolating operators are constructed directly from the local fields in the lattice Lagrangian, then the coupling to the high energy modes is strong. A widely adopted means of suppressing this coupling is through the use of spatially extended, or smeared, quark fields. Here, this smearing was accomplished through the adoption of the *distillation* technique [1], in which the distillation operator, i.e., the
smoothing function, of the following form:

$$\Box_{x,y}(t) = \sum_{k=1}^{N_{\text{vecs}}} \xi_x^{(k)}(t)\xi_y^{(k)\dagger}(t),$$

(3.41)

is applied to the quark fields on the appropriate time slice. Here $\xi^{(k)} (k = 1, \ldots, N_{\text{vecs}})$ are the $N_{\text{vecs}}$ eigenvectors of the gauge-covariant lattice Laplacian, $-\nabla^2$, corresponding to the $N_{\text{vecs}}$ lowest eigenvalues, evaluated on the background of the spatial gauge-fields of time slice $t$. With this, a meson interpolating operator acts now on smeared quark fields $\tilde{\psi} = \Box \psi$ and has the general form

$$\mathcal{O} = \tilde{\psi}(t)\Gamma\tilde{\psi}(t),$$

(3.42)

and a correlation function between operators $\mathcal{O}_i$ and $\mathcal{O}_j$ can be written as

$$C_{ij}(t) = \langle \tilde{\psi}(t)\Box(t)\Gamma^i(t)\Box(t)\psi(t) \cdot \tilde{\psi}(0)\Box(0)\Gamma^j(0)\Box(0)\psi(0) \rangle. \quad (3.43)$$

Due to the small rank of the smearing operator, distillation has major benefit over other smearing techniques in significantly reducing the computational cost related to the construction of all elements of the correlation matrix, whilst enabling a time sliced sum to be performed both at the sink and at the source.

The construction of the correlation functions from operators smeared both at the sink and the source has been described in detail in Ref. [1], but the extension to the calculation of the smeared-local two-point functions needed here is straightforward. The starting point is the solution of the Dirac equation from the the eigenvectors at time slice $t'$, which without loss of generality we take to be on time slice $t' = 0$

$$\tilde{\tau}_{\alpha\beta}^{(k)}(\bar{x}, t; t' = 0) = M_{\alpha\beta}^{-1}(\bar{x}, t; t' = 0)\xi^{(k)}(t' = 0). \quad (3.44)$$
Then one constructs

\[ C_{\mu,i}(t,0) = \frac{1}{V^3} \sum_{\vec{x},\vec{y}} \langle 0 | A\mu(\vec{x},t)\mathcal{O}_i^\dagger(\vec{y},0) | 0 \rangle \]

\[ = \sum_{\vec{x}} \text{Tr} [\gamma_\mu \tilde{\tau}(\vec{x},t;0) \Phi(0) \gamma_5 \tilde{\tau}(\vec{x},t;0) \dagger], \quad (3.45) \]

where the trace is over spin, color and eigenvector indices, and $\Phi$ is the representation of the operator $\mathcal{O}_i$ in terms of the eigenvectors $\xi$. The correlator onto the optimal operator for the $N^{th}$ excited state immediately follows from Eqn. (4.16).

### 3.3.4 “Ideal” operators.

The different interpolators used in the variational approach serve as an operator basis for the system. At the same time, the eigenvectors $v^{(N)}$ in the solution of the generalized eigenvalue problem can be interpreted as the relative weights of the basis elements. Thus, once the $v^{(N)}$s are obtained from the solution of the generalized eigenvalue problem (3.32) at some $t = t_{\text{ref}}$, weighting the basis operators by this vector produces an optimal, or ideal, operator \cite{55} for the state $N$:

\[ \Omega^N = \sqrt{2m_N}e^{-m_N t_0/2}v^{(N)}_i \mathcal{O}_i. \quad (3.46) \]

Note that the operators $\Omega^N$ are normalized here in a manner which accounts for the value of $t_0$ (see \cite{55}). These new interpolators are optimal within the given basis of interpolators in the sense that they give rise to orthogonal correlation functions,

\[ \langle \Omega^M(t)\Omega^N_\dagger(0) \rangle = \lambda^N(t)\delta_{NM}. \quad (3.47) \]
Thus the variational method determines through the eigenvectors which linear combinations of the basis interpolators best describe a physical state, and these optimized operators are used in the study of hadronic excitations presented below.

The combination of the variational method, novel approach to operator construction, and the distillation technique applied to the anisotropic lattice ensembles has been shown to be very effective in studies of excited light isovector mesons [4, 3], isoscalar mesons [37, 56], mesons containing charmed quarks [57, 58] and of baryons [59, 60, 61, 62]. For the research presented here, the use of anisotropic lattices with a finer temporal than spatial resolution enables the time-sliced correlators to be examined at small Euclidean times. The variational method with a large basis of operators derived from a continuum construction yet which satisfy the symmetries of the lattice, together with an efficient means of computing the necessary correlation functions through the use of “distillation”, enables us to overcome some challenges arising in the study of the hadronic excitations. In the next chapter, I will demonstrate how this toolkit has been exploited in order to extract the vacuum-to-hadron matrix elements of excited states, and hence for the study of the decay constant of the ground-state pion and its excitations.
In this chapter, I will provide details of a calculation of the leptonic decay constant of the pion - the lightest system with a valence quark-antiquark structure - and its excitations. A knowledge of the decay constants of the excited states, as well as of the ground state, is important in delineating between different QCD-inspired pictures of the meson spectrum, as well as demonstrating the feasibility of studying the properties of highly excited states within lattice QCD.

4.1 Pseudoscalar leptonic decay constants

Charged mesons can decay, through quark-antiquark annihilations via a virtual $W$ boson, to a charged lepton and (anti-)neutrino. The decay width for any pseudo-scalar meson $P$ of a quark content $q_1 \bar{q}_2$ with mass $m_P$ is given by [34]

$$
\Gamma(P \to l\nu) = \frac{G_F^2}{8\pi} f_P^2 m_l^2 m_P \left(1 - \frac{m_l^2}{m_P^2}\right)^2 |V_{q_1q_2}|^2. \quad (4.1)
$$
Here $m_l$ is the mass of the lepton $l$, $G_F$ is the Fermi coupling constant, $V_{q_1q_2}$ is the Cabibbo-Kobayashi-Moskawa (CKM) matrix element between the constituent quarks in $P$, and $f_P$ is the decay constant related to the wave function overlap at the origin of the quark and antiquark. A charged pion can decay as $\pi \rightarrow l\nu$ (the notation here assumes $\pi^+ \rightarrow l^+\nu_l$ or $\pi^- \rightarrow l^-\bar{\nu}_l$), and its decay constant $f_\pi$, which dictates the strength of these leptonic pion decays, has a significance in many areas of modern physics. Thus a knowledge of $f_\pi$ is important for the extraction of certain CKM matrix elements, where the leptonic decay width $\Gamma$ in Eqn. (4.1) is proportional to $f_P|V_{q_1q_2}|$. The pion decay constant, through its role in determining the strength of $\pi\pi$ interactions, also serves as an expansion parameter in Chiral Perturbation Theory [63, 64]. As $|V_{ud}|$ has been quite accurately measured in super-allowed $\beta$-decays, measurements of $\Gamma(\pi^+ \rightarrow \mu^+\nu)$ yield a value of $f_\pi$. According to PDG [34], the most precise value of $f_\pi$ is

$$f_{\pi^-} = (130.41 \pm 0.03 \pm 0.20) \text{ MeV.} \quad (4.2)$$

Lattice QCD enables ab initio computations of the mass spectrum and decay constants of pseudo-scalar mesons, and the calculation of the decay constant for ground-state mesons has been an important endeavor in lattice calculations for the reasons cited above. Recent lattice predictions [65, 66, 67, 68] for the ratio $f_K/f_\pi$ of $K^-$ and $\pi^-$ decay constants were used in order to find a value for $|V_{us}|/|V_{ud}|$ which, together with the precisely measured $|V_{ud}|$, provides an independent measure of $|V_{us}|$.

The leptonic decay constant has a further role in hadronic physics in representing the wave function at the origin, and therefore a knowledge of the decay constant not only of the lowest-lying state but of some of the excitations is important in confronting QCD-inspired descriptions of the meson spectrum. The pion excited states decay predominantly through strong decays, and therefore experimental data on their decay constants are lacking. A
study based on Schwinger-Dyson equations [69] predicted significant suppression of the
excited-state pion decay constant in comparison to that of the ground state. Similar
predictions, based on the QCD-inspired models and sum rules, also propose remarkably
small values for the decay constant of the first pion excitation $f_{\pi_1}$; e.g., [70] proposed the
ratio $\frac{f_{\pi_1}}{f_{\pi_0}}$ to be of the order of one percent. The authors of Ref. [71] in their review of
meson properties also note that some suppression of the leptonic decay constants might
be expected; for $S$-wave states, the decay constant is proportional to the wave function at
the origin, and for excited states the configuration-space wave function is broader.

The only lattice studies of the decay constants of the excited state of the pion are those of
the UKQCD Collaboration [72] using a non-perturbatively improved clover fermion action
with two mass-degenerate quark flavors, and of the RBC collaboration, using a Domain-
Wall Fermion action with two mass-degenerate quark flavors [73]; both exhibit a strong
suppression of $f_{\pi_1}$ in the chiral limit. I will discuss these results in further detail later.

### 4.1.1 Calculation of pion decay constant

The procedure for extracting energies and hadron-to-vacuum matrix elements from a
lattice calculation is, as described in previous chapter, to evaluate numerically Euclidean
correlation functions of operators $O_i$ and $O_j$ of given quantum numbers, which are then
expressed through their spectral representation

$$C_{ij}(t, 0) = \sum_N \frac{Z_i^N Z_j^N}{2E_N} e^{-E_N t},$$

(4.3)

where $E_N$ is the energy of the state. In the case of pion, the overlap factor $Z_N$ of the $N^{th}$
state in the spectrum, $\pi_N$, is defined as

$$Z_i^N \equiv \langle \pi_N | O_i^t(0) | 0 \rangle.$$ 

(4.4)
For a pseudoscalar at rest, its decay constant $f_P$ can be calculated from the matrix element of the local axial vector current:

$$\langle 0 | A_L^\mu(0) | P \rangle = f_P m_P,$$

(4.5)

with $A_L^\mu = \bar{\psi} \gamma_\mu \gamma_5 \psi$ and $P = \bar{\psi} \gamma_5 \psi$. The decay constant of the $N$th excitation of the pion, $\pi_N$, is given by the hadron-to-vacuum matrix element of the axial vector current,

$$\langle 0 \mid A_\mu(0) \mid \pi_N \rangle = p_\mu f_{\pi_N},$$

(4.6)

where $A_\mu = \bar{\psi} \gamma_\mu \gamma_5 \psi$; for a state at rest, considered here, only the temporal component of the matrix element is non-zero. The flavor-non-singlet axial-vector Ward-Takahashi identity relates the decay constant to the matrix element of the pseudoscalar density $P$ through

$$f_{\pi_N} m_N^2 = 2m_q \langle 0 \mid P \mid \pi_N \rangle,$$

(4.7)

and it is this expression that gives rise to the expectation $f_{\pi_N} \equiv 0$ for $N > 0$ in the chiral limit. It is important to note, however, that away from the chiral limit any suppression of $f_{\pi_N}$ could be due to a small value of the matrix element $\langle 0 \mid P \mid \pi_N \rangle$.

In our study, we determine the decay constant by calculating correlation function using smeared (S) source and local (L) sink:

$$\langle 0 \mid A_{LA}(t) P_S(0) \mid 0 \rangle = \frac{1}{2m_N} \langle 0 \mid A_LA(0) \mid N \rangle \langle N \mid P_S(0) \mid 0 \rangle e^{-m_N t}.$$  

(4.8)

Here $\langle N \mid P_S \mid 0 \rangle$ is the overlap factor $Z_N$, i.e.

$$\langle 0 \mid A_{LA}(t) P_S(0) \mid 0 \rangle = \frac{e^{-m_N t}}{2m_N} m_P f_P Z_N.$$  

(4.9)
These factors $Z_N$ may be found from the variational method, using the orthogonality condition:

$$v^{(N)} C(t_0) v^{(M)} = \delta_{MN}, \quad (4.10)$$

or

$$\langle 0 | \sum_i v_i^{(N)} \mathcal{O}^i(t_0) \sum_j v_j^{(M)} \mathcal{O}^j(0) | 0 \rangle = \delta_{NM}. \quad (4.11)$$

As already pointed out in the previous Chapter, the normalized “optimal” operators $\Omega_N$ were used in these calculations:

$$\Omega_N \equiv B_N v_i^{(N)} \mathcal{O}^i, \quad (4.12)$$

where $B_N$ is the normalization coefficient: $B_N = \sqrt{2m_ne^{-m_N t_0}}$. Thus, in the case $N = M$ one has:

$$\langle 0 | \Omega_n(t_0) \Omega_n(0) | 0 \rangle = \frac{Z_N^2 e^{-m_N t_0}}{B_N^2} \frac{2m_N}{2m_N} = 1, \quad (4.13)$$

so that the final expression for overlaps $Z_N$ is the following:

$$Z_N = B_N \sqrt{2m_N e^{-m_N t_0}}. \quad (4.14)$$

Substituting this result back into the initial formula for the decay constant, one obtains:

$$\langle 0 | A_L(t) P_S(0) | 0 \rangle = e^{-m_n t} m_P f_P. \quad (4.15)$$

Therefore, in order to find the lattice value of the pion decay constant $f_\pi$, we fit the combination $e^{m_N t} m_n \langle 0 | A_L(t) P_S(0) | 0 \rangle$ to a constant plus exponent function. Armed with the optimal interpolating operator for the $N^{th}$ excited state, we now extract its lattice decay
constant $\tilde{f}_{\pi N}$ through the two-point correlation function

$$C_{A_{4,N}}(t) = \sum_{\vec{x},\vec{y}} \langle 0 | A_{4}(\vec{x},t) \Omega_{N}^{\dagger}(\vec{y},0) | 0 \rangle,$$

(4.16)

by forming the following combination:

$$\frac{e^{m_{N}t}}{m_{N}} C_{A_{4,N}}(t) \to \tilde{f}_{\pi N} + B_{N} e^{-\Delta m_{N}t},$$

(4.17)

where $A_{4}$ is the temporal component of the axial-vector current. Finally, we note that whilst the sign of the decay constants has been discussed in Refs. [74] and [75], the matrix element $\langle 0 | A_{\mu} | \pi_{N} \rangle$ for both the improved and unimproved currents, obtained through Eqn. (4.16), is defined only up to a phase, since the corresponding eigenvector $u^{(N)}$ can be multiplied by an arbitrary phase. We therefore quote the absolute values of the decay constants in our subsequent analyses.

Finally, to obtain the physical value of the decay constant from the lattice value, we have [76]

$$f_{\pi N} = \xi^{-3/2} a_{t}^{-1} \tilde{f}_{\pi N},$$

(4.18)

where $\tilde{f}_{\pi N}$ is the dimensionless value obtained in our calculation.

### 4.1.2 Axial-vector Current

The decay constant of the $N^{\text{th}}$ excitation of the pion, $\pi_{N}$, is given by the hadron-to-vacuum matrix element of the axial vector current,

$$\langle 0 | A_{\mu}(0) | \pi_{N} \rangle = p_{\mu} f_{\pi N},$$

(4.19)
where $A_\mu = \bar{\psi} \gamma_\mu \gamma_5 \psi$; for a state at rest, considered here, only the temporal component of the matrix element is non-zero.

We have established in the previous section that, in order to calculate the pseudoscalar decay constant, one needs to deal with the axial-vector current $A_\mu = \bar{\psi} \gamma_\mu \gamma_5 \psi$. The matrix element of this current, determined on an isotropic lattice is related to that in some specified continuum renormalization scheme through an operator matching coefficient $Z_A$:

$$A_\mu = Z_A A^\text{lat}_\mu. \quad (4.20)$$

$Z_A$ is unity to tree level in perturbation theory, and furthermore the mixing with higher-dimension operators at $\mathcal{O}(a)$ only occurs at one-loop. However, on an anisotropic lattice, mixing with higher dimension operators occurs at tree level [77]. For the action employed here, the following improved formula was derived:

$$A^I_4 = (1 + ma_t \Omega_m) \left[ A^V_4 - \frac{1}{4}(\xi - 1) a_t \partial_4 P \right]. \quad (4.21)$$

Here $A^I_4 = \bar{\psi} \gamma_4 \gamma_5 \psi$ is the temporal component of the unimproved local axial-vector current introduced earlier, and $P = \bar{\psi} \gamma_5 \psi$ is the pseudoscalar current; the details of derivation are provided in the Appendix.

There is an ambiguity in the values of the parameters $m, \Omega_m, \xi$ at tree level, and in this work we take $\xi$ to have its target renormalized value of 3.5. It is important to note that the mixing at tree level vanishes for an isotropic action, $\xi = 1$, and therefore is an artefact of the anisotropic action used in this work. In our subsequent analysis, we will consider the ratios of the decay constant of an excited state and that of the ground state; both the matching coefficient of $Z_A$ of Eqn. (4.20) and the mass improvement term $(1 + ma_t \Omega_m)$ of Eqn. (4.21) cancel in these ratios.
4.2 Results

4.2.1 Mass spectrum

The determination of the excited-state spectrum using the variational method has been described in detail in Refs. [3, 4]; here, the results for the spectrum of the lowest lying states are represented as the first row for each ensemble in Table 4.1. Only the lowest-lying four states in the spectrum are quoted, since the next state is identified as having spin 4, as will be discussed later. In practice, the coefficients giving rise to the "optimal" operator for the $N^{th}$ excited states must be determined at some value $t_{\text{ref}}>t_0$; we take the value of $t_{\text{ref}}$ as that which gives the best reconstruction of the correlation matrix used in the variational method, following the technique described in Ref. [3]. The mass spectrum obtained from a two-exponential fits to the correlation functions $C_{A_4,N}(t)$, using the unimproved axial-vector current at the sink, is listed in the second row for each ensemble in Table 4.1. The consistency between the resultant spectra is encouraging. Finally, in the third row of the same Table 4.1 we presented the masses of pion and its excitations in physical units (MeV) for each ensemble.

4.2.2 Decay constants

As I already mentioned, the decay constants $f_{\pi N}$ are also obtained through the correlation function $C_{A_4,N}(t)$ of Eqn. (4.16), using the optimal operator determined above. A three-parameter fit in $\{\tilde{f}_{\pi N}, B_N, \Delta m_N\}$ (see Eqn. (4.17)) then yields the value of the decay constant. In Table 4.2 we present, as the first line for each ensemble, our results for the absolute, unrenormalized values of the pion decay constants $a_t f_{\pi N}$ for the ground ($N = 0$) and first three excited states ($N = 1, 2, 3$), obtained using the unimproved axial-vector current. As discussed earlier, the use of an anisotropic lattice introduces mixing with
TABLE 4.1: The first line for each ensemble lists the masses of the pion and its first three excitations in lattice units \((a_m \pi_x)\) obtained from the variational method. The second line lists the pion masses in lattice units obtained from a two-exponential fit to the correlator \(C_{A_3,N}(t)\) using the optimal interpolating operator from the variational method at the source, and the unimproved axial-vector current at the sink. In the third line the pion masses in physical units (MeV) obtained from the variational method are presented.

<table>
<thead>
<tr>
<th>(m_\pi)</th>
<th>(N = 0)</th>
<th>(N = 1)</th>
<th>(N = 2)</th>
<th>(N = 3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(m_\pi) [MeV]</td>
<td>0.1483(1)</td>
<td>0.3619(11)</td>
<td>0.4439(34)</td>
<td>0.5199(61)</td>
</tr>
<tr>
<td></td>
<td>0.1482(4)</td>
<td>0.3600(84)</td>
<td>0.3664(975)</td>
<td>0.5569(506)</td>
</tr>
<tr>
<td></td>
<td>702.0(1)</td>
<td>1713(5)</td>
<td>2101(16)</td>
<td>2461(29)</td>
</tr>
<tr>
<td>(m_\pi) [MeV]</td>
<td>0.0999(5)</td>
<td>0.3118(31)</td>
<td>0.4028(43)</td>
<td>0.4493(149)</td>
</tr>
<tr>
<td></td>
<td>0.1008(4)</td>
<td>0.3134(99)</td>
<td>0.4047(683)</td>
<td>0.4361(460)</td>
</tr>
<tr>
<td></td>
<td>524(3)</td>
<td>1635(16)</td>
<td>2113(23)</td>
<td>2357(78)</td>
</tr>
<tr>
<td>(m_\pi) [MeV]</td>
<td>0.0694(2)</td>
<td>0.2735(31)</td>
<td>0.3665(34)</td>
<td>0.4209(99)</td>
</tr>
<tr>
<td></td>
<td>0.0709(10)</td>
<td>0.2626(93)</td>
<td>0.3592(688)</td>
<td>0.4270(75)</td>
</tr>
<tr>
<td></td>
<td>391(1)</td>
<td>1541(17)</td>
<td>2065(19)</td>
<td>2371(56)</td>
</tr>
</tbody>
</table>

Higher dimension operators, even at tree level. Thus the decay constants of Eqn. (4.16) were calculated, but using the improved axial-vector current of Eqn. (4.21). The partial derivative of the pseudoscalar current contributing to the improved current could be evaluated in two ways: by replacing it with energy of the state, \(\partial_4 P \rightarrow E_N P\), and through the use of a finite difference between successive time slices, \(\partial_4 P \rightarrow P(t + 1) - P(t)\). These are presented as the second and third rows for each ensemble in Table 4.2. The two methods of computing the temporal derivative are in general consistent, and the finite-difference method will be used in the subsequent discussion. Finally, as an illustration of the quality of the calculation procedure, in Figure 4.1 there are shown data for Eqn. (4.17), together with the values of \(a_t f_{\pi_N}\) obtained from the three-parameter fit, for the \(N_f = 3\) ensemble. The decay constants \(a_t f_{\pi_N}\) for each of our ensembles computed using the unimproved and improved axial-vector currents are presented in Figures 4.2 and 4.3, respectively. One can observe a decrease in the value of the decay constant up to and including that for the second excited state on all three ensembles, irrespective of the use of the unimproved or improved
FIG. 4.1: The data for $a_t f_{\pi N}$ in units of the temporal lattice spacing from Eqn. (4.17), for the ensemble at $m_\pi = 702$ MeV; the line corresponds to the value of $a_t f_{\pi N}$ obtained from a three-parameter fit to the data as discussed in the text. The optimal operators are obtained from the variational method with $t_0 = 7$ and the eigenvectors determined at $t_{\text{ref}} = 15$. 
FIG. 4.2: The unrenormalized pion decay constants $a_t f_{\pi N}$ on each of our ensembles obtained using the unimproved axial-vector current.
TABLE 4.2: The unrenormalized values of $a_t f_{\pi N}$ for the ground state and first three excitations. For each ensemble, the first line are the values computed using the unimproved axial-vector current, while the second and third lines employ the improved axial-vector current of Eqn. (4.21) with the derivative of the pseudoscalar current computed using the corresponding energy of the state, and a finite time difference, respectively.

<table>
<thead>
<tr>
<th>$m_\pi$ [MeV]</th>
<th>$N = 0$</th>
<th>$N = 1$</th>
<th>$N = 2$</th>
<th>$N = 3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>702</td>
<td>0.0551(3)</td>
<td>0.0319(10)</td>
<td>0.0005(12)</td>
<td>0.0307(23)</td>
</tr>
<tr>
<td></td>
<td>0.0716(6)</td>
<td>0.0556(52)</td>
<td>0.0041(23)</td>
<td>0.0565(54)</td>
</tr>
<tr>
<td></td>
<td>0.0710(4)</td>
<td>0.0543(8)</td>
<td>0.0017(21)</td>
<td>0.0466(54)</td>
</tr>
<tr>
<td>524</td>
<td>0.0441(5)</td>
<td>0.0261(12)</td>
<td>0.0057(3)</td>
<td>0.0315(31)</td>
</tr>
<tr>
<td></td>
<td>0.0565(18)</td>
<td>0.0465(27)</td>
<td>0.0065(4)</td>
<td>0.0493(13)</td>
</tr>
<tr>
<td></td>
<td>0.0564(6)</td>
<td>0.0476(62)</td>
<td>0.0083(10)</td>
<td>0.0483(91)</td>
</tr>
<tr>
<td>391</td>
<td>0.0369(7)</td>
<td>0.0218(15)</td>
<td>0.0062(18)</td>
<td>0.0256(5)</td>
</tr>
<tr>
<td></td>
<td>0.0476(8)</td>
<td>0.0429(113)</td>
<td>0.0138(28)</td>
<td>0.0508(11)</td>
</tr>
<tr>
<td></td>
<td>0.0473(9)</td>
<td>0.0398(90)</td>
<td>0.0140(67)</td>
<td>0.0462(11)</td>
</tr>
</tbody>
</table>

axial-vector current. In Figure 4.4, the ratio of the decay constant of the first excited state to that of the ground state is plotted, a combination in which the matching factor cancels, for both the unimproved (green) and improved (red) currents. Figure 4.4 also shows the linear and constant fits in $m_\pi^2$ to this ratio. Whilst it is notable that the improvement term represents a significant contribution at each quark mass, once again, the qualitative behavior of the ratios remains the same for both currents. It was already pointed out that the experimental leptonic decay rate for the ground-state pion is known very accurately. For the pion excitations, knowledge of the decay constant still lacks experimental data and needs careful theoretical consideration. So far, all lattice QCD predictions for the decay constant of the excitations of the pion have been made for the first excited state only. Within this project, the previous work was extended through the calculation of the decay constant of higher excitations, up to that of the third excited state. The ratios $f_{\pi N}/f_{\pi 0}$ of decay constants for the 1st, 2nd and 3rd excited states to that of the ground state $f_{\pi 0}$ are shown using the unimproved and improved currents respectively in Figures 4.5 and 4.6,
FIG. 4.3: The unrenormalized pion decay constants $a_t f_{\pi N}$ on each of our ensembles obtained using the improved axial-vector current.
FIG. 4.4: Lattice values for the ratio of the "improved" decay constants for the first excited $f_{\pi_1}$ and ground-state $f_{\pi_0}$ pion as a function of the pion mass squared. The green points represent unimproved values, while data in red color correspond to the ratios of improved decay constants. We present linear (upper) and constant (bottom) fits in $m_{\pi}^2$ to the ratio of decay constants.
respectively.

FIG. 4.5: Ratios of the excited-state decay constants $f_{\pi^N}$ to the ground-state decay constant $f_{\pi_0}$ for the first three pion excitations ($N = 1, 2, 3$), using the unimproved current.

4.2.3 Discussion

The results above indicate the value of $\frac{f_{\pi_1}}{f_{\pi_0}}$ to be largely independent of the pion mass in the explored region of 400 – 700 MeV. These conclusions differ from the previously mentioned studies performed by UKQCD Collaboration [72] and by the RBC Collaboration [73]. In the former, using an isotropic clover fermion action, they find in particular that their results show a strong dependence on the current used. A simple linear fit to the ratio of the improved decay constants obtained through the implementation of the full ALPHA Collaboration method [78] gave $|f_{\pi_1}/f_{\pi_0}| = 0.078(93)$ in the chiral limit, showing
FIG. 4.6: Ratios of the excited-state decay constants $f_\pi^N$ to the ground-state decay constant $f_\pi^0$ for the first 3 pion excitations ($N = 1, 2, 3$), using the improved current.
a significant suppression of the decay constant for the first pion excitation. Meanwhile, for the unimproved decay constants, they obtained $|f_{\pi_1}/f_{\pi_0}| = 0.38(11)$ in the chiral limit. We have also employed an improved current, but the improvement term we include arises at tree level and is an artefact of the use of an anisotropic lattice. The RBC calculation, using domain-wall fermions, explores the spectrum of the flavor-singlet pseudoscalar mesons, and amongst the compendium of results presents the leptonic decay constant of the ground-state and first-excited-state pion. There, the decay constants are obtained by relating the matrix elements of the axial-vector current to those of the pseudoscalar density through the axial-vector Ward-Takahashi identity, and a linear extrapolation in the quark mass yields a value of $f_{\pi_1}$ consistent with zero in the chiral limit.

A particularly striking observation in our calculation is the strong suppression of the decay constant of the second excitation. The quark and gluon content of the excitations of the pion spectrum has been investigated earlier using the overlaps of the operators of the variational basis with the states in the spectrum as signatures for their partonic content [3, 4], and a phenomenological interpretation provided in Ref. [36]. Of the lowest four states in the spectrum that we study here, each was identified as corresponding to a state of spin 0 rather than of spin 4, with the first excitation an $S$-wave radial excitation, but with the second excited state having a significant hybrid content represented by a strong overlap onto operators comprising a quark and antiquark coupled to a chromomagnetic field, as we illustrate for the lightest ensemble in Figure 4.7 (for the convenience, I also included a Table 4.3 which clarifies the specific operator naming scheme). Thus the strong suppression of the decay constant for the second-excited state, but the far more moderate suppression of the first excited state, is quite understandable within this phenomenology.
FIG. 4.7: The histogram shows the overlap of the operators of the variational basis to the five lowest-lying states in the spectrum, for the data corresponding to a pion mass of 391 MeV, as described in Refs. [3, 4]. The yellow bar denotes the overlap onto an operator derived from a $J = 4$ continuum construction; we associate the fourth excitation with a state of spin 4, and do not discuss further. Grey bars denote overlaps onto “hybrid” operators, as discussed in the text.
TABLE 4.3: Naming scheme of the $A_1^{-+}$ basis operators obtained from the variational method $f_{\pi N}$.

<table>
<thead>
<tr>
<th>operator label as in Figure 4.7</th>
<th>operator name</th>
</tr>
</thead>
<tbody>
<tr>
<td>a0 x D3.131.J0.J0.A1</td>
<td>$(a_0 \times D_{j=3}^{[3]}_{j=1,J=0})^{J=0}$</td>
</tr>
<tr>
<td>a1 x D3.131.J1.J0.A1</td>
<td>$(a_1 \times D_{j=3}^{[3]}_{j=1,J=1})^{J=0}$</td>
</tr>
<tr>
<td>b1 x D1.J1.J0.A1</td>
<td>$(b_1 \times D_{j=1}^{[1]}_{J=0})^{J=0}$</td>
</tr>
<tr>
<td>b1 x D3.J130.J1.J0.A1</td>
<td>$(b_1 \times D_{j=3=0,J=1})^{J=0}$</td>
</tr>
<tr>
<td>b1 x D3.J132.J1.J0.A1</td>
<td>$(b_1 \times D_{j=3=2,J=2})^{J=0}$</td>
</tr>
<tr>
<td>pion_2 x D0.J0.J0.A1</td>
<td>$(\pi_2 \times D_{j=0}^{[0]})^{J=0}$</td>
</tr>
<tr>
<td>pion_2 x D2.J0.J0.A1</td>
<td>$(\pi_2 \times D_{j=2}^{[2]})^{J=0}$</td>
</tr>
<tr>
<td>pion x D0.J0.J0.A1</td>
<td>$(\pi \times D_{j=0}^{[0]})^{J=0}$</td>
</tr>
<tr>
<td>pion x D2.J0.J0.A1</td>
<td>$(\pi \times D_{j=2}^{[2]})^{J=0}$</td>
</tr>
<tr>
<td>rho_2 x D2.J1.J0.A1</td>
<td>$(\rho_2 \times D_{j=1}^{[2]})^{J=0}$</td>
</tr>
<tr>
<td>rho x D2.J1.J0.A1</td>
<td>$(\rho \times D_{j=1}^{[2]})^{J=0}$</td>
</tr>
</tbody>
</table>

4.2.4 Leptonic decay constants: some concluding remarks and future challenges.

In this research, the first steps were undertaken in investigating the properties of the excited meson states in QCD by computing the decay constants both of the pion, and of its lowest three excitations. Final results [79] show that the optimal operators obtained through the variational method are effective interpolating operators when calculating the hadron-to-vacuum matrix elements of local operators. The picture that emerges is that for the lowest two excitations, the decay constants are indeed suppressed, but largely independent of the quark mass, and that the strong suppression for the second excited state is indicative of the predominantly hybrid nature of the state.

The work presented here is highly encouraging and demonstrates clearly that the properties of the excited state hadrons are accessible to lattice calculation, but there are
certain caveats. Firstly, the basis of interpolating operators used here includes only “single-hadron” operators, whose coupling to multi-hadron decay states is expected to be suppressed by the volume, and thus results obtained here effectively ignore that higher excitations become unstable under the strong interactions. The Hadron Spectrum Collaboration’s previous work on the isovector spectrum [3] suggested that the single-particle energy levels at these values of the quark mass are somewhat insensitive to the volume, but that has not been checked for the decay matrix elements. None-the-less, the fact that the decay constant ratios themselves show a limited quark-mass dependence, despite large differences in $m_\pi L$ ($L$ being the length of the lattice), leads credence to the results presented here. Secondly, the improvement term we include in the axial vector current is that arising at tree level through the use of an anisotropic action; mixings beyond tree level, and the matching coefficients, which cancel in the ratios of decays constants, have not been included. As well as addressing these issues, possible future work would extend the calculation to obtain the moments of the quark distribution amplitudes, and will investigate the decay constants and distribution amplitudes for both the $\rho$ and nucleon excitations.
CHAPTER 5

Lattice Perturbation Theory

In lattice QCD, a discretized space-time lattice can be considered as a non-perturbative regularization scheme which has a unique advantage over other known regularizations: dimensional regularization or Pauli-Villars can only be defined order by order in perturbation theory, while lattice regularization is not tied to any specific calculational method and, with the help of various specially developed numerical and analytical methods, it allows one to perform calculations from first principles. The main reason for the introduction of the lattice was to study the non-perturbative aspects of QCD, like confinement, and LQCD proved to be very successful in corresponding calculations, demonstrating, for example, that only a small fraction of the proton mass is due to the quark masses, while its majority comes from the non-Abelian interactions between quarks and gluons. Lattice QCD also revealed that only about half of the proton momentum comes from the momentum of the constituent quarks, and the fact that only a small part of its spin is due to the spin of the quarks. Therefore, lattice computations are crucial ingredient on our way to better understanding of the strong interactions.

Although LQCD is essentially non-perturbative in its nature, perturbative calculations
also contribute significantly to lattice studies, and play an essential role in connecting the results of Monte Carlo simulations to the continuum. Detailed pedagogical introduction to lattice perturbation theory can be found in [80, 81, 82], and later in this chapter, I will introduce the main methods and techniques used in lattice perturbation theory. In particular, I will discuss lattice Feynman rules and various aspects of the analytic calculations and evaluations of lattice integrals.

5.1 Lattice perturbation theory: why?

Once again, lattice QCD was invented originally for the study of non-perturbative phenomena, like quark confinement, hadron masses, etc. But then the obvious question arises: why is there any interest in developing perturbation theory within lattice QCD? It turns out that there are several important reasons for lattice perturbation theory (LPT) to be developed, and one of them is to serve as a test for the results of numerical lattice simulations. The perturbative region must be explored in order to reach the continuum limit where, in fact, because of asymptotic freedom, one has $g_0 \rightarrow 0$ as $a \rightarrow 0$ [80]. From the other side, the short-distance physics becomes "hidden" in the renormalization parameters while one studies long distance phenomena nonperturbatively within lattice QCD, and lattice perturbation theory helps to make a connection between the low energy and high energy QCD regimes. Also, by introducing a lattice, one breaks Poincare invariance, and perturbation theory can help to investigate the important question of the approach to symmetry restoration.

Results obtained from experiment are expressed typically in the continuum using the standard modified minimally subtracted $\overline{\text{MS}}$ dimensional regularization, therefore another, and more practically important, reason is the use of LPT calculations aimed toward the determination of the renormalization factors converting the results obtained within the
lattice scheme to the one in the continuum. There is a great variety of different lattice actions, each one of which defines its own regularization scheme, so if one wants to be able to use the results obtained in Monte Carlo simulations and compare them with existing or forthcoming experimental data, one needs to obtain a complete set of matching coefficients for each action. These renormalization factors are particularly important for QCD matrix elements and for fixing masses and the couplings presented in the Lagrangian, as well as for matching between the lattice regularization scale $\Lambda$ to the familiar $\Lambda_{QCD}$. Such perturbative lattice renormalization can also serve as a guide for the cases where renormalization constants might be determined non-perturbatively, using the method proposed by Martinelli et al [83]. According to their approach, the numerical extraction of the renormalization factors can be done in limited cases when a plateau is observed over a large enough range of momenta; this might be quite difficult and computationally demanding, in which case lattice perturbation methods serve as the only possibility to evaluate matching coefficients. An alternative approach which allows to perform precise non-perturbative evaluation of renormalized coupling constants, masses and operators for a wide range of momenta is the so-called Schrödinger functional scheme, but computations within this method are much more involved and require also usually large computational resources [80].

To justify completely the application of perturbation theory to a non-perturbative formulation of QCD, one can refer to [84]. When introducing a lattice by dividing space and time into a grid with some lattice spacing $a$, one excludes ultraviolet modes with momenta higher than $\frac{\pi}{a}$. P. Lepage showed that the perturbative renormalisation factors account for the momenta excluded by the lattice cutoff. The current lattice spacings, which are about 0.1 fm, correspond to the ultraviolet cutoff of 6 GeV, and the coupling constant at these energies is small enough for perturbation theory to be valid and to be able to describe the effects excluded by lattice regularization of momenta. Thus, as one can see, lattice
perturbation theory is a powerful technique that can provide much valuable information, and in some cases it is irreplaceable.

5.2 Renormalization in LQCD

As we have learned from the previous Section, the matrix elements of lattice operators computed using numerical simulations require a renormalization in order to be converted into meaningful physical quantities. To perform such a matching to a continuum scheme, one has to look for numbers connecting the bare lattice results to physical continuum renormalized numbers. It turns out that the extraction of the physical continuum matrix elements from Monte Carlo simulations is possible using both lattice and continuum perturbative techniques. At tree level, lattice and original continuum operators have the same matrix elements, and at 1 loop one has, according to [80],

\[
\langle q | O^\text{lat}_i | q \rangle = \sum_j \left( \delta_{ij} + \frac{g_0^2}{16\pi^2} (-\gamma_{ij}^{(0)} \log a^2 p^2 + R^\text{lat}_{ij}) \right) \langle q | O^\text{tree}_j | q \rangle, \tag{5.1}
\]

\[
\langle q | O^\text{MS}_i | q \rangle = \sum_j \left( \delta_{ij} + \frac{g_{\text{MS}}^2}{16\pi^2} (-\gamma_{ij}^{(0)} \log \frac{p^2}{\mu^2} + R^\text{MS}_{ij}) \right) \langle q | O^\text{tree}_j | q \rangle. \tag{5.2}
\]

Here \( g_0 \) and \( g_{\text{MS}} \) are correspondingly lattice and continuum coupling constants, and \( \mu \) is the scale brought in by renormalization. Due to the fact that lattice propagators and vertices differ from their continuum partners (as we will see later in this Chapter), the lattice \( R^\text{lat}_{ij} \) and continuum \( R^\text{MS}_{ij} \) 1-loop constants are not the same. From these equations, one can find the relation between lattice and continuum results,

\[
\langle q | O^\text{MS}_i | q \rangle = \sum_j \left( \delta_{ij} - \frac{g_0^2}{16\pi^2} (-\gamma_{ij}^{(0)} \log a^2 \mu^2 + R^\text{lat}_{ij} - R^\text{MS}_{ij}) \right) \langle q | O^\text{lat}_j | q \rangle. \tag{5.3}
\]
In this expression the lattice coupling constant $g_0$ is used, as advocated in [85], since the choice of a particular coupling constant only makes a difference for 2-loop calculations. It is obvious from Eqn. (5.3) that the main focus of calculations within lattice perturbation theory is on the evaluation of so-called matching factors

$$Z_{ij}(a\mu, g_0) = \delta_{ij} - \frac{g_0^2}{16\pi^2} \left(-\gamma_i^{(0)} \log a^2 + \Delta R_{ij}\right),$$

(5.4)

depending on the differences $\Delta R_{ij} = R_{ij}^{\text{lat}} - R_{ij}^{\overline{\text{MS}}}$ between lattice and continuum constants from (5.3). In other words, matching between the bare lattice results, obtained in the Monte Carlo simulations, to the physical results in the $\overline{\text{MS}}$ scheme, means calculation of the renormalization factor $Z(a\mu)$ which converts the lattice operator $\mathcal{O}^{\text{lat}}(a)$ into the physical renormalized operator $\mathcal{O}^{\text{phys}}(\mu)$:

$$\mathcal{O}^{\text{phys}}(\mu) = Z(a\mu)\mathcal{O}^{\text{lat}}(a).$$

(5.5)

While matching to the continuum scheme, the lattice cutoff must be removed, which means the consideration of the continuum limit $a \to 0$, so that only some suitable quantity (the scale $\mu$) is kept fixed:

$$\mu < \frac{1}{a}.$$ 

(5.6)

Here the lower bound ensures the validity of the perturbation theory, while the upper bound guarantees that cutoff effects, proportional to positive powers of $a$, are small [80]. In general, every lattice action defines a different regularization scheme, which means that renormalization factors are also different for each particular lattice formulation of QCD.
5.3 Feynman rules on the lattice: general approach

Similarly to the continuum case, the calculation of Feynman diagrams on the lattice is done usually in two steps. Firstly, one makes a perturbative Taylor expansion of the lattice action, dividing it into a free field part (i.e. terms quadratic in the fields), and interaction vertices (everything else). From such an expansion, expressions for propagators and vertices that form the Feynman rules can be derived in momentum space. After that, one can construct Feynman diagrams of interest from these rules, and evaluate them eventually by integrating over phase space.

One of the unpleasant surprises is that, despite similarities between lattice and continuum perturbation theories, the lattice one is much more involved than that of the continuum formulation. The lattice actions include some irrelevant vertices, which have no analog in the continuum theory. Some number of these vertices make actual contributions to the Green functions at a given order of the perturbation theory in the limit of vanishing lattice spacing $a \to 0$. So the number of Feynman diagrams on the lattice is greater than that in the continuum formulation.

The main difficulties at the stage of evaluating Feynman diagrams arise due to the presence of terms violating Lorentz symmetry, as well as due to the additional complications which come with replacing momentum integrals by discrete sums. That is why these computationally intensive calculations are done usually using specially developed mathematical packages, like, for example, HiPPy/HPsrc [86]. Meanwhile, the first step of the lattice perturbation program, i.e. the derivation of Feynman diagrams, is also rather involved: lattice gauge fields are elements of the Lie group, rather than the algebra of the gauge group, therefore one needs to do the expansion of exponentials of non-commuting fields.

The discussion later in this chapter will be devoted to the details of the derivation of lattice Feynman rules for the improved anisotropic action introduced for the non-perturbative
study of pion decay constants, which was described in chapter 4. After outlining the main steps of the derivation, I will present the final expressions for the perturbatively calculated propagators and vertices for this specific improved lattice action.

5.4 Details of calculation

5.4.1 An anisotropic lattice action

Even though the improved gauge and quark anisotropic lattice actions were already introduced in the previous chapter, I would like to recall their forms here, since the whole of the following discussion will be based on these expressions. The anisotropic LQCD action is simply the sum of the gauge action $S^\xi_G$ and the fermion action $S^\xi_F$:

$$S^\xi = S^\xi_G + S^\xi_F. \quad (5.7)$$

Here $S^\xi_G[U]$ is a Symanzik-improved action with tree-level tadpole-improved coefficients [41]:

$$S^\xi_G[U] = \frac{\beta}{N_c \gamma_g} \left\{ \sum_{x,s \neq s'} \left[ \frac{5}{6u_s^4} \Omega_{P_{s's'}}(x) - \frac{1}{12u_s^6} \Omega_{R_{s's'}}(x) \right] + \sum_{x,s} \gamma_g^2 \left[ \frac{4}{12u_s^2u_t^2} \Omega_{P_{s't}}(x) - \frac{1}{12u_s^4u_t^2} \Omega_{R_{s't}}(x) \right] \right\} \quad (5.9)$$
and $S^F_\xi[U, \bar{q}, q]$ is the anisotropic clover fermion action:

$$
S^F_\xi[U, \bar{q}, q] = a_t a_s x \sum_x \bar{q}(x) \left[ m_0 + \nu_1 [\gamma_t \nabla_t - \frac{a_t}{2} \Delta_t] + \nu_s \sum_s [\gamma_s \nabla_s - \frac{a_s}{2} \Delta_s] - \\
- \frac{1}{2} [C_{sw} a_s \sum_s \sigma_{ts} F_{ts} + C_{sw} a_s \sum_{s<s'} \sigma_{ss'} F_{ss'}] \right] q(x) 
$$

(5.10)

Some standard definitions in lattice perturbation theory for the covariant first- and second-order lattice derivatives $\nabla_\mu$ and $\Delta_\mu$, the form of the clover-leaf discretization of the field tensor $F_{\mu\nu}(x)$, as well as all variety of different parameters used in this particular action can be found in Appendices C.2 and C.3.

To perform the subsequent derivations of expressions for propagator and vertices, it is convenient to work with the explicit form of the fermion action. We found it is easier to obtain such a form by considering each term of the action separately; we provided expressions for each of these terms, as well as the explicit form of the total expression for the fermion anisotropic lattice action in the Appendix C.4. One can see at this point, that lattice actions are indeed much more complicated than their continuum counterparts, and any derivations corresponding to these actions are going to be rather involved.

### 5.4.2 Fourier transforms on the lattice

To calculate Feynman diagrams in momentum space, the Fourier transforms on the lattice need to be defined. In infinite volume, which is the standard setting in perturbation theory, they are given by the following expressions: - for fermion fields $\psi(x)$:

$$
\psi(x) = \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{d^4 p}{(2\pi)^4} e^{ipx} \tilde{\psi}(p), 
$$

(5.11)

$$
\tilde{\psi}(x) = \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{d^4 p}{(2\pi)^4} e^{-ipx} \psi(p), 
$$

(5.12)
- for gauge fields $A^a_\mu(x)$, that are naturally associated with the middle point of the link $(x, x + \hat{\mu})$:

$$A^a_\mu(x) = \int_{-\pi/\mu}^{\pi/\mu} \frac{d^d p}{(2\pi)^d} e^{i p \cdot (x + \frac{\hat{\mu}}{2})} \tilde{A}^a_\mu(p).$$  \hspace{1cm} (5.13)

Obviously, on a lattice of finite volume the allowed momenta are a discrete set. However, in perturbation theory one always consider the limit of infinite volume. The corresponding formulae for inverse Fourier transforms on the lattice can be found in Appendix C.1.

### 5.4.3 Quark propagator

In order to derive the expression for a quark propagator, one needs terms from the fermion action $S_F$ which quadratic in quark fields, i.e. $\sim \bar{q}(x)q(x))$. Gauge links $U_\mu(x)$ and $U^\dagger_\mu(x)$ can be expanded perturbatively as following:

$$U_\mu(x) = e^{iga_\mu A_\mu} \sim 1 + i g a_\mu A_\mu + \cdots$$

$$U^\dagger_\mu(x) = e^{-iga_\mu A_\mu} \sim 1 - i g a_\mu A_\mu + \cdots,$$  \hspace{1cm} (5.14)

so for the problem of obtaining the quark propagator, we can safely assume $U_\mu(x) = U^\dagger_\mu(x) \sim 1$. Then the only non-zero terms contributing to the propagator are:

$$S_{qq} = \sum_x \left\{ \bar{q}(x) a t_3 m_0 q(x) + \bar{q}(x) \frac{a^3}{2} \nu_t q(x + t) - \bar{q}(x) \frac{a^3}{2} \nu_t q(x - t) - \bar{q}(x) \frac{a^3}{2} \nu_t q(x + t) - \bar{q}(x) \frac{a^3}{2} \nu_t q(x - t) + \bar{q}(x) \frac{a^3}{2} \nu_t q(x) + \bar{q}(x) \sum_s \frac{a t_3}{2} \nu_s q(x + s) - \bar{q}(x) \sum_s \frac{a t_3}{2} \nu_s q(x - s) - \bar{q}(x) \sum_s \frac{a t_3}{2} \nu_s q(x + s) - \bar{q}(x) \sum_s \frac{a t_3}{2} \nu_s q(x - s) + \bar{q}(x) \sum_s \frac{a t_3}{2} \nu_s q(x) \right\}$$  \hspace{1cm} (5.15)
Substituting here the Fourier transforms for \( q(x) \) and \( \bar{q}(x) \),

\[
q(x) = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{d^4 p}{(2\pi)^4} e^{ip_x q(p)} ,
\]

\[
\bar{q}(x) = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{d^4 p'}{(2\pi)^4} e^{-ip'_x \bar{q}(p')},
\]

one obtains

\[
S_{qq} = \sum_s \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{d^4 p'}{(2\pi)^4} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{d^4 p}{(2\pi)^4} \left\{ e^{-ip'_x \bar{q}(p')} a_t q_m e^{ip_x q(p)} + e^{-ip'_x \bar{q}(p')} a^3_s \nu t (e^{ip(x + a_t t)} - e^{ip(x - a_t t)}) q(p) - e^{-ip'_x \bar{q}(p')} a^3_t \nu t (e^{ip(x + a_t t)} + e^{ip(x - a_t t)} - 2e^{ip_x}) q(p) + e^{-ip'_x \bar{q}(p')} \sum_s \frac{a_t a^2_s}{2} \nu s \gamma_s (e^{ip(x + a_s s)} - e^{ip(x - a_s s)}) q(p) - e^{-ip'_x \bar{q}(p')} \sum_s \frac{a_t a^2_s}{2} \nu s (e^{ip(x + a_s s)} + e^{ip(x - a_s s)} - 2e^{ip_x}) q(p) \right\} .
\]

Using the formula for the momentum-space delta function,

\[
\frac{a^4}{(2\pi)^4} \sum_x e^{-ix(p' - p)} = \delta^{(4)}(p' - p),
\]

\( S_{qq} \) can be written as

\[
S_{qq} = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{d^4 p'}{(2\pi)^4} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{d^4 p}{(2\pi)^4} (2\pi)^4 \delta^{(4)}(p' - p) \bar{q}(p') \left\{ a_t a^3_s q_m + \frac{a^3_t}{2} \nu t (e^{ipa_t t} - e^{-ipa_t t}) - \frac{a^3_s}{2} \nu s (e^{ipa_s s} + e^{-ipa_s s} - 2) + \sum_s \frac{a_t a^2_s}{2} \nu s \gamma_s (e^{ipa_s s} - e^{-ipa_s s}) - \sum_s \frac{a_t a^2_s}{2} \nu s (e^{ipa_s s} + e^{-ipa_s s} - 2) \right\} q(p).
\]
Recalling

\[ \sin(p) = \frac{1}{2i} (e^{ip} - e^{-ip}), \quad \cos(p) = \frac{1}{2} (e^{ip} + e^{-ip}), \]

we get:

\[
S_{qq} = \int_{-\pi}^{\pi} \frac{d^4 p'}{(2\pi)^4} \int_{-\pi}^{\pi} \frac{d^4 p}{(2\pi)^4} (2\pi)^4 a^3 \delta^{(4)}(p' - p) \tilde{q}(p') \left\{ a_t a_s^3 m_0 + \frac{a^3}{2} \nu \gamma_t 2i \sin(a_t p_t) - \frac{a^3}{2} \nu_t (2 \cos(a_t p_t) - 2) + \sum_s a_t a^2_s \nu_s \gamma_s 2i \sin(a_s p_s) - \sum_s a_t a^2_s \nu_s (2 \cos(a_s p_s) - 2) \right\} q(p) = \\
\int_{-\pi}^{\pi} \frac{d^4 p'}{(2\pi)^4} \int_{-\pi}^{\pi} \frac{d^4 p}{(2\pi)^4} (2\pi)^4 a^3 \delta^{(4)}(p' - p) \tilde{q}(p') \left\{ a_t a_s^3 m_0 + i a^3_s \nu \gamma_t \sin(a_t p_t) - a^3 \nu_t (\cos(a_t p_t) - 1) + i \sum_s a_t a^2_s \nu_s \gamma_s \sin(a_s p_s) - \sum_s a_t a^2_s \nu_s (\cos(a_s p_s) - 1) \right\} q(p).
\]

Here \( 1 - \cos(p) = 2 \sin^2(\frac{p}{2}) \), then

\[
S_{qq} = \int_{-\pi}^{\pi} \frac{d^4 p'}{(2\pi)^4} \int_{-\pi}^{\pi} \frac{d^4 p}{(2\pi)^4} (2\pi)^4 a^3 \delta^{(4)}(p' - p) \tilde{q}(p') \left\{ a_t a_s^3 m_0 + i a^3_s \nu \gamma_t \sin(a_t p_t) + 2a^3 \nu \sin^2(\frac{a_t p_t}{2}) + i \sum_s a_t a^2_s \nu_s \gamma_s \sin(a_s p_s) + 2 \sum_s a_t a^2_s \nu_s \sin^2(\frac{a_s p_s}{2}) \right\} q(p).
\]
Therefore the final expression for the quark propagator, which is the inverse of the quadratic part of the action, has the following form:

\[
Q = \left\{ \frac{1}{a_t a_s^3} \left( a_t a_s m_0 + i a_s^3 \gamma_t \sin(a_t p_t) + 2 a_s^3 \nu_t \sin^2\left(\frac{a_t p_t}{2}\right) + \right.ight.
\]
\[
\left. + i \sum_s a_t a_s^2 \nu_s \gamma_s \sin(a_s p_s) + 2 \sum_s a_t a_s^2 \nu_s \sin^2\left(\frac{a_s p_s}{2}\right) \right) \right\}^{-1}.
\] (5.23)

In order to check the correctness of this novel result, we compared it with the well-known expression for the isotropic Wilson action quark propagator [87]. For this case of an unimproved isotropic action, we take

\[
a_t = a_s = a;
\]
\[
\gamma_t = \gamma_s = 1;
\]
\[
\nu_t = \nu_s = 1.
\] (5.24)

Under these simplifications, the quark propagator \( Q \) turns into

\[
Q_w = \left\{ \frac{1}{a^4} \left( a^4 m_0 + i a^3 \gamma_t \sin(a p_t) + \right. \right.
\]
\[
\left. + 2 a^3 \sin^2\left(\frac{a p_t}{2}\right) + i \sum_s a^3 \gamma_s \sin(a p_s) + 2 \sum_s a^3 \sin^2\left(\frac{a p_s}{2}\right) \right) \right\}^{-1} = \left\{ \frac{1}{a} \left( a m_0 + i \gamma_t \sin(a p_t) + i \sum_s \gamma_s \sin(a p_s) + 2 \sin^2\left(\frac{a p_t}{2}\right) + 2 \sum_s \sin^2\left(\frac{a p_s}{2}\right) \right) \right\}^{-1} = \left\{ \frac{1}{a} \left( a m_0 + i \sum_\mu \gamma_\mu \sin(a p_\mu) + 2 \sum_\mu \sin^2\left(\frac{a p_\mu}{2}\right) \right) \right\}^{-1} = \frac{1}{a m_0 + i \sum_\mu \gamma_\mu \sin(a p_\mu) + 2 \sum_\mu \sin^2\left(\frac{a p_\mu}{2}\right)} = a \frac{am_0 + 2 \sum_\mu \sin^2\left(\frac{a p_\mu}{2}\right) - i \sum_\mu \gamma_\mu \sin(a p_\mu)}{\left( \sum_\mu \gamma_\mu \sin(a p_\mu) \right)^2 + \left( 2 \sum_\mu \sin^2\left(\frac{a p_\mu}{2}\right) + a m_0 \right)^2},
\] (5.25)
which is the correct form of the quark propagator for the Wilson action.

5.4.4 Quark-quark-gluon vertex

To derive the Feynman rule for the quark-quark-gluon vertex, we first need to find terms in the action which are proportional to $\bar{q}(x)A(x)q(x)$, so in this case we will keep $U_\mu(x) \approx i\gamma_\mu A_\mu(x)$.

It is convenient to represent the total fermion anisotropic action $S_F^\xi$ as a sum of two terms $S_{q1}$ and $S_{q2}$

$$S_F^\xi = S_{q1} + S_{q2},$$

whose explicit form can be found in Appendix C.

Applying here, as in the previous case, the Fourier transforms (5.16) for the fermion fields, together with the following Fourier transform for the gauge field:

$$A_\mu(x) = \int_{-\pi a}^{\pi a} \frac{d^4 k}{(2\pi)^4} e^{i(x + \frac{a_\mu}{2})k} A_\mu(k),$$

and using

$$\frac{1}{(2\pi)^4} \sum_x e^{ix(-p'+k+p)} = \frac{1}{a_t a_s^3} \delta^{(4)}(-p' + k + p),$$

one obtains the terms contributing to the quark-quark-gluon vertex from $S_{q1}$ as:

$$S_{\bar{q}qq} = ig \sum_{x} \int_{-\pi a}^{\pi a} \frac{d^4 p'}{(2\pi)^4} \int_{-\pi a}^{\pi a} \frac{d^4 p}{(2\pi)^4} \int_{-\pi a}^{\pi a} \frac{d^4 k}{(2\pi)^4} \delta^{(4)}(-p' + k + p) \times
\times \bar{q}(p') \left\{ \cos \left[ a_t \left( \frac{k_t}{2} + p_t \right) \right] \nu_t \gamma_t A_t(k) - i \sin \left[ a_t \left( \frac{k_t}{2} + p_t \right) \right] \nu_t A_t(k) +
+ \sum_s \nu_s \gamma_s \cos \left[ a_s \left( \frac{k_s}{2} + p_s \right) \right] A_s(k) -
- i \sum_s \nu_s \sin \left[ a_s \left( \frac{k_s}{2} + p_s \right) \right] A_s(k) \right\} q(p).$$
In the case of $S_{q2}$, after following a similar procedure, where we first apply the *Baker-Campbell-Hausdorff* (BCH) formula to the terms containing products of four gauge links (see Appendix B), and then substitute Fourier transforms for the quark and gluon fields, we obtain:

$$S_{qq2} = g \int_{-\pi/2}^{\pi/2} \frac{d^4p'}{(2\pi)^4} \int_{-\pi/2}^{\pi/2} \frac{d^4p}{(2\pi)^4} \int_{-\pi/2}^{\pi/2} \frac{d^4k}{(2\pi)^4} \delta^{(4)}(-p' + k + p) \bar{q}(p') \times$$

$$\left\{ C_s^{\alpha} \frac{1}{a_t} \sum_s \sigma_{ts} \frac{1}{2} \left[ a_s \cos \left( \frac{a_s k_s}{2} \right) \sin(a_t k_t) A_s(k) - a_t \sin(a_s k_s) \cos \left( \frac{a_t k_t}{2} \right) A_t(k) \right] + \right.$$  

$$+ C_s^{\alpha} \frac{1}{a_s} \sum_{s < s'} \sigma_{ss'} \frac{1}{2} \left[ a_{s'} \cos \left( \frac{a_{s'} k_{s'}}{2} \right) \sin(a_s k_s) A_{s'}(k) - a_s \sin(a_s k_s) \cos \left( \frac{a_s k_s}{2} \right) A_s(k) \right] \right\} q(p).$$  

(5.30)

With these two expressions, we obtained the desired Feynman rule for the quark-quark-gluon vertex:

$$V_{qqg} = g \left\{ i \nu_t \gamma_t \cos \left( \frac{(p + p')_t}{2} \right) + \nu_t \sin \left( \frac{(p + p')_t}{2} \right) + \right.$$  

$$+ i \nu_s \sum_s \gamma_s \cos \left( \frac{(p + p')_s}{2} \right) + \nu_s \sum_s \sin \left( \frac{(p + p')_s}{2} \right) + \right.$$  

$$+ \frac{C_s^{\alpha}}{a_t} \sum_s \sigma_{ts} \frac{1}{2} \left[ a_s \sin \left( \frac{a_t (p' - p)_t}{2} \right) \cos \left( \frac{(p' - p)_t}{2} \right) - \right.$$  

$$- a_t \sin \left( \frac{a_s (p' - p)_s}{2} \right) \cos \left( \frac{(p' - p)_s}{2} \right) \right\}.$$

(5.31)

As was the case with the quark propagator, we “checked” this result by comparing it with the quark-quark-gluon vertex for an isotropic Wilson action [87]. After applying (5.24),
our improved anisotropic Feynman rule turned into

$$ V_{qg} = g \left\{ i \gamma_t \cos \left[ a \left( \frac{(p + p')_t}{2} \right) \right] + \sin \left[ a \left( \frac{(p + p')_t}{2} \right) \right] + \right. $$

$$ + i \sum_s \gamma_s \cos \left[ a \left( \frac{(p + p')_s}{2} \right) \right] + \sum_s \sin \left[ a \left( \frac{(p + p')_s}{2} \right) \right] + $$

$$ + \sum_s \sigma_{ts} \left( \sin[a(p' - p)_t] \cos \left[ a \frac{(p' - p)_s}{2} \right] \right) - $$

$$ - \sin[a(p' - p)_s] \cos \left[ a \frac{(p' - p)_t}{2} \right] \right) + $$

$$ + \sum_{s < s'} \sigma_{ss'} \left( \sin[a(p' - p)_s] \cos \left[ a \frac{(p' - p)_{s'}}{2} \right] \right) - $$

$$ - \sin[a(p' - p)_{s'}] \cos \left[ a \frac{(p' - p)_s}{2} \right] \right) \right\} = $$

$$ = g \left\{ \sin \left[ a \frac{(p + p')_t}{2} \right] + i \gamma_t \cos \left[ a \frac{(p + p')_t}{2} \right] \right\}. \quad (5.32) $$

### 5.4.5 Gluon propagator

In order to derive the Feynman rule for the gluon propagator, one needs to find the inverse of the quadratic part of the gauge action, i.e. to take into account terms of the action proportional to $A_\mu(x)A_\nu(x)$. After sorting these relevant terms out, with the use of the BCH formula, gauge fixing has to be introduced. Gauge fixing is not necessary, in general, for Monte Carlo simulations within non-perturbative lattice QCD, where one works with actions expressed directly in terms of the fundamental gauge fields of the theory $U_\mu(x)$. This is due to the fact that the lattice functional integrals are well defined, and correlation functions can be computed without fixing the gauge. But in the case of perturbative LQCD one works, after Taylor expansion of the gauge link, with different actual degrees of freedom, i.e. $A_\mu(x)$. Here, gauge fixing is necessary in order to eliminate the zero modes in the quadratic part of the action [80]. Therefore, following the discussion of [88], we add to the initial gauge action an anisotropic gauge fixing term, which in
Feynman gauge looks like

\[ S_{G\, \text{fix}} = \frac{1}{2} a_s^3 a_t \sum_x \left[ \frac{1}{a_t} \partial_t A_t + \frac{1}{a_s} \sum_j \partial_j A_j \right]^2 = \]
\[ = \frac{1}{2\xi} \sum_x \left[ \xi^2 \partial_t(a_t A_t) + \sum_j \partial_j(a_s A_j) \right]^2, \quad (5.33) \]

where

\[ \partial_\mu A_\mu(x) \equiv A_\mu(x + \frac{a_\mu}{2}) - A_\mu(x - \frac{a_\mu}{2}). \quad (5.34) \]

Then the gauge action becomes

\[ S_G + S_{G\, \text{fix}} = \frac{1}{2} \sum_{\mu\nu} \int_{-\pi}^{\pi} \frac{d^4 k}{(2\pi)^4} A_\mu(k) M_{\mu\nu}(k) A_\nu(-k), \quad (5.35) \]

with \( A_\mu(k) \) being the Fourier transform of the dimensionless gauge fields \( a_\mu A_\mu \), and the free gauge propagator has the structure

\[ G_{\mu\nu}(k) = (M^{-1})_{\mu\nu}. \quad (5.36) \]

We found the elements of the matrix \( M_{\mu\nu} \) to be consistent with [88]:

\[ M_{tt} = \left( \frac{a_s}{a_t} \right)^3 \hat{k}_t^2 + \frac{a_s}{a_t} \sum_s \hat{k}_s^2 \left( 1 + \frac{1}{12} \hat{k}_s^2 \right), \]
\[ M_{ss} = \frac{a_t}{a_s} \hat{k}_s^2 + \frac{a_s}{a_t} \hat{k}_t^2 \left( 1 + \frac{1}{12} \hat{k}_s^2 \right) + \frac{a_t}{a_s} \sum_{s' \neq s} \left[ 1 + \frac{1}{12} \left( \hat{k}_{s'}^2 + \hat{k}_s^2 \right) \right], \]
\[ M_{s' \neq s} = -\frac{1}{12} \frac{a_t}{a_s} \hat{k}_{s'} \hat{k}_s \left( \hat{k}_{s'}^2 + \hat{k}_s^2 \right), \]
\[ M_{st} = M_{ts} = -\frac{1}{12} \frac{a_s}{a_t} \hat{k}_t \hat{k}_s, \quad (5.37) \]
where \( \hat{k}_\mu = 2 \sin \left( \frac{k_\mu}{2} \right) \).

In our derivations, we did not take into account the additional improvement of the lattice action - stout smearing of the gauge fields, introduced in chapter 3, where one replaces all gauge links by

\[
U_\mu(x) \rightarrow \tilde{U}_\mu(x) = e^{i Q_\mu(x)} U_\mu(x).
\]  

(5.38)

Nevertheless, this improvement can be added easily, as was shown in [89]. In our simulations, we have used the three-dimensional smearing with the following choice of staple weights,

\[
\rho_{ij} = \rho, \quad \rho_{tm} = 0, \quad \rho_{tt} = 0,
\]

(5.39)

i.e. the smearing in the spatial directions only. Following [89], where authors shifted \( x \rightarrow x - \frac{i}{2} \), this yields for the smeared field (up to terms of order \( O(a^2) \))

\[
A'_i(x) = A_i(x) + \rho \sum_j [A_i(x + j) - 2A_i(x) + A_i(x - j)] + \\
+ \rho \sum_j [A_j(x - \frac{i}{2} + \frac{j}{2}) - A_j(x - \frac{i}{2} - \frac{j}{2}) - \\
- A_j(x + \frac{i}{2} + \frac{j}{2}) + A_j(x + \frac{i}{2} - \frac{j}{2})].
\]

(5.40)

According to [90], the final relation for the iterated smearing \( n > 1 \) in \( d \) dimensions is of
the form

\[
\tilde{A}_\mu^{(n)}(q) = \sum \left\{ \left( \left[ 1 - \frac{\rho}{2(d-1)} \hat{q}^2 \right]^n \left( \delta_{\mu,\nu} - \frac{\hat{q}_\mu \hat{q}_\nu}{\hat{q}^2} \right) + \frac{\hat{q}_\mu \hat{q}_\nu}{\hat{q}^2} \right) A_\nu(q) \right\},
\]  

(5.41)

so in our case \( n = 2 \) we have

\[
\begin{align*}
\tilde{A}_t(q) &= A_t(q), \\
\tilde{A}_i(q) &= \sum_j \left\{ \left[ 1 - \rho \hat{q}_s^2 \right]^2 \left( \delta_{ij} - \frac{\hat{q}_i \hat{q}_j}{\hat{q}_s^2} \right) + \frac{\hat{q}_i \hat{q}_j}{\hat{q}_s^2} \right) A_j(q) \right\},
\end{align*}
\]

(5.42)

where we replaced \( \hat{q}^2 = \sum_\nu \hat{q}_\nu^2 \) from Eq. (5.41) with the spatial terms \( \hat{q}_s^2 = \sum_j \hat{q}_j^2 \). Ref. [90] shows that for the gluon propagator the effect of smearing is equivalent to the introduction of the form factor \( f_{\mu\nu} \), so that

\[
G_{\mu\nu} \rightarrow \sum_{\kappa\sigma} f_{\mu\kappa} G_{\kappa\sigma} f_{\sigma\nu},
\]

(5.43)

where \( f_{tt} = 1, f_{t\mu} = 0, \) and \( f_{ij} \) equals to the factor in front of \( A_j(q) \) in Eq. (5.42).

The Feynman rules presented here represent novel results which have not been derived before for this particular kind of lattice action. These results can be used eventually for the evaluation of the corresponding Feynman diagrams and for the consequent perturbative renormalization of the fermion rest mass or wave function. Applicable to the previous chapter case of the pion decay constants, such perturbative evaluation of the renormalization parameters can help to bridge the gap between numerical results obtained in the lattice simulations and corresponding experimental data.
CHAPTER 6

Conclusion and Outlook

Understanding the hadron spectrum in the light and heavy quark sectors of QCD remains one of the fundamental aims of strong interaction physics. The lattice approach, discussed within this thesis in great detail, offers, among others, a well-developed method for performing computations of the QCD spectrum from first principles. Experiments have revealed already a rich spectrum of excited states, and more studies are on the way: for instance, a detailed investigation of the spectrum of mesons composed of light quarks is the goal of Jefferson Lab GlueX experiment at 12 GeV, which aims to photoproduce mesons with exotic quantum numbers and reveal the role of gluonic degrees of freedom in the spectrum. Within this realm of research, lattice calculations are able to identify properties of hadronic excitations, and produce useful guidance for experiment.

Our desire to describe the wealth of existing experimental data on the spectrum and to predict the outcomes of future experiments poses numerous challenges and always comes at a price. In particular, obtaining an accurate resolution of excited states using lattice QCD calculations is complicated due to the faster decay of excited-states correlation functions in Euclidean time in comparison with those of ground states. A means to overcome
this difficulty is through the use of anisotropic lattices with a finer temporal than spatial discretization; in this work we used a particular type of improved anisotropic lattice action, which helps to resolve the spectrum of hadronic excitations and also reduces greatly systematic errors associated with numerical simulations.

The focus of the current study was on applying LQCD methodology to go beyond the spectrum to discern the structure of the states. This was done with the use of the variational method which employs a large basis of interpolating operators satisfying the symmetries of the lattice and allows to extract the excited-state spectrum of hadrons. In particular, we explored the properties of the pion and its excitations by computing their decay constants for different excitations and for different quark masses. This work presents several new results: it contains calculations of the decay constants both of the pion, and of its lowest three excitations, while previous similar lattice calculations have never been extended further than the first excitation. There are projects that would extend the work outlined in this part of thesis. In the improvement for the axial vector current, discussed in chapter 4, the mixings beyond the tree level can be included. Another direction is to extend the calculations to look at the leptonic decay constants for other channels, such as the rho meson.

The second part of the work presented here is devoted to lattice perturbation theory, which provides us with a method for systematically matching regularization schemes so that we can establish the appropriate connection between results obtained within a particular lattice scheme and physical continuum theory (or, in other words, between lattice simulations and experimental data). For the results obtained in numerical lattice simulations to be directly compared to experiment, one needs to calculate corresponding matching factors. This text provides a detailed step-by-step description of the derivation of the Feynman rules using perturbation theory for the improved anisotropic-clover fermion action which was employed in our numerical studies of excited states. As emphasized in
chapter 5, such perturbative calculations represent a highly demanding task, since Feyn-
man rules on the lattice are much more complicated than those on the continuum due
to the breaking of Lorentz symmetry; moreover, they differ for different lattice actions.
Their evaluation for this particular type of action have never been done before, and the
future application of these rules for the calculation of lattice Feynman diagrams will be a
significant advance.
APPENDIX A

Notation and Conventions

A.1 Natural units, notation, and Euclidean space

In this dissertation, I employ the use of natural units that simplify notation considerably:

\[\hbar = c = 1.\]  \hspace{1cm} (A.1)

I use Greek letters \(\alpha, \beta, \gamma, \ldots\), which run from 0 to 3, for four-dimensional Lorentz indices. Latin letters \(i, j, k, \ldots\), which run from 1 to 3, denotes three-dimensional indices (I reserve \(a, b, c, \ldots\) for color indices).

Four-vectors with real time \(\tau\) correspond to Minkowski metric \(g_{\mu\nu} = diag(1, -1, -1, -1)\). When one switches to imaginary time \(t = i\tau\), the relative minus sign between time- and space-components vanishes and the metric becomes Euclidean \(\delta_{\mu\nu} = diag(1, 1, 1, 1)\). The change from real to imaginary time is often referred to as Wick rotation.

The Euclidean gamma matrices \(\gamma_\mu (\mu = 1, 2, 3, 4)\) can be constructed from the
Minkowski gamma matrices $\gamma^M_\mu (\mu = 0, 1, 2, 3)$. Minkowski gamma matrices obey

$$\{\gamma^M_\mu, \gamma^M_\nu\} = 2g_{\mu\nu} \mathbb{1}, \quad (A.2)$$

with the metric tensor given by $g_{\mu\nu} = \text{diag}(1, -1, -1, -1)$ and $\mathbb{1}$ is the $4 \times 4$ unit matrix.

Thus when we define the Euclidean matrices $\gamma_\mu$ by setting

$$\gamma_i = -i\gamma_1^M, \quad \gamma_4 = \gamma_0^M, \quad (A.3)$$

we obtain the Euclidean anti-commutation relations

$$\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu} \mathbb{1} \quad (A.4)$$

In addition to the matrices $\gamma_\mu$, we define the matrix $\gamma_5$ as the product

$$\gamma_5 = \gamma_1\gamma_2\gamma_3\gamma_4. \quad (A.5)$$

The matrix $\gamma_5$ anti-commutes with all other gamma matrices $\gamma_\mu$ and obeys $\gamma_5^2 = \mathbb{1}$. The Euclidean gamma matrices also obey

$$\gamma_\mu = \gamma_\mu^\dagger = \gamma_\mu^{-1}. \quad (A.6)$$

### A.2 $SU(N)$ algebra generators

Each element of $SU(N)$ can be represented in the following form:

$$\Lambda = e^{\sum_{a=1}^{N-1} i Tr a^a}. \quad (A.7)$$
Here $\omega^a \in \mathcal{R}$, and $N \times N$ matrices $T_a$ are the traceless and Hermitian generators of the Lie algebra

$$\text{Tr} \ T_a = 0, \quad T_a^\dagger = T_a. \quad (A.8)$$

They are normalized as

$$\text{Tr} \ (T_a T_b) = \frac{1}{2} \delta_{ab}, \quad (A.9)$$

and satisfy

$$[T_a, \ T_b] = i f_{abc} T_c, \quad (A.10)$$

where $f_{abc}$ are real antisymmetric structure constants. $SU(N)$ algebra generators can also be written using Gell-Mann matrices $\lambda_a$:

$$T_a = \frac{\lambda_a}{2}, \quad (a = 1, 2, \ldots, N^2 - 1). \quad (A.11)$$
APPENDIX B

Improvement

B.1 Axial-vector current improvement

Here we provide the derivation of the formula for the improved axial-vector current that we use in our computations. Following closely the discussion on classical improvement of the anisotropic action introduced in Ref. [77], we start with the naive fermion action that has manifestly no $O(a)$ discretization errors

$$\bar{\psi}_c(m_c + \nabla)\psi_c;$$

the bare quark mass $m_c$ here is the same as in the continuum. The $O(a)$-improved anisotropic quark action can be derived by applying the field redefinition $\bar{\psi}_c = \bar{\psi} \Omega$ ($\psi_c = \psi \Omega$), where

$$\Omega = 1 + \frac{\Omega_m}{2} a_t m_c + \frac{\Omega_t}{2} a_t \nabla_t + \frac{\Omega_s}{2} a_s \nabla_s,$$

$$\bar{\Omega} = 1 + \frac{\bar{\Omega}_m}{2} a_t m_c + \frac{\bar{\Omega}_t}{2} a_t \nabla_t + \frac{\bar{\Omega}_s}{2} a_s \nabla_s,$$

(B.1)
with $\Omega_{m.t.s}$ (and $\bar{\Omega}_{m.t.s}$) being mass-dependent pure numbers, and where the covariant lattice derivatives $\nabla_\mu$ are defined as

$$\nabla_\mu \psi(x) = \frac{1}{2a_\mu} [U_\mu(x)\psi(x + \mu) - U_{-\mu}(x)\psi(x - \mu)].$$

The application of this field redefinition to the anisotropic action is discussed in detail in Ref. [77]. Here we will focus on the improved quark-bilinear operators, given by

$$J^I = \bar{\psi}_c \Gamma \psi_c = \bar{\psi} \bar{\Omega} \Omega \psi,$$  \tag{B.2}

which, after substitution the formulae from Eqn. (B.1) and requiring $\Omega_m = \bar{\Omega}_m$, $\Omega_t = \bar{\Omega}_t$ and $\Omega_s = \bar{\Omega}_s$ (see [77]) turns into

$$J^I = (1 + m_c a_t \Omega_m) J^U + \frac{1}{2} \Omega t a_t [\bar{\psi} \Gamma \nabla_t \psi - \bar{\psi} \nabla_t \Gamma \psi] +$$

$$+ \frac{1}{2} \Omega s a_s [\bar{\psi} \Gamma \nabla_s \psi - \bar{\psi} \nabla_s \Gamma \psi],$$  \tag{B.3}

where $J^U \equiv \bar{\psi} \Gamma \psi$ is the unimproved operator.

For the case of the axial-vector current we have $\Gamma = \gamma_\mu \gamma_5$, and the improved axial-vector current current $A_\mu^I$ is given by

$$A_\mu^I = (1 + \Omega_m a_t m_c) A_\mu^U + \frac{\Omega t a_t}{2} (\bar{\psi} \Gamma \nabla_t \psi - \bar{\psi} \nabla_t \Gamma \psi) +$$

$$+ \frac{\Omega s a_s}{2} (\bar{\psi} \Gamma \nabla_s \psi - \bar{\psi} \nabla_s \Gamma \psi) =$$

$$= (1 + \Omega_m a_t m_c) A_\mu^U + \frac{\Omega t a_t}{2} (\bar{\psi} \gamma_\mu \gamma_5 \gamma_4 \nabla_4 \psi) -$$

$$- \bar{\psi} \gamma_4 \gamma_\mu \gamma_5 \nabla_4 \psi \psi + \frac{\Omega s a_s}{2} (\bar{\psi} \gamma_\mu \gamma_5 \gamma_j \nabla_j \psi -$$

$$- \bar{\psi} \gamma_j \gamma_\mu \gamma_5 \nabla_j \psi).$$  \tag{B.4}
Using the relationship between the Euclidean gamma matrices and the Dirac matrices,

$$\gamma_\mu \gamma_\nu = \delta_{\mu\nu} + \sigma_{\mu\nu},$$  \hspace{1cm} \text{(B.5)}

where

$$\sigma_{\mu\nu} = \frac{1}{2} [\gamma_\mu, \gamma_\nu],$$  \hspace{1cm} \text{(B.6)}

Eqn. (B.4) can be re-written as:

\[
A_\mu^I = (1 + \Omega_m a_t m_c) A_{\mu}^U - \\
- \frac{\Omega_t a_t}{2} (\bar{\psi}(\delta_{\mu4} + \sigma_{\mu4}) \gamma_5 \overleftrightarrow{D}_4 \psi + \bar{\psi}(\delta_{4\mu} + \sigma_{4\mu}) \gamma_5 \overleftrightarrow{D}_4 \psi) - \\
- \frac{\Omega_s a_s}{2} (\bar{\psi}(\delta_{\mu j} + \sigma_{\mu j}) \gamma_5 \overleftrightarrow{D}_j \psi + \bar{\psi}(\delta_{j\mu} + \sigma_{j\mu}) \gamma_5 \overleftrightarrow{D}_j \psi), \hspace{1cm} \text{(B.7)}
\]

or

\[
A_\mu^I = (1 + \Omega_m a_t m_c) A_{\mu}^U + \\
+ \frac{\Omega_t a_t}{2} (- \delta_{\mu4} \partial_4 \bar{\psi} \gamma_5 \psi - \sigma_{\mu4} \bar{\psi} \gamma_5 \overleftrightarrow{D}_4 \psi - \sigma_{4\mu} \bar{\psi} \gamma_5 \overleftrightarrow{D}_4 \psi) + \\
+ \frac{\Omega_s a_s}{2} (- \delta_{\mu j} \partial_j \bar{\psi} \gamma_5 \psi - \sigma_{\mu j} \bar{\psi} \gamma_5 \overleftrightarrow{D}_j \psi - \sigma_{j\mu} \bar{\psi} \gamma_5 \overleftrightarrow{D}_j \psi), \hspace{1cm} \text{(B.8)}
\]

To simplify this expression, we make use of the equations of motion which (to the lowest order) are written as:

\[
(m_0 + \nu_t \overleftrightarrow{\Phi}_t + \nu_s \overleftrightarrow{\Phi}_s) \psi = 0, \hspace{1cm} \text{(B.9)}
\]
\[
\bar{\psi}(m_0 - \nu_t \overleftrightarrow{\Phi}_t - \nu_s \overleftrightarrow{\Phi}_s) = 0. \hspace{1cm} \text{(B.10)}
\]
From the first equation:

\[ m_0 \gamma_\rho \psi + \nu_\ell \gamma_\rho \gamma_4 \vec{D}_4 \psi + \nu_s \gamma_\rho \gamma_j \vec{D}_j \psi = 0, \]  

(B.11)

and therefore

\[ \nu_s \sigma_{\rho j} \vec{D}_j \psi + \nu_\ell \sigma_{\rho 4} \vec{D}_4 \psi = -m_0 \gamma_\rho \psi - \nu_\ell \delta_{\rho 4} \vec{D}_4 \psi - \nu_s \delta_{\rho j} \vec{D}_j \psi. \]  

(B.12)

Similarly, from Eqn. (B.10) we get:

\[ m_0 \bar{\psi} \gamma_\rho - \nu_\ell \bar{\psi} \gamma_4 \gamma_\rho \vec{D}_4 - \nu_s \bar{\psi} \gamma_j \gamma_\rho \vec{D}_j = 0, \]  

(B.13)

and

\[ \nu_\ell \bar{\psi} \sigma_{\rho 4} \vec{D}_4 + \nu_s \bar{\psi} \sigma_{\rho j} \vec{D}_j = m_0 \bar{\psi} \gamma_\rho - \nu_\ell \bar{\psi} \delta_{\rho 4} \vec{D}_4 - \nu_s \bar{\psi} \delta_{\rho j} \vec{D}_j. \]  

(B.14)

Here we consider the temporal component of the axial-vector current (\( \mu = 4 \)), so Eqn. (B.8) becomes

\[ A_4' = (1 + \Omega_m a t m_c)A_4^U - \frac{\Omega_t a t}{2} \delta_{\rho 4} \partial_4 \bar{\psi} \gamma_5 \psi - \frac{\Omega_s a_s}{2} (\sigma_{4j} \bar{\psi} \gamma_5 \vec{D}_j \psi + \sigma_{j4} \bar{\psi} \gamma_5 \vec{D}_j \psi) \]  

(B.15)

and, after applying Eqns. (B.12) and (B.14), we obtain:

\[ A_4' = (1 + \Omega_m a t m_c)A_4^U + \frac{a_t}{2} (\Omega_s a_s \nu_t - \Omega_t) \partial_4 \bar{\psi} \gamma_5 \psi. \]  

(B.16)

We choose the case with \( \nu_\ell = 1 \) (so-called “\( \nu_s \)-tuning”), where \( \nu_s \) is tuned via the dispersion
relation between meson energy and momentum, yielding

$$\nu_s = \frac{1 + \frac{1}{2} a_t m_c}{1 + \frac{1}{2} a_s m_c}.$$  \hfill (B.17)

The parameters $\Omega_t$ and $\Omega_s$ are set as in Ref. [77]:

$$\Omega_s = -\frac{1}{2} \left(1 + \frac{1}{2} a_t m_c\right), \quad \Omega_t = -\frac{1}{2}. \quad \hfill (B.18)$$

The value for the anisotropy parameter in our calculations is $\xi = \frac{\alpha_s}{a_t} \approx 3.5$, so the final expression for the time component of the improved axial-vector current takes the form:

$$A_4^I = (1 + \Omega_m a_t m_c)A_4^U - 0.625 a_t \partial_4 \bar{\psi} \gamma_5 \psi, \quad \hfill (B.19)$$

or, up to leading order in $a$,

$$A_4^I = (1 + \Omega_m a_t m_c) \left[A_4^U - \frac{1}{4}(\xi - 1) a_t \partial_4 P\right].$$
C.1 Fourier transformations on the lattice

The Fourier transforms on the lattice, which are necessary for calculations of Feynman diagrams in momentum space, are given as follows:

- for fermion fields \( \psi(x) \):

\[
\psi(x) = \int_{-\pi/a}^{\pi/a} \frac{d^4p}{(2\pi)^4} e^{ipx} \tilde{\psi}(p),
\]

\( \tilde{\psi}(x) = \int_{-\pi/a}^{\pi/a} \frac{d^4p}{(2\pi)^4} e^{-ipx} \psi(p), \) (C.0)

- for gauge fields \( A_\mu^a(x) \), that are naturally associated with the middle point of the link \((x, x + \hat{\mu})\):

\[
A_\mu^a(x) = \int_{-\pi/a}^{\pi/a} \frac{d^4p}{(2\pi)^4} e^{ip(x + \frac{\hat{\mu}}{2})} \tilde{A}_\mu^a(p),
\]

\( \tilde{A}_\mu^a(p), \) (C.0)
such choice is made for the general economy of the calculations. The inverse Fourier transforms are given by

\[ \tilde{\psi}(p) = a^4 \sum_x e^{-ipx} \psi(x), \]

\[ \tilde{\bar{\psi}}(p) = a^4 \sum_x e^{ipx} \bar{\psi}(x), \]

\[ \tilde{A}_\mu^a(p) = a^4 \sum_x e^{-ip(x + a^\mu)} A^a_\mu(x). \]

Here

\[ \delta^4(p) = \frac{a^4}{(2\pi)^4} \sum_x e^{-ipx}, \]

(the momentum-space lattice \( \delta \)-function is zero except at the values \( p_n = 2\pi n \) of the momenta). The \( \delta \)-function in position space is

\[ \delta_{xy} = a^4 \int_{-\pi/a}^{\pi/a} \frac{d^4p}{(2\pi)^4} \sum_x e^{ip(x-y)}. \]

### C.2 Some standard definitions: derivatives and field strength

#### C.2.1 Continuum gauge fields

The gauge field \( A_\mu \) is defined as

\[ A_\mu(x) = -igA^a_\mu(x)T_a, \]

where \( g \) is the coupling constant. The gauge covariant derivative and the field strength are correspondingly

\[ D_\mu = \partial_\mu + A_\mu(x) \]
and
\[ F_{\mu\nu}(x) = [D_{\mu}, D_{\nu}] = \partial_{\mu} A_{\nu}(x) - \partial_{\nu} A_{\mu}(x) + [A_{\mu}(x), A_{\nu}(x)], \quad \text{(C.0)} \]
\[ F_{\mu\nu}(x) = -igF_{\mu\nu}^a(x)T_a. \quad \text{ (C.0)} \]

**C.2.2 Lattice derivatives and strength tensor**

The lattice forward and backward derivatives of the function \( f(x) \):
\[ \Delta^+_\mu f(x) = f(x + \hat{\mu}) - f(x), \quad \text{(C.1)} \]
\[ \Delta^-_\mu f(x) = f(x) - f(x - \hat{\mu}). \quad \text{(C.2)} \]

The Laplace and d’Alembert operators on the lattice are:
\[ \Delta f(x) = -\Box f(x) = \Delta^+_\mu \Delta^-_\mu f(x) = \Delta^-_\mu \Delta^+_\mu f(x) = \sum_{\mu=1}^{4} [f(x + \hat{\mu}) + f(x - \hat{\mu}) - 2f(x)]. \quad \text{(C.2)} \]

The covariant first- and second-order lattice derivatives \( \nabla_{\mu} \) and \( \Delta_{\mu} \) are defined through their operations on the quark field \( \psi(x) \).
\[ \nabla_{\mu} \psi(x) = \frac{1}{2a_{\mu}} \left[ U_{\mu}(x)\psi(x + \mu) - U_{-\mu}(x)\psi(x - \mu) \right] \]
\[ \Delta_{\mu} \psi(x) = \frac{1}{a_{\mu}^2} \left[ U_{\mu}(x)\psi(x + \mu) + U_{-\mu}(x)\psi(x - \mu) - 2\psi(x) \right]. \quad \text{(C.1)} \]

Here link variables are denoted by \( U_{\mu}(x) \), and we employ the notation \( U_{-\mu}(x) \equiv U_{\mu}(x - \mu)^\dagger \).
for the parallel transporter from $x$ to $x - \mu$. So we can rewrite:

$$\nabla_\mu \psi(x) = \frac{1}{2a_\mu} \left[ U_\mu(x)\psi(x + \mu) - U_\mu^\dagger(x - \mu)\psi(x - \mu) \right]$$

$$\Delta_\mu \psi(x) = \frac{1}{a_\mu^2} \left[ U_\mu(x)\psi(x + \mu) + U_\mu^\dagger(x - \mu)\psi(x - \mu) - 2\psi(x) \right] \quad (C.1)$$

The clover-leaf discretization of the field tensor $F_{\mu\nu}(x)$:

$$F_{\mu\nu}(x) = \frac{1}{8a^2}[Q_{\mu\nu}(x) - Q_{\mu\nu}^\dagger(x)]$$

$$Q_{\mu\nu}(x) = P_{\mu,\nu}(x) + P_{\nu,-\mu}(x) + P_{-\mu,-\nu}(x) + P_{-\nu,\mu}(x) \quad (C.1)$$

Here $P_{\alpha,\beta}(x)$ are plaquettes, so

$$Q_{\mu\nu}(x) = U_\mu(x)U_\nu(x + \mu)U_\mu^\dagger(x + \nu)U_\nu^\dagger(x) +$$

$$+ U_\nu(x)U_\mu^\dagger(x - \mu + \nu)U_\mu(x - \mu) +$$

$$+ U_\mu^\dagger(x - \mu)U_\nu^\dagger(x - \mu - \nu)U_\mu(x - \mu - \nu)U_\nu(x - \nu) +$$

$$+ U_\nu^\dagger(x - \nu)U_\mu(x - \nu)U_\nu(x + \mu - \nu)U_\mu^\dagger(x). \quad (C.-1)$$

### C.3 Anisotropic clover action

The anisotropic QCD action is the sum of the gauge action $S_G^\xi$ and the fermion action $S_F^\xi$

$$S^\xi = S_G^\xi + S_F^\xi, \quad (C.-1)$$
where $S^\xi_G$ is a so-called Symanzik-improved action with tree-level tadpole-improved coefficients:

\[
S^\xi_G[U] = \frac{\beta}{N_c \gamma_g} \left\{ \sum_{x,s \neq s'} \left[ \frac{5}{6u_s^4} \Omega_{P_{s'}}(x) - \frac{1}{12u_s^6} \Omega_{R_{s'}}(x) \right] + \sum_{x,s} \gamma_g^2 \left[ \frac{4}{12u_s^2u_t^2} \Omega_{P_{st}}(x) - \frac{1}{12u_s^4u_t^2} \Omega_{R_{st}}(x) \right] \right\},
\]

(C.0)

and $S^\xi_F$ is the anisotropic clover fermion action:

\[
S^\xi_F[U, \bar{q}, q] = a_t a_s^3 \sum_x \bar{q}(x) \left[ m_0 + \nu_t [\gamma_t \nabla_t - a_t^2 \Delta_t] + \nu_s \sum_s [\gamma_s \nabla_s - a_s^2 \Delta_s] - \frac{1}{2} \left[ C_{sw}^t a_s \sum_s \sigma_{ts} F_{ts} + C_{sw}^s a_s \sum_{s < s'} \sigma_{ss'} F_{ss'} \right] \right] q(x).
\]

(C.0)

Here $\Omega_W = ReTr(1 - W)$ and $W = P$, the plaquette, or $R_{\mu\nu}$, the $2 \times 1$ rectangular Wilson loop (length two in the $\mu$ direction and one in the $\nu$ direction) with $\{s, s'\} \in \{x, y, z\}$. The parameter $\gamma_g$ is the bare gauge anisotropy, $N_c = 3$ indicates number of colors, $\beta$ is related to the coupling $g^2$ through $\beta = 2N_c/g^2$, and $u_s$ and $u_t$ are the spatial and temporal tadpole factors. This action has leading discretization error at $O(a_s^4, a_t^2, g^2 a_s^2)$ and possesses a positive-definite transfer matrix, since there is no length-two rectangle in time.
C.4 Explicit form of the fermion action $S_F^\xi[U, \bar{q}, q]$

The fermion action

$$S_F^\xi = \sum_x \left\{ \bar{q}(x) a_t a_s^3 m_0 q(x) + a_t a_s^3 \nu t \bar{q}(x) [\gamma_t \nabla_t - \frac{a_t}{2} \Delta_t] q(x) + a_t a_s^3 \bar{q}(x) \sum_s [\gamma_s \nabla_s - \frac{a_s}{2} \Delta_s] - a_t a_s^3 \bar{q}(x) \frac{1}{2} C_{st}^a a_s \sum_s \sigma_{ts} F_{ts} q(x) - a_t a_s^3 \bar{q}(x) \frac{1}{2} C_{st}^a a_s \sum_{s < s'} \sigma_{ss'} F_{ss'} q(x) \right\}$$

(C.1)

can be written explicitly as the sum of the following five terms:

$$S_F^\xi = S_{F_1} + S_{F_2} + S_{F_3} + S_{F_4} + S_{F_5}.$$  (C.1)

Here the first term is

$$S_{F_1} = \bar{q}(x) a_t a_s^3 m_0 q(x);$$  (C.1)

the second term:

$$S_{F_2} = \bar{q}(x) a_t a_s^3 \nu t \gamma_t \nabla_t - \frac{a_t}{2} \Delta_t] q(x) =$$

$$= \bar{q}(x) a_t a_s^3 \nu t \gamma_t \frac{1}{2a_t} \left[ U_t(x) q(x + t) - U_t^t(x - a_t) q(x - t) \right] -$$

$$- \bar{q}(x) a_t a_s^3 \nu t \frac{1}{2} a_t^2 \left[ U_t(x) q(x + t) + U_t^t(x - a_t) q(x - t) - 2q(x) \right] =$$

$$= \bar{q}(x) a_t a_s^3 \nu t \gamma_t \left[ U_t(x) q(x + t) - U_t^t(x - a_t) q(x - t) \right] -$$

$$- \bar{q}(x) a_t a_s^3 \nu t \frac{1}{2} \left[ U_t(x) q(x + t) + U_t^t(x - a_t) q(x - t) - 2q(x) \right];$$  (C.4)
the third term:

\[ S_{F_{3}} = \bar{q}(x) \sum_{s} a_{t} a_{s}^{3} \nu_{s} \gamma_{s} \nabla_{s} - \frac{a_{s}}{2} \Delta_{s}] q(x) = \]

\[ = \bar{q}(x) \sum_{s} a_{t} a_{s}^{3} \nu_{s} \frac{1}{2a_{s}} \left[ U_{s}(x)q(x + s) - U_{s}^{\dagger}(x - a_{s}s)q(x - s) \right] - \]

\[ - \bar{q}(x) \sum_{s} a_{t} a_{s}^{3} \nu_{s} \frac{a_{s}}{2 a_{s}^{2}} \left[ U_{s}(x)q(x + s) + U_{s}^{\dagger}(x - a_{s}s)q(x - s) - 2q(x) \right] = \]

\[ = \bar{q}(x) \sum_{s} \frac{a_{t} a_{s}^{2}}{2} \nu_{s} \gamma_{s} \left[ U_{s}(x)q(x + s) - U_{s}^{\dagger}(x - a_{s}s)q(x - s) \right] - \]

\[ - \bar{q}(x) \sum_{s} \frac{a_{t} a_{s}^{2}}{2} \nu_{s} \left[ U_{s}(x)q(x + s) + U_{s}^{\dagger}(x - a_{s}s)q(x - s) - 2q(x) \right]; \quad \text{(C.-7)} \]

the fourth term:

\[ S_{F_{4}} = \bar{q}(x) a_{t} a_{s}^{3} \frac{1}{2} C_{sw} a_{s} \sum_{s} \sigma_{ts} F_{ts} q(x) = \]

\[ = \bar{q}(x) \frac{a_{t} a_{s}^{4}}{2} C_{sw} \sum_{s} \sigma_{ts} \frac{1}{8a_{t} a_{s}} \left[ Q_{ts}(x) - Q_{st}(x) \right] q(x) = \]

\[ = \bar{q}(x) \frac{a_{s}^{3}}{2} C_{sw} \sum_{s} \sigma_{ts} \frac{1}{8a_{t} a_{s}} \left[ U_{t}(x)U_{s}(x + a_{t}t)U_{t}^{\dagger}(x + a_{s}s)U_{s}^{\dagger}(x) + \right. \]

\[ + U_{s}(x)U_{t}^{\dagger}(x - a_{t}t + a_{s}s)U_{s}^{\dagger}(x - a_{t}t)U_{t}(x - a_{t}t) + \]

\[ + U_{t}^{\dagger}(x - a_{t}t)U_{s}^{\dagger}(x - a_{t}t - a_{s}s)U_{t}(x - a_{t}t - a_{s}s)U_{s}(x - a_{s}s) + \]

\[ + U_{s}^{\dagger}(x - a_{s}s)U_{t}(x - a_{s}s)U_{s}(x + a_{t}t - a_{s}s)U_{t}^{\dagger}(x) - \]

\[ - U_{s}(x)U_{t}(x + a_{s}s)U_{s}^{\dagger}(x + a_{t}t)U_{t}^{\dagger}(x) - \]

\[ - U_{t}(x)U_{s}^{\dagger}(x - a_{s}s + a_{t}t)U_{t}^{\dagger}(x - a_{s}s)U_{s}(x - a_{s}s) - \]

\[ - U_{s}^{\dagger}(x - a_{s}s)U_{t}^{\dagger}(x - a_{s}s - a_{t}t)U_{s}(x - a_{s}s - a_{t}t)U_{t}(x - a_{t}t) - \]

\[ - U_{t}^{\dagger}(x - a_{t}t)U_{s}(x - a_{t}t)U_{t}(x + a_{s}s - a_{t}t)U_{s}^{\dagger}(x) \right] q(x); \quad \text{(C.-15)} \]
and the fifth term is

\[ S_{F_5} = \bar{q}(x) a_0 a_s^2 \frac{1}{2} C_{sw}^s a_s \sum_{s < s'} \sigma_{s s'} F_{s s'} q(x) = \]

\[ = \bar{q}(x) a_0 a_s^2 \frac{1}{2} C_{sw}^s a_s \sum_{s < s'} \sigma_{s s'} \frac{1}{8a_s a_s'} \left[ Q_{s s'}(x) - Q_{s s'}(x) \right] q(x) = \]

\[ = \bar{q}(x) a_0 a_s^2 \frac{1}{2} C_{sw}^s a_s \sum_{s < s'} \sigma_{s s'} \frac{1}{8} \left[ U_s(x) U_{s'}(x + a_s s) U_{s'}^\dagger(x + a_s' s') U_{s'}^\dagger(x) + 
+ U_{s'}(x) U_{s'}^\dagger(x - a_s s + a_s' s') U_{s'}^\dagger(x - a_s s) U_{s}(x - a_s s) + 
+ U_{s}^\dagger(x - a_s s) U_{s'}^\dagger(x - a_s s - a_s' s') U_{s'}(x - a_s s - a_s' s') U_{s'}^\dagger(x - a_s' s') + 
+ U_{s'}^\dagger(x - a_s' s') U_{s}(x - a_s' s') U_{s'}(x + a_s s - a_s' s') U_{s}^\dagger(x) - 
- U_{s'}(x) U_{s}(x + a_s' s') U_{s'}^\dagger(x + a_s s) U_{s}^\dagger(x) - 
- U_{s}(x) U_{s'}^\dagger(x - a_s s' + a_s s) U_{s'}^\dagger(x - a_s' s') U_{s'}(x - a_s' s') - 
- U_{s'}^\dagger(x - \mu) U_{\nu}^\dagger(x - \mu - \nu) U_{\mu}(x - \mu - \nu) U_{\nu}(x - \nu) - 
- U_{s}^\dagger(x - a_s s) U_{s'}(x - a_s s) U_{s}(x + a_s' s' - a_s s) U_{s'}^\dagger(x) \right] q(x). \]  

(C.-23)

This is the explicit form of the total expression for fermion anisotropic lattice action.
(here $a_{s'} \equiv a_s$):

\[
S^x_{t'} = \sum_x \left\{ \bar{q}(x) a_t a^3 t m_0 q(x) + \bar{q}(x) q^3 2 \nu t \left[ U_t(x) q(x + t) - U^t_t(x - a_t t) q(x - t) \right] - q(x) a^3 2 \nu t \left[ U_t(x) q(x + t) + U^t_t(x - a_t t) q(x - t) - 2q(x) \right] + \bar{q}(x) \sum_s \frac{a_s a^2 s}{2} \nu s \left[ U_s(x) q(x + s) - U^s_t(x - a_s s) q(x - s) \right] - \bar{q}(x) \sum_s \frac{a_s a^2 s}{2} \nu s \left[ U_s(x) q(x + s) + U^s_t(x - a_s s) q(x - s) - 2q(x) \right] - \bar{q}(x) \sum_s \frac{a_s a^2 s}{2} C_{t'sw} \sum_s \sigma_{ss'} \frac{1}{8} \left[ U_t(x) U_s(x + a_t t) U^t_t(x + a_s s) U^s_t(x) + U_s(x) U^t_t(x - a_t t + a_s s) U^t_t(x - a_t t) + U^t_t(x - a_t t) U^t_s(x - a_s s) U_t(x - a_t t - a_s s) U_s(x - a_s s) + U^t_s(x - a_s s) U_t(x - a_s s) U_s(x + a_t t - a_s s) U^t_t(x) - U_s(x) U_t(x + a_s s) U^s_t(x + a_t t) U^t_t(x) - U_t(x) U^t_s(x - a_s s + a_t t) U^t_t(x - a_s s) U_s(x - a_s s) - U^t_t(x - a_s s) U^t_t(x - a_s s) U_t(x - a_t t - a_s s) U_s(x - a_t t) - U^t_t(x - a_t t) U_s(x - a_t t) U_t(x + a_s s - a_t t) U^t_t(x) \right] q(x) - \bar{q}(x) \sum_s \frac{a_s a^2 s}{2} C_{t'sw} \sum_s \sigma_{ss'} \frac{1}{8} \left[ U_s(x) U^s_t(x + a_s s) U^t_t(x + a_s s) U^t_s(x) + U^s_t(x - a_s s + a_s s') U^s_t(x - a_s s) U_s(x - a_s s) + U^t_s(x - a_s s) U^t_s(x - a_s s - a_s s') U^t_t(x - a_s s) U^s_t(x - a_s s') + U^t_s(x - a_s s) U^t_s(x - a_s s' - a_s s') U^t_t(x - a_s s) U^s_t(x - a_s s') - U^t_t(x) U_s(x + a_s s) U^t_s(x + a_s s) U^t_t(x) - U^t_t(x) U_s(x - a_s s') U^t_t(x) U^s_t(x - a_s s') U^t_t(x) - U^t_t(x - a_s s') U^t_t(x - a_s s') U^t_t(x - a_s s') U^t_t(x) - U^t_t(x) U^t_s(x + a_s s) U^t_s(x + a_s s) U^t_t(x) - U^t_t(x) U^t_s(x - a_s s') U^t_t(x - a_s s') U^t_t(x) - U^t_t(x - a_s s') U^t_t(x - a_s s') U^t_t(x - a_s s') U^t_t(x) \right] q(x) \right\}.
\]
C.4.1 Derivation of the Feynman rule for the quark-quark-gluon vertex

For the purpose of deriving the Feynman rule for the quark-quark-gluon vertex, it is convenient to represent the total fermion anisotropic action $S_F^\xi$ as a sum of two terms:

$$S_F^\xi = S_{q1} + S_{q2},$$  \hspace{1cm} (C.-41)

where

\begin{align*}
S_{q1} &= \sum_x \left\{ \bar{q}(x) a_t a_s^3 m_0 q(x) + \bar{q}(x) \frac{a_s^3}{2} \nu_t \gamma_t \left[ U_t(x)q(x + t) - U_t^\dagger(x - a_t t)q(x - t) \right] - \\
&\quad - \bar{q}(x) \frac{a_s^3}{2} \nu_t \left[ U_t(x)q(x + t) + U_t^\dagger(x - a_t t)q(x - t) - 2q(x) \right] + \\
&\quad + \bar{q}(x) \sum_s \frac{a_s a_t^2}{2} \nu_s \gamma_s \left[ U_s(x)q(x + s) - U_s^\dagger(x - a_s s)q(x - s) \right] - \\
&\quad - \bar{q}(x) \sum_s \frac{a_s a_t^2}{2} \nu_s \left[ U_s(x)q(x + s) + U_s^\dagger(x - a_s s)q(x - s) - 2q(x) \right] \right\}, \hspace{1cm} (C.-43)
\end{align*}
and

\[
S_{q2} = \sum_x \left\{ -\bar{q}(x) \frac{a_t^2}{2} C_{sw} \sum_s \sigma_{ts} \frac{1}{8} \left[ U_t(x) U_s(x + a_t s) U_t^\dagger(x + a_t s) U_s^\dagger(x) + U_s(x) U_t^\dagger(x - a_t t + a_s s) U_t^\dagger(x - a_t t) U_t(x - a_t t) + U_t^\dagger(x - a_t t) U_s^\dagger(x - a_t t - a_s s) U_s(x - a_t t - a_s s) + U_s^\dagger(x - a_s s) U_t(x - a_s s) U_s(x + a_t t - a_s s) U_t^\dagger(x) - U_s(x) U_t(x + a_s s) U_t^\dagger(x + a_t t) U_t^\dagger(x) - U_t(x) U_s(x - a_s s + a_t t) U_t^\dagger(x - a_s s) U_s(x - a_s s) - U_t^\dagger(x - a_s s) U_t^\dagger(x - a_s s - a_t t) U_s(x - a_s s - a_t t) U_t(x - a_t t) - U_t^\dagger(x - a_t t) U_s(x - a_t t) U_t(x + a_s s - a_t t) U_s^\dagger(x) \right] q(x) - \bar{q}(x) \frac{a_t a_s^2}{2} C_{sw} \sum_{s < s'} \sigma_{ss'} \frac{1}{8} \left[ U_s(x) U_{s'}(x + a_s s) U_t^\dagger(x + a_s' s') U_t^\dagger(x) + U_{s'}(x) U_s^\dagger(x - a_s s + a_s' s') U_t^\dagger(x - a_s s) U_s(x - a_s s) + U_s^\dagger(x - a_s s) U_{s'}^\dagger(x - a_s s' - a_s' s') U_s(x - a_s s - a_s' s') U_{s'}(x - a_s' s') + U_{s'}^\dagger(x - a_s' s') U_{s'}^\dagger(x - a_s' s') U_{s'}(x + a_s s - a_s' s') U_s^\dagger(x) - U_{s'}^\dagger(x) U_s(x + a_s' s') U_{s'}^\dagger(x + a_s s) U_s^\dagger(x) - U_s(x) U_{s'}^\dagger(x - a_s' s' + a_s s) U_{s'}^\dagger(x - a_s' s) U_{s'}(x - a_s' s') - U_{s'}^\dagger(x - a_s' s) U_{s'}^\dagger(x - a_s' s) U_s^\dagger(x + a_s' s' - a_s s) U_{s'}^\dagger(x) \right] q(x) \right\}. \tag{C.-57} \]
The relevant for $\bar{q}qq$ vertex terms from $S_{q1}$ are the following:

\[
S_{qq1} = \sum_x \left\{ \bar{q}(x) \frac{a_s^2}{2} \nu_\tau \gamma_{\tau i} q \gamma_4 a_i A_i(x) q(x + t) - \bar{q}(x) \frac{a_s^3}{2} \nu_\tau \gamma_{\tau}(-i) g a_t A_t(x - a_t t) q(x - t) - \right. \\
- \bar{q}(x) \frac{a_s^3}{2} \nu_\tau \gamma_{\tau} i g a_t A_t(x) q(x + t) - \bar{q}(x) \frac{a_s^3}{2} \nu_\tau \gamma_{\tau}(-i) g a_t A_t(x - a_t t) q(x - t) + \\
+ \bar{q}(x) \sum_s \frac{a_t a_s^2}{2} \nu_s \gamma_s i g a_s A_s(x) q(x + s) - \\
- \bar{q}(x) \sum_s \frac{a_t a_s^2}{2} \nu_s \gamma_s (-i) g a_s A_s(x - a_s s) q(x - s) - \\
- \bar{q}(x) \sum_s \frac{a_t a_s^2}{2} \nu_s i g a_s A_s(x) q(x + s) - \\
- \bar{q}(x) \sum_s \frac{a_t a_s^2}{2} \nu_s (-i) g a_s A_s(x - a_s s) q(x - s) \right\} = \\
= i g \frac{a_t a_s^3}{2} \sum_x \left\{ \bar{q}(x) \nu_\tau \gamma_{\tau} A_t(x) q(x + t) + \bar{q}(x) \nu_\tau \gamma_{\tau} A_t(x - a_t t) q(x - t) - \\
- \bar{q}(x) \nu_\tau A_t(x) q(x + t) + \bar{q}(x) \nu_\tau A_t(x - a_t t) q(x - t) + \\
+ \bar{q}(x) \sum_s \nu_s \gamma_s A_s(x) q(x + s) + \bar{q}(x) \sum_s \nu_s \gamma_s A_s(x - a_s s) q(x - s) - \\
- \bar{q}(x) \sum_s \nu_s A_s(x) q(x + s) + \bar{q}(x) \sum_s \nu_s A_s(x - a_s s) q(x - s) \right\}. \tag{C.65}
\]

After applying here the Fourier transforms for fermion and gauge fields, and taking into account

\[
\frac{1}{(2\pi)^4} \sum_x e^{i x (-p' + k + p)} = \frac{1}{a_t a_s^3} \delta^{(4)}(-p' + k + p), \tag{C.65}
\]
we obtain

\[ S_{qq_1} = ig \frac{a_t a_s^3}{2 a_t a_s^2} \sum_{x} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{d^4p'}{(2\pi)^4} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{d^4p}{(2\pi)^4} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{d^4k}{(2\pi)^4} \delta^{(4)}(-p' + k + p) \times \]

\[ \times \bar{q}(p') \left\{ \left[ e^{iat(x + pt)} + e^{-iat(x + pt)} \right] \nu_t \gamma_t A_t(k) - \right. \]
\[ \left. - \left[ e^{iat(x + pt)} - e^{-iat(x + pt)} \right] \nu_t A_t(k) + \right. \]
\[ + \sum_s \nu_s \gamma_s \left[ e^{ia_s(x + pt)} + e^{-ia_s(x + pt)} \right] A_s(k) - \]
\[ - \sum_s \nu_s \left[ e^{ia_s(x + pt)} - e^{-ia_s(x + pt)} \right] A_s(k) \right\} q(p) = \]

\[ = ig \sum_{x} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{d^4p'}{(2\pi)^4} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{d^4p}{(2\pi)^4} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{d^4k}{(2\pi)^4} \delta^{(4)}(-p' + k + p) \times \]

\[ \times \bar{q}(p') \left\{ \cos \left[ a_t \left( \frac{k_t}{2} + p_t \right) \right] \nu_t \gamma_t A_t(k) - i \sin \left[ a_t \left( \frac{k_t}{2} + p_t \right) \right] \nu_t A_t(k) + \right. \]
\[ + \sum_s \nu_s \gamma_s \cos \left[ a_s \left( \frac{k_s}{2} + p_s \right) \right] A_s(k) - \]
\[ - i \sum_s \nu_s \sin \left[ a_s \left( \frac{k_s}{2} + p_s \right) \right] A_s(k) \right\} q(p). \quad (C.-72) \]

In the expression for \( S_{q2} \), one has to deal with a sum of terms with product of four links, for example

\[ U_t(x)U_s(x + a_s t)U_t^\dagger(x + a_s x)U_s^\dagger(x), \quad (C.-72) \]

i.e. we have terms of general form \( e^A e^B e^C e^D \). Using the Baker-Campbell-Hausdorff (BCH) formula,

\[ e^A e^B = \exp \left\{ A + B + \frac{1}{2} (AB - BA) + \right. \]
\[ + \frac{1}{12} (A^2 B - 2ABA + BA^2 - 2BAB + B^2 A + AB^2) + \]
\[ + \frac{1}{24} (A^2 B^2 - B^2 A^2 + 2BABA - 2ABAB) + \cdots \right\}, \quad (C.-73) \]
the approximate expression for $e^A e^B e^C e^D$ can be derived. From (C.-73),

$$e^A e^B \approx \exp \left\{ A + B + \frac{1}{2} (AB - BA) \right\}.$$  \hspace{1cm} (C.-73)

Then

$$e^A e^B e^C = \exp \left\{ A + B + C + \frac{1}{2} (AB - BA) + \frac{1}{2} (AC + BC - CA - CB) + \cdots \right\} =$$

$$= \exp \left\{ A + B + C + \frac{1}{2} (AB - BA + AC - CA + BC - CB) + \cdots \right\}, \hspace{1cm} (C.-73)$$

and

$$e^A e^B e^C e^D = \exp \left\{ A + B + C + D + \frac{1}{2} (AB - BA + AC - CA + BC - CB) + \right.$$ \hspace{1cm} (C.-73)

$$\left. + \frac{1}{2} (AD + BD + CD - DA - DB - DC) + \cdots \right\}.$$  

So for the product of four non-commuting exponents we will use

$$e^A e^B e^C e^D \approx \exp \left\{ A + B + C + D \right\} \approx 1 + A + B + C + D, \hspace{1cm} (C.-73)$$

or $e^A e^B e^C e^D \approx A + B + C + D$ for the vertex of interest. Then the relevant terms in $S_{q2}$
are the following:

\[
S_{qqg} = -i g \sum_{x} \bar{q}(x) C_{sw} a^{3}_{s} \sum_{s} \sigma_{ts} \frac{1}{8} \left[ a_{s} A_{s}(x + at) - a_{t} A_{t}(x + as) - \\
- a_{t} A_{t}(x - at + as) - a_{s} A_{s}(x - at) - a_{s} A_{s}(x - at - as) + \\
+ a_{t} A_{t}(x - at - as) + a_{t} A_{t}(x - as) + a_{s} A_{s}(x + at - as) \right] - \\
- i g \sum_{x} \bar{q}(x) C_{sw} a^{2}_{t} \sum_{s < s'} \sigma_{ss'} \frac{1}{8} \left[ a_{s'} A_{s'}(x + a_{s}) - a_{s} A_{s}(x + a_{s'} s') - \\
- a_{s} A_{s}(x + a_{s'} s' - as) - a_{s} A_{s'}(x - as) - \\
- a_{s} A_{s'}(x - a_{s'} s' - as) + a_{s} A_{s}(x - a_{s'} s' - as) + \\
+ a_{s} A_{s}(x - a_{s'} s') + a_{s} A_{s'}(x - a_{s'} s' + as) \right]. \quad (C.78)
\]
After applying, once again, Fourier transforms, we obtain:

\[
S_{qq2} = \int \frac{d^4 p'}{(2\pi)^4} \int \frac{d^4 p}{(2\pi)^4} \int \frac{d^4 k}{(2\pi)^4} \delta^{(4)}(-p' + k + p) \tilde{q}(p') \times \\
\times \left\{ -C_{sw} \frac{a^2}{a_1 a_3} \sum_s \sigma_{ts} \cdot \frac{1}{8} \left[ a_s e^{i \left( \frac{a_s k_s}{2} + a_t k_t \right)} A_s(k) - a_s e^{i \left( \frac{a_s k_s}{2} - a_t k_t \right)} A_s(k) - a_t e^{i \left( \frac{a_t k_t}{2} + a_s k_s \right)} A_t(k) + a_t e^{i \left( \frac{a_t k_t}{2} - a_s k_s \right)} A_t(k) + a_s e^{i \left( \frac{a_s k_s}{2} + a_t k_t \right)} A_s(k) - a_s e^{i \left( \frac{a_s k_s}{2} - a_t k_t \right)} A_s(k) + \right] q(p) \right\} = \\
ge g \int \frac{d^4 p'}{(2\pi)^4} \int \frac{d^4 p}{(2\pi)^4} \int \frac{d^4 k}{(2\pi)^4} \delta^{(4)}(-p' + k + p) \tilde{q}(p') \times \\
\times \left\{ C_{sw} \frac{1}{a_t} \sum_s \sigma_{ts} \cdot \frac{1}{4} \left[ a_s \left( \sin \left( \frac{a_s k_s}{2} + a_t k_t \right) - \sin \left( \frac{a_s k_s}{2} - a_t k_t \right) \right) A_s(k) + a_t \left( -\sin \left( \frac{a_t k_t}{2} + a_s k_s \right) + \sin \left( \frac{a_t k_t}{2} - a_s k_s \right) \right) A_t(k) \right] + \\
+ C_{sw} \frac{1}{a_s} \sum_{s' < s} \sigma_{ss'} \cdot \frac{1}{4} \left[ a_s \left( \sin \left( \frac{a_s k_s}{2} + a_s k_s' \right) - \sin \left( \frac{a_s k_s}{2} - a_s k_s' \right) \right) A_s(k) + a_s \left( -\sin \left( \frac{a_s k_s}{2} + a_s k_s' \right) + \sin \left( \frac{a_s k_s}{2} - a_s k_s' \right) \right) A_s(k) \right] q(p) \right\} (C.-90)
\]

We can simplify this expression by making use of the formula

\[
\sin (\alpha \pm \beta) = \sin(\alpha) \sin(\beta) \pm \cos(\alpha) \cos(\beta),
\]

(C.-90)
then

\[
S_{qq2} = g \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{d^4p}{(2\pi)^4} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{d^4p}{(2\pi)^4} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{d^4k}{(2\pi)^4} \delta^{(4)}(-p' + k + p)q(p') \times
\]

\[
\times \left\{ C^{t}_{sw} \frac{1}{a_t} \sum_s \sigma_{ts} \frac{1}{2} \left[ a_s \cos \left( \frac{a_s k_s}{2} \right) \sin (a_t k_t) A_s(k) - a_t \sin (a_s k_s) \cos \left( \frac{a_t k_t}{2} \right) A_t(k) \right] +
\right.
\]

\[
+ C^{s}_{sw} \frac{1}{a_s} \sum_{s' < s'} \sigma_{ss'} \frac{1}{2} \left[ a_s \cos \left( \frac{a_{s'} k_{s'}}{2} \right) \sin (a_s k_s) A_{s'}(k) - a_s \sin (a_s k_s) \cos \left( \frac{a_{s'} k_{s'}}{2} \right) A_s(k) \right] \right\} q(p).
\]

(C.-93)

Therefore the total expression with the relevant to a quark-quark-gluon vertex terms is:

\[
S_{qq} = S_{qq1} + S_{qq2} =
\]

\[
\begin{align*}
&= g \sum_x \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{d^4p}{(2\pi)^4} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{d^4p}{(2\pi)^4} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{d^4k}{(2\pi)^4} \delta^{(4)}(-p' + k + p)q(p') \times \\
&\times \left\{ i \cos \left[ a_t \left( \frac{k_t}{2} + p_t \right) \right] \nu_t \gamma_t A_t(k) + \sin \left[ a_t \left( \frac{k_t}{2} + p_t \right) \right] \nu_t A_t(k) +
\right.
\end{align*}
\]

\[
+ \sum_s \nu_s \gamma_s i \cos \left[ a_s \left( \frac{k_s}{2} + p_s \right) \right] A_s(k) + \sum_s \nu_s \sin \left[ a_s \left( \frac{k_s}{2} + p_s \right) \right] A_s(k) +
\]

\[
+ C^{t}_{sw} \frac{1}{a_t} \sum_s \sigma_{ts} \frac{1}{2} \left[ a_s \cos \left( \frac{a_s k_s}{2} \right) \sin (a_t k_t) A_s(k) - a_t \sin (a_s k_s) \cos \left( \frac{a_t k_t}{2} \right) A_t(k) \right] +
\]

\[
- a_t \sin (a_s k_s) \cos \left( \frac{a_t k_t}{2} \right) A_t(k) +
\]

\[
+ C^{s}_{sw} \frac{1}{a_s} \sum_{s' < s'} \sigma_{ss'} \frac{1}{2} \left[ a_s \cos \left( \frac{a_{s'} k_{s'}}{2} \right) \sin (a_s k_s) A_{s'}(k) - a_s \sin (a_s k_s) \cos \left( \frac{a_{s'} k_{s'}}{2} \right) A_s(k) \right] -
\]

\[
- a_s \sin (a_s k_s) \cos \left( \frac{a_{s'} k_{s'}}{2} \right) A_s(k) \right\} q(p),
\]

(C.-99)
and the corresponding Feynman rule for the this vertex is

\[
V_{qqg} = g \left\{ i \nu_t \gamma_t \cos \left[ a_t \left( \frac{k_t}{2} + p_t \right) \right] + \nu_t \sin \left[ a_t \left( \frac{k_t}{2} + p_t \right) \right] + 
\right.
\]

\[
+ i \nu_s \sum_s \gamma_s \cos \left[ a_s \left( \frac{k_s}{2} + p_s \right) \right] + \nu_s \sum_s \sin \left[ a_s \left( \frac{k_s}{2} + p_s \right) \right] + 
\]

\[
+ \frac{C^t_{sw}}{a_t} \sum_s \sigma_{ts} \frac{1}{2} \left[ a_s \cos \left( \frac{a_s k_s}{2} \right) \sin \left( a_t k_t \right) - a_t \sin \left( a_s k_s \right) \cos \left( \frac{a_t k_t}{2} \right) \right] + 
\]

\[
+ \frac{C^s_{sw}}{a_s} \sum_{s < s'} \sigma_{ss'} \frac{1}{2} \left[ a_{s'} \cos \left( \frac{a_{s'} k_{s'}}{2} \right) \sin \left( a_s k_s \right) - 
\right.
\]

\[
- a_s \sin \left( a_{s'} k_{s'} \right) \cos \left( \frac{a_s k_s}{2} \right) \right\} \right. 
\]

(C.-102)

In our notation \( p' = p + k \), i.e. \( k = p' - p \). Then the previous expression can be rewritten in the following form:

\[
V_{qqg} = g \left\{ i \nu_t \gamma_t \cos \left[ a_t \left( \frac{(p + p')_t}{2} \right) \right] + \nu_t \sin \left[ a_t \left( \frac{(p + p')_t}{2} \right) \right] + 
\right.
\]

\[
+ i \nu_s \sum_s \gamma_s \cos \left[ a_s \left( \frac{(p + p')_s}{2} \right) \right] + \nu_s \sum_s \sin \left[ a_s \left( \frac{(p + p')_s}{2} \right) \right] + 
\]

\[
+ \frac{C^t_{sw}}{a_t} \sum_s \sigma_{ts} \frac{1}{2} \left[ a_s \sin \left[ a_t (p' - p)_t \right] \cos \left[ a_t \left( \frac{p' - p}{2} \right) \right] \right] - 
\]

\[
- a_t \sin \left[ a_s (p' - p)_s \right] \cos \left[ a_t \left( \frac{p' - p}{2} \right) \right] \right) + 
\]

\[
+ \frac{C^s_{sw}}{a_s} \sum_{s < s'} \sigma_{ss'} \frac{1}{2} \left[ a_{s'} \sin \left[ a_s (p' - p)_s \right] \cos \left[ a_{s'} \left( \frac{p' - p}{2} \right) \right] \right] - 
\]

\[
- a_s \sin \left[ a_{s'} (p' - p)_{s'} \right] \cos \left[ a_s \left( \frac{p' - p}{2} \right) \right] \right\}. \quad (C.-106)\]
BIBLIOGRAPHY


VITA

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Ekaterina Valentinovna Mastropas was born in Rostov-on-Don, Russia, in 1981. She grew up and attended the public schools in the same city, and after graduation from high school she began undergraduate studies at the Physics Department of Rostov State University (RSU). She remained at RSU from 1997 to 2003, acquiring Bachelor of Science (B.S.) and Master of Science (M.S.) degrees in theoretical and computational physics. During the next five years, she worked in various private companies while teaching part-time undergraduate courses at Rostov State Pedagogical University.

In August 2008, Ekaterina moved to Williamsburg, VA, to begin her graduate study at the College of William and Mary. She received her M.S. degree in physics in January of 2010, and soon after that she started working under the advisory of Prof. David Richards within Nuclear and Hadronic Theory group at William and Mary and Lattice QCD group at Jefferson Lab. Her Ph.D. thesis is devoted to the exploration of the decay constant of the pion and its excitations using methods of lattice quantum chromodynamics.