Hadronic Matrix Elements for Weak Transitions Beyond the Standard Model

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Dedicated to

My wife, Esther, who with her support and understanding made this thesis possible.
Abstract

In this work we calculate the matrix elements of the electromagnetic and chromomagnetic operators between a kaon and a pion state. The calculation is performed on the lattice using the Wilson maximally twisted mass fermion action and the Symanzik tree-level improved gluon action. The calculation is unquenched with two dynamic quarks, with pion masses down to 270 MeV. The fermion propagators are calculated by a stochastic all-to-all method which improves accuracy, and with twisted boundary conditions which allow arbitrarily small momentum probing.

This is the first unquenched calculation of the $K^-\pi$ matrix element of the electromagnetic operator. We use a non-perturbative RI-MOM renormalization obtained in a previous work. We compare our results to a previous (quenched) $K^-\pi$ matrix element, and to a recent $\pi-\pi$ calculation. The results show a good agreement, and higher accuracy in this work. Our final continuum-extrapolated result differs significantly from the previous one, mainly because of more realistic pion mass range and unquenched simulation.

The $K^-\pi$ matrix element of the chromomagnetic operator has never been calculated before on the lattice. Its renormalization entails subtraction of operators mixing with power divergences. We present the analysis of the mixing operators, a non-perturbative method for the subtraction; we also present a perturbative method for the multiplicative renormalization, as required by the presence of logarithmic divergences, along with the initial 1-loop results of the quark-quark-gluon amplitude for the perturbative renormalization.
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Chapter 1

Introduction: weak decays in the Standard Model and beyond

The standard model (SM) of elementary particles has been highly successful in describing observed phenomena. It encloses all known matter and interactions, apart from gravity, into one elegant theory. However, there are indications that the SM is incomplete [1]. We list here some of these indications (this is not an exhaustive list):

- The large hierarchy problem – quantum corrections to the Higgs mass diverge as the UV cutoff scale: $\Delta m_H^2 \propto \Lambda_{UV}^2$, a situation which requires extreme fine tuning.

- Dark matter has gravitational effects which are observed in astrophysics, and other effects possibly observed through collisions frequency variation in the DAMA experiment. However, dark matter is not included in the SM.

- Charge and Parity symmetry (CP) violation in the SM is too small to account for baryogenesis, i.e. the matter-antimatter asymmetry in the universe.

- The small hierarchy problem – the wide separation of quark masses over many orders of magnitude is unnatural in the SM.

These considerations make us suspect the existence of a more general theory, of which the standard model is but a low-energy effective theory.

Electroweak processes have proven to be a unique window through which we can probe the SM and the subtle effects of new physics, whether by detecting rare processes, violation of symmetries previously thought to be exact, or by precision measurements which tightly bind theory and experiment. The weak interactions and Higgs mechanism were not immediately understood when discovered. In fact, the Higgs boson itself has not been detected yet, and neutrino mixing (and mass) was only recently discovered, and has not yet been incorporated into the model. Weak decays can be calculated and measured with extreme precision, when leptons are the interacting particles. However, hadronic matrix elements still suffer from large theoretical uncertainties, and the unitarity matrix is not known to a high precision.
Effective electroweak action and weak decays

Electroweak hadronic processes can be studied most effectively in the framework of the Wilson operator product expansion of the weak Hamiltonian, \( \mathcal{H}_{\text{weak}} \), where the long-distance contributions of the effective operators \( Q_i^{\text{eff}} \) are separated from the short-distance Wilson coefficients, \( C_i \),

\[
\mathcal{H}_{\text{weak}} = \sum_i C_i(\mu) Q_i^{\text{eff}}(\mu),
\]

(1.1)

where \( \mu \) is the renormalization scale. Both the high-energy \( C_i \) coefficients and the low-energy \( Q_i^{\text{eff}} \) operators have to be transformed according to the renormalization scale. We treat these two effects separately: due to the large scale differences, the high-energy interactions (including new-physics contributions) are taken into account through the Wilson coefficients and integrated out, while the large distance hadronic evolution is treated on the lattice. We introduce the electromagnetic (EM) and chromomagnetic (CM) effective operators.

\[
\begin{align*}
Q_{\text{EM}}^+ &= \bar{s}F_{\mu\nu}\sigma^{\mu\nu}d, \\
Q_{\text{CM}}^+ &= \bar{s}G_{\mu\nu}\sigma^{\mu\nu}d,
\end{align*}
\]

(1.2)

where \( F_{\mu\nu} \) and \( G_{\mu\nu} \) are the EM and CM field tensors, respectively, and \( \sigma^{\mu\nu} \) is defined as \( \frac{i}{2}[\gamma^\mu\gamma^\nu - \gamma^\nu\gamma^\mu] \), where \( \gamma_\mu \) are the gamma matrices acting in the fermion spinor space.

These two operators can induce flavor-changing \( K \to \pi \pi \) hadronic decay and \( K \to \pi \ell \ell \) semileptonic decay (in the case of the electromagnetic operator). These two decays offer a wealth of insight into the weak sector of the SM and beyond, in particular on CP violation and baryogenesis which are fundamental questions still open today. These decays are calculable non perturbatively in lattice QCD through the \( K \to \pi \) matrix element. The \( K \to \pi \pi \) matrix element is not directly calculable in Monte-Carlo simulations due to the Maiani-Testa no-go theorem \([3]\) for Euclidean space.

In this work we are concerned with the “long distance” part of the weak interaction – the matrix element of the electromagnetic and chromomagnetic operators – between a kaon and pion states, on the lattice. We also treat the renormalization of the chromomagnetic operator, which requires taking into account its mixing with other operators.

The “short distance” part contained in the coefficients \( C_i \) comprises the exclusive \( s \to d + X_i \) interaction. In the SM, these flavor changing neutral currents (FCNC’s) are mediated through the \( W^+ \) gauge boson at the order of 1-loop and higher in perturbation theory. The short-distance coefficient can be calculated in continuum perturbation theory, and is suppressed by the Glashow-Iliopoulos-Maiani (GIM) mechanism \([4]\). Beyond the SM other processes contribute, as will be discussed below. In the present work we do not concern ourselves with this calculation, which has been carried out in detail elsewhere, see for example \([5, 6]\).

\(^1\)Peskin & Schroeder [2], Ch. 18.3
Weak rare decays are particularly favorable testing tools for the standard model. They are rare because in the SM they are subject to a suppression mechanism. The suppression may be due to highly effective cancellations, such as the GIM mechanism, which suppresses flavor-changing neutral currents, or it may be due to the conservation of a fundamental or approximate symmetry, such as lepton number or CP symmetry. New physics models may greatly enhance such processes. In such models rare decays are potentially large, and therefore provide a direct constraint on the parameters of any new theory. Precision measurements of frequent weak decays may serve the same purpose, by constraining the bounds on the SM and on new physics models.

The calculations of these decays suffer from major hadronic uncertainties, since experimentally they can only be measured between hadronic states, while the theory basically has quark fields as its elementary degrees of freedom. Lattice QCD enables us to make contact between theory and experiment by calculating the hadronic matrix elements of the various weak operators.

To give a taste of rare decays and their significance, we show values of the branching-ratios of semileptonic rare decays, and compare theory and experiment. Current experimental upper bounds are \[\text{[7]}:\]

\[
\begin{align*}
BR(K_L \rightarrow \pi^0 e^+ e^-)_{\text{exp}} &< 2.8 \cdot 10^{-10}, \\
BR(K_L \rightarrow \pi^0 \mu^+ \mu^-)_{\text{exp}} &< 3.8 \cdot 10^{-10}, \\
BR(K_L \rightarrow \pi^0 \nu \bar{\nu})_{\text{exp}} &< 6.7 \cdot 10^{-8}.
\end{align*}
\]

while the SM estimates are \[\text{[8]}:\]

\[
\begin{align*}
BR(K_L \rightarrow \pi^0 e^+ e^-)_{\text{SM}} &\sim 3 \cdot 10^{-11}, \\
BR(K_L \rightarrow \pi^0 \mu^+ \mu^-)_{\text{SM}} &\sim 1 \cdot 10^{-11}, \\
BR(K_L \rightarrow \pi^0 \nu \bar{\nu})_{\text{SM}} &= 2.49 \pm 0.39 \times 10^{-11}.
\end{align*}
\]

\subsection*{Supersymmetry}

One of the most successful theories beyond the standard model is supersymmetry (SUSY). Supersymmetry defines new operators which transform fermions to bosons and vice-versa.\footnote{For a comprehensive taste of supersymmetry from the phenomenological point of view, see Martin’s 1997 review \[\text{[1]}\].} These operators and their algebra introduce a host of new fields and interactions into the model: every SM field gets a super-partner, besides other fields being produced, and also weak processes are generalized and no longer constrained by one phase, as is the case in the Cabibbo Kobayashi Maskawa (CKM) matrix of the standard model. In fact SUSY introduces too many processes to naturally derive measured interactions, so that restrictions are necessary. The two important ones are 1) R-parity, which creates super-partners only by pairs, thereby conserving lepton and baryon numbers which are otherwise broken; and 2) the “universality”, “alignment” or “irrelevancy” solutions which semi-diagonalize the quark mixing
matrix with the mass matrix, cutting down on the arbitrarily large flavour mixing and CP violation of supersymmetry. Supersymmetry has potentially large CP violating processes, which are not experimentally ruled out. In particular, $\bar{s} \to d\gamma$ and $\bar{s} \to dg$ can be enhanced with respect to the SM value, through the electromagnetic and chromomagnetic effective operators. Perturbatively, this happens through gauginos in loop processes, in penguin and box diagrams. These interactions are suppressed in SUSY by the loop factor $(\alpha_{EW}^2)$ and SUSY particles mass, but enhanced by arbitrary interaction angles unless one imposes also a kind of “super GIM” mechanism.

**Previous results**

The $K \to \pi$ chromomagnetic matrix element has not been previously calculated on the lattice. It has, however, been previously calculated in heavy quark effective theory for heavy→light mesons [9], which is not applicable to kaon decays. In addition the renormalizations previously performed for the chromomagnetic operator either have not taken into account operator mixing, or did not consider power divergences, and they were not performed in methods suitable for the lattice. Thus the full renormalization of the chromomagnetic operator on the lattice is a novel and complex problem.

Previous work on the electromagnetic operator includes the $K \to \pi$ electromagnetic matrix-element, which was computed in 2001 by Becirevic et al. [10]. The results were obtained using a quenched Monte-Carlo, with relatively high sea-quark masses and on one lattice spacing. We aimed to make use of the improved twisted-mass action, new algorithms and enhanced computing power to improve the statistical accuracy and range of parameters. Another work by Brömmel et al. (2008) [11] dealt with the $\pi - \pi$ electromagnetic matrix element. We show that our results compare well with previous estimates.

**Present work**

We calculated in a Monte-Carlo simulation on the lattice the $K \to \pi$ matrix elements of the chromomagnetic and electromagnetic operators. The matrix elements are parameterized using chiral perturbation theory to lowest order.

The electromagnetic operator includes a photon field $F_{\mu\nu}$, which is external to the lattice, so that the remaining part on the lattice has a tensor form, whose $K \to \pi$ matrix element reads

$$\langle \pi^0 | \bar{s} \sigma_{\mu\nu} d | K^0 \rangle = i \left( p_{K\pi}^\mu p_{K\pi}^\nu - p_{K\pi}^\nu p_{K\pi}^\mu \right) \frac{2f_T}{m_K + m_\pi}.$$  \hspace{1cm} (1.5)

The tensor form-factor has a momentum dependence well-approximated by a pole form,

$$f_T(q^2) = \frac{f_T(0)}{1 - q^2\lambda},$$  \hspace{1cm} (1.6)

where the two coefficients $f_T(0)$ and $\lambda$ are the results which we report.
The chromomagnetic operator on the lattice includes the gluon field $G_{\mu\nu}$, and its $K \to \pi$ matrix element in lowest-order chiral perturbation theory is

$$
\langle \pi^0 | sG_{\mu\nu}\sigma^{\mu\nu}d | K^0 \rangle = -\frac{11B_m}{32\sqrt{2}\pi^2} \frac{m_K^2}{m_s + m_d} p_\pi \cdot p_K ,
$$

where $B_m$ is the coefficient which includes all the lattice information which we need to calculate.

Our principal result is:

$$f_T(0) = 0.443 \pm 0.037^{\text{stat}} \pm 0.050^{\text{syst}}, \quad \lambda = 1.57 \pm 0.18^{\text{stat}} \pm 0.18^{\text{syst}} [\text{GeV}^{-2}] .
$$

Unfortunately we do not have yet enough lattice Monte-Carlo data to present results for the chromomagnetic operator.

We also discuss the renormalization of the CM operator and the operators which mix in the renormalization, and display the renormalization constants obtained through perturbative and non-perturbative calculations\(^3\). We present preliminary results from the perturbative calculation\(^4\).

**This thesis is organized as follows:** In the second chapter we introduce lattice QCD and its main relevant aspects: we show how the naïve discretization of the Hamiltonian brings about the doubling of fermion energy eigenvalues, and how the Wilson term evades it. We describe the Symanzik and twisted-mass (TM) improved actions, and how they enable the calculation of values which are free of errors of the first order in the lattice spacing.

In the third chapter we describe the main lattice techniques used in our calculations: how we extract matrix elements and form factors from correlation functions, the twisted boundary conditions used to access very small momenta, the stochastic fermion-propagator calculation which improves accuracy and efficiency, the jackknife statistical error estimation and also our non-standard systematic error estimate. We present the RI-MOM method, which is used for nonperturbative (and also perturbative) renormalization, and its application in previous work to the electromagnetic operator. We present chiral perturbation theory and lowest order expansions which give us a relation between meson mass and constituent quarks mass, and also a parameterization of the chromomagnetic and electromagnetic operators.

In the fourth chapter we present our results for the electromagnetic matrix element. We display our procedure, plateau fit, momentum dependence fit, extrapolations to physical strange and light quark masses, and extrapolation to the continuum. We show how we minimized the total error, systematic and statistical, and we also compare our results to previous results for the $K \to \pi$ transitions and for $\pi - \pi$ interactions.

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\(^4\)For the perturbative chromomagnetic operator renormalization I thank Haralambos Panagopoulos and Apostolos Skouroupathis from the University of Cyprus.
The fifth chapter describes the renormalization of the chromomagnetic operator, which is a novel and complex problem. We describe lattice perturbation theory and how we can use it to calculate the renormalization coefficients for the chromomagnetic operator. We explain in detail how the renormalization was performed, the 1-loop diagrams we calculated and the calculation methods. Feynman rules are given in the appendix. We further analyze the method that we use to renormalize non-perturbatively the chromomagnetic operator. We show how the actual renormalization can be performed by taking into account operator mixing through proper analysis of the symmetries and chiral structure, of the maximally twisted mass lattice action and matrix elements. We present the analysis result for the operator mixing and preliminary perturbative results.
Chapter 2

Lattice QCD

Lattice theory is a way of regularizing quantum field theory. The regularization is achieved both in the low-energy (InfraRed, IR) regime using a finite lattice size $L$, and in the high-energy (UltraViolet, UV) by using a finite lattice spacing $a$ (see Fig. 2.1). The lattice regularization does not depend on a particular approximation method, and is therefore suitable for non-perturbative methods as well as perturbative ones, in contrast with, for example, the dimensional regularization scheme which is defined for the perturbative expansion in the Feynman diagram formalism. The lattice is used in practice for both perturbative and non-perturbative calculations. The discretization automatically breaks Lorentz invariance, keeping the internal symmetry intact (for example, the QCD SU(3) local gauge symmetry).

Non-perturbative calculations are essential for studying several aspects of QCD. One such fundamental property is infrared slavery, which is an increase of the coupling constant at low energies, and its counterpart asymptotic freedom, which is the vanishing coupling at high energies. The consequence of IR slavery is confinement, which means that quarks in experiments are never observed alone, rather they come in color-singlet combinations, which are called hadrons. Due to the large coupling constant perturbative methods fail, because the amplitude cannot be expanded in the coupling constant, and higher order terms are larger than previous terms. As a consequence, analysis of hadronic processes requires non-perturbative methods.

Figure 2.1. An example of a lattice in 2+1 dimensions (our lattices are d=3+1). the lattice step $a$ and lattice sizes $L$ and $T$ are shown.
Since single quarks are not experimentally observed but only hadrons are, in order to calculate real-world processes one must use hadronic asymptotic states, and not quarks. Parton processes (asymptotic quarks and gluons) are suitable for hard (high energy) scattering processes, where perturbation theory holds.

In lattice Monte-Carlo simulations, correlation functions are explicitly calculated using field configurations chosen with the probability density which is dictated by the exponential of the action. Usually one carries out explicitly the functional integral over the fermion degrees of freedom, thus arriving at an effective action for gauge bosons which is used to generate gauge configurations; these simulated configurations are then used to calculate hadronic propagators and correlation functions. The importance sampling technique used to select the gauge configurations in the Monte-Carlo simulation imposes the use of Euclidean time, \( \tau \equiv x^4 \), such that \( x^0 \equiv t = -i \tau \). Euclidean quantities are denoted by a subscript \( E \). The Euclidean action is related to the Minkowski action by \( S = iS_E \).

Lattice QCD is a way to solve exactly the theory from first principles, without any assumptions, to the desired precision. However, in practice the calculation power is limited, which requires us to use smartly the available resources. We need to choose an action which gives the maximum physical content and minimum errors with the available computational power. The computing time scales roughly according to [12]

\[
\text{cost} \propto \left( \frac{L}{a} \right)^4 \left( \frac{1}{a} \right) \left( \frac{1}{m^2_m a} \right).
\]  

(2.1)

The limited computer resources force us to use physical constants which are different from their true physical values. The lattice discretization obviously forces a finite lattice spacing and size which do not exist in the continuum, but the limited resources force us to use smaller physical lattices and larger lattice spacing than wanted in order to minimize errors. In addition we introduce unphysical quark masses and most notoriously flavour quenching. In order to compensate for the errors we improve the lattice action in various ways, to minimize mainly finite spacing \((a)\) errors.

Quarks on the lattice cannot be described today with sufficient accuracy. This is partly for fundamental reasons, such as flavour doubling or chiral symmetry breaking, and partly because of computer limitations. Simulations typically include at least 2 dynamical (unquenched) quarks. Less dynamical flavours are slightly more computationally advantageous, since the quark determinant is smaller, and also because more massive quarks require a smaller lattice spacing to simulate accurately. Heavy flavours are less important for most lattice simulations, since at at lower energy scales they contribute less, while at high energy scales processes can also be calculated accurately using perturbation theory. Our simulations include two dynamical flavors. More dynamical flavors would not be computationally expensive but would cause theoretical difficulties, because of our twisted-mass fermion action. Light quark \((u\) and \(d)\) masses are steadily going down in recent years. Simulating the light quarks at their physical mass is still problematic. The main reason is that the fermion matrix becomes singular, thus iterative methods to invert it converge
much more slowly. Another reason is that finite size effects become larger at small quark masses, because the pions are “larger”, i.e. $m_\pi L$ is smaller.

### 2.1 Gauge and fermion fields on the lattice

In the following introduction we follow the outline in [13].

We start by defining the lattice derivative operators: forward derivative

$$\Delta^f_\mu f(x) = \frac{1}{a}(f(x + a\hat{\mu}) - f(x)) , \quad (2.2)$$

backwards derivative

$$\Delta^b_\mu f(x) = \frac{1}{a}(f(x) - f(x - a\hat{\mu})) , \quad (2.3)$$

and the d’Alembert operator

$$\Box f(x) \equiv -\Delta^b_\mu \Delta^f_\mu f(x) = \sum_\mu \frac{1}{a^2}(2f(x) - f(x + a\hat{\mu}) - f(x - a\hat{\mu})) . \quad (2.4)$$

The parallel transporter defines the gauge field. The link variable is the parallel transporter of any vector between two adjacent lattice points:

$$U_{x\mu} \equiv U(x, x + a\hat{\mu}) : V_{x+a\hat{\mu}} \rightarrow V_x , \quad (2.5)$$

is hermitian and unitary,

$$U(y, x) = U^{-1}(x, y) = U^+(x, y) , \quad (2.6)$$

and transforms under a gauge transformation as

$$U_{x\mu} \rightarrow \Lambda^{-1}(x)U_{x\mu}\Lambda(x + a\hat{\mu}) . \quad (2.7)$$

The gauge field $A_\mu$ is defined as

$$U_{x\mu} \equiv e^{-iagA^a_\mu(x)T^a} = 1 - iagA^a_\mu(x)T^a - \frac{(ag)^2}{2}[A^a_\mu(x)T^a]^2 + ... . \quad (2.8)$$

This definition has a form such that the lattice gauge action, expanded in the field $A_\mu$ in the continuum limit, will have the standard form of $F^{\mu\nu}F_{\mu\nu}$, as we also show below. We further introduce the covariant forward and backward derivatives:

$$D^f_\mu f(x) = \frac{1}{a}[U_{x\mu}f(x + a\hat{\mu}) - f(x)] ,$$

$$D^b_\mu f(x) = \frac{1}{a}\left[f(x) - U_{x-a\hat{\mu},\mu}^+f(x - a\hat{\mu})\right] . \quad (2.9)$$

A gauge-invariant combination of links is composed of a closed loop of links (“Wilson loop”); the smallest closed loop on the lattice is the plaquette, which is a simple square in the $\hat{\mu}$ and $\hat{\nu}$ directions:

$$U_p = U(x, x + a\hat{\nu})U(x + a\hat{\mu}, x + a\hat{\mu} + a\hat{\nu})U(x + a\hat{\mu} + a\hat{\nu}, x + a\hat{\mu})U(x + a\hat{\mu}, x) . \quad (2.10)$$
The plaquette action, proposed by Wilson, is the sum on all the plaquettes:

\[ S \supset \sum_p \beta \left( 1 - \frac{1}{N} \text{Re Tr } U_p \right). \]  

(2.11)

We can write this in a form similar to the continuum action: if we define

\[ F_{\mu\nu}(x) = \Delta^t_{\mu} A_{\nu}(x) - \Delta^t_{\nu} A_{\mu}(x) + [A_{\mu}(x), A_{\nu}(x)], \]  

(2.12)

then by expanding the plaquette sum in \( aA \) we get

\[ S = -\frac{\beta}{4N} \sum_x a^4 \text{Tr } F_{\mu\nu}(x) F^{\mu\nu}(x) + \mathcal{O}(a^5). \]  

(2.13)

The coupling constant \( \beta \) can be related to the continuum coupling \( g \), by imposing the equality in the continuum limit of this action to the continuum Yang-Mills action. This equality yields

\[ \beta = \frac{2N}{g^2}. \]  

(2.14)

For fermions we start from the usual free-theory Dirac operator (symmetrized) in three dimensional momentum space,

\[ H = \int d^3x \bar{\psi}(\vec{x}) \left\{ m \gamma_4 + \frac{i}{2} (\vec{\partial}_k - \vec{\partial}_k) \alpha_k \right\} \psi(\vec{x}) \]  

(2.15)

where \( \gamma_4 = \text{diag}[1, 1, -1, -1] \), \( \alpha_k \equiv i \gamma_4 \gamma_k = \left( \begin{array}{cc} 0 & \sigma_k \\ \sigma_k & 0 \end{array} \right) \), \( \gamma_\mu \) are the Euclidean gamma matrices and \( \sigma_k \) are the Pauli matrices.

We discretize the Dirac operator (the so-called “naïve discretization”),

\[ H = \sum_x a^3 \left\{ \bar{\psi}_x m \gamma_4 \psi_x + \frac{i}{2} \sum_{k=1}^3 \left[ \bar{\psi}_{x+k} \alpha_k \psi_x - \bar{\psi}_x \alpha_k \psi_{x+k} \right] \right\} \psi. \]  

(2.16)

Fourier transforming to 3-momentum space, we get

\[ H = \frac{1}{(aL)^3} \sum \bar{\psi}_q \left\{ m \gamma_4 + \frac{1}{a} \sum_k \alpha_k \sin q_k \right\} \psi_q. \]  

(2.17)

In one dimension, the “naïve” Dirac operator, written above in curly brackets, has two eigenvalues,

\[ E_q^2 = m^2 + \frac{1}{a^2} \sum_k \sin^2 q_k. \]  

(2.18)

In the continuum limit \( (a \to 0) \) the second term dominates. Due to \( \sin(q + \pi) = -\sin(q) \), we have

\[ E_q^2 = E_{q+\pi}^2, \]  

(2.19)

where, in three dimensions,

\[ \vec{q}_\pi = \{(0,0,0), (\pi,0,0), (0,\pi,0), (0,0,\pi), (\pi,\pi,0), (\pi,0,\pi), (0,\pi,\pi), (\pi,\pi,\pi)\}. \]  

(2.20)
In our 4-dimensional Euclidean space we have therefore 16 different fermion solutions for the same eigenvalue, which are unphysical extra fermions which the naïve discretization automatically introduced. This result of the simple discretization is called the “doubling problem”. The first solution, introduced by Wilson in 1975, makes the extra fermions infinitely heavy in the continuum limit, thereby eliminating their contribution. The Wilson Hamiltonian has an additional term multiplied by \( r \) – the Wilson constant. In 3-space:

\[
H = \sum_{\vec{x}} a^3 \left\{ \bar{\psi}_{\vec{x}} \left( m + \frac{3r}{a} \right) \gamma_4 \psi_{\vec{x}} + \frac{1}{2a} \sum_k \left[ i(\bar{\psi}_{\vec{x}+\hat{k}} \alpha_k^\dagger \psi_{\vec{x}} - \bar{\psi}_{\vec{x}} \alpha_k \psi_{\vec{x}+\hat{k}}) - r(\bar{\psi}_{\vec{x}+\hat{k}} \gamma_4 \psi_{\vec{x}} - \bar{\psi}_{\vec{x}} \gamma_4 \psi_{\vec{x}+\hat{k}}) \right] \right\},
\]

(2.21)

and in 3-momentum space:

\[
H = \frac{1}{(aL)^3} \sum_{\vec{q}} \bar{\psi}_{\vec{q}} \left\{ m \gamma_4 + \frac{1}{a} \sum_k \left[ \alpha_k \sin q_k + r \gamma_4 (1 - \cos q_k) \right] \right\} \psi_{\vec{q}},
\]

(2.22)

which has the eigenvalues

\[
E_q^2 = \left[ m + \frac{r}{a} \sum_k (1 - \cos q_k) \right]^2 + \frac{1}{a^2} \sum_k \sin^2 q_k.
\]

(2.23)

These two eigenvalues are unique even under periodic boundary conditions. The Wilson action is derived from this by the partition function \( Z \), in 4-space:

\[
Z = \text{Tr} e^{-\beta H} = \int [d\bar{\psi} \, d\psi] e^{-S}
\]

(2.24)

\[
S = \sum_{\vec{x}} a^4 \left\{ \left( m + \frac{4r}{a} \right) \bar{\psi}_{\vec{x}} \psi_{\vec{x}} - \frac{1}{2a} \sum_{\pm \mu} \bar{\psi}_{\vec{x}+\hat{\mu}} [r + \gamma_\mu] \psi_{\vec{x}} \right\}.
\]

(2.25)

The fields can be normalized by a constant:

\[
\sqrt{a^4 \left( m + \frac{4r}{a} \right)} \psi \rightarrow \psi,
\]

(2.26)

producing

\[
S = \sum_{\vec{x}} \left\{ \bar{\psi}_{\vec{x}} \psi_{\vec{x}} - K \sum_{\pm \mu} \bar{\psi}_{\vec{x}+\hat{\mu}} [r + \gamma_\mu] \psi_{\vec{x}} \right\} \equiv \sum_{\vec{x} \vec{y}} \bar{\psi}_{\vec{y}} Q_{\vec{y} \vec{x}} \psi_{\vec{x}},
\]

(2.27)

where \( K \) is the hopping parameter,

\[
K \equiv \frac{1}{2am + 8r},
\]

(2.28)

and \( Q_{\vec{y} \vec{x}} \) is the fermion matrix,

\[
Q_{\vec{y} \vec{x}} \equiv \delta_{\vec{y} \vec{x}} - K \sum_{\pm \mu} \delta_{\vec{y}, \vec{x}+\hat{\mu}} (r + \gamma_\mu).
\]

(2.29)
For the calculation of correlation functions we use the fermion determinant, which is the determinant of this matrix. The Wilson action is by no means the only solution to the doubling problem; This was the first solution, and also the one which serves as a basis for the twisted-mass action, which is the one we use in our Monte-Carlo simulations.

### 2.2 Symanzik tree-level improved gluon action

Symanzik suggested in \[14\] a programme aimed to create actions with decreased cutoff effects. The idea is to identify a “physical” quantity – a Green’s function, and calculate it in perturbation theory. One should then identify the lowest order in \(a\), and subtract its contribution by adding an “irrelevant” effective operator to the action. Irrelevant in this context means that the term goes to zero in the continuum limit \((a \to 0)\). This method does not completely eliminate the lowest order cutoff dependence, since that dependence comes also from non-perturbative sources. Nevertheless, the perturbative Symanzik improvement method was found in practice to greatly improve lattice Monte-Carlo simulations \[12\]. A similar method, in which the \(a\) dependence is subtracted non-perturbatively \[15\], can be also applied. A non-perturbative improvement is more accurate in principle, but requires additional lattice simulations.

In \[16\] Weisz applied the perturbative Symanzik programme to the Yang-Mills action, by calculating the gluon propagator – the 2-point Green function of the gauge field – and canceling the \(O(a^2)\) dependence. The terms added were constructed by calculating, in addition to the plaquette (4 links) term also 6 links long closed curves, shown in fig. 2.2.

![Figure 2.2. Four and six link curves](image-url)

From this analysis Weisz recovered a general higher-order gluon action

\[
S_g = \beta \sum_{i=0}^{3} \sum_{\wp_i} c_i(\beta) \left( 1 - \text{Tr} \, U_{\wp_i} \right),
\]

(2.30)

where \(\wp_i\) is a path of type \(i\), as numbered in fig. 2.2. This action is quite general, and can define various improved actions, by choosing appropriate constants \(c_i\). An overall normalization condition is defined by setting the constant, appearing in the quadratic (in the gluon field) part of the action, to one:

\[
c_0 + 8c_1 + 16c_2 + 8c_3 = 1 \quad \text{(for all orders of } g^2).\]

(2.31)
2.3 Improvement of the fermion action

The elimination of the lowest order terms in the propagator gives us the coefficients which define tree-level Symanzik improved action:

\begin{align}
  c_2 + c_3 &= 0, \\
  c_1 &= -\frac{1}{12}. \\
\end{align}  \tag{2.32}

\section*{2.3 Improvement of the fermion action}

The $\mathcal{O}(a)$ improvement of the fermion action follows a completely different approach. We do not add an “irrelevant” operator in order to cancel lattice artifacts, but instead exploit the symmetry of the action itself. Following the arguments in [17], we see that the Wilson action can yield $\mathcal{O}(a)$ improved matrix elements, of operators which are: multiplicatively-renormalizable, gauge-invariant, multi-local. The idea is to define a chiral transformation $R_5$, which is a symmetry of the action, acting on the fields as well as on the masses and Wilson constant $r$ (spurionic symmetry)

\[ R_5 : \psi \to \gamma_5 \psi, \quad \bar{\psi} \to \bar{\psi} \gamma_5, \quad r \to -r, \quad m_q \to -m_q, \]  \tag{2.33}

where $m_q \equiv m_0 - m_{cr}$ is called the excess quark mass. Parity under $R_5$ of an operator $Q$ will be denoted by $P_5(Q)$.

An operator can generally mix with other operators of lower or equal dimension. We expand the bare operator $Q$ in powers of $a$ (up to first order) in terms of renormalized continuum operators,

\[ \langle Q \rangle = \langle \zeta(r) + am_q \xi(r) \rangle_{\text{cont}} + a \sum_j (m_q)^n \eta_j(r) \langle Q_j \rangle_{\text{cont}} + \mathcal{O}(a^2), \]  \tag{2.34}

where the superscript $\text{cont}$ denotes continuum renormalized operators. The logarithmic divergence in $a$ was eliminated by a multiplicative renormalization constant, which is itself an even function of $r$ and can be calculated non-perturbatively with only $\mathcal{O}(a^2)$ discretization errors.

If the operator is not multiplicatively-renormalizable, and the mixing coefficients have power divergences in $1/a$, the following discussion does not hold.

The operator $Q$ can be taken to have a definite parity in $R_5$ without loss of generality. The continuum-renormalized operators have the same $P_5$ parity as the lattice operators,

\[ \langle Q \rangle_{m_q}^{\text{cont}} = (-1)^{P_5(Q)} \langle Q \rangle_{-m_q}^{\text{cont}}. \]  \tag{2.35}
We apply the $R_5$ transformation on the operator:

$$
\langle Q \rangle = (-1)^{P_5(Q)} \langle Q \rangle \bigg|_{R_5}
= (-1)^{P_5(Q)} \left\{ \left[ \zeta(-r) - am_q \xi(-r) \right] \langle Q \rangle \bigg|_{m_q}^{\text{cont}} 
+ a \sum_j (m_q)^{n_j} \eta_j(-r) \langle Q_j \rangle \bigg|_{m_q}^{\text{cont}} + \mathcal{O}(a^2) \right\}
= (-1)^{P_5(Q)} \left\{ \left[ \zeta(-r) - am_q \xi(-r) \right] \langle Q \rangle \bigg|_{m_q}^{\text{cont}} 
+ a \sum_j (m_q)^{n_j} \eta_j(-r) (-1)^{P_5(Q)} + P_5(Q_j + n_j) \langle Q_j \rangle \bigg|_{m_q}^{\text{cont}} + \mathcal{O}(a^2) \right\}. \quad (2.36)
$$

It can be shown [17] that

$$P_5(Q) + P_5(Q_j) + n_j = 1 \mod(2). \quad (2.37)$$

If we equate Eqs. (2.36) and (2.34) by powers of $a$ we get

$$
0 = \zeta(r) - \zeta(-r),
0 = am_q[\xi(r) + \xi(-r)] \langle Q \rangle |_{m_q}^{\text{cont}} + a \sum_j (m_q)^{n_j} [\eta_j(r) + \eta_j(-r)] \langle Q_j \rangle |_{m_q}^{\text{cont}}. \quad (2.38)
$$

The last equation is exactly the $\mathcal{O}(a)$ term which we get by averaging the correlator calculated with $r$ and $-r$, which is the Wilson averaging:

$$
\langle Q \rangle |_{m_q,r}^{WA} = \frac{1}{2} \left[ \langle Q \rangle |_{m_q,r}^{\text{cont}} + \langle Q \rangle |_{m_q,r}^{\text{cont}} \right] = \zeta(r) \langle Q \rangle |_{m_q}^{\text{cont}} + \mathcal{O}(a^2). \quad (2.39)
$$

This is not directly applicable in the Wilson action since it is not defined for $r < 0$. Instead we use this symmetry in the improvement of the twisted-mass action, as described below.

### 2.3.1 Maximally twisted mass action and $O(a)$ improvement

A twisted-mass term was first introduced by Aoki [18] ([19]) as an order parameter used for probing the QCD phase structure. Aoki and Bär [20] later realized that a nonzero quark twisted-mass eliminates zero-modes from which the Wilson action suffers. Zero-modes are very small eigenvalues of the Dirac operator, which cause a divergence in the propagator and therefore in the correlation functions [21]. This notably happens in the quenched approximation, but also in unquenched actions with light dynamical fermions. Zero modes, however, are absent from the QCD continuum action.

Following [17], we introduce the axial rotation, which transforms the fermions from the untwisted ("physical") basis $\psi$ to the twisted basis $\chi$

$$
\chi = \exp\{-\frac{i}{2} \gamma_5 \tau_3 \omega\} \psi, \quad \bar{\chi} = \bar{\psi} \exp\{-\frac{i}{2} \gamma_5 \tau_3 \omega\}, \quad (2.40)
$$
where $\omega$ is the twist angle and $\tau_3$ is the third Pauli matrix in flavor space. The $\tau_3$ is responsible for arranging the fermions in pairs with opposite twist, and for the positivity of the fermion determinant. The twisted-mass (TM) action is a Wilson action which contains an extra term, and is written in the twisted basis as

$$S^{TM} = a^4 \sum_x \bar{\chi}_x \left\{ \frac{1}{2} \gamma_\mu \left( D_\mu + D^b_\mu \right) - \frac{ar}{2} D_\mu D^b_\mu + m_0 + i\gamma_5 \tau_3 \mu q \right\} \chi_x ,$$  \hspace{1cm} (2.41)$$

where we recall that $D_\mu$ and $D^b_\mu$ are the forward and backward covariant lattice derivatives, a sum over $\mu$ is understood, $m_0$ is the bare untwisted mass and $\mu q$ is the bare twisted mass.

In terms of gauge fields instead of covariant derivatives, the action reads

$$S = a^4 \sum_x \left\{ \bar{\chi}_x \left[ m_0 + i\gamma_5 \tau_3 \mu q \right] \chi_x + \frac{1}{2a} \bar{\chi}_x \left[ U_{x,\mu}(\gamma_\mu - r) \chi_{x+\bar{\mu}} + U^+_{\bar{x}-\bar{\mu},\mu}( -\gamma_\mu - r) \chi_{x-\bar{\mu}} \right] \right\} .$$  \hspace{1cm} (2.42)$$

In terms of the physical, i.e. untwisted, fermion fields, the action is

$$S = a^4 \sum_x \bar{\psi}_x^{phys} \left\{ \frac{1}{2} \gamma_\mu \left( D_\mu + D^b_\mu \right) + \left( -\frac{ar}{2} D_\mu D^b_\mu + M_{cr}(r) \right) e^{-i\omega\gamma_5 \tau_3} + m_q \right\} \psi_x^{phys} .$$  \hspace{1cm} (2.43)$$

Note that the action has the usual Dirac form in the continuum limit, since the rotation acts only on the Wilson (unphysical) term, which is why this basis is called “physical”. The fermion determinant can be decomposed by flavor:

$$\det Q = \det \left[ (D_{W}^r + m_q \cos \omega)^+ (D_{W}^r + m_q \cos \omega) + m_q^2 \sin^2 \omega \right] ,$$  \hspace{1cm} (2.44)$$

where $D_{W}^r$ is the Dirac operator of the Wilson action with the critical mass,

$$D_{W}^r = \frac{1}{2} \gamma_\mu \left( D_\mu + D^b_\mu \right) - \frac{ar}{2} D_\mu D^b_\mu + M_{cr}(r) .$$  \hspace{1cm} (2.45)$$

We can see how the determinant is real and positive, and no zero-modes occur for $m_q, \omega \neq 0$.

Furthermore, we can see that the action with physical fermions is invariant under

$$[r \rightarrow -r] \times [\omega \rightarrow \omega + \pi]$$  \hspace{1cm} (2.46)$$

($M_{cr}(-r) = -M_{cr}(r)$), which leads to a prescription similar to the Wilson average, described above in Ch. 2.4: we showed that correlators with the Wilson action have $\mathcal{O}(a)$ terms odd in $r$, so that averaging correlators calculated with $r$ and $-r$ gives a quantity which is free from $\mathcal{O}(a)$ terms. Equivalently, because of the invariance to (2.46), if we calculate a correlator with $\omega$ and $\omega + \pi$, the average is $\mathcal{O}(a)$ improved. More specifically, in maximally-twisted mass action, which is defined by $\omega = \pm \pi/2$, quantities which are even in $\omega$ are automatically $\mathcal{O}(a)$ improved, since $\omega + \pi = -\omega$.
The critical mass is chosen in such a way that we get an $O(a)$ improved theory for correlators of operators with odd parity, and free of IR divergences \cite{22}. The critical mass is tuned by setting the PCAC mass

$$m_{PCAC} = \frac{\sum_x \langle \partial_0 A_0(x) \pi(0) \rangle}{2 \sum_x \langle \pi(x) \pi(0) \rangle}$$

(2.47)

to zero, in the limit $\mu_q \to 0$ \cite{23}.
Chapter 3

Lattice techniques

3.1 Correlation functions and matrix elements

In the following discussion we show how physical quantities of interest can be calculated from lattice Monte-Carlo simulations. For additional material the interested reader can look at, e.g., [24] or [13] (Ch. 5.2, hadron spectroscopy). Physical observables in Quantum field theory are calculated from expectation values, which are n-point correlation functions of suitable operators or fields $\Gamma$,

$$C_n(x_1,..,x_n) = \langle \Gamma(\phi, x_1,..,x_n) \rangle = \frac{\int d[\phi(x)] \exp\{-S(\phi)\} \Gamma(\phi, x_1,..,x_n)}{\int d[\phi(x)] \exp\{-S(\phi)\}} \ , \quad (3.1)$$

where $S$ is the action.

3.1.1 2-point correlation functions

Usually we use time-slices of the correlators, which are sums of the local operators over the 3-space. We look at the time evolution of a 2-point correlation function, of two local operators $A(\tau_A)$ and $B(\tau_B)$ which have the same quantum numbers,

$$C_2 = \sum_n \frac{1}{2E_n} \langle 0|A(\tau_A)|\alpha_n\rangle \langle \alpha_n|B(\tau_B)|0\rangle \ . \quad (3.2)$$

where we assume $\tau_A \geq \tau_B$.

Inserting a full basis of states, $\alpha_n$, with the same quantum numbers of $A$ and $B$, we get

$$C_2 = \sum_n \frac{1}{2E_n} \langle 0|A(\tau_A)|\alpha_n\rangle \langle \alpha_n|B(\tau_B)|0\rangle \ . \quad (3.3)$$

After extracting the time evolution of the operators, we can see that the 2-point correlator timeslice has the form

$$C_2 = \sum_n \frac{1}{2E_n} \langle 0|A(0)|\alpha_n\rangle e^{-E_n(\tau_A-\tau_B)} \langle \alpha_n|B(0)|0\rangle \ . \quad (3.4)$$
The correlator at times which are close to the sources \((\tau_A \sim \tau_B)\) involves the mixing of an infinite tower of states. If we fix the momenta of the operators, the energy of the different states \((E_n^2 = m_n^2 + p^2)\) differs according to the mass of the states. We can therefore separate the ground state, by choosing large time separations, \(\tau_A - \tau_B \to \infty\), where all modes with mass (and therefore energy) higher than the ground state are exponentially suppressed,

\[
\lim_{\tau_A - \tau_B \to \infty} C_2 = \frac{\sqrt{Z_A Z_B}}{2E} e^{-E(\tau_A - \tau_B)},
\]

where the \(Z_{A,B}\) constants are given by the matrix element between the vacuum and the lowest state, \(\sqrt{Z_A} = \langle 0 | A(0) | \alpha_0 \rangle\), \(\sqrt{Z_B} = \langle 0 | B(0) | \alpha_0 \rangle\).

For hadron spectroscopy we can use the zero-momentum correlator of two identical hadronic operators, which at large times is proportional to the exponent of the time difference times the mass of the particle. For example, in the case of a pion operator \(\pi = \bar{d} \gamma_5 u\),

\[
\lim_{\tau_1 - \tau_2 \to \infty} C_2(\pi(\tau_1), \pi(\tau_2)) = \frac{\sqrt{Z_{\pi}}}{2E} e^{-E(\tau_1 - \tau_2)}.
\]

In the stochastic calculations, the 2-point correlator at time \(t\) is defined by two operator injections, one at time \(\tau = 0\) and the other at time \(t\), and two fermion propagators between 0 and \(t\). Due to the periodic boundary conditions, the sources propagate backwards as well as forwards. The correlator is the sum of the forwards and backwards propagating source from time \(\tau = 0 = T\) (\(T\) is the lattice size in the time dimension), which for a pion (kaon) takes the form

\[
C_2^{(K)}(t) \propto \frac{Z_{\pi(K)}}{2E(\pi(K))} \left[ e^{-E_\pi(K)t} + e^{-E_\pi(K)(T-t)} \right].
\]

When we fit the lattice data at large times to this function, we can recover the zero matrix element \((Z)\), and the energy and mass (which is energy at zero spatial momentum) of the ground states – which are pions (or kaons).

### 3.1.2 3-point correlation functions

A weak decay process can be simulated using a 3-point correlation function of an appropriate weak current operator between external fields. 3-point correlators can be also used for the calculation of hadron structure function and form factors and \(K^0 - \bar{K}^0\) mixing, to cite a few examples. A 3-point correlator is the expectation value of 3 injected local operators, which we call \(A(\tau_1), Q(t)\) and \(B(\tau_2)\), where we later identify \(Q\) with our weak decay operators, and \(A\) and \(B\) with the mesons which are involved in the process. We show the propagator triangle diagram which corresponds to a weak meson decay in Fig. 3.1. 4-fermion operators or baryonic processes in 3-point correlators are more involved, since they require additional propagators which can be combined in several different ways, as can be seen in the

\(^1\)Although most frequently one looks at the lowest-state only, other approaches measure also excited states, see e.g. \([25]\).
3.2 Twisted boundary conditions

The usual boundary conditions of
\[ \psi(x + \hat{e}_j L) = \psi(x) , \]  
(3.10)
where \( \hat{e}_j \) is a unit vector in the spatial direction \( j \), lead to the possible momentum values being quantized as
\[ p_j = n_j \frac{2\pi}{L} . \]  
(3.11)
Our typical lattice sizes, \( a^{-1} \sim 2.3 \text{ GeV} \) and \( L = 32a \) lead to a smallest nonzero momentum \( p \sim 0.45 \text{ GeV} \). This constitutes a limitation on probing the momentum region of interest.

A method for probing small momenta was proposed in [26], where it was suggested to phase shift the fields, by coupling to a background \( U(1) \) gauge field. This is effectively equivalent to reformulating the boundary conditions to include a phase shift
\[ \tilde{\psi}(x + \hat{e}_j L) = e^{2\pi i \theta_j} \psi(x) , \]  
(3.12)

\[ C_3 = \langle A(\tau_1) Q(t) B(\tau_2) \rangle \]
\[ = \sum_{n,m} \frac{1}{4E_{An}E_{Bm}} \langle 0 | A(\tau_1) | \alpha_n(t) \rangle \langle \alpha_n(t) | Q(t) | \beta_m(t) \rangle \langle \beta_m(t) | B(\tau_2) | 0 \rangle \]
\[ = \sum_{n,m} \frac{1}{4E_{An}E_{Bm}} \sqrt{Z_{An}} e^{-E_{An}(\tau_1-t)} \langle \alpha_n | Q | \beta_m \rangle e^{-E_{Bm}(t-\tau_2)} \sqrt{Z_{Bm}} . \]  
(3.8)
As before, at large times modes higher than the ground state are exponentially suppressed,
\[ C_3 \to \frac{\sqrt{Z_A Z_B}}{4E_A E_B} e^{-E_A(\tau_A-t)} \langle A | Q | B \rangle e^{-E_B(t-\tau_B)} . \]  
(3.9)

Figure 3.1. A triangle diagram, corresponding to the schematic propagators in a 3-point correlator.

collection of diagrams in, e.g., [24]. However, these operators are beyond the scope of this work.

In order to calculate the desired matrix elements from the 3-point correlators, we use a derivation similar to the 2-point correlators, where we insert two complete sets of states with quantum numbers equal to those of \( A \) and \( B \), and extract the evolution in time of the time-slices
\[ C_3 = \langle A(\tau_1) Q(t) B(\tau_2) \rangle \]
\[ = \sum_{n,m} \frac{1}{4E_{An}E_{Bm}} \langle 0 | A(\tau_1) | \alpha_n(t) \rangle \langle \alpha_n(t) | Q(t) | \beta_m(t) \rangle \langle \beta_m(t) | B(\tau_2) | 0 \rangle \]
\[ = \sum_{n,m} \frac{1}{4E_{An}E_{Bm}} \sqrt{Z_{An}} e^{-E_{An}(\tau_1-t)} \langle \alpha_n | Q | \beta_m \rangle e^{-E_{Bm}(t-\tau_2)} \sqrt{Z_{Bm}} . \]  
(3.8)
As before, at large times modes higher than the ground state are exponentially suppressed,
\[ C_3 \to \frac{\sqrt{Z_A Z_B}}{4E_A E_B} e^{-E_A(\tau_A-t)} \langle A | Q | B \rangle e^{-E_B(t-\tau_B)} . \]  
(3.9)
3. Lattice techniques

where $\tilde{\psi}$ is the shifted field. This shifts the momentum to

$$\tilde{p}_j = (n_j + \theta_j) \frac{2\pi}{L}.$$  \hspace{1cm} (3.13)

These boundary conditions were implemented in our stochastic calculation of all-to-all propagators [27], with the maximally twisted mass action. As was noted before, this is equivalent to defining a new gauge transformation and a rotated quark field, with periodic boundary conditions

$$\psi_\theta(x) = e^{-2\pi i \theta \cdot x / L} \psi(x),$$  \hspace{1cm} (3.14)

where $\theta = (L/2T, \vec{\theta})$ is the 4-vector twist. We rephase similarly the gluon gauge field

$$\tilde{U}_\mu(x) = e^{2\pi i \theta \cdot L / U_\mu(x)}.$$  \hspace{1cm} (3.15)

We can see that the twisted mass action in (2.42) is invariant under this transformation. Our action is calculated with periodic boundary conditions but shifted fields, where the quark propagator $S_\theta$ is calculated from the shifted Dirac operator $D_\theta$, by solving the equation

$$\sum_z D_\theta(x, z) S_\theta(z, y) = \delta_{x, y},$$  \hspace{1cm} (3.16)

and then shifted back to the twisted boundary conditions by

$$\tilde{S}(x, y) = e^{2\pi i \theta \cdot (x - y) / L} S_\theta(x, y).$$  \hspace{1cm} (3.17)

Quantities not depending on final state interactions, i.e. the gluon propagator, gauge configurations and sea quarks, are modified by exponentially small finite volume effects, and need not be recalculated [28].

This method allows us in practice to achieve an arbitrarily small momentum for the external mesons $q_{\text{min}} = \frac{2\pi}{L} \theta$. This minimal value was the momentum we used in the simulation, taking several values of $\theta$ and therefore of $q$. We checked that this represents a physical momentum by comparing the dispersion relation $E(q)$ taken from the 2-point correlation function, with the energy $E^2 = m^2 + q(\theta)^2$ – which compare very well, up to simulation errors, as can be seen in Fig. 3.2.

3.3 Stochastic all-to-all propagators

The quark propagator between two arbitrary points on the lattice (all-to-all propagator) can be directly evaluated in principle by inversion of the Dirac operator, which is a very costly procedure. A cheaper alternative is to evaluate the point-to-all propagator, which has a much lower complexity, but also computes correlators with a lower precision. A better solution is to calculate the all-to-all propagator, which exploits the information contained in the gauge configurations more fully, by introducing stochastic sources. We follow the introduction and notation in [23].
3.3 Stochastic all-to-all propagators

The degrees of freedom of the fermions are denoted by subscripts indices from 1 to V, the volume of the system. These vary between stochastic procedures and need to be defined: initially the indices are set to include space, time, flavour, color and spin. The random sources $\xi_r^i$ are created $R$ times, and their average over $r$ is required to satisfy

$$\lim_{R \to \infty} \langle \xi_r^i \xi_r^j \rangle = \delta_{ij}.$$  (3.18)

We introduce the $\phi$-propagator

$$\phi_j^i = D_{jk}^{-1} \xi_k^r$$  (3.19)

where $D$ is the Dirac operator. The fermion propagator is the inverse of the Dirac operator, estimated by

$$\langle \xi_r^i \phi_j^r \rangle = \frac{1}{R} \sum_{r,k} \xi_r^i D_{jk}^{-1} \xi_k^r = \frac{1}{R} \sum_{r,k} D_{jk}^{-1} (\delta_{ik} + \mathcal{N}(1)) = \frac{1}{R} D_{ji}^{-1} (R + \mathcal{N}(\sqrt{VR}))$$

$$= D_{ji}^{-1} (1 + \mathcal{N}(\sqrt{VR})),$$  (3.20)

where $\mathcal{N}(c)$ is random noise of the order of magnitude of $c$.

We can see that the all-to-all propagator can be calculated without inverting the full matrix, but at the cost of a very large noise, which forces many random sets for a reasonable error and overall does not improve efficiency.

A more sophisticated approach, called the ‘one-end trick’ corrects this behavior. We calculate a product of $\phi$-propagators to recover the product of two fermion propagators joined at one point $k$. The sources are non-zero only at one point in

Figure 3.2. Comparison between the pion energy directly calculated from the correlation function $E_\pi$, and the energy calculated from the twisted 3-momentum $E_\pi(\theta) = \sqrt{m_\pi^2 + p_\pi^2(\theta)}$. In the abscissa is the 3-momentum. The smallest “classic” momentum $a \cdot 2\pi/L$ in this case is $\sim 0.26$. 

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure3_2.png}
\caption{Comparison between the pion energy directly calculated from the correlation function $E_\pi$, and the energy calculated from the twisted 3-momentum $E_\pi(\theta) = \sqrt{m_\pi^2 + p_\pi^2(\theta)}$. In the abscissa is the 3-momentum. The smallest “classic” momentum $a \cdot 2\pi/L$ in this case is $\sim 0.26$.}
\end{figure}
time, \( t = t_0 \).

\[
< \phi_i^r \phi_j^s > = \frac{1}{R} \sum_{r,k,m} \xi_k^r D_{ki}^{-1s} D_{jm}^{-1s} = \sum_k D_{jk}^{-1} D_{ki}^{-1s} \left( 1 + \mathcal{N} \left( \sqrt{V/R} \right) \right). \tag{3.21}
\]

Contracting with \( \delta_{ij} \) and summing over \( j \) and over space point of we get

\[
\sum < \phi_i^r \phi_i^s > = \sum_{i,k} D_{ik}^{-1} D_{ki}^{-1s} \left( 1 + \mathcal{N} \left( \sqrt{V/R} \right) \right). \tag{3.22}
\]

The signal in this case is of order \( V \), and so is the noise. This allows us to use only one random source to calculate the correlator.

### 3.4 Fits, extrapolations and systematic errors

All the fits were performed in Fortran using MINUIT [29], which is a package designed for multi-variable search and minimization. The fits were performed for each jackknife separately, where the fit looks to minimize the squared error \( \chi^2 \), between the fitted points \((x_i, y_i)\) with error \( \Delta y_i \) and the function \( f \) calculated at the points \( x_i \),

\[
\chi^2 = \sum_i \left( \frac{y_i - f(x_i)}{\Delta y_i} \right)^2. \tag{3.23}
\]

The process is calculated at a range of transferred momenta \( q \). In our case the momentum is defined through twisted boundary conditions, which enable the probing of an arbitrarily small momentum, as described in Ch. 3.2. The momentum dependence of form factors is approximated by a pole fit,

\[
f(q^2) = \frac{f(0)}{1 - \lambda q^2}, \tag{3.24}
\]

which was found to fit quite well our form factors. An eventual error due to this fit can be estimated from a quadratic fit and from a variation in the number of momentum values. We report on the \( f(0) \) values and the slope, \( \lambda \). The zero form factor is actually an interpolation, since we always have momentum values near and around \( q^2 = 0 \), which contributes to a low error.

The next step is an interpolation to the physical strange mass, which is achieved by keeping the pion mass fixed and extrapolating in the kaon mass. We fit the simulated form factor as a function of kaon mass and extrapolate to the physical (i.e., experimentally measured) kaon mass. This procedure also contributes a very small systematic error. The extrapolation to the physical strange mass will be described in more detail in Sec. 4.3.1.

The next steps are extrapolation to the physical pion mass, and to the continuum limit, \( a \to 0, \ L \to \infty \). Our lowest simulated pion masses are 270 MeV, which are still too high compared to the 135 MeV physical mass. The \( L \to \infty \) limit was not actually done, since we deemed that the finite volume does not contribute a
significant error. This was motivated physically by the fact that the lattice is large with respect to the pion, \( m_\pi L \gtrsim 3.3 \), and motivated also by the actual results, which were consistent to within statistical errors for two different lattice sizes \( L = 24 \) and \( L = 32 \) (at the same lattice spacing \( \beta = 3.9 \)).

Extrapolation was done in two ways: 1) separately, to the physical pion mass for each lattice spacing, then combining the results for a fit to \( a = 0 \), and 2) fitting together all pion masses and lattice spacings.

For the lattice spacing we assumed a linear dependence on \( a^2 \). For the pion masses, we extrapolated using a linear fit, a quadratic fit and a log-linear fit in \( m_\pi^2 \) (described below). In the separate extrapolation (1) we typically have 3 mass values, so only a linear fit is feasible.

The combined fits take the forms:

(a) quadratic \( f(a^2, m_\pi^2) = C' + A'm_\pi^2 + B'm_\pi^4 + D'a^2 + H'a^2m_\pi^2 \)

(b) log-linear \( f(a^2, m_\pi^2) = C'' + A''m_\pi^2 + B''m_\pi^2 \ln m_\pi^2 + D''a^2 + H''a^2m_\pi^2 \)

These extrapolations typically add a large statistical and systematic error, which can be taken into account by comparing the various fits.

**Statistical errors**

The statistical error due to the Monte-Carlo simulation is computed in the Bootstrap method, but an initial estimate was computed using the jackknife method. Basically the statistical error is computed by taking into account the variation and correlations between the results obtained with each gauge configuration. We have 240 separate gauge configurations.

In the jackknife approach we divide the configuration into \( N \) groups (typically 24 in our calculation). The \( i \)'th jackknife \( C_i \) is the mean of the correlation functions of all the gauge configurations except for those in the \( i \)'th group. Every subsequent value \( V \) is calculated from each jackknife separately, \( V_i(C_i) \), and then averaged. The mean and error is estimated using

\[
\bar{V} = \frac{1}{N} \sum_i V_i \quad (3.25)
\]

\[
\Delta V = \sqrt{\frac{N - 1}{N} \sum_i (V_i - \bar{V})^2}. \quad (3.26)
\]

### 3.5 Electromagnetic operator renormalization in the RI-MOM method

We calculate on the lattice the electromagnetic (EM) operator,

\[
Q_{EM} = \bar{q}_i \sigma_{\mu\nu} q_j , \quad (3.27)
\]
where $\sigma_{\mu\nu} = i/2(\gamma_{\mu}\gamma_{\nu} - \gamma_{\nu}\gamma_{\mu})$. The calculation suffers from logarithmic divergences in the regulator, $a$, which require a renormalization to eliminate. The divergence and subsequent renormalization can be expressed by the renormalization constant, $Z_T$, which is applied multiplicatively to the Monte-Carlo results. This constant was calculated non-perturbatively in a previous work by Constantinou et al. (2010) \cite{30} in the RI-MOM method (described below). The result is automatically $O(a)$ improved due to the maximally twisted mass action, while $O(a^2)$ terms were calculated in lattice perturbation theory and subtracted, making the resulting renormalization constant $O(a^2)$ improved. We try here to give an idea of the method they used, and the main advantages and limitations of this method.

Lattice perturbation theory, described in Ch. 5.3.1, can be successfully used to calculate the electromagnetic renormalization constant. However, a non-perturbative scheme is usually more desirable since the errors are generally smaller. As an aside, we remark that a non-perturbative scheme is necessary in those cases where perturbation theory cannot be applied, such as in mixing with power divergences (as in the case of the chromomagnetic operator), and where the QCD coupling constant $g$ is large.

### 3.5.1 RI-MOM

The regularization independent momentum subtraction (RI-MOM) renormalization scheme \cite{31} imposes renormalization conditions on the amplitudes with off-shell quark and gluon external states (and not hadrons), such that the resulting renormalization depends on the external states and gauge. On the other hand, the method produces by construction the same renormalized operators in all regularization schemes. The simplest condition is defined such that the renormalized amplitude is set to be equal to its tree-level value. For a multiplicatively-renormalizable bilinear operator,

$$ Q_\Gamma = \bar{q}_i \Gamma q_j, \quad (3.28) $$

where $q_i$ and $q_j$ represent the external quarks and $\Gamma$ is some combination of gamma matrices. If we slightly abuse the $\langle bra|ket \rangle$ notation, and use it to denote a Green function between off-shell fields, instead of a matrix element between physical states as usual, the renormalization condition can be written as

$$ Z_\Gamma \langle q_i(p)|Q_\Gamma|q_j(p)\rangle \bigg|_{p^2=-\mu^2} = \langle q_i(p)|Q_\Gamma|q_j(p)\rangle_{\text{tree}}. \quad (3.29) $$

As we can see, the right-hand-side is the same regardless of the regularization used for calculating quantum corrections on the left-hand-side. In order to write the condition in a more convenient way, we define the amputated Green function

$$ \Lambda_\Gamma(p) = S^{-1}_{q_i}(p) \langle q_i(p)|Q_\Gamma|q_j(p)\rangle S^{-1}_{q_j}(p), \quad (3.30) $$

which at tree level is simply the gamma matrix, $\Lambda_\Gamma(p) = \Gamma$. We also define the projected amputated Green function

$$ \mathcal{V}(p) \equiv \text{Tr} \left[ \Lambda(p) P_\Gamma \right], \quad (3.31) $$
where the projector is defined such that $\text{Tr } [P \Gamma] = 1$. The projector, for a vertex which is a combination of gamma matrices, is $\Gamma$ divided by an appropriate normalization constant, $P = \Gamma / c$. The quark field renormalization constant is given by the a renormalization condition similar to the one above, for the projected amputated Green function of the conserved vector current in Euclidean space,

$$Z_q^{-1} \mathcal{V}_{\mu}(p) \bigg|_{p^2 = \mu^2} = 1 . \quad (3.32)$$

We can now write the same renormalization condition for a general vertex $\Gamma$ in a different form, for the projected amputated Green function $\mathcal{V}$ in Euclidean space,

$$Z_{\Gamma}(\mu a, g(a))Z_q^{-1}(\mu a, g(a))\mathcal{V}_{\Gamma}(p a) \bigg|_{p^2 = \mu^2} = 1 , \quad (3.33)$$

where we have written explicitly the dependence upon the renormalization scale, $\mu$, upon the coupling $g$ and upon the lattice step $a$.

### 3.5.2 Electromagnetic operator renormalization

We present here the method of the renormalization of the electromagnetic operator, $\Gamma = \sigma_{\mu\nu}$ of [30], performed in RI-MOM, in the maximally twisted mass action, with $r_u = -r_d = 1$.

In order to write the RI-MOM conditions more specifically, one defines the following Green functions in momentum space:

- the quark propagator

$$S_q(p) = a^4 \sum_x e^{-ip \cdot x} \langle q(x) \bar{q}(0) \rangle , \quad (3.34)$$

which in the maximal twisted-mass basis follows the relations $S_d(0, y) = \gamma_5 S_u(y, 0)^+ \gamma_5$ and $S_d(p) = \sum_y e^{-ip \cdot y} S_d(0, y) = \gamma_5 S_u(p)^+ \gamma_5$ ,

- the vertex function

$$G_{\Gamma}(p) = a^8 \sum_{x,y} e^{-ip \cdot (x-y)} \langle u(x) Q_{\Gamma}(0) \bar{d}(y) \rangle , \quad (3.35)$$

the amputated Green function

$$\Lambda_{\Gamma}(p) = S_u(p)^{-1} G_{\Gamma}(p) S_d(p)^{-1} , \quad (3.36)$$

the twisted basis vertex

$$\bar{\Gamma} = e^{-i\gamma_5 \pi/4} \Gamma e^{i\gamma_5 \pi/4} , \quad (3.37)$$

and the projected amputated Green function

$$\mathcal{V}(p) \equiv \text{Tr } [\Lambda(p) P_T] , \quad (3.38)$$
where $P_{\Gamma}$ is the projector in spin space satisfying $\text{Tr} [\Gamma P_{\Gamma}] = 1$. We can see that this relation is very similar to the original one, although the quantities which enter it are different due to the twisted mass action.

For the quark field renormalization condition, we write the general structure of the quark propagator in the twisted mass action

$$S_q^{-1}(p) = i\Sigma_1(p^2) + \Sigma_2(p^2) - i\gamma_5 \Sigma_3(p^2) ,$$

where $\Sigma_1$, $\Sigma_2$ and $\Sigma_3$ are functions to be calculated which may contain quantum corrections. Their tree-level values are taken from the twisted-mass action in the twisted basis,

$$\Sigma_1(p^2) = 1, \quad \Sigma_2(p^2) = \mu_q, \quad \Sigma_3(p^2) = \frac{ar_q}{2} p^2 .$$

In the RI-MOM scheme, the quark field renormalization condition, which is written in Euclidean space, reads

$$Z_q^{-1} \frac{i}{48} \text{Tr} \left[ \frac{\partial S_q(p)^{-1}}{\partial \mu^2} \right]_{p^2=\mu^2} = 1 .$$

However, in order to avoid a derivative with respect to the discrete variable, the renormalization constant that they used in practice is slightly altered, and is called $Z'$ scheme after the $Z'$ constants introduced in Martinelli et al. The condition is written

$$Z'_q^{-1} \Sigma_1(p) \bigg|_{p^2=\mu^2} \equiv Z'_q^{-1} \frac{i}{12} \text{Tr} \left[ \frac{pS_q(p)^{-1}}{p^2} \right]_{p^2=\mu^2} = 1 .$$

The two schemes are equal up to discretization errors, or as Constantinou et al. report, they differ in the Landau gauge at the next-to-next-to-leading order.

One can now write the renormalization condition for the vertex function

$$Z_q^{-1} Z_{\Gamma} \mathcal{V}_{\Gamma}(p) |_{p^2=\mu^2} = 1 .$$

### 3.5.3 Errors and corrections to the non-perturbative renormalization

The renormalization of [30] suffers from several main uncertainties: first there is the usual statistical error of the gauge configurations. In addition, there is a discretization error associated to the renormalization scale, and then the error coming from the calculation at finite quark-mass of the scheme which is basically defined in the chiral limit (massless). Since the calculation is done in the maximally twisted mass action the results are $\mathcal{O}(a)$ improved, and the error enters at the $\mathcal{O}(a)$ level.

The chiral extrapolation performed in [30] assumes a linear plus inverse (due to the Goldstone pole) behaviour in the quark masses,

$$\mathcal{V}(p^2, m_\pi^2) = A(p^2) + B(p^2)m_\pi^2 + \frac{D(p^2)}{m_\pi^2} ,$$

where $A(p^2)$, $B(p^2)$, and $D(p^2)$ are functions of the Wilson mass $p^2$. The coefficients $A(p^2)$, $B(p^2)$, and $D(p^2)$ are determined from the analysis of the chiral extrapolation in the maximally twisted mass action.
where the first two terms are used to extrapolate to the continuum, while the last term represents the Goldstone pole, which was subtracted from the amplitude for each momentum and mass before the extrapolation. The first term, $A$, represents the amplitude at the chiral limit. We note that the fit assumes the chiral relation $m_{\pi}^2 \propto (\mu_1 + \mu_2)$, where $\mu_{1,2}$ are the twisted quark masses. The results were calculated also assuming different mass dependences and were found to be consistent, and therefore fairly independent of the extrapolation method. The renormalization constants were also found to be weakly dependent upon quark mass.

The scale dependence evolution is calculated using a $C_\Gamma$ function dependent upon the beta function $\beta(\alpha)$ and the anomalous dimension $\gamma_\Gamma(\alpha)$,

$$ C_\Gamma(\mu_0, \mu) = \exp \int_{\alpha(\mu_0)}^{\alpha(\mu)} \frac{\gamma_\Gamma(\alpha)}{\beta(\alpha)} d\alpha, \quad (3.45) $$

where $\mu_0 = 1/a$ is a reference scale. The renormalization constant scale dependence is

$$ Z_\Gamma(a, \mu_0) = C_\Gamma(\mu_0, \mu) Z_\Gamma(a, \mu). \quad (3.46) $$

The scale dependence in the Monte-Carlo simulation was found to be practically linear in $a^2 p^2$, as was expected. Here the results were improved with the help of lattice perturbation theory, By Constantinou et al. (2009) [32]. The same amplitudes were calculated in perturbation theory, and the ensuing results which multiply the $a^2 p^2$ terms were collected and subtracted from the Monte-Carlo results.

The final numerical results which they obtained are presented here in Table 4.2 (Ch. 4.3).

As an aside result, Constantinou et al. (2010) demonstrate analytically that the renormalization constants are automatically $O(a^{2m+1})$ (odd powers of $a$) improved, at a general twist angle, including zero.

### 3.6 Chiral perturbation theory

Chiral perturbation theory (ChPT) is an effective framework for studying low-energy hadronic processes. As a result of confinement, in low-energy processes the effective degrees of freedom are not quarks and gluons but hadrons, represented in the theory by effective pseudoscalar fields. These are used to construct an effective Lagrangian. We follow here the introductions in [33] and [34], leading to some results which we used in our analysis. Mainly, we get the first-order relation between meson and quark masses, and first order expansions in momentum of the electromagnetic and chromomagnetic operators.

We collect the meson fields inside a unitary matrix $U$,

$$ U = \exp(i2\Phi/f_\pi), \quad \Phi = \begin{pmatrix} \frac{\pi^0}{\sqrt{2}} + \frac{\eta_8}{\sqrt{6}} & \pi^+ & K^+ \\ -\frac{\pi^0}{\sqrt{2}} + \frac{\eta_8}{\sqrt{6}} & \eta_8 & K^0 \\ \sqrt{2} & K^0 & -2\eta_8 \sqrt{6} \end{pmatrix}, \quad (3.47) $$
where $f_\pi = 132$ MeV is the pion decay constant in the chiral limit, rows and columns represent $u$, $d$, $s$ quarks and their anti-partners, respectively, and instead of $\sqrt{2}$ in the exponent of $[33]$ we use 2, which is corrected in $f_\pi$ accordingly. In addition we have external fields $s$, $p$ (scalar, pseudoscalar) and $v_\mu$, $a_\mu$ (vector, axial-vector) which have the same quantum numbers as the corresponding quark currents, to which they couple in the action. The vector and axial external fields can be combined into chiral fields

$$r_\mu = v_\mu + a_\mu, \quad l_\mu = v_\mu - a_\mu,$$

(3.48)

to form the covariant derivative

$$D_\mu U = \partial_\mu U - i r_\mu U + i U l_\mu.$$

(3.49)

The scalar and pseudo-scalar external fields combine into

$$\chi = 2B(s + ip), \quad \chi^+ = 2B(s - ip),$$

(3.50)

where $B$ is a parameter of dimension 1 tied to the quark masses. The dynamic scalar field can be separated from the vacuum-value $m_q$ which is the quark mass matrix: $s \to s + m_q$. The Lagrangian is constructed by imposing the $SU(3)_L \times SU(3)_R$ chiral symmetry, which is spontaneously broken to conform to QCD physics. To the lowest order, $O(p^2)$, the Lagrangian reads

$$L = \frac{f_\pi^2}{4} \left( D_\mu UD^\mu U^+ + \chi U^+ + \chi^+ U \right).$$

(3.51)

$U$ can be expanded in powers of $\Phi$

$$U = 1 + i2 \frac{\Phi}{f_\pi} - 2 \frac{\Phi^2}{f_\pi^2} - i \frac{4}{3} \frac{\Phi^3}{f_\pi^3} + O(\Phi^3).$$

(3.52)

The first order expansion in the fields $\Phi$, when inserted in the equations of motion derived from the Lagrangian, in the limit of zero external field, $\chi \to m_q$, produces the lowest-order relation between meson and quark masses $[35]$

$$m_{\pi^0}^2 = B(m_u + m_d) + O(m_q^2),$$

$$m_{K^+}^2 = B(m_u + m_s) + O(m_q^2),$$

(3.53)

which we later use in the form-factor extrapolations.

The chromomagnetic operator

In the chiral quark model, we write the chromo-magnetic operator contribution in $O(p^4)$ $[36]$

$$Q^{CM} = -\frac{11}{4} \langle \bar{q}q \rangle \frac{B_{CM}}{16\pi^2} \text{Tr} [(U^+ M_q \lambda_- + \lambda_- M_q^+ U) D_\mu U^+ D^\mu U],$$

(3.54)
where $M_q = \text{diag}(m_u, m_d, m_s)$ is the quark mass matrix, $\langle \bar{q}q \rangle = -f_\pi^2 B[1 + \mathcal{O}(m_q)]$ is the quark condensate, and $\lambda_- = (\lambda_6 - i\lambda_7)/2$ are Gell-Mann matrices in flavor space, where all $(\lambda_-)_{ij} = 0$ except for $(\lambda_-)_{32} = 1$. The relevant part of the operator is between $\bar{s}$ and $d$, such that

$$Q_{23}^{CM} = \frac{11}{256\pi^2} \frac{f_\pi^2 m_K^2 B_{CM}}{m_s + m_d} [(UD_\mu U^+ D^\mu U + D_\mu U^+ D^\mu UU^+)_{23}].$$  \hspace{1cm} (3.55)

Expanding the matrices, using Matlab and Mathematica, the expectation value between $K$ and $\pi$ reads

$$\langle \pi^0 | Q_{CM} | K^0 \rangle = -\frac{11B_{CM}}{32\sqrt{2}\pi m_s + m_d} p_\pi \cdot p_K .$$  \hspace{1cm} (3.56)

We later use this parameterization for the chromo-magnetic operator form-factor, $B_{CM}$.

### The electromagnetic operator

The electromagnetic (EM) operator

$$Q^{EM} = \bar{s}\sigma^{\mu\nu}d$$  \hspace{1cm} (3.57)

is written in ChPT notation as [37]

$$Q_{23}^{EM} = -i\frac{\alpha_T f_\pi^2}{2} [\partial^\mu U^+ \partial^\nu UU^+ - \partial^\nu U^+ \partial^\mu UU^+ + \partial^\mu U \partial^\nu U^+ U - \partial^\nu U \partial^\mu U^+ U]_{23}. $$  \hspace{1cm} (3.58)

Expanding the matrices, using Matlab and Mathematica, the expectation value between $K$ and $\pi$ reads

$$\langle \pi^0 | Q_{EM} | K^0 \rangle = -i\frac{\alpha_T f_\pi^2}{2} \frac{4\sqrt{2}}{f_\pi^2} (p_\pi^\mu p_K^\nu - p_\pi^\nu p_K^\mu)$$

$$= i2\sqrt{2}\alpha_T (p_K^\mu p_\pi^\nu - p_K^\nu p_\pi^\mu) ,$$ \hspace{1cm} (3.59)

where [10, 37]

$$\alpha_T(q^2) = \frac{B_T(q^2)}{2m_K} = \frac{f_T(q^2)}{m_K + m_\pi} ,$$ \hspace{1cm} (3.60)

and $q = p_K - p_\pi$ is the transferred momentum.

This expansion agrees with the form used in [10]. We later use this parameterization for the EM (tensor) form-factor, $f_T$. 

Chapter 4

Numerical results: the electromagnetic form factor

In this chapter we present the first unquenched lattice results for the $K - \pi$ electromagnetic (EM) matrix element. A previous calculation was done in 2001 by Becirevic et al. [10]. We describe the formulae and process of extracting the matrix element and form-factor from the stochastic 2- and 3-point correlators double ratio, at large times of the time-slices. We show how we extrapolate the form factor to the physical masses of the quarks and to the continuum. We discuss the various systematic errors which are generated in the process. The statistical errors were evaluated using the jackknife prescription, which was discussed in Ch. 3.4.

First we describe here the extrapolation procedure of the previous calculation of Becirevic et al. (2001) [10], which may serve as an insightful introduction. Our procedure follows a similar road. We present the results for the form-factor at zero transferred momentum and the slope of the form-factor at zero momentum, and compare our results to Becirevic’s calculation. We find that our results are compatible with the previous calculation, although when extrapolated to the physical light quark masses, the numerical results of the zero-momentum form factor are different. The two results actually converge at the higher light quark masses, as we show in Fig. 4.20 in the discussion. We conclude that our results mainly differ in the extrapolation to physical light quark masses, and by the presence of the sea quarks which were not included in the previous quenched simulation.

4.1 Previous lattice calculation of the tensor form factor

Becirevic et al. (2001)

First we describe here the extrapolation procedure of the previous calculation of Becirevic et al. (2001) [10], which may serve as an insightful introduction. They obtain a form factor from the correlation function of a quenched Monte-Carlo simulation, which is calculated for a range of transferred momenta $q^2$, 6 combinations
of light quarks and strange quark masses, at one lattice spacing ($a^{-1} = 2.7 \pm 0.1$ GeV, $a = 0.0731 \pm 0.0027$ fm). First, they perform a momentum fit assuming a linear behaviour in the squared momentum,

$$ f_T(q^2) = f_T(0) \left(1 + \frac{\lambda_T}{m^2} q^2\right) . $$

They use only the two lowest momenta for the fit, since the quality of the signal in the other points is rather poor. Next, they extrapolate to the physical masses, assuming two different models:

- Ignoring $SU(3)$ chiral symmetry breaking effects,

$$ f = C + A m_{K}^2 . $$

- Including $SU(3)$ breaking effects,

$$ f = C + B m_{K}^2 + D m_{\pi}^2 . $$

They find that the difference between the results in the two cases is small, and conclude that $SU(3)$ breaking effects are quite small. They take into account the difference in the systematic error, and average over the two results. Their renormalization constant $Z_T$ was calculated non-perturbatively in [38] in the RI-MOM method, and was found to be $Z_T^{RI-MOM}(\mu = 2 GeV) = Z_T^{RMS}(\mu = 2 GeV) = 0.87(2)$. Finally, they calculate the ratio between the tensor and vector form factor,

$$ \frac{f_T(0)}{f_+(0)} , $$

which is needed for, e.g., the calculation of the semileptonic decay $K^0 \rightarrow \pi^0 e^+ e^-$, or more specifically in the $\langle \pi^0 e^+ e^- | Q_{EM} | K^0 \rangle$ electromagnetic matrix element. The form-factor ratio is a fully theoretical prediction, which therefore has a lower systematic error than a ratio between the theoretical tensor form factor and experimental $f_+$, and is better suited for comparison with experiments. From the ratio they obtain another prediction for the tensor form factor, which is the ratio multiplied by the experimental vector form factor.

Their final $f_T(0)$ result is the average of the one obtained directly with that obtained from the ratio,

$$ 0.770 \pm 0.057^{\text{stat}} \pm 0.025^{\text{syst}} , $$

while the final slope they report is given without systematic error consideration, from the direct $f_T$ calculation, with the fit which takes into account $SU(3)$ symmetry breaking,

$$ \lambda_T = 0.022 \pm 0.001 . $$

**Brommel et al. (2008)**

In [11] Brömmel et al. calculated in an unquenched ($N_f = 2$) lattice simulation the $\pi - \pi$ matrix element of the electromagnetic operator, which they call the transverse spin structure of the pion. They calculate the matrix element

$$ \langle \pi^+(p')|q \sigma^{\mu\nu} q|\pi^+(p)\rangle = i (p^\rho p'^\nu - p'^\rho p^\nu) \frac{B_{10}}{m_{\pi}} , $$

\[4.6\]
which translates $B_{πτ}^{π}$ equal to our $f_T$ described below, in the case of the $π − π$ transition, which is achieved with us technically by setting $m_s = m_d$, or equivalently $m_K = m_π$. The lattice sizes employed were $16^3 \times 32$ and $24^3 \times 48$, and lattice spacings between 0.07 and 0.115 fm.

### 4.2 Lattice details

Lattice Monte-Carlo simulations were conducted by the European twisted-mass collaboration. The action used is the Symanzik tree-level improved gluon action with the maximally twisted mass fermion action, and two dynamical flavors of the same mass. We used 240 gauge configurations for each parameter set. The lattices used are of sizes $24^3 \times 48$ and $32^3 \times 64$, with 3 lattice spacings. We simulated between two and five sea quark masses for each lattice spacing, and many valence masses covering approximate ranges of sea masses, strange mass, and heavy quarks. The parameters of the various runs are shown in Tab. 4.1.

<table>
<thead>
<tr>
<th>$β$</th>
<th>$a$ [fm]</th>
<th>$a^{-1}$ [GeV]</th>
<th>$L/a$</th>
<th>$T/a$</th>
<th>$m_π$ [MeV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.8</td>
<td>0.10033±0.00150</td>
<td>1.97±0.03</td>
<td>24</td>
<td>48</td>
<td>409, 478, 583</td>
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<tr>
<td>3.9</td>
<td>0.08500±0.000067</td>
<td>2.32±0.02</td>
<td>24</td>
<td>48</td>
<td>318, 392, 455, 488, 597</td>
</tr>
<tr>
<td>3.9</td>
<td>0.08500±0.000067</td>
<td>2.32±0.02</td>
<td>32</td>
<td>64</td>
<td>271, 308</td>
</tr>
<tr>
<td>4.05</td>
<td>0.06781±0.00042</td>
<td>2.91±0.02</td>
<td>32</td>
<td>64</td>
<td>304, 413, 477</td>
</tr>
</tbody>
</table>

Table 4.1. The parameters of the Monte-Carlo simulations used for the electromagnetic matrix element calculation.

### 4.3 Electromagnetic matrix elements

In Ch. 3.1 we showed how matrix elements are calculated from 2- and 3-point correlation functions. In particular, we saw that the 2-point correlator for a pion (kaon) created at time $\tau = 0$ and destroyed at time $\tau = t$, at times $t$ far from the creation operator, takes the form

$$C_2^{π(K)}(t) \xrightarrow{t,T-t\to\infty} \frac{Z_{π(K)}}{2E_{π(K)}} \left[ e^{-E_{π(K)}t} + e^{-E_{π(K)}(T-t)} \right], \quad (4.7)$$

where $Z_{π(K)}$ is the matrix element between the vacuum and the lowest state of the pion (kaon), and $T$ is the lattice size in the time dimension. We use the 2-point correlation functions to find the mass and energy of the mesons, in addition to the $Z$ constant which we need in order to calculate the 3-point matrix element.
The 3-point correlator of the time-slices of an operator $Q$, between the hadronic states $A$ and $B$, at times $t$ far from the sources at $\tau_1$ and $\tau_2$, was shown to be

$$ C_3(t) \equiv \langle A(\tau_1)Q(t)B(\tau_2) \rangle - \sqrt{Z_AZ_B} \frac{E_A E_B}{4E_A E_B} e^{-E_A(\tau_1-t)} \langle A|Q|B \rangle e^{-E_B(t-\tau_2)}. \quad (4.8) $$

Our 3-point correlators are calculated between a kaon and a pion and vice-versa. The operator $Q$ is defined at a variable time $t$, while the kaon (pion) is fixed at $\tau = 0$ and the pion (kaon) at $\tau = t_y = T/2$. To obtain the 3-point matrix element from the correlators, we use both of the 3-point correlators at large time separations:

$$ C_3^{K\pi}[\pi(t_y), Q(t), K(0)] \rightarrow \frac{Z_KZ_\pi}{4E_K E_\pi} \langle \pi|Q|K \rangle e^{-E_K t - E_\pi (t_y-t)} , $$

$$ C_3^{\pi K}[K(t_y), Q(t), \pi(0)] \rightarrow \frac{Z_KZ_\pi}{4E_K E_\pi} \langle K|Q|\pi \rangle e^{-E_\pi t - E_K (t_y-t)} . \quad (4.9) $$

Their product, assuming reciprocity of the matrix element, is

$$ C_3^{K\pi}C_3^{\pi K} \rightarrow \frac{Z_KZ_\pi}{(4E_E E_\pi)^2} \langle \pi|Q|K \rangle^2 e^{-(E_K + E_\pi)t_y} , \quad (4.10) $$

where we recall that $t_y$ is a fixed point $t_y = T/2$.

The 2-point correlators at the fixed time $t = t_y = T/2$ are

$$ C_2^{\pi(K)}(t = t_y) = \frac{Z_\pi(K)}{2E_\pi(K)} \left[ e^{-E_\pi(K) \frac{T}{2}} + e^{-E_\pi(K)(T - \frac{T}{2})} \right] = \frac{Z_\pi(K)}{E_\pi(K)} e^{-E_\pi(K) \frac{T}{2}}. \quad (4.11) $$

By combining the 3 and 2-point correlators we get the matrix element for the operator $Q$ between a kaon and a pion state,

$$ \frac{C_3^{K\pi}(t)C_3^{\pi K}(t)}{C_2^{\pi(K)}(t_y)C_2^{K\pi}(t_y)} \rightarrow \frac{\langle \pi|Q|K \rangle^2}{16E_K E_\pi}. \quad (4.12) $$

The $K - \pi$ matrix element of the operator $Q$, which is constant in time, is therefore extracted from this double ratio of correlation functions, at times far from the sources, $t, T/2 - t \rightarrow \infty$. Due to the periodic boundary conditions and the sources positions, we have a symmetry or anti-symmetry about $T/2$, and we average accordingly the correlation functions at points $t$ and $T - t$.

As we saw earlier in Eq. (3.59), the electromagnetic (EM) matrix element has a tensor structure

$$ \left\langle \frac{\pi^0}{\sqrt{2}} | \bar{s}\sigma^{\mu\nu}d | K^0 \right\rangle = i (p_K^\mu p_\pi^\nu - p_K^\nu p_\pi^\mu) \frac{\sqrt{2} f_T}{m_K + m_\pi}. \quad (4.13) $$

In our stochastic correlator calculations we use twisted boundary conditions. This means that our momenta are defined by the twist angle $\theta$. Calculating different momenta for the pion and kaon might get complicated. We have chosen to calculate
the propagators in the Breit frame of reference, in which the pion and kaon have opposite 3-space momenta
\[
\vec{p}_K = \vec{p}, \quad \vec{p}_\pi = -\vec{p}.
\] (4.14)
This choice enables using one twist angle and simplifies the stochastic calculation. In this frame of reference the 00 and ij components of the matrix element cancel, while the 0i components remain nonzero,
\[
\langle \pi^0 | \bar{s} \sigma^0 d | K^0 \rangle = i \left( E_K p_i^\pi - p_i^K E_\pi \right) \frac{2f_T}{m_K + m_\pi} = -ip^i (E_K + E_\pi) \frac{2f_T}{m_K + m_\pi}.
\] (4.15)
The 3-component \(\langle \pi^0 | \bar{s} \sigma^0 d | K^0 \rangle\) matrix element is projected to a scalar quantity \(\langle VTK \rangle\), by performing a scalar product with the momentum \(p^i\),
\[
\langle VTK \rangle \equiv 2p^i \langle \pi^0 | \bar{s} \sigma^0 d | K^0 \rangle = \vec{p}^2 (E_K + E_\pi) - 4i f_T \frac{m_K + m_\pi}{m_K + m_\pi}.
\] (4.16)
The 3-point correlator in our Monte-Carlo simulation includes the projected matrix element \(\langle VTK \rangle\) instead of the tensor matrix element. This is an internal detail of the calculation which does not affect the results, but is included here for future reference. The 3-point correlator in terms of the projected matrix element is given by
\[
C_{3\pi}^{K} = \sqrt{Z_{K} Z_{\pi}} \langle VTK \rangle e^{-E_K t - E_\pi (t_y - t)} ,
\] (4.17)
similarly to Eq. (4.9) above. The \(\langle VTK \rangle\) matrix element is calculated, as shown above for a general 3-point matrix element, using
\[
\langle VTK \rangle^2 = 16E_K E_\pi \lim_{t, t_y \to -\infty} \frac{C_3^{K}(t) C_3^{\pi}(t)}{C_2^{\pi}(t_y) C_2^{K}(t_y)}.
\] (4.18)
From \(\langle VTK \rangle\) we recover
\[
f_T = \frac{i}{4} Z_T \langle VTK \rangle \frac{1}{\vec{p}^2} \frac{m_K + m_\pi}{E_K + E_\pi}.
\] (4.19)
where we multiply by the renormalization constant \(Z_T\), which was calculated non-perturbatively in a previous work by Constantinou et al. [30] in the RI-MOM method [31]. The results that they obtained are displayed in Table 4.2.

<table>
<thead>
<tr>
<th>(\beta)</th>
<th>3.8</th>
<th>3.9</th>
<th>4.05</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Z_T) ((\overline{MS}, 2) GeV)</td>
<td>0.733±0.009</td>
<td>0.743±0.005</td>
<td>0.777±0.006</td>
</tr>
</tbody>
</table>

Table 4.2. The EM operator renormalization constant, from Constantinou et al. [30].

In Ch. 3.5 we described how their results were obtained, the extrapolations to the chiral limit, and how discretization effects were taken into account, including the \(a^2 p^2\) dependence which were subtracted analytically from perturbative results. The errors are predominantly statistical errors from the gauge configurations.
4. Numerical results: the electromagnetic form factor

4.3.1 Extrapolations and fits

We describe below the procedure we followed in order to obtain the physical form factor, which should be independent of all calculation artifacts. In short, this is achieved by fitting a plateau far from the injected operator sources, modelling the momentum dependence by a pole fit, and finally extrapolating to the physical quark masses and to the continuum.

All our fits are performed for each jackknife separately, as discussed in Ch. 3.4. The error bars of the single points, and the errors on the extrapolated value, are all statistical errors evaluated using the jackknife prescription, also discussed in Ch. 3.4.

Plateau

In order to extract the matrix element from the correlators, we take the weighted average (plateau) of the double ratio described above in Eq. (4.18), for each lattice momentum, strange and light quark mass, lattice spacing and jackknife. In order to keep valid the exponential operator time-dependence described above, the time-slices $t$ of the correlators need to be as far as possible from the sources ($0$ and $T/2$), i.e. around the $T/4$ point. For the plateau average we do not use all the time point available but only those in a range within a certain distance from the $T/4$ point. A plateaux is shown in Figs. 4.1, 4.2, for typical values of parameters in the simulation. We can see how the signal deteriorates for a higher momentum.

![Figure 4.1](image.png)

Figure 4.1. The electromagnetic form factor, time plateau average. Parameters: $m_K = 558$ MeV, $m_\pi = 318$ MeV, $\beta = 3.9$, $L = 24a$, $T = 48a$, transferred momentum $q^2 = 0.2$ MeV$^2$. 
### 4.3 Electromagnetic matrix elements

**Figure 4.2.** The electromagnetic form factor, time plateau average. Parameters: $m_K = 558$ MeV, $m_\pi = 318$ MeV, $\beta = 3.9$, $L = 24a$, $T = 48a$, $q^2 = -832$ MeV$^2$.

#### Momentum dependence

Usually, one parameterizes the momentum dependence with the transferred momentum, $q \equiv p_K - p_\pi$. The transferred momentum dependence of the operators can be parameterized in several different ways, of which the most typical are: a linear function, a quadratic function or a pole function –

$$f_T(q^2) = \frac{f_T(0)}{1 - q^2 \lambda}, \quad (4.20)$$

which has two parameters, $f_T(0)$ and $\lambda$. We found that the pole function resembles most closely the momentum dependence of the EM matrix element. We therefore interpolate in momentum assuming a pole behaviour. In Fig. 4.3 we can see a typical pole fit in momentum. In all the following results we report these two fit coefficients, $f_T(q^2 = 0)$ (abbreviated as $f_T(0)$, dimensionless) and $\lambda$ [GeV$^{-2}$], the slope. As for the systematic errors which the fit induces, the $f_T(0)$ parameter has a negligible error, since in the interpolated range the fit is typically very precise. On the other hand, the $\lambda$ parameter (the slope) is much more sensitive and depends upon the exact fit method chosen. The difference between the results obtained with different fit methods is an indication of the systematic error, which we estimate as described in the discussion of systematic errors in Ch. 4.3.2.

**Extrapolation of the strange mass to the physical value**

Our results were calculated for a range of light and strange quark masses. We first extrapolate the form factor to the physical (i.e., experimentally measured) strange
Figure 4.3. The electromagnetic form factor, momentum pole fit. In this example the fit parameters obtained were: $f_T(0) = 0.551 \pm 0.012$, $\lambda = 1.11 \pm 0.11 \text{GeV}^{-2}$.

Quark mass. We can connect the renormalized quark masses to the meson masses by using the relation that we presented in chiral perturbation theory (Ch. 3.6),

$$
\begin{align*}
m^2_\pi &= B(2m_\ell) + O(m^2_q), \\
m^2_K &= B(m_\ell + m_s) + O(m^2_q),
\end{align*}
$$

where $\ell$ denotes a light quark, and $B$ is a constant of the theory. From these relations we can calculate a quantity proportional to the renormalized strange quark mass on the lattice,

$$
2m^2_K - m^2_\pi = 2Bm_s.
$$

It follows that the physical strange mass is connected to the physical masses of the kaon and pion by

$$
(2m^2_K - m^2_\pi)_{\text{phys}} = 2B(m_s)_{\text{phys}}.
$$

In practice, in order to find the form factor at the physical strange mass, we plot the form factor against $2m^2_K - m^2_\pi$, keeping the pion mass fixed and varying only $m_K$, and perform a fit. We use the parameters of the fit to find the value of the form factor at the physical pion and kaon masses $(2m^2_K - m^2_\pi)_{\text{phys}}$, which is also the form factor at the physical strange mass.

For the fit, we assume a quadratic behaviour if the number of strange masses is $n \geq 4$ (in order to keep the fit over-constrained), and linear otherwise. In Figs. 4.4-4.7 we can see linear and quadratic $m_s$ fits, for the form factor and slope. Like the momentum fit, the $m_s$ fit is typically very precise, such that this interpolation induces yet another small source of systematic error. We examined the error by changing the function which models the momentum behavior (linear, quadratic, quartic), and found that this error is in practice negligible.
4.3 Electromagnetic matrix elements

Figure 4.4. The EM form factor (at $q^2 = 0$), $m_s$ linear fit and extrapolation to $m^\text{phys}_s$, at a fixed pion mass $m_\pi = 318$ MeV, $\beta = 3.9$ and $L = 24a$.

Figure 4.5. The EM form factor (slope), $m_s$ linear fit and extrapolation to $m^\text{phys}_s$, at a fixed pion mass $m_\pi = 318$ MeV, $\beta = 3.9$ and $L = 24a$.

We can see that the strange masses in our simulations are close to the physical point, defined by $m^\text{phys}_\pi = 135$ MeV and $m^\text{phys}_K = 494.4$ MeV, such that $(2m^2_K - m^2_\pi)^\text{phys} = 0.4706\text{GeV}^2$.

Extrapolation in the light quark mass, lattice spacing and finite volume

In lattice simulations, two main quantities cannot be simulated at their physical value. One is the light quarks mass, $m_\ell$, which at its physical value entails a huge calculational cost, and is therefore typically higher – this situation has gradually
4. Numerical results: the electromagnetic form factor

Figure 4.6. The EM form factor (at $q^2 = 0$), $m_s$ quadratic fit and extrapolation to $m_s^{\text{phys}}$, at a fixed pion mass $m_\pi = 304$ MeV, $\beta = 4.05$ and $L = 32a$.

Figure 4.7. The EM form factor (slope), $m_s$ quadratic fit and extrapolation to $m_s^{\text{phys}}$, at a fixed pion mass $m_\pi = 304$ MeV, $\beta = 4.05$ and $L = 32a$.

improved and we can hope that in the future simulations will contain quarks at their physical mass. Our light quark masses are much larger than the physical value – the lowest value in our simulations is 4 times larger than the physical mass, which is a typical situation in contemporary lattice simulations.

The other main artifact is the lattice itself, which cannot be removed in the Monte-Carlo simulation, but its effect can be minimized using an improved action, such as the maximally twisted mass action, and extrapolated to the continuum, as we describe shortly. As an aside, we recall that any divergences as $a \rightarrow 0$ should be removed in the renormalization procedure, and are not regarded as discretization errors in this context, although the renormalization procedure itself introduces $a$-
dependent errors, which are hopefully small (as is the case for $Z_T$, as can be seen in Table 4.2).

As regards the finite lattice size $L$ errors, we found that both from physical considerations, and as demonstrated in our results below, the corrections are small, and were ignored in our calculations.

In practice, after the calculation of the matrix elements at the simulated unphysical lattice parameters, we extrapolate the lattice step $a$, lattice size $L$ and quark masses to their physical values. These extrapolations may be carried out consecutively – one after the other – or all together. We will show the results of both approaches: the consecutive, separate approach allows to gain more insight, while results from the whole extrapolation are more numerically robust. We anticipate that both approaches produced very similar results and statistical errors.

Separate extrapolation in the light quark mass

The light quark mass is connected to the squared pion mass by the chiral perturbation theory relation

$$m^2_\pi = 2Bm_\ell + O(m^2_q) .$$

(4.24)

We fit our data in $m^2_\pi$ and extrapolate to $m^\text{phys}_\pi = 135$ MeV, which is equivalent to a fit and extrapolation of $m_\ell \to m^\text{phys}_\ell$, for each lattice spacing. We take into account the following models:

- linear $f = Am^2_\pi + C$
- quadratic $f = A'm^4_\pi + B'm^2_\pi + C''$
- log-linear $f = A''m^2_\pi ln(m^2_\pi) + B''m^2_\pi + C''$

Unfortunately, we do not always have enough light quark masses to perform a 3-parameter fit: for $\beta = 3.8$ and $\beta = 4.05$ we only have 3 masses, which makes the fit fully-constrained and too sensitive to variations. We can only perform the quartic and log-linear fits for $\beta = 3.9$, and we show the fit results and extrapolation to physical mass in Figs. 4.8-4.9. The linear extrapolations for the other lattice sizes are shown in Figs. 4.10-4.13. We can see that the extrapolated results from the different fit models, for $\beta = 3.9$, are consistent within the statistical error, and the difference between them estimates the error which is due to the unphysical quark masses in the simulations. We can further see that for the same lattice spacing $\beta$, the different lattice sizes $L = 24a$, $L = 32a$ give practically the same results (they are compatible with the fit). This suggests small finite lattice size errors, which is further discussed below. In the plots we can see the disparity between the mass of the simulated light quark and the physical one. We can see how all plots are essentially consistent with a linear behaviour, which is encouraging regarding the validity of the procedure.

Finite size dependence
4. Numerical results: the electromagnetic form factor

Figure 4.8. The EM form factor (at $q^2 = 0$), $m_\pi^2$ fits and extrapolation to $m_{\pi}^{\text{phys}}$, for $\beta = 3.9$, $L = 24, 32$.

Figure 4.9. The EM form factor (slope), $m_\pi^2$ fits and extrapolation to $m_{\pi}^{\text{phys}}$, for $\beta = 3.9$, $L = 24, 32$.

As we can see in Figs. 4.8-4.9, results from two different lattice sizes at the same lattice spacing are compatible, which suggests small finite lattice size errors. Another consideration that brings to the same conclusion is that our lattice size is much greater than the pion “size”: $Lm_\pi \gtrsim 3.3$, which complements our argument. It would seem that extrapolating to an infinite lattice size $L \to \infty$ is superfluous, and we do not concern ourselves further with finite lattice size errors.

Separate extrapolation to the continuum

We now use the extrapolated form-factors at physical masses, at the three different
4.3 Electromagnetic matrix elements

Figure 4.10. The EM form factor (at $q^2 = 0$), $m^2$ fits and extrapolation to $m^{\text{phys}}$, for $\beta = 3.8, L = 24$.

Figure 4.11. The EM form factor (slope), $m^2$ fits and extrapolation to $m^{\text{phys}}$, for $\beta = 3.8, L = 24$.

lattice spacings, to estimate the continuum result. We use an $O(a)$ improved action, which prompts us to expect $O(a^2)$ lattice artifact, so that we fit linearly in $a^2$, and extrapolate to $a^2 \to 0$,

$$f = Aa^2 + B.$$  \hspace{1cm} (4.25)

In Figs. 4.14-4.15 we plot the form factor and slope against $a^2$, along with the linear fits and extrapolated form factor at $a = 0$.

We can see that the zero-momentum form factor is very well described by a linear behaviour. The slope is less so, mainly due to a very large statistical error in the
4. Numerical results: the electromagnetic form factor

\[ f_T(0) = 0.430 \pm 0.066 \], \quad \lambda = 1.61 \pm 0.41 \text{ [GeV}^{-2}] . \quad (4.26)

\[ q^2 = 0 \), \[ m_\pi^2 \] fits and extrapolation to \[ m_{\pi}^{\text{phys}} \], for \[ \beta = 4.05, L = 32 \].

\[ \beta = 4.05 \text{ run}, \] which corresponds to our smallest lattice spacing \[ a = 0.068 \text{ fm} \]. We note that the \[ \beta = 3.9 \] results extrapolated to the physical pion mass have a very small statistical error, as we can expect due to the large number of pion masses which we have in the simulation. The final numerical results obtained in the separate extrapolation, with the statistical jackknife errors, are

Coupled extrapolation to continuum and physical light mass
4.3 Electromagnetic matrix elements

Figure 4.14. The EM form factor (at $q^2 = 0$), $a^2$ fits and extrapolation to $a^2 \to 0$.

Figure 4.15. The EM form factor (slope), $a^2$ fits and extrapolation to $a^2 \to 0$.

An alternative to the separate pion mass and lattice interval extrapolations is a combined fit which takes into account a unified behaviour in mass and lattice interval. This approach is better justified theoretically, since the parameters in the fit are then tied to physical ones instead of changing independently for every lattice interval. A combined fit is also better from a numerical point of view, since we have less parameters to fit, and therefore the fit is more constrained and less susceptible to individual errors. As in previous fits, it was performed for each jackknife separately, from which the average and statistical error was estimated. The combined $a$ and $m_\pi$ fit was evaluated through the models

- $f_T(0)_{\text{quadratic}} = A' + B'm_\pi^2 + C'm_\pi^4 + D'a^2 + E'a^2m_\pi^2$
- $f_T(0)_{\text{logarithmic}} = A + Bm_\pi^2 + Cm_\pi^2 \log(m_\pi^2) + Da^2 + Ea^2m_\pi^2$. 
These fits have 5 parameters, to compare with a total of $2 \cdot 3 + 2 = 8$ parameters for the separate linear fits presented above. This makes the combined fits more robust and less sensitive to stray points. The fits are presented graphically in Figs. 4.16-4.17. In the plots we show also the fitted values for the simulated points (in the lines), for the logarithmic fit only, which is nearly identical to the quadratic

**Figure 4.16.** The EM form factor (at $q^2 = 0$), coupled fit for both $a$ and $m_\pi$. The lines represent the fit results for the same mass and lattice spacing as the fitted points for the logarithmic fit.

**Figure 4.17.** The EM form factor (slope), coupled fit for both $a$ and $m_\pi$. The lines represent the fit results for the same mass and lattice spacing as the fitted points for the logarithmic fit.
4.3 Electromagnetic matrix elements

fit for those points. The fits become separate only when extrapolated far from the simulated points, e.g., at $m_s^{\text{phys}}$ and $a = 0$, as we can see in the plots. Numerically, the results obtained in the combined fit and extrapolation shown in Figs. 4.16-4.17, are

\[
\text{quadratic: } f_T(0) = 0.499 \pm 0.058, \quad \lambda = 1.44 \pm 0.38 \text{ [GeV}^{-2}] \\
\text{logarithmic: } f_T(0) = 0.465 \pm 0.058, \quad \lambda = 1.49 \pm 0.39 \text{ [GeV}^{-2}] .
\]

4.3.2 Systematic errors and optimization

We have several sources of systematic error:

- Proximity to the sources – minimized by using for the plateau a range of points far from the sources.
- Transferred momentum squared fit – expressed in the range of momentum points considered.
- $m_s$ fit – negligible.
- Finite lattice size $L$ – negligible.
- Finite lattice spacing and unphysical quark masses – $a$ and $m$ extrapolations – evaluated by the difference in the various fit models, described above.

In this list we also see the parameters which enter the various fits and extrapolations and influence the results.

The statistical error is estimated using the jackknife procedure, which was described above in 3.4, and is a measure of the difference between the correlation function calculated with different gauge configurations. Values calculated with the same gauge configurations are correlated, which means that their statistical errors are highly interdependent. In general, extrapolations on correlated values will produce results with statistical errors similar to the ones in the fit, with little dependence on the fit method, which will induce a very small systematic error.

The $a$ and $m$ fits are performed over uncorrelated values. This can also be seen graphically in Figs. 4.8-4.15, where the extrapolated error is very different from the errors on the fitted values: in some cases it is significantly larger than the individual errors, while in others it is smaller. On the other hand, the extrapolation in momentum to $f_T(0)$ and in $m_s$ to the physical strange mass have correlated errors, where interpolation does not increase the error. For this reason the $f_T(0)$ and $m_s^{\text{phys}}$ interpolated values have an error equal to the surrounding points.

The final fits give of themselves an error increase. To estimate our sensitivity to the fits, we tried 3 approaches, as described above. Our results are a weighted average and error of these three approaches. In addition, we remark that the logarithmic combined fit was found to have the smallest statistical error, but this does not influence our final results since we average over the individual methods. We note that we do not report any systematic error.
4.3.3 Extrapolated results

In Table 4.3 we give the numerical results obtained from the separate $m_\pi$ and $a$ extrapolations, along with the previous prediction, of [10], described above. In Figs. 4.18-4.19 we show the same results in a graphical form.

<table>
<thead>
<tr>
<th>fit</th>
<th>$f_T(0)$</th>
<th>$\lambda$ [GeV$^{-2}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Becirevic (2001)</td>
<td>0.770 ± 0.062</td>
<td>1.207 ± 0.055</td>
</tr>
<tr>
<td>linear, separate</td>
<td>0.430 ± 0.066</td>
<td>1.61 ± 0.41</td>
</tr>
<tr>
<td>logarithmic</td>
<td>0.465 ± 0.058</td>
<td>1.49 ± 0.39</td>
</tr>
<tr>
<td>quadratic</td>
<td>0.499 ± 0.058</td>
<td>1.44 ± 0.38</td>
</tr>
</tbody>
</table>

Table 4.3. Results for the EM form-factor, after extrapolations to $m_\pi^{\text{phys}}$ and $a \to 0$.

Figure 4.18. Comparison of the EM form factors (at $q^2 = 0$): those obtained in this work with different methods, and previous result.

Figure 4.19. Comparison of the EM form factors (slope): those obtained in this work with different methods, and previous result.

We note that the momentum slope of Becirevic et al. is evaluated assuming a linear behaviour in the square momentum,

$$f_T(q^2) = f_T(0) \left( 1 + \frac{\lambda_T}{m_\pi^2} q^2 \right).$$  \hspace{1cm} (4.28)
4.3 Electromagnetic matrix elements

Our definition is similar for small momenta, since the first order Taylor expansion of the pole fit will give a linear term in $q^2$ with the same coefficient,

$$f_T(q^2)^{\text{(new)}} = \frac{f_T(0)}{1 - q^2 \lambda} = f_T(0) \left(1 + \lambda q^2 + O(q^4)\right). \quad (4.29)$$

The two coefficients are connected by the pion mass,

$$\lambda = \frac{\lambda_T}{m_\pi^2}. \quad (4.30)$$

Our results seem fairly compatible, irrespectively of the extrapolation method we used, and have a similar statistical accuracy. We performed a simple average on each jackknife and calculated the jackknife error described before. The values are correlated, and the statistical error after averaging decreases. We report as our final result

$$f_T(0) = 0.458 \pm 0.074, \quad \lambda = 1.53 \pm 0.25 \, [\text{GeV}^{-2}]. \quad (4.31)$$

### 4.3.4 Discussion

The 2001 results by Becirevic et al. [10] were obtained using a quenched ($n_f = 0$) Monte-Carlo, with high sea-quark masses ($530 < m_\pi < 800 \text{MeV}$) and one lattice spacing ($a^{-1} = 2.7(1) \, \text{GeV}$). We were able to make use of the improved twisted-mass action, new algorithms and enhanced computing power to improve the statistical accuracy and range of parameters. The slope of the form factor at zero momentum is compatible (within accuracy) to the results of 2001. However, we can see a large discrepancy between the form-factor calculated by us and that calculated by Becirevic et al. We tried to investigate the difference in the results by plotting the Monte-Carlo results before extrapolations: our results and previous ones side by side. The 2001 results have a different pion and kaon mass range, and one way of comparing the results would be to use only $m_K = m_\pi$, or in other words the $\pi - \pi$ form-factors. We show this comparison in Figs. 4.20-4.21. Comparing also with the results of Brommel et al. [11], we show in Fig. 4.22 all results for $f_T(0)$ of the three collaborations superimposed.

We can see that the results are actually compatible to within statistical accuracy. In addition, our direct Monte-Carlo results have a better statistical accuracy of $f_T(0)$ and a comparable accuracy of the slope, which worsens at lower sea-quark mass and also worsens after the extrapolations. This plot shows that a major discrepancy is due to a “bend” in the curve of the form factor as a function of pion mass, in the range of our smaller light quark masses, which was not visible in the previous simulation due to the larger masses available.

Another major possible source of error is the quenched approximation. We (and Brommel et al.) are using $n_f = 2$, where the strange quark is not present, while the previous result was quenched. Understanding the difference between our and Becirevic’s results would require additional quenched simulations at lower quark masses.
Figure 4.20. The EM $\pi - \pi$ form factor (at $q^2 = 0$), our results compared with Becirevic et al. (2001) results.

Figure 4.21. The EM $\pi - \pi$ form factor (slope), our results compared with Becirevic et al. (2001) results.
Figure 4.22. The EM $\pi - \pi$ form factor (at $q^2 = 0$), our results compared with Becirevic et al. (2001) and Brommel et al. (2008) results.
Chapter 5

Renormalization of the chromomagnetic operator

5.1 Operator mixing

We have calculated in a lattice Monte-Carlo simulation the matrix element of the chromomagnetic (CM) effective operator between kaon and pion states, \( \langle K | Q^R_{CM} | \pi \rangle \), where

\[
Q_{CM} = g \bar{s} t^a G^{\mu \nu} \sigma_{\mu \nu} d .
\]

(5.1)

A general discussion of the operator product expansion and of the renormalization of effective operators can be found in [2] (Ch.18). The constant

The need to renormalize comes from divergences which arise when we try to remove the dependence of the matrix element on regulator, and set it to its continuum value \( a \rightarrow 0 \). From a perturbative point of view, the divergences arise from quantum corrections (1-loop and up) to the matrix element. In addition to the divergence of the operator itself, which is corrected by the “multiplicative” renormalization constant \( Z_{CM} \), quantum corrections to the amplitude will contain contributions from mixing with other operators. We need to identify these operators and subtract their contributions, which are possibly divergent. The operators will mix in a linear combination of operators and “additive” renormalization constants. A general relation between the bare operator and the renormalized one can be written as

\[
Q^R_{CM} = Z_{CM} \left[ Q_{CM} + \sum_i Z_i Q_i \right] .
\]

(5.2)

The chromomagnetic operator is of dimension \( d_{CM} = 5 \) (1.5 for every fermion field and 2 from \( F_{\mu \nu} \)). From dimensional analysis we can see that operators of dimension equal to the chromomagnetic operator dimension will contribute, at most, divergences which are logarithmic in \( a \). Lower dimension \( d \) operators, however, will induce power-divergent contributions in \( a \), which are at worst of order \( 1/a^{(5-d)} \), and are of lower order when the operators are multiplied by some combination of quark masses, as will be seen shortly.
Renormalization of the CM operator in previous works

In [39] the chromomagnetic operator was renormalized perturbatively in the continuum dimensional regularization, where the operator was considered to mix only with other 5D operators. The CM operator was renormalized non-perturbatively, multiplicatively (without taking into account operator mixing) in heavy quark effective theory [40]. Non perturbative renormalization for 6D operators, where the chromomagnetic operator is one of the mixing operators was done in [41]. We lay out a plan for the renormalization of the CM operator in the spirit of these works, and we thank R. Frezzotti [43] for his help in this analysis.

5.1.1 Analysis

The mixing operators $Q_i$ are those with the same quantum numbers as the chromomagnetic operator, of equal or lower mass dimension $1$. We write here the considerations which have to be taken into account for the identification of these operators:

- The relevant operators are those which have a non-vanishing $\langle K | Q_i | \pi \rangle$ matrix element.
- The operators need have $\bar{s}d$ external legs.
- The mass dimension should be $d \leq 5$. Terms with lower mass dimension will contribute power divergences, $1/a^{(5-d)}$.
- The operators with their coefficients should obey the same symmetries as the action, which is the maximally twisted mass action in our case. The symmetries are written in short below and analyzed in App. B.
- The operators should be gauge invariant, since the CM operator is gauge invariant, and the renormalization procedure maintains the gauge invariance.
- The matrix element is calculated on-shell. All the dependence on external momenta is accompanied by a gluon field to preserve gauge-invariance into $D_{\mu}$, and all $D$ become masses due to the equations of motion. In this case also, the renormalization procedure maintains the on-shell relation. Note that when the RI-MOM renormalization procedure is applied, both non-gauge-invariant operators and operators vanishing by the equations of motion should be taken into account. The operators must still respect, however, the BRST symmetry, which is an exact symmetry of the action.

Symmetries of the action

The symmetries depend on the particular form chosen for the action, which in our case is the maximally twisted mass action. This discussion follows [17, 42, 43, 44]. In continuum QCD, we have CPS spurionic symmetry,

$$CPS : \quad C \times P \times (s \leftrightarrow d) ,$$

$1$ Peskin & Schroeder, p.430.
where the “spurionic” requirement imposes that also constants such as the mass change under the symmetry, for example, \( m_s \leftrightarrow m_d \). The continuum chiral structure is invariant under the transformation

\[
R_5 : \quad \psi \rightarrow \psi' = \gamma_5 \psi, \quad \bar{\psi} \rightarrow \bar{\psi}' = \gamma_5 \bar{\psi}.
\]

In the Wilson action we have the spurionic symmetry

\[
R_5^W = R_5 \times [r \rightarrow -r] \times [m \rightarrow -m].
\]

The twisted mass action in the physical quark basis (Eq. (2.43)) in maximal twist \( \omega = \pi/2 \) is

\[
S = a^4 \sum_x \bar{\psi}_x^{\text{phys}} \left\{ \frac{1}{2} \gamma_\mu \left( D_\mu + D_\mu^b \right) - i \gamma_5 \tau_3 \left( - \frac{ar}{2} D_\mu D_\mu^b + M_{cr}(r) \right) + m_q \right\} \psi_x^{\text{phys}}. \tag{5.6}
\]

This action is symmetric under the particular spurionic symmetry transformations \[43\]

\[
C \times [s \leftrightarrow d] \times [m_s \leftrightarrow m_d], \tag{5.7}
\]

\[
P \times D_d \times [\text{all } m \leftrightarrow -m]. \tag{5.8}
\]

The symmetries are written in detail in App. B, where we also analyze the transformation under these symmetries, of the operators which possibly mix with the chromomagnetic operator.

The above considerations lead to the following mixing operators:

- \( Q_s = \bar{s}d \) (scalar operator)
- \( Q_{ps} = \bar{s}\gamma_5 d \) (pseudo-scalar operator)

which can mix with the chromomagnetic operator multiplied by the following mass combinations \[43\]

\[
\begin{align*}
\text{Dimension 3} & - a^{-2} \bar{s}d, \tag{5.9} \\
\text{Dimension 4} & - a^{-1} (m_s + m_d) \bar{s}\gamma_5 d, \tag{5.10} \\
\text{Dimension 5} & - (m_s^2 + m_d^2) \bar{s}d, \tag{5.11} \\
&m_s m_d \bar{s}d. \tag{5.12}
\end{align*}
\]

Note that the pseudoscalar operator \( \bar{s}\gamma_5 d \) mixes with the chromomagnetic operator, although their parity is opposite. This mixing is only allowed with twisted mass fermions, which explicitly break parity at finite lattice spacing.

The “wrong chirality” operator \( Q_{CM5} = \bar{s}G^{\mu\nu} \sigma_{\mu\nu} \gamma_5 d \) would mix multiplied by a factor \( (m_s - m_d) \), which makes it a 6-dimensional operator, and therefore not relevant here.

Another operator which comes to mind is the electromagnetic one,

\[
Q_{EM} = \bar{s}F^{\mu\nu} \sigma_{\mu\nu} d. \tag{5.13}
\]
This operator has the photon as external boson instead of the gluon in the chromomagnetic operator. We do not have photons on our QCD lattice, therefore this mixing, which would appear at $\mathcal{O}(\alpha_s\alpha_{EM})$, is absent.

The fully renormalized operator can be written with its explicit dependence on the bare operators

$$Q_{CM}^R = Z_{CM} \left[ Q_{CM} + \bar{s}d \left( \frac{c_1}{a^2} + c_2(m_s^2 + m_d^2) + c_3m_sm_d \right) + \bar{s}\gamma_5d \frac{c_4}{a}(m_s + m_d) \right].$$

(5.14)

The calculation of the $\langle s|Q_{CM}|dg \rangle$ matrix element (between a gluon and strange and down quarks), in lattice perturbation theory can produce in principle the full renormalization pattern of the operator, including its mixing with all other operators. However, as we mentioned before, renormalization coefficients of lower-dimension operators have a power divergence. They are not accurate in perturbation theory due to a non-expandable factor of $\frac{1}{\alpha_e} e^{-\frac{\alpha}{\alpha_e}}$, consequently they will have to be calculated non-perturbatively. The renormalization coefficients of 5D operators, on the other hand, have no power divergence, only a logarithmic one. These can be calculated in lattice perturbation theory. Even though the numerical coefficients are not accurate, the perturbative matrix element can give analytically the quark masses dependence and pattern of the mixing operators, which can serve as a check of our analysis.

### 5.2 Non-perturbative subtraction

We have shown the mixing pattern of the renormalized chromomagnetic operator in Eq. (5.14) above, which follows from the symmetry of the action,

$$Q_{CM}^R = Z_{CM} \left[ Q_{CM} + \bar{s}d \left( \frac{c_1}{a^2} + c_2(m_s^2 + m_d^2) + c_3m_sm_d \right) - \bar{s}\gamma_5d \frac{c_4}{a}(m_s + m_d) \right] + \mathcal{O}(a).$$

(5.15)

What remains is to calculate the coefficients. As we mentioned before, the power divergent coefficients need to be calculated non-perturbatively. We show here how the coefficients can be calculated, up to finite discretization errors, from our Monte-Carlo correlation functions. Due to the particular construction of the continuum chromomagnetic operator, which we can see in chiral perturbation theory in Eq. (3.56), the matrix element between two particles $K$ and $K'$ at rest is proportional to $m_K \cdot m_{K'}$. We recall here the full form

$$\langle \pi^0|Q_{CM}^R|K^0 \rangle = -\frac{11B_{CM}}{32\sqrt{2}\pi^2} \frac{m_K^2}{m_s + m_d} p_\pi \cdot p_K.$$

(5.16)

There are several ways to find the coefficients, depending on the specific relations that we impose. We delineate two possible ways below.
5.2 Non-perturbative subtraction

5.2.1 Separate coefficient subtraction

First, we can see that in the chiral limit, for two particles at rest, the renormalized matrix element is null. The $c_1$ parameter can thus be calculated by

$$c_1 \frac{a}{a^2} = \frac{\langle K | Q^b_{CM} | \pi \rangle}{\langle K | \bar{s}d | \pi \rangle} \bigg|_{p_s=p_d=0},$$

(5.17)

noting that zero 4-dimensional momentum means also zero mass (chiral limit). Thus, we get the first subtracted operator

$$Q_{CM}^{\text{sub}} \equiv Q_{CM}^{\text{bare}} - c_1 \frac{a}{a^2} \bar{s}d.$$

(5.18)

Next, in order to eliminate $c_4$, we use the $K - 0$ matrix element, noting that up to $O(a^2)$, both the renormalized chromomagnetic operator and $\bar{s}d$ contribute zero to this matrix element,

$$c_4 \frac{a}{a^2} (m_s + m_d) = \frac{\langle K | Q_{CM}^{\text{sub}} | 0 \rangle}{\langle K | \bar{s}\gamma_5 d | 0 \rangle},$$

(5.19)

assuming that $r_s = r_d$. After subtracting the $c_4$ contribution we call the operator $Q_{CM}^{\text{sub}14}$. The two non-divergent coefficients can be subtracted by noting that the chromomagnetic operator cannot have an on-shell contribution for two particles at rest, i.e., for an off-shell process. We impose the following condition for two separate mass combinations,

$$0 = \langle K | Q_{CM}^{\text{sub}14} | \pi \rangle \bigg|_{\bar{p}_s=\bar{p}_d=0, \ m_s=bm_d},$$

(5.20)

where arbitrarily $b = 1, 3$ for example. Solving the two equations we get the coefficients $c_2$ and $c_3$. We can then subtract these two contributions to get the fully subtracted chromomagnetic operator $Q_{CM}^{\text{sub}}$, which does not mix with other operators and diverges only logarithmically with $a$. It is connected to the renormalized operator by

$$Q_{CM}^{R} = Z_{CM} Q_{CM}^{\text{sub}}.$$

(5.21)

5.2.2 Combined coefficient fit

A second approach involves the chiral perturbation theory expansion to first order of the renormalized operator of Eq. (5.16). For particles at rest ($\bar{p}_s = \bar{p}_d = 0$), we assume a constant $B_{CM}$ for all masses. We can use these properties to construct an equation which connects the renormalized and bare chromomagnetic matrix elements, with those of the scalar and pseudoscalar with the mixing pattern mentioned above. In this way we get an equation with 5 coefficients, which we can fit for all mass combinations, as we describe below.

In our Monte-Carlo simulation, the particles are mesons composed of one valence quark (which participates in the flavor-changing operator) and one light sea quark
Renormalization of the chromomagnetic operator

(spectator), with opposite $r$ constants. The mesons can be written as $K = \bar{q}_1 \gamma_5 q_\ell$, $K' = \bar{q}_2 \gamma_5 q_\ell$. Manipulating the equation we get

$$\frac{\langle K | Q_{CM}^b | K' \rangle}{\langle K | \bar{q}_1 q_2 | K' \rangle} = \frac{c_1}{a^2} + c_2 (m_1^2 + m_2^2) + c_3 m_1 m_2 + \frac{\langle K | \bar{q}_1 \gamma_5 q_2 | K' \rangle}{\langle K | \bar{q}_1 q_2 | K' \rangle} \frac{c_4}{a} (m_1 + m_2) + O(a),$$

(5.22)

which is a linear equation connecting two ratios of matrix elements. We call these ratios $R_1$ and $R_2$,

$$R_1 \equiv \frac{\langle K | Q_{CM}^b | K' \rangle}{\langle K | \bar{q}_1 q_2 | K' \rangle}, \quad R_2 \equiv \frac{\langle K | \bar{q}_1 \gamma_5 q_2 | K' \rangle}{\langle K | \bar{q}_1 q_2 | K' \rangle}.$$

(5.23)

We can perform the matrix element extraction for each mass combination calculated on the lattice and fit the functional form above. Such a fit, if it is successfully performed with small error, can confirm our analysis and renormalization procedure. However, at one lattice spacing the discretization errors cannot be seen, and only by plotting the coefficients obtained from the fit as a function of $a$ one can see whether these errors are present. Furthermore, it is not clear that setting one renormalization condition can define all the coefficients, although one can argue that there are many conditions, i.e. one for every mass combination, which are admittedly all of the same kind.

Unfortunately, Monte-Carlo runs are still underway, and we do not have yet ready enough results to perform good fits.

5.3 Perturbative renormalization

5.3.1 Lattice perturbation theory

Lattice perturbation theory is an approximation method that is used to calculate correlation functions in the lattice regularization. For further reading on lattice perturbation theory, see for example [45]. Although the lattice was initially introduced by Wilson as a framework for studying strongly coupled theories, such as QCD, non-perturbatively, it was found to be a regularization also suitable for perturbative calculations. Perturbation theory involves an expansion in the coupling constant, and is well-justified in high-energy QCD where the coupling constant is small, while it fails completely when the coupling is large and higher order corrections are larger that lower orders in the perturbative series. In this region non-perturbative methods, such as Monte-Carlo sampling of the correlation function, are necessary. Lattice perturbation theory is very important for several reasons. Since it involves high energy and small distances, it is a natural way to match the lattice action to the continuum – hence it is one of the simpler ways to renormalize non-perturbative lattice calculations. Although perturbation theory is more involved in lattice regularization than, e.g., using dimensional regularization in the continuum, it is in some cases essential to complete the non-perturbative lattice calculations. For example, when calculating a renormalization constant of a non-perturbative lattice
5.3 Perturbative renormalization

Simulation, the renormalization constant must be calculated with the same lattice action for consistence. A thorough treatment of continuum perturbation theory can be found in [2, 46].

Lattice perturbation theory may even provide invaluable insight into condensed matter theory, in calculations where the lattice represents the real atomic crystal. In this case the lattice step $a$ is a physical value and not an artifact to be removed, and a quantum field theory can be formulated and solved on the physical lattice. See e.g. [47] for a recent work in this spirit, applied to a mono-layer hexagonal graphene lattice.

5.3.2 Perturbative renormalization method

The perturbative, multiplicative renormalization (the $Z_{CM}$ coefficient of Eq. (5.14)) eliminates the $\log(a)$ divergences which remain after the power-divergences subtraction. To the best of our knowledge the chromomagnetic operator has never been renormalized before in lattice perturbation theory. We chose to calculate the multiplicative renormalization coefficient $Z_{CM}$ in lattice perturbation theory, up to leading order – 1-loop, $g^2$ order. The formalism entails calculating the amplitude as a sum of Feynman diagrams. For consistence, we need to use the Feynman rules of the same action that we used in the Monte-Carlo calculation of the correlator, which is the maximally twisted mass fermion action with the Symanzik tree-level improved gluon action. We chose to renormalize using RI-MOM, which connects the tree-level and 1-loop amplitude, while the amplitude chosen was the quark-quark-gluon Green function, since it seems the simplest choice. We could have equally chosen the 2-quarks-2-gluons Green function, which would require a larger number of 1-loop diagrams.

Definitions

The RI-MOM scheme was described above in Ch. 3.5.1, for the case of bilinear operators of the form

$$Q_\Gamma = \bar{q}_i \Gamma q_j ,$$

where $q_i$ and $q_j$ represent the external quarks and $\Gamma$ is some combination of gamma matrices.

We need to write the renormalization conditions in an explicit form specific to the chromomagnetic operator. The bare operator is

$$Q_{CM} = g s t^a G^a_{\mu \nu} \sigma_{\mu \nu} d .$$

As we mentioned above, the simplest implementation is to impose the renormalization condition on the quark-quark-gluon 3-point Green function,

$$G(p) = \left\langle s(p_s) A^\nu(p_A) Q_{CM} d(p_d) \right\rangle .$$

The method is defined for one single momentum scale which we call $\mu$. This leads naturally to the so-called “democratic” choice of external momenta

$$p_A^2 = p_s^2 = p_d^2 = p^2 = \mu^2 .$$
With this symmetric choice the method has been called RI/SMOM [48]. The 1-loop calculation is performed in the twisted basis, so we need to rotate the action as well as the effective operators to this basis. The twisted basis rotation of the quark fields from physical quark doublets \( \Psi \) to twisted quarks \( X \) is

\[
X = \exp\left\{-\frac{i}{2} \gamma_5 t_3 \omega \right\} \Psi, \quad \bar{X} = \bar{\Psi} \exp\left\{-\frac{i}{2} \gamma_5 t_3 \omega \right\},
\]

where

\[
t_3 = \begin{pmatrix}
1 & 0 \\
0 & -1
\end{pmatrix}
\]

is the twisted flavor matrix which multiplies quark weak \( SU(2) \) doublets. We now separate the doublets and write the relation for each flavor. The singlet spinors are denoted by \( \psi \) (physical basis) and \( \chi \) (twisted basis). The \( t_3 \) matrix contributes a constant that multiplies every quark flavour,

\[
r_u = +1, \quad r_d = -1, \quad r_c = +1, \quad r_s = -1,
\]

such that the rotation for the single quarks is

\[
\chi = \exp\left\{-r_u \frac{i}{2} \gamma_5 \omega \right\} \psi, \quad \bar{\chi} = \bar{\psi} \exp\left\{-r_s \frac{i}{2} \gamma_5 \omega \right\}.
\]

For \( s, d \) quarks, in the maximal twist (\( \omega = \pi/2 \)), the rotation is

\[
\chi = e^{\frac{i \pi}{4} \gamma_5} \psi, \quad \bar{\chi} = \bar{\psi} e^{\frac{i \pi}{4} \gamma_5}.
\]

The vertex in the twisted basis absorbs the rotation,

\[
\tilde{\Gamma} = e^{i \gamma_5 \pi/4} \Gamma e^{i \gamma_5 \pi/4},
\]

which for our operator \( \Gamma_{CM} = gG^{\mu\nu} \sigma_{\mu\nu} \) becomes

\[
\tilde{\Gamma} = e^{i \gamma_5 \pi/4} gG^{\mu\nu} \sigma_{\mu\nu} e^{i \gamma_5 \pi/4} = ig \gamma_5 G^{\mu\nu} \sigma_{\mu\nu}.
\]

The tree level values of all our propagators and vertices, which are required for the tree-level values of the RI-MOM renormalization, are given in App. A. The gluon renormalization constant \( Z_A \) is found from setting the renormalized inverse propagator equal to its tree-level value,

\[
Z_A^{-2}(\mu)[S_A^{-1}(p)]_{\mu\rho} = [S_A^{-1}(p)]_{\mu\rho}^{\text{tree}}.
\]

For the quark field renormalization condition, we write the general structure of the quark propagator in the twisted mass action,

\[
S_q^{-1}(p) = i\tilde{\rho}_q \Sigma_3(p) + \Sigma_2(p^2) - i\gamma_5 \Sigma_3(p^2),
\]

which is exact at tree level and for quantum corrections up to \( O(a^2) \) terms, and where \( \tilde{\rho}_q \equiv \frac{1}{a} \sin(\alpha p_\nu) \), and the tree-level values of \( \Sigma_1, \Sigma_2 \) and \( \Sigma_3 \) are taken from the twisted-mass action in the twisted basis,

\[
\Sigma_1(p^2) = 1, \quad \Sigma_2(p^2) = \mu_q, \quad \Sigma_3(p^2) = \frac{ar_q}{2} \tilde{p}^2.
\]
We can see that $\Sigma_2$ is mainly due to the quark bare mass which is zero in massless conditions, while $\Sigma_3$ is mainly a discretization artifact. $\Sigma_1$ is

$$\Sigma_1(p) = -i \text{Tr} \left[ \hat{P}_\nu S_q^{-1}(p) / \hat{p}_\nu \right], \quad (5.38)$$

where the projector $\hat{P}_\nu = \gamma_\nu / 4 N_c$, where $N_c = 3$ is the number of colors, such that $\text{Tr} \left[ \hat{P}_\nu \hat{p} / p_\nu \right] = 1$. We impose the quark renormalization condition on $\Sigma_1$ as defined above,

$$Z_q^{-1}(\mu) \Sigma_1(p) \bigg|_{p^2 = \mu^2} = 1. \quad (5.39)$$

The renormalization condition we impose, in the spirit of RI-MOM, is that the renormalized amplitude is set to be equal to its tree-level value, in Euclidean space,

$$G_\rho(p) \bigg|_{p^2 = \mu^2} = \langle s(p_s) A_\rho(p_A) | Q_{CM} | d(p_d) \rangle \bigg|_{p_A^2 = p_s^2 = p_d^2 = \mu^2} = \langle s(p_s) A_\rho(p_A) | Q_{CM} | d(p_d) \rangle \bigg|_{p_A^2 = p_s^2 = p_d^2 = \mu^2}. \quad (5.40)$$

We note that the amplitude here was not projected or amputated. Projectors are necessary for renormalization of a numerical Monte-Carlo amplitude, since otherwise one cannot identify the various operators in the expression. However, in our analytic calculation in perturbation theory, projectors are not mandatory because we can explicitly see the operators, gamma matrices, Lorenz indices, spin elements and so on. The condition will be projected on to the chromomagnetic operator when we make contact with a non-perturbative renormalization.

### 5.3.3 1-loop amplitude calculation

The perturbative calculation starts with obtaining the Feynman rules from the action. The action is Symanzik tree-level improved for gluons – which defines the gluon propagator and gluonic vertices (and ghosts), and maximally twisted mass Wilson fermion action – which defines the quark propagator and quark-gluon vertices. The fermion action also included the Sheikholeslami-Wohlert (SW or clover) term [49] – which contributes to the gluon-fermion vertices. The SW term is always found multiplied by a constant $c_{SW}$ which is tuned in order to improve the action. We do not have this term in the Monte-Carlo lattice action since the maximally twisted mass action is already improved, yet in the perturbative calculation it costs negligible additional effort, and we included it in order to get more general results. All the Feynman rules have been published previously, but are included here in App. A for completeness. The relevant vertices up to $O(g^3)$ are: 2-fermion vertices with one or two gluons, a 3-gluon vertex, 4 gluon vertex, gluon-gluon-ghost and 2-gluons-2-ghosts vertices, plus the chromomagnetic operator itself with external legs of 2 fermions and one, two or three gluons.

We have identified 11 diagrams for the amputated, one-loop, $s - d$-gluon 3-point Green function, which are shown in Fig. 5.1. The sign $\otimes$ in the diagrams indicates the chromomagnetic operator insertion. These diagrams were also shown in [39].

In addition, we have the 1-particle reducible diagrams in Fig. 5.2, which can be described as an $sd$ propagator insertion which describes effective flavour mixing, or
Figure 5.1. The Feynman diagrams which contribute to the perturbative renormalization of the chromomagnetic operator.
as a non flavor diagonal effective propagator, or as mixing with the scalar operator $\bar{s}d$. This insertion is not considered part of the quark renormalization. We do not calculate these full diagrams, since the 1-loop calculation for $12a$, $13a$ is redundant, as well as for $14a$, $15a$. We therefore calculate at 1-loop only the two 2-point diagrams of Fig. 5.3.

![Diagram 12a and 13a](image1)

**Figure 5.2.** 1-particle reducible 3-point Feynman diagrams which contribute to the perturbative renormalization of the CM operator, with the loop indicating mixing with the scalar operator.

![Diagram 14a and 15a](image2)

**Figure 5.3.** Scalar operator mixing Feynman diagrams which contribute to the perturbative renormalization of the CM operator.

Another diagram which comes to mind is the one shown in Fig. 5.4, which indicates mixing with the gluonic operator $G^{\mu\nu}G_{\mu\nu}$. This diagram does not exist for our $s \rightarrow d$ flavor changing chromomagnetic operator, since the quark-quark-gluon

![Diagram 12 and 13](image3)

**Figure 5.4.** 1-particle reducible 3-point diagram indicating mixing with the gluonic operator, exists only for a singlet chromomagnetic operator, which is not our case.
vertices below are flavor diagonal in QCD. This diagram would exist for a singlet chromomagnetic operator,

\[ Q_{CM}^{\text{singlet}} = g \bar{q}_i G^{\mu \nu} \sigma_{\mu \nu} q_i. \]  

The remaining 1-loop diagrams include the quark propagator renormalization in Fig. 5.5, and the gluon propagator renormalization in Fig. 5.6.

**Figure 5.5.** Diagrams which contribute to the renormalization of the quark propagators.

**Figure 5.6.** Diagrams which contribute to the renormalization of the gluon. The ⋄ insertion is the measure part of the action, which is the Jacobian of the functional integral, added when changing variables from links \( U_{x,\mu} \) to vector fields \( A_\mu(x) \).

The calculation itself was performed in Mathematica, using a specialized routine set developed by H. Panagopoulos [32]. The routines are used to manually construct in analytical form the amplitudes for each Feynman diagram, and then manipulate semi-automatically the terms until all can be evaluated either analytically or numerically. In the manipulation, Mathematica is used for “book-keeping” and none of the advanced, “black-box” functions, such as Simplify and Integrate, are used. Where integrals, limits, simplifications etc. are needed, they are performed by substitution, as we describe below. Thus the procedure combines the advantages from
both hand-manipulation and computer processing, while simplifications of Mathematica which may make the calculation easier are not used, in favor of total control over the output. The terms evaluated numerically are transformed to a Fortran code which performs a numerical integration as described below. The results, numerical and analytical, are re-combined in Mathematica to give the final result.

**Simplifications**

We treated each term of the amplitude until it could be either integrated numerically on the lattice (“lattice convergent terms”) or has IR divergences which have to be evaluated analytically. We denote by $q_i$ an external momentum and by $p$ the internal momentum over which we integrate. No UV divergences occur because of momentum periodicity, which imposes integration over momentum up to $ap_{\text{max}} = \pi/2$. The IR behaviour is determined by power counting of momenta with $p, q \to 0$. The general form of the terms to be evaluated is, in this limit,

$$\int_{-\pi}^{\pi} \frac{d^4p}{(2\pi)^4} \frac{A(p, q)}{(p^2)^a((p + q_2)^2)^b},$$

where $q$ is an external momentum, and $A(p, q)$ is a polynomial of momenta. The denominator shown is only one example of the denominators that appear, which can also have different external momenta dependence.

The term shown above is written in a simple form, which is not available from the start. The terms had to be expanded and simplified, using well-known techniques: trigonometric expansion to the simplest argument, Taylor expanding in powers of $q$ while keeping only one power for our order of calculation (only in convergent terms; for diverging terms all powers of $q$ are kept). In order to get to the simplest denominator we used the convergent difference between the term and a divergent simpler term with the same power counting:

$$I = [I - I_{\text{simple}}]^{(\text{convergent})} + [I_{\text{simple}}]^{(\text{divergent})}.$$  

(5.43)

Another simplification substitutes the gluon propagator of the Symanzik improved action into a sum of the simple plaquette gluon propagator and a difference,

$$D(q) = D_{\text{plaq}}(q) + D(q) - D_{\text{plaq}}(q)$$

$$= D_{\text{plaq}}(q) + D_{\text{plaq}}(q) \left[ D^{-1}_{\text{plaq}}(q) - D^{-1}(q) \right] D(q),$$

(5.44)

where the plaquette propagator retains the higher IR degree of divergence, and the term with the difference of inverse propagator has a $+2$ degree of IR divergence in the momentum with respect to the propagator, which in our case makes it convergent and calculable numerically. This means that we do not need to use the analytical form of the gluon propagator which is quite involved, but can use the inverse form which is much more compact.

IR convergent terms are those which have a power count of $P > -3$, not counting the momentum from the Jacobian ($d^4p$). These convergent integrals were calculated
numerically on several lattices of sizes up to $128^4$, and the result was extrapolated to infinite lattice size.

IR non-convergent terms are those which have a power count of $P \leq -3$, and in our calculation IR divergent terms all have a power count of exactly -3. For example, a divergent term can be one of

$$\int_{-\pi}^{\pi} \frac{d^4 p}{(2\pi)^4} \frac{p^2 p_\mu ; q^2 p_\mu ; q^2 q_\mu}{p^2((p + q)^2)^2}.$$  (5.45)

We now separated the superficially divergent integrals according to the powers of the external momentum $q$ in the numerator.

“Lattice” divergent terms have one or zero powers of $q$ in the numerator, and cannot be converted to the continuum since they would diverge also in the UV. For their calculation we use tabulated divergent lattice integrals, which give rise to $\log(q)$ terms.

“Continuum” integrals contain more than one power of $q$, and has no UV divergence even if calculated between $-\infty < p < \infty$, i.e., on the continuum. These integrals actually converge both on the lattice and on the continuum, but cannot be calculated numerically on the lattice. The conversion to continuum is performed using

$$\int_{-\pi}^{\pi} I = \int_{-\pi}^{\pi} (I - I^{p=0} + I^{p=0}) = \int_{-\pi}^{\pi} \Delta I_0 + q^2 \left( \int_{-\pi}^{\pi} J - \int_{-\infty}^{\pi} J + \int_{-\infty}^{\pi} J \right)$$

$$= \int_{-\pi}^{\pi} \Delta I_0 + q^2 \Delta \int J + q^2 \int_{-\infty}^{\pi} J,$$  (5.46)

where $\Delta I_0 = I - I^{p=0}$ and $J = I^{p=0}/q^2$. The first term on the r.h.s., $\Delta I_0$, is a finite integral which can be calculated numerically. The second term, $q^2 \Delta \int J$, is a finite number times $q^2$, which goes to zero as $q \rightarrow 0$. The last term, $q^2 \int_{-\infty}^{\pi} J$, is a continuum converging integral which presents no conceptual difficulty, and will be calculated with Feynman parameters and dimensional regularization.

We found that the terms contributing to the divergent (logarithmic or power divergent) in a Green’s function have a relatively simple form which can be calculated analytically with no further assumptions. However, in the finite terms (in $a$) there arise integrals of

$$d^4 p \frac{A(p, q)}{(p^2)^2(p + q_1)^2(p + q_2)^2},$$  (5.47)

which have an unwieldy and uninformative structure, involving Spence functions.

In order to simplify the analytical continuum integrals, we want to reduce the number of external momenta. Our renormalization scheme (RI’) allows a freedom of choice of the external momenta. A typical choice would be to set all to zero. However, in our case it is not directly possible since the momentum appears in the operator definition, so setting $q_i = 0$ would lead to a Green function vanishing identically. There are possible workarounds for this problem, such as identifying all linear dependence of the amplitude on the momentum and recombining it as a derivative before setting momentum to zero. We nevertheless chose another external
momenta setting, the so-called “democratic” choice. This sets all momenta squared to a single value

\[ q_1^2 = q_2^2 = q_3^2 = \mu^2, \]  

as anticipated in Eq. (5.27), still keeping momentum conservation

\[ q_1 - q_2 + q_3 = 0, \]  

Where \( q_1 \) is the incoming gluon, \( q_2 \) is the outgoing fermion, and \( q_3 \) is the incoming fermion.

**Continuum divergent integrals**

As we described above, terms which IR-diverge in the continuum limit were reduced to a simple form,

\[ \int_{-\infty}^{\infty} \frac{d^d p}{(2\pi)^d} f(p,q) \left(\frac{2}{p^2(p+q)^6}\right), \]  

which has only one external momentum. We use dimensional regularization, \( \varepsilon = \frac{1}{2}(4 - d) \), where \( d \) is the number of dimensions.

These integrals can be solved for all non-negative integer \( a \) and \( b \) using the Chetyrkin [50] formula.

\[ I(f(p,q)) = \int_{-\infty}^{\infty} \frac{d^d p}{(2\pi)^d} f(p,q) \]  

We use a general covariant gauge, such that the gluon propagator has a free parameter \( \alpha \), as described in the Feynman rules in App. A. The general gauge enables a powerful inside check for the results, which have to be gauge invariant.

### 5.3.4 Perturbative results

We give here the 1-loop results of the perturbative calculation. The external momenta are depicted in Fig. 5.7.

![Figure 5.7](image)

**Figure 5.7.** Definition of the quark-quark-gluon 3-point Green function.

The tree-level amputated 3-point amplitude, in the maximally twisted mass basis, in the limit \( a \to 0 \), is

\[ G_{\nu}^{\text{tree}} = igt^a \gamma_5 (-2i\gamma_\mu q_1^\mu) \sigma_{\mu\nu} = 2gt^a \gamma_5 (q_1^\mu) \left(\frac{1}{2}(\gamma_\mu \gamma_\nu - \gamma_\nu \gamma_\mu)\right) = gt^a \gamma_5 (q_1) = 2 \partial^\mu A^\nu \sigma_{\mu\nu} = -2i q_1^\mu A^\nu \sigma_{\mu\nu}. \]  

noting that \( (\partial^\mu A^\nu - \partial^\nu A^\mu) \sigma_{\mu\nu} = 2 \partial^\mu A^\nu \sigma_{\mu\nu} = -2i q_1^\mu A^\nu \sigma_{\mu\nu} \). We use color symmetry \( SU(N_c) \), where \( N_c = 3 \). The amputated 1-loop Amplitude, with only the 1-particle-irreducible 11 Feynman diagrams, was calculated to lowest order in \( a \) and \( g \). We
set here the clover $c_{SW}$ term to zero. Decimal numbers are the result of numerical integration on the lattice (as described above), and are typically of a precision of $10^{-10} - 10^{-11}$. We truncated the numbers accordingly. We reduced the expression, using gamma matrix algebra and momentum conservation $(q_1 - q_2 + q_3 = 0)$, to terms proportional to $q_2 q_3 (q_2 + q_3)_\nu / \mu^2$, $q_1^\mu \sigma_{\mu \nu}$ and $(q_2 + q_3)_\nu$ only,

$$
G_{11}^{\alpha \ell} = g^3 \gamma_5 t^\alpha \left\{ \frac{\bar{q} \gamma_5 q (q_2 + q_3)_\nu}{\mu^2} \right. \\
\times \left[ \beta (-0.000181485/N_c - 8.370 \cdot 10^{-6} N_c) + (0.000527714/N_c + 0.000263857 N_c) \right] \\
+ q_1^\mu \sigma_{\mu \nu} \left[ \beta (0.006349525/N_c - 0.00788994 N_c) + 0.038657867/N_c - 0.040008287 N_c \\
- 0.000791572 \beta^2 N_c + \beta (- \frac{1}{64 N_c \pi^2} + \frac{3 N_c}{128 \pi^2} - \frac{1}{64 N_c \pi^2} - \frac{17 N_c}{256 \pi^2}) \log (\mu^2) \right] \\
+ (q_2 + q_3)_\nu \left[ \frac{3}{64 N_c \pi^2} - \frac{9 N_c}{256 \pi^2} \log (\mu^2) + \beta (0.000709199/N_c - 0.001578959 N_c) \\
- 0.010365494/N_c + 0.008121153 N_c \right] \}, 
$$

The next step is analyzing the various operators. Operators which may mix with the chromomagnetic one are, as analyzed in Tab. B.1 in the appendix,

$$
\bar{s} D \gamma_\mu d, \quad \bar{s} \gamma^\nu D^\nu d, \quad (m_a + m_d) \bar{s} D d, \quad (m_a + m_d) \bar{s} \gamma^\nu d, 
$$

where $D_\mu$ is the forward covariant derivative and $D^\nu_\mu$ is the backward one. These operators will reduce on-shell to the 5-dimensional operators of Eqs. (5.11) and (5.12), $(m_s^2 + m_a^2)s d$ and $m_s m_d s d$. However, RI-MOM renormalization is not performed on-shell, and these operators give a logarithmically divergent contribution to the amplitude, which can be confused with the chromomagnetic operator, as we will show shortly. The last two operators do not contribute, since the 3-point amplitude is calculated for massless quarks. This is not the case for our calculation of the 2-point $s d$ amplitude which featured massive quarks, where we expect that they will contribute. The first three operators, which have two covariant derivatives, are actually identical, up to momentum conservation (integration by parts). Their tree-level contribution to the gluon-quark-quark amplitude, in the twisted basis (see above in Sec. 5.3.2), is

$$
\langle \psi_2 (q_2) | Q_{DD} | A (q_1) \psi (q_3) \rangle = \bar{u}_2 (q_2) \gamma_5 \gamma_5 D u_3 (q_3) \\
= \bar{u}_2 (q_2) g \gamma_5 ((q_2 + q_3)_\nu - q_1^\mu \sigma_{\mu \nu}) A^\nu u_3 (q_3),
$$

for $D_\mu = \partial_\mu + i g A_\mu$.

We call $G_{em}$ the expression $q_2 q_3 (q_2 + q_3)_\nu$. In the amplitude it has a finite coefficient. We expect that $G_{em}$ will cancel out when we make contact with the continuum renormalized amplitude, i.e. in the difference with the continuum amplitude, so that it will not affect the renormalization and mixing pattern.
We re-write the 1-loop results using the three quantities,

\[ G_{\nu CM} = 2g\gamma_5 q_1^\mu \sigma_{\mu \nu} , \]  
\[ G_{\nu DD} = g\gamma_5 [(q_2 + q_3)_{\nu} - q_1^\mu \sigma_{\mu \nu}] , \]  
\[ G_{\nu em} = g\gamma_5 \ell_3 (q_2 + q_3)_{\nu} . \] (5.56)  
(5.57)  
(5.58)

After substitution, the 1-loop amplitude reads

\[ G_{\nu}^{1\ell} = g^2 t^a \left\{ G_{\nu CM} \left[ \left( \beta \left( -\frac{1}{128 N_c \pi^2} + \frac{3 N_c}{256 \pi^2} \right) + \frac{1}{64 N_c \pi^2} - \frac{13 N_c}{256 \pi^2} \right) \log(\mu^2) \right. 
\quad - 0.000395786 \beta^2 N_c + \beta (0.003529362/N_c - 0.004683977 N_c) 
\quad + 0.014146186/N_c - 0.015943567 N_c \right] 
\quad + G_{\nu DD} \left[ \beta (0.000709199/N_c - 0.001578959 N_c) \right. 
\quad + \left( \frac{3}{64 N_c \pi^2} - \frac{9 N_c}{256 \pi^2} \right) \log(\mu^2) 
\quad - 0.010365494/N_c + 0.008121153 N_c \right] 
\quad + G_{\nu em} \left[ \beta (-0.00181485/N_c - 8.370 \cdot 10^{-6} N_c) \right. 
\quad + 0.000527714/N_c + 0.000263857 N_c \left. \right] \right\} . \] (5.59)

The mixing with lower-dimensional operators can be calculated in perturbation theory from the 2-point diagrams shown in Fig. 5.3. The analysis of the 2-point results is in progress.

The renormalization constant in RI-MOM is obtained by combining the result of Eq. (5.59) projected on the chromomagnetic operator, with the renormalization constants of the quark and gluon fields \( Z_q \) and \( Z_A \) and coupling constant \( Z_g \), as described above in Eq. (5.40). This calculation is underway.
Appendix A

Feynman rules

We give here the Feynman rules used in the perturbative calculation. The chromo-
magnetic operator is essentially the clover term in the action, without $c_{SW}$ and $g$.
The Feynman rules for the fermion propagator and fermion-gluon vertices can be
also found in, e.g., [51], for Wilson fermions and Symanzik tree-level improved glu-
ons. The Wilson quarks are suitable in the massless case, otherwise one needs the
propagator of [17]. In [52] is written the full tree-level gluonic lagrangian, including
the gluon propagator, 3 and 4 gluon vertices, the gluon measure (Jacobian), ghost
propagator and ghost pair vertex with one or two gluons.

Fermionic part of the action

Definitions:

$$\sigma_{\mu\nu} = \frac{i}{2}(\gamma^\mu \gamma^\nu - \gamma^\nu \gamma^\mu) \quad (A.1)$$

The chromomagnetic operator is

$$Q_m = -\frac{i}{4}\gamma_5 \sigma_{\mu\nu} F^{\mu\nu} \quad (A.2)$$

The gluon 2-fermions chromomagnetic vertex is given by

$$V_{\mu}^{\gamma g CM} = \frac{r}{2} T^a i \gamma_5 \sum \sigma_{\mu\rho} \cos(k_{1\mu}/2) \sin(k_{1\rho}) \quad (A.3)$$

The gluon 2-fermions Wilson vertex is

$$V_{\mu}^{\gamma g W} = -g T^a \{ i \gamma_\mu \cos((k_{2\mu} + k_{3\mu})/2) + r \sin((k_{2\mu} + k_{3\mu})/2) \} \quad (A.4)$$

The 2-gluon 2-fermions chromomagnetic vertex,

$$V_{\mu\nu}^{\gamma gg CM} = -\frac{ag r T^a T^b}{4} \gamma_5 \left\{ \sigma_{\mu\nu} \left[ -\cos(k_{1\mu}/2) \cos(k_{2\nu}/2) + \cos(k_{1\nu}/2) \cos(k_{1\mu} + k_{2\nu}/2) \\ + \cos(k_{2\nu}/2) \cos(k_{1\mu}/2 + k_{2\mu}) + \cos(k_{1\nu} + k_{2\nu}/2) \cos(k_{1\mu}/2 + k_{2\mu}) \right] \\ + \delta_{\mu\nu} \sigma_{\mu\rho} \sin((k_{1\mu} + k_{2\mu})/2)[-\sin(k_{1\rho}) + \sin(k_{2\rho})] \right\} \quad (A.5)$$
The 2-gluon 2-fermions Wilson vertex,
\[ V_{\mu
u
\rho
\tau}^{2gg2f} W = \frac{ag^2 \{ T^a, T^b \}}{4} \delta_{\mu\nu} \{ i\gamma_\mu \sin((k_{2\mu} + k_{3\mu})/2) - r \cos((k_{2\mu} + k_{3\mu})/2) \} \] (A.6)

The 3-gluon 2-fermions chromomagnetic vertex,
\[ V_{\mu\nu\rho}^{ggg} CM = \frac{g^2 a^2 r}{16} T^a T^b T^c \gamma_5 \sigma_{\mu\nu} \left\{ 2\delta_{\mu\rho} \delta_{\nu\lambda} \delta_{\tau\lambda} c_2 (2k_2 + k_3) \lambda s_2 (k_1 + k_2) \rho 
- 2\delta_{\mu\rho} \delta_{\nu\lambda} \delta_{\tau\lambda} c_2 (k_1 + 2k_2) \rho s_2 (k_2 + k_3) \lambda 
+ \delta_{\mu\rho} \delta_{\nu\lambda} \delta_{\tau\lambda} [c_2 (k_1) + c_2 (k_1 + 2k_2 + 2k_3) \rho] 
\times [s_2 (k_2 + k_3) \lambda - s_2 (2k_1 + k_2 + k_3) \lambda] 
- 2\delta_{\mu\rho} \delta_{\nu\lambda} \delta_{\tau\rho} [c_2 (2k_1 + k_2) \lambda + c_2 (k_2 + 2k_3) \lambda] s_2 (k_1 + k_2 + k_3) \rho 
+ \delta_{\mu\rho} \delta_{\nu\lambda} \delta_{\tau\rho} [c_2 (k_3 \lambda) + c_2 (k_1 + 2k_2 + k_3) \lambda] 
\times [-s_2 (k_1 + k_2) \rho + s_2 (k_1 + k_2 + 2k_3) \rho] 
+ \delta_{\mu\rho} \delta_{\nu\lambda} \delta_{\tau\rho} c_2 (k_1 + k_2 + k_3) \rho 
\times [-s_2 (2k_1 \lambda) + s_2 (2k_1 + 2k_2) \lambda - s_2 (2k_3 \lambda) + s_2 (2k_2 + 2k_3) \lambda] 
+ \frac{2}{3} \delta_{\mu\lambda} \delta_{\nu\lambda} \delta_{\tau\lambda} c_2 (k_1 + k_2 + k_3) \lambda s_2 (2k_1 + 2k_2 + 2k_3) \rho \right\}, \] (A.7)

where \( s_2 (p) \equiv \sin (p/2) \) and \( c_2 (p) \equiv \cos (p/2) \).

The twisted mass inverse quark propagator, with regular mass \( m \) and twisted mass \( \mu \) is in the twisted basis
\[ S_{q^{-1}} (p) = 2r \sum_\nu \sin^2 (p_{\nu}/2) + m + i \sum_\nu \sin (p_{\nu}) + i \mu \gamma_5. \] (A.8)

The quark twisted-mass propagator is therefore
\[ S_q (p, m, \mu) = \frac{m + 2r \sum_\nu \sin^2 (p_{\nu}/2) - i \sum_\nu \gamma_\nu \sin (p_{\nu}) - i \mu \gamma_5}{[m + 2r \sum_\nu \sin^2 (p_{\nu}/2)]^2 + [\sum_\nu \gamma_\nu \sin (p_{\nu})]^2 + \mu^2}. \] (A.9)

**Gluonic part of the action**

We define \( \hat{\mu} = \frac{2}{a} \sin (p_{\mu}/2) \). The gluon plaquette propagator is
\[ S_{g \mu \nu}^{\text{plaq}} (p) = \frac{\delta_{\mu\nu}}{\hat{p}^2} - (1 - \alpha) \frac{\hat{p}_{\mu\nu}}{(\hat{p}^2)^2}, \] (A.10)
where \( \alpha \) is the gauge parameter, setting \( \alpha = 1 \), for example, defines the Feynman–’t Hooft gauge, and setting \( \alpha = 0 \) sets the Landau gauge. The gluon 6-links improved inverse propagator is
\[ S_{g \mu \nu}^{-1} (k) = \frac{1}{\alpha} \hat{k}_{\mu \nu} + \sum_\rho (\hat{k}_{\rho \mu \nu} - \hat{k}_{\mu \nu} \delta_{\rho\mu}) q_{\mu \rho} \hat{k}_{\rho}, \] (A.11)
where
\[ q_{\mu\nu} = (1 - \delta_{\mu\nu})[1 - (c_1 - c_2 - c_3)(\hat{k}_{\mu}^2 + \hat{k}_{\nu}^2) - (c_2 + c_3) \hat{k}_{\mu}^2]. \] (A.12)
The direct propagator in analytical form can be found in [16] and [51], but is not used in our calculations, as explained above in Ch. 5.3.1. The 3-gluon vertex, to quote Weisz and Wohlert\[cosine of half angle). The gluon measure, which is the Jacobian of the variable transfer," which they write in their paper but we do not show here. The 4-gluon vertex, used in our calculations, as explained above in Ch. 5.3.1, the 2-ghosts-2-gluons vertex is

\[
V_{\mu\nu\tau}^{gg} = a^3 g\delta(k_1 + k_2 + k_3) f_{abc} \left\{ -c_{\text{plaq}} \delta_{\mu\nu} c_2(k_1 + k_2) s_2(-k_1 + k_2)_\tau 
- 4c_{\text{rect}} \delta_{\mu\nu} c_2(k_1)_\mu c_2(k_2)_\nu c_2(2k_1 + 2k_2)_\mu s_2(-k_1 + k_2)_\tau 
- 2c_{\text{rect}} \delta_{\mu\nu} c_2(k_1 + k_2)_\mu c_2(k_1 + k_2)_\nu s_2(-2k_1 + 2k_2)_\tau 
+ 2c_{\text{rect}} \delta_{\mu\tau} s_2(k_1)_\mu s_2(2k_1)_\nu s_2(-k_2 + k_3)_\nu 
+ 2c_{\text{rect}} \delta_{\mu,\nu,\tau} s_2(2k_1)_\mu s_2(-k_2 + k_3)_\rho s_2(k_2 + k_3)_\rho 
+ 4c_{\text{chair}} \delta_{\mu\nu} c_2(k_1 - k_2)_\rho c_2(k_1 + k_2)_\rho s_2(k_1 - k_2)_\tau 
- 4c_{\text{chair}} \delta_{\mu\nu} c_2(k_1 + k_2)_\mu c_2(k_1 + k_2)_\nu s_2(-k_1 + k_2)_\tau 
+ 4c_{\text{chair}} s_2(k_1)_\mu s_2(k_2)_\nu s_2(-k_1 + k_2)_\tau 
+ 4c_{\text{chair}} \delta_{\mu\nu} c_2(k_3)_\mu s_2(k_1 - k_2)_\rho s_2(k_1 + k_2)_\rho s_2(k_1 + k_2)_\rho s_2(k_1 + k_2)_\rho 
- 4c_{\text{paral}} \delta_{\mu\nu} c_2(k_1 - k_2)_\rho c_2(k_1 + k_2)_\rho c_2(k_1 + k_2)_\rho s_2(-k_1 + k_2)_\tau 
+ 2c_{\text{paral}} s_2(k_1)_\mu s_2(k_2)_\nu s_2(-k_1 + k_2)_\tau 
+ \frac{2}{3} c_{\text{paral}} s_2(-k_1 + k_2)_\rho s_2(k_1 - k_3)_\nu s_2(k_2 - k_3)_\mu \right\}, \tag{A.13}
\]

where \(\delta_{\mu,\nu,\tau} = \delta_{\mu,\nu,\tau}\), and \(c_{\text{plaq}} = c_0 = 5/3\), \(c_{\text{rect}} = c_1 = -1/12\), \(c_{\text{chair}} = c_2 = 0\) and \(c_{\text{paral}} = c_3 = 0\) are the constants of the symanzik tree-level improved action (the \(c_2\) constant is not to be confused with that in the Feynman rule which denotes a cosine of half angle).

The 4-gluon vertex, to quote Weisz and Wohlert [52], is given by “horrendous expressions” which they write in their paper but we do not show here. The gluon measure, which is the Jacobian of the variable transformation from links \(U_{x,\mu}\) to vector fields \(A_\mu(x)\), is

\[
V_{\mu\nu}^{\text{measure}} = \frac{g^2 N}{12} \delta_{\mu\nu}. \tag{A.14}
\]

The ghost propagator is

\[
S_h = \frac{1}{\bar{p}^2}, \tag{A.15}
\]

the ghost-ghost-gluon vertex is

\[
V_{\mu}^{hhg} = ig f_{\text{cah}} \tilde{p}_1 \mu \cos(p_{2\mu}/2), \tag{A.16}
\]

and the 2-ghosts-2-gluons vertex is

\[
V_{\mu\nu}^{hhg} = \frac{g^2}{12} f_{\text{cah}} f_{\text{deh}} \tilde{p}_1 \mu \tilde{p}_2 \nu \delta_{\mu\nu}. \tag{A.17}
\]
Appendix B

Operator analysis

We give here a detailed analysis of the spurionic symmetry properties of the operators which possibly mix with the chromomagnetic operator [43]. The symmetries of the maximally twisted mass action are

\[ P \times D_d \times [\text{all } m \leftrightarrow -m] , \quad (B.1) \]

\[ D_d \times R_5 , \quad (B.2) \]

\[ C \times [s \leftrightarrow d] \times [m_s \leftrightarrow m_d] , \quad (B.3) \]

where \( R_5 \) is the parity transformation

\[ R_5 : \quad \psi \rightarrow \gamma_5 \psi , \quad \bar{\psi} \rightarrow \bar{\psi} \gamma_5 , \quad (B.4) \]

and

\[ D_d = \begin{cases} 
U_\mu(x) \rightarrow U_\mu^+(x - a\hat{\mu}) , \\
\psi(x) \rightarrow e^{3i\pi/2} \psi(-x) , \\
\bar{\psi}(x) \rightarrow e^{3i\pi/2} \bar{\psi}(-x) .
\end{cases} \quad (B.5) \]

Under these transformations, the operators transform as shown in Tab. B.1. We can see that the symmetry (B.2) plays no role in the selection of operators since they are all even under the transformation.
### Table B.1.
The dimension 3 to 5 operators which can possibly mix with the chromomagnetic operator, and their transformation under the symmetries of the maximally twisted mass action. Note that $D$ denotes generically either the forward or the backward covariant derivative.
Bibliography


[38] D. Becirevic et al., arXiv:hep-lat/9809129.


