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Isospin-breaking Corrections to Light Pseudoscalar Leptonic Decays Rates

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Abstract

The Cabibbo-Kobayashi-Maskawa (CKM) matrix is a 3×3 unitary matrix in the Standard Model of particle physics. It characterises the transmutation of quarks in flavor-changing weak decays. In flavor physics, a precise determination of its matrix elements represents a crucial test of the limits of the Standard Model. One of the major theoretical challenges in this enterprise is the inclusion of low energy hadronic quantities. In this non-perturbative regime, Lattice Quantum Chromodynamics remains the *ab initio* approach for first principle calculations of the hadronic observables required. Traditionally, the Euclidean n -point correlation functions from these Monte-Carlo simulations are calculated in the isospin-symmetric limit, where $\alpha = 0$ and $m_u - m_d = 0$. In recent years, however, lattice calculations of f_π and f_K , which are necessary for the determination of V_{ud} and V_{us} from leptonic decays, respectively, have reached an impressive precision of $\mathcal{O}(1\%)$ or better. To make further progress, lattice simulations can no longer neglect percent-level isospin-breaking effects.

In this thesis, isospin-breaking corrections to the inclusive rate $K^+/\pi^+ \rightarrow \mu^+ \nu_\mu [\gamma]$ and an update to V_{us}/V_{ud} are presented. A distinct feature of this work is the amplitude correction arising from a virtual photon coupling the initial pseudoscalar to the final state charged lepton. The non-perturbative, electro-quenched result comes from the RBC-UKQCD $2 + 1$ flavor Domain Wall fermion simulations with near-physical quark masses. The QED interactions are introduced via a perturbative expansion of the action in α and the photon propagators are implemented in the Feynman gauge and QED_L formulation. The isospin-breaking corrections obtained from the lattice are then corrected for finite volume effects and combined with the analytic real photon emission term to remove the IR divergence. For this latter term, all possible photon energies are integrated over. The phenomenological quantity V_{us}/V_{ud} determined in this thesis is discussed in light of the latest published results.

Lay Summary

The Standard Model of particle physics is a mathematical framework that describes Nature at its fundamental level. It comprises quarks and leptons - which, the most stable of them make up the atom - and the particles that mediate their electromagnetic and nuclear interactions. To date, all the contents of the Standard Model have been experimentally verified, making this one of the most successful applications of quantum theory and the theory of special relativity.

Nevertheless, the Standard Model is incomplete. For example, it is unable to fully account for the absence of naturally-occurring anti-matter in the Universe. Thus, there is a need to extend this framework. One of the avenues to search for physics beyond the Standard Model is to compare high precision measurements and theoretical predictions. In quantum theory, hitherto unknown particles can contribute to observables (*e.g.* the magnetic moment of an electron) and these quantum effects can be detected in experiments. This will manifest as a discrepancy to theoretical predictions based on the Standard Model.

The Cabibbo-Maskawa-Kobayashi matrix contains information about how quarks transmute into one another. The elements of this matrix are fundamental parameters of the Standard Model and their precise determination is an ongoing enterprise. The ratio of matrix elements central to this thesis is V_{us}/V_{ud} . This requires experimental measurement of the mean lifetimes of the K and π meson and theoretical prediction of their decay probability. The latter must be evaluated in large numerical simulations due to the highly non-linear nature of Quantum Chromodynamics. Until recently, simulations relied on an approximation known as isospin symmetry, which regards the quark content of the proton and neutron in the same way. The error of this approximation is expected to be $\sim 1\%$. Given that the precision of recent theoretical predictions has reached percent level, this thesis predicts V_{us}/V_{ud} that includes isospin symmetry-breaking effects.

Declaration

I declare that this thesis was composed by myself, that the work contained herein is my own except where explicitly stated otherwise in the text, and that this work has not been submitted for any other degree or professional qualification except as specified.

The contents of Chapters 4-5 are currently under peer review [1], with Peter Boyle, Matteo Di Carlo, Felix Erben, Vera Gülpers, Maxwell Hansen, Tim Harris, Nils Hermansson-Truedsson, Raoul Hodgson, Andreas Jüttner, Fionn Ó hÓgáin, Antonin Portelli and James Richings as co-authors.

Parts of this work have been published in [2] and [3].

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As a sojourner in Edinburgh, I am grateful for my extended family at Chalmers. The names are innumerable, but these brothers- and sisters-in-Christ have been a source of encouragement through their prayers and fellowship during the pandemic and beyond. Thank you.

Above all, I am eternally thankful for the Lord Jesus, who saw fit to make a Universe His creatures can comprehend and find delight in seeing His glory in it.

*When I look at your heavens, the work of your fingers,
the moon and the stars, which you have set in place,
what is man that you are mindful of him,
and the son of man that you care for him?*

Psalm 8v3-4

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Chapter 1

Introduction

Quantum field theory, a union of 20th century quantum physics, principles of relativity and the concept of fields, forms the backbone of modern fundamental physics. In terms of experimental verification, its most successful application to date is the Standard Model of particle physics. Over the past five decades, with the advent of high energy colliders, experimental measurements have been able to test Standard Model predictions to a high degree of precision.

At its core, the Standard Model is a description of the constituents that make up the observable Universe and how they interact via three fundamental forces of Nature. Beginning with the atomic picture, the nucleons (protons and neutrons) are composed of the up- and down-quarks. Together with the electron and its neutrino partner, they form the first generation of spin- $\frac{1}{2}$ particles known as *fermions*. Subsequent collider experiments up to the 1990s have led to the discovery of two more generations. In total, there are six *flavors* of quarks and leptons. The interactions between fermions are mediated by spin-1 particles called (vector) gauge *bosons*. The electromagnetic interaction between electrically-charged fermions are due to *photon* exchanges. Quarks may transmute between flavors via the weak nuclear force, which is responsible for the (inverse) β -decay, and this is mediated by the $W^\pm$ boson. Note that although the Z boson also carries the weak force, it does not induce a change of flavor. Quarks also experience the strong nuclear force, which binds them together into triplets (baryons) or quark-anti-quark pairs (mesons). The mediator boson for this force is aptly called the *gluon*.

The mediator bosons are manifestations of the $SU(3)_C \times SU(2)_L \times U(1)_Y$ Lie

groups. Gauge theory expects these bosons to be massless, while massive weak force mediators¹ were discovered at the Super Proton Synchrotron in 1983. This discrepancy between prediction and measurement is explained by the *Higgs mechanism*, proposed independently by P. Higgs [5], F. Englert and R. Brout [6], G. Guralnik, C. Hagen and T. Kibble [7]. The details of spontaneous symmetry breaking of the $SU(2)_L \times U(1)_Y \rightarrow U(1)_{EM}$ are relegated to Chapter 2. Here, it suffices to comment that this mass-generating mechanism predicts the existence of an additional spin-0 (scalar) boson, dubbed the *Higgs boson*. On 4th July 2012, Higgs-boson-like events were confirmed at both ATLAS and CMS experiments at the Large Hadron Collider. In the following year, the Nobel Prize in Physics was awarded to P. Higgs and F. Englert and with that, the family of fundamental particles known to date is illustrated in Figure 1.1.

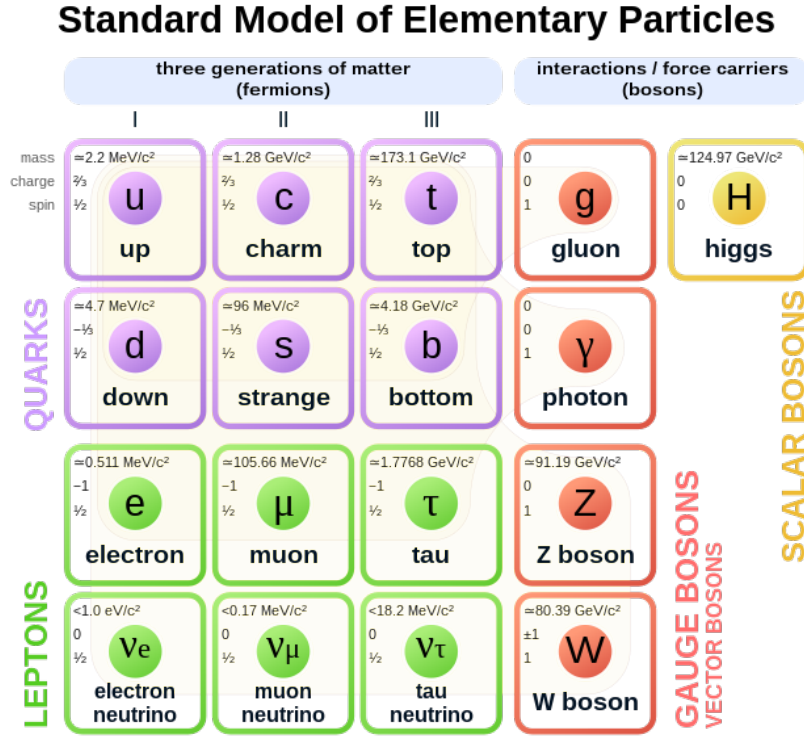


Figure 1.1 *The Standard Model of particle physics, beginning in 1897 with the discovery of the electron in Cambridge, completed in 2012 with the confirmation of the Higgs boson at the Large Hadron Collider.*

Indeed, at the time of writing, we have arrived at the decennial since the discovery of the Higgs boson. Despite its successes, the Standard Model is far from being a complete description of Nature at the fundamental scale. For

¹ $W^\pm = 80.379(12)\text{GeV}$, $Z = 91.1876(21)\text{GeV}$ [4]

example, there is still no viable dark matter candidate that can stand against the stringent constraints set by recent experimental measurements. Even within the flavor sector, there is insufficient CP -violation to satisfy one of the three Sakharov conditions [8], which are necessary to account for the matter-anti-matter asymmetry observed in the Universe.

One of the avenues to search for physics beyond the Standard Model (BSM) relies on the fact that the Standard Model contents may interact with BSM particles from an inaccessible energy scale via virtual loop corrections in perturbation theory. Thus, any inconsistencies between prediction and measurement are expected to be small; so the control of uncertainties on the experimental and theoretical frontier becomes paramount in this age of precision physics. An example of present effort is to test the unitarity of the Cabibbo-Kobayashi-Maskawa (CKM) matrix. The matrix elements of this 3×3 matrix represent the interaction strength of flavor-changing weak currents and their uncertainties are notoriously difficult to control, owing to the non-perturbative effects of the strong nuclear force. To date, the lattice formulation of *Quantum Chromodynamics* (QCD) - the theory of quarks and gluons - remains the only *ab initio* method for calculating and controlling the uncertainties of QCD quantities through numerical simulations. Indeed, with the prevalence of high performance computers (HPC's) and also the advent of graphic processing units (GPU's) in the arena of scientific computing, lattice QCD is becoming an increasingly accessible method to meet the demands of precision physics. The timing is serendipitous since an aggressive push to control theoretical uncertainties from non-perturbative hadronic effects can better inform the experimental frontier at CERN of any measurements which are due an improvement in statistics ahead of the high luminosity upgrade, due to complete in 2029.

In this thesis, our main goal is to provide a precise determination of the hadronic contribution to the ratio of CKM matrix elements, $\frac{|V_{us}|}{|V_{ud}|}$. We begin with an overview of the Standard Model of particle physics. In particular, the origin of the CKM matrix and how to extract its elements. Then, we introduce the methodology of lattice QCD, followed by a practical implementation in light of leptonic decays. This leads us to the presentation of the original work that is central to this thesis. Finally, we conclude with key outcomes from this work and an outlook on future prospects for this search beyond the Standard Model.

Chapter 2

The Standard Model & the CKM Matrix

In the early Universe, the electromagnetic and weak nuclear force can be described by a single unified gauge theory known as the *electroweak theory*. Its formulation was developed by Glashow[9], Weinberg[10] and Salam[11], which earned them their Nobel Prize in Physics in 1979. The gauge bosons associated to the electroweak theory were postulated to be massless. That the weak interaction is short-ranged today suggests that their mediating boson, $W^\pm$ and Z are massive. This is explained by the spontaneous breaking of the gauge symmetry associated to the electroweak force. The Higgs mechanism, triggered at the electroweak phase transition during the early evolution of the Universe, is responsible for their mass generation and we review it in the first section of this chapter.

Moreover, the Higgs mechanism also gives rise to quark masses. The theoretical developments in obtaining the mass terms via this mechanism leads to the important concept of quark flavor mixing. We will review this in the second section and briefly study the non-perturbative nature of Quantum Chromodynamics. In the final two sections, we will focus on decays involving hadrons in the weak sector and how improvements in the theoretical prediction can be made.

For this thesis, we will work in natural units, setting $\hbar = c = 1$.

2.1 The Electroweak Sector

2.1.1 Breaking of Global Symmetry

Let us warm up by reviewing the spontaneous breaking of a global symmetry and its effects. Consider the simple model involving a complex scalar field ϕ . Suppressing spacetime arguments, the Lagrangian is¹

$$\begin{aligned}\mathcal{L} &= \frac{1}{2}\partial_\mu\phi(\partial^\mu\phi)^* - V(\phi), \\ &= \frac{1}{2}\partial_\mu\phi(\partial^\mu\phi)^* - \frac{1}{2}\mu^2\phi\phi^* - \frac{1}{4}\lambda(\phi\phi^*)^2.\end{aligned}\tag{2.1}$$

We see that this Lagrangian is invariant under a $U(1)$ global transformation $\phi \rightarrow e^{i\alpha}\phi, \phi^* \rightarrow e^{-i\alpha}\phi^*$, where α is a constant. Now, let $\phi = \phi_1 + i\phi_2$, where $\phi_{1,2}$ are real-valued fields. The Lagrangian can then be factorised into

$$\mathcal{L} = \frac{1}{2}\partial_\mu\phi_1\partial^\mu\phi_1 + \frac{1}{2}\partial_\mu\phi_2\partial^\mu\phi_2 - \frac{1}{2}\mu^2(\phi_1^2 + \phi_2^2) - \frac{1}{4}\lambda(\phi_1^2 + \phi_2^2)^2.\tag{2.2}$$

Written in this manner, the first two term on the RHS are the kinetic term for each field while the last two terms form the potential $V(\phi_1, \phi_2)$. This is illustrated in Figure 2.1. To study the vacuum of this potential, one simply takes the derivative with respect to each field and solve for the extremum, *i.e.* for $\mu < 0$,

$$\left.\frac{\partial V}{\partial\phi_1}\right|_{\phi_2} = \mu^2\phi_1 + \lambda(\phi_1^2 + \phi_2^2)^2 = 0,\tag{2.3}$$

$$\left.\frac{\partial V}{\partial\phi_2}\right|_{\phi_1} = \mu^2\phi_2 + \lambda(\phi_1^2 + \phi_2^2)^2 = 0,\tag{2.4}$$

$$\Rightarrow \phi_1^2 + \phi_2^2 = -\frac{\mu^2}{\lambda} = v^2\tag{2.5}$$

where v is the vacuum expectation value. We see that there is an infinite number of field values which satisfy Equation (2.5). Let $\phi_1 = v$ and $\phi_2 = 0$. By making this choice, we have broken the symmetry at the ground state. Now, to perturb the vacuum, we introduce the following shifted fields $\eta = \phi_1 - v, \zeta = \phi_2$. Then, denoting with subscript ‘0’, the complex scalar field in the vacuum is

$$\phi_0 = \frac{1}{\sqrt{2}}(\eta + v + i\zeta).\tag{2.6}$$

¹Here and everywhere in the thesis, repeated indices imply a summation, unless otherwise stated

We may rewrite Equation (2.2) as

$$\mathcal{L} = \frac{1}{2}\partial_\mu\eta\partial^\mu\eta - \lambda v^2\eta^2 + \frac{1}{2}\partial_\mu\zeta\partial^\mu\zeta + \dots, \quad (2.7)$$

where the ellipses denote the constant and higher order terms. This Lagrangian gives us two equations of motion: one for the field η with mass $m^2 = \lambda v^2$ and another for the massless field ζ .

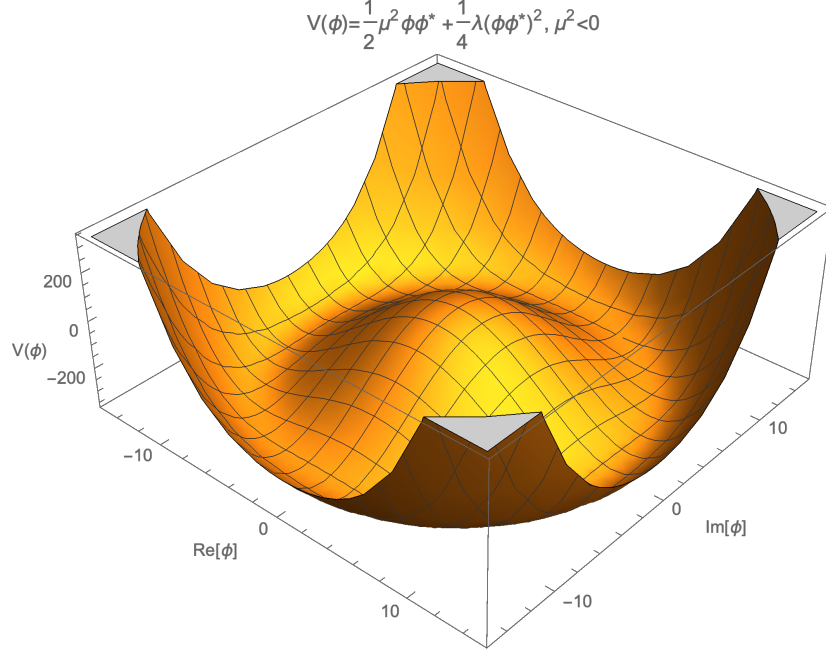


Figure 2.1 *An example plot of a potential with complex scalar field ϕ , using $\mu^2 < 0$.*

2.1.2 Breaking of Local Gauge Symmetry

Let us now move to the breaking a local gauge symmetry and its consequences for the gauge fields in the theory. For a concrete yet simple case study, let us consider a Lagrangian that includes a $U(1)$ gauge field A_μ (*e.g.* QED):

$$\mathcal{L} = (D^\mu\phi)^\dagger(D_\mu\phi) - \frac{1}{4}F^{\mu\nu}F_{\mu\nu} - V(\phi), \quad (2.8)$$

where $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ is the field strength tensor and the covariant derivative

$$\partial_\mu \rightarrow D_\mu = \partial_\mu - ieA_\mu \quad (2.9)$$

ensures the Lagrangian is invariant under the following local gauge transformation²

$$A_\mu \rightarrow A'_\mu = A_\mu + \frac{1}{e} \partial_\mu \alpha. \quad (2.10)$$

With the same potential as in the previous study (see Equation (2.2)), we re-write the Lagrangian in Equation (2.8) using ϕ_0 from Equation (2.6):

$$\begin{aligned} \mathcal{L} = & \frac{1}{2}(\partial_\mu \eta)(\partial^\mu \eta) - \lambda v^2 \eta^2 + \frac{1}{2}(\partial_\mu \zeta)(\partial^\mu \zeta) \\ & - \frac{1}{4}F^{\mu\nu}F_{\mu\nu} + \frac{1}{2}e^2 v^2 A^\mu A_\mu \\ & - ev A_\mu \partial^\mu \zeta + \dots \end{aligned} \quad (2.11)$$

In the first line, we have again the equation of motion for a massive η field of mass $m = \sqrt{\lambda}v$ and a massless ζ , whereas in the second line the gauge field acquires a mass term $m_\gamma = \sqrt{ev}$. To interpret the term in the third line, we rewrite as

$$\frac{1}{2}(\partial_\mu \zeta)(\partial^\mu \zeta) + \frac{1}{2}e^2 v^2 A^\mu A_\mu - ev A_\mu \partial^\mu \zeta = \frac{1}{2}e^2 v^2 \left(A_\mu - \frac{1}{ev} \partial_\mu \zeta \right)^2. \quad (2.12)$$

The Lagrangian becomes

$$\begin{aligned} \mathcal{L} = & \frac{1}{2}(\partial_\mu \eta)(\partial^\mu \eta) - \lambda v^2 \eta^2 \\ & - \frac{1}{4}F^{\mu\nu}F_{\mu\nu} + \frac{1}{2}e^2 v^2 \left(A_\mu - \frac{1}{ev} \partial_\mu \zeta \right)^2 + \dots \end{aligned} \quad (2.13)$$

We can define a shifted gauge field

$$A'_\mu = A_\mu - \frac{1}{ev} \partial_\mu \zeta, \quad (2.14)$$

which we identify from our original local gauge transformation that $\alpha(x) \rightarrow \zeta(x)/v$. Such a choice is called the *unitary gauge*. A shift in the gauge will affect both the field and the Lagrangian. In the former, we have, neglecting cross terms

²Here, α is understood to be spacetime-dependent, $\alpha = \alpha(x)$.

and higher order terms,

$$\begin{aligned}
\phi_0 &\rightarrow \phi'_0 = e^{-i\zeta/v} \phi_0, \\
&= e^{-i\zeta/v} \frac{1}{\sqrt{2}} (v + \eta + i\zeta), \\
&= e^{-i\zeta/v} \frac{1}{\sqrt{2}} (v + \eta) e^{i\zeta/v} \\
\phi'_0 &= \frac{1}{\sqrt{2}} (v + h),
\end{aligned} \tag{2.15}$$

where in the final line, h is a real-valued field in this shifted ϕ . Since the field strength tensor remains unchanged under this gauge shift, we now only consider the scalar part of the Lagrangian. First, the kinetic piece

$$\begin{aligned}
(D^\mu \phi)^\dagger (D_\mu \phi) &= \left[(\partial^\mu + ieA^\mu) \frac{1}{\sqrt{2}} (v + h) \right] \cdot \left[(\partial_\mu - ieA_\mu) \frac{1}{\sqrt{2}} (v + h) \right], \\
&= \frac{1}{2} \partial^\mu h \partial_\mu h + \frac{1}{2} e^2 (v + h)^2 A^\mu A_\mu.
\end{aligned} \tag{2.16}$$

Meanwhile, the scalar potential is

$$\begin{aligned}
V(\phi) &= -\frac{1}{2} \lambda v^2 (v + h)^2 + \frac{1}{4} \lambda (v + h)^4, \\
&= \lambda v^2 h^2 + \lambda v h^3 + \frac{1}{4} \lambda h^4,
\end{aligned} \tag{2.17}$$

where we have made the substitution $\mu^2 = -\lambda v^2$. Then, the full Lagrangian is

$$\begin{aligned}
\mathcal{L} &= \frac{1}{2} \partial^\mu h \partial_\mu h - \lambda v^2 h^2 \\
&\quad - \frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \frac{1}{2} e^2 v^2 A^\mu A_\mu \\
&\quad + e^2 v A^\mu A_\mu h + \frac{1}{2} e^2 A^\mu A_\mu h^2 \\
&\quad - \lambda v h^3 - \frac{1}{4} \lambda h^4.
\end{aligned} \tag{2.18}$$

We began with a Lagrangian with $U(1)$ symmetry. That this symmetry does not hold for the ground state is called *spontaneous symmetry breaking*. According to Goldstone's theorem[12, 13], when a symmetry group G is broken into $H \subset G$, one expects $\dim H$ massless (Goldstone) modes or masses and $\dim G - \dim H$ massive modes. In the unitary gauge, the gauge field has ‘eaten’ the massless field ζ (see gauge shift in Equation (2.14)) and gains a mass term $m_\gamma = ev$. The h field in the vacuum acquires its usual mass $m = \sqrt{2\lambda}v$ and interaction terms with the A_μ and itself.

2.1.3 Higgs Mechanism in the Standard Model

We have learned that the spontaneous breaking of a local $U(1)$ symmetry gives rise to a massive gauge boson as well as a mass to the scalar particle associated to the potential. When spontaneous symmetry breaking occurs in the electroweak sector of the Standard Model, the Higgs mechanism is responsible for the mass generation of the weak boson and fermions. We will discuss the former in this section, dedicating an entire section to the fermion masses later.

The electroweak sector has a $SU(2)_L \times U(1)_Y$ symmetry, where Y is the hypercharge. There are 4 generators associated to this symmetry. As such, let the scalar field be an isospin doublet with hypercharge $Y = \frac{1}{2}$,

$$\phi = \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix} = \begin{pmatrix} \phi_1 + i\phi_2 \\ \phi_3 + i\phi_4 \end{pmatrix}. \quad (2.19)$$

The Lagrangian for the scalar field is

$$\mathcal{L} = (D^\mu \phi)^\dagger (D_\mu \phi) + \lambda(\phi^\dagger \phi)^2, \quad (2.20)$$

with the usual potential

$$V(\phi) = \mu^2 \phi^\dagger \phi + \lambda(\phi^\dagger \phi)^2, \quad \mu^2 < 0 \quad (2.21)$$

and $SU(2)_L \times U(1)_Y$ covariant derivative is

$$D_\mu = \partial_\mu + \frac{i}{2}g\mathbf{W}_\mu \cdot \boldsymbol{\sigma} + \frac{i}{2}g'B_\mu, \quad (2.22)$$

where $\boldsymbol{\sigma} = (\sigma^1, \sigma^2, \sigma^3)$ are the Pauli matrices in vector notation. Following the procedure before in minimising the potential and choosing the vacuum to be $\phi_1 = \phi_2 = \phi_4 = 0, \phi_3 = v$, we have

$$\phi_0 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v + h \end{pmatrix} \quad (2.23)$$

for a real-valued field h .

As before, the mass terms for the gauge fields will arise from the covariant

derivative in the Lagrangian:

$$\begin{aligned}
D_\mu \phi_0 &= \left[\frac{i}{2} g \mathbf{W}_\mu \cdot \boldsymbol{\sigma} + \frac{i}{2} g' B_\mu \right] \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v+h \end{pmatrix}, \\
&= \frac{i}{2\sqrt{2}} \begin{pmatrix} gW_{3\mu} + g'B_\mu & g(W_{1\mu} - iW_{2\mu}) \\ g(W_{1\mu} + W_{2\mu}) & -gW_{3\mu} + g'B_\mu \end{pmatrix} \begin{pmatrix} 0 \\ v+h \end{pmatrix}, \\
&= \frac{i}{2\sqrt{2}} \begin{pmatrix} g(W_{1\mu} - iW_{2\mu}) \\ -gW_{3\mu} + g'B_\mu \end{pmatrix} (v+h).
\end{aligned} \tag{2.24}$$

Studying only the terms that couple to the vacuum expectation value v , the kinetic piece is

$$(D_\mu \phi_0)^\dagger (D^\mu \phi_0) = \frac{v^2}{8} [g^2(W_1^2 + W_2^2) + (g'B_\mu - gW_3)^2]. \tag{2.25}$$

Let us rewrite these gauge fields in terms of physical fields. Analogous to the raising and lowering operators in $SU(2)_L$, *i.e.* $\sigma^\pm = \frac{1}{2}(\sigma_1 \pm i\sigma_2)$, we express the first term on the RHS of Equation 2.25 in a similar linear combination:

$$W^\pm = \frac{1}{\sqrt{2}}(W_1 \mp iW_2). \tag{2.26}$$

Inverting this relation, we find

$$g^2(W_1^2 + W_2^2) = g^2(W^{+2} + W^{-2}). \tag{2.27}$$

The second term in Equation (2.25) can be decomposed as

$$(g'B_\mu - gW_3)^2 = \begin{pmatrix} W_3 & B_\mu \end{pmatrix} \begin{pmatrix} g^2 & -gg' \\ -gg' & g'^2 \end{pmatrix} \begin{pmatrix} W_3 \\ B_\mu \end{pmatrix}. \tag{2.28}$$

The matrix of couplings,

$$G = \begin{pmatrix} g^2 & -gg' \\ -gg' & g'^2 \end{pmatrix} \tag{2.29}$$

can be diagonalised as $G = PDP^{-1}$. Using the eigenvalues λ_j and eigenvectors v_j of G

$$\begin{aligned}
\lambda_1 &= 0, \quad v_1 = \frac{1}{\sqrt{g^2 + g'^2}} \begin{pmatrix} g' \\ g \end{pmatrix} \\
\lambda_2 &= (g^2 + g'^2), \quad v_2 = \frac{1}{\sqrt{g^2 + g'^2}} \begin{pmatrix} g \\ -g' \end{pmatrix}
\end{aligned} \tag{2.30}$$

we can construct P and its inverse

$$P = \frac{1}{\sqrt{g^2 + g'^2}} \begin{pmatrix} g' & g \\ g & -g' \end{pmatrix}, \quad P^{-1} = \frac{1}{\sqrt{g^2 + g'^2}} \begin{pmatrix} -g' & g \\ g & g' \end{pmatrix} \quad (2.31)$$

and the diagonal matrix of eigenvalues

$$D = \begin{pmatrix} 0 & 0 \\ 0 & g^2 + g'^2 \end{pmatrix}. \quad (2.32)$$

This gives us

$$\begin{aligned} \begin{pmatrix} W_3 & B_\mu \end{pmatrix} P &= \frac{1}{\sqrt{g^2 + g'^2}} \begin{pmatrix} W_3 & B_\mu \end{pmatrix} \begin{pmatrix} g' & g \\ g & -g' \end{pmatrix}, \\ &= \frac{1}{\sqrt{g^2 + g'^2}} \begin{pmatrix} g'W_3 + gB_\mu & gW_3 - g'B_\mu \end{pmatrix} \end{aligned} \quad (2.33)$$

and similarly for $P^{-1}(W_3 \ B_\mu)^T$. Let

$$\begin{aligned} A_\mu &= \frac{1}{\sqrt{g^2 + g'^2}} (g'W_3 + gB_\mu), \\ Z_\mu &= \frac{1}{\sqrt{g^2 + g'^2}} (gW_3 - g'B_\mu). \end{aligned} \quad (2.34)$$

Then, the second term in Equation (2.25) becomes

$$(g'B_\mu - W_3)^2 = (g^2 + g'^2)Z_\mu^2 + 0 \cdot A_\mu^2. \quad (2.35)$$

Re-writing the covariant derivative with respect to the physical gauge fields, the kinetic term becomes

$$(D^\mu \phi_0)^\dagger (D_\mu \phi_0) = \frac{v^2}{8} [g^2 W^{+2} + g^2 W^{-2} + (g^2 + g'^2)Z_\mu^2 + 0 \cdot A_\mu^2]. \quad (2.36)$$

Written in this manner, we observe that with spontaneous symmetry breaking of $SU(2)_L \times U(1)_Y \rightarrow U(1)_{EM}$, we have $\dim U(1)_{EM} = 1$ massless Goldstone boson, which we identify as the photon, and $\dim [SU(2)_L \times U(1)_Y] - \dim U(1)_{EM} = (2^2 - 1) + 1 - 1 = 3$ massive Goldstone bosons. These are the weak force carriers $W^\pm$ and Z , with masses

$$m_{W^\pm} = \frac{1}{2}vg \quad m_Z = \frac{1}{2}\sqrt{g^2 + g'^2}. \quad (2.37)$$

As before, the mass of the scalar (Higgs) particle is also predicted by this mechanism

$$m_H = \sqrt{2\lambda}v. \quad (2.38)$$

The experimental discovery of the Z and $W^\pm$ came in 1973 and 1983, respectively. The existence of the Higgs boson was confirmed at CERN in July 2012.

2.2 The Flavor Sector

2.2.1 Quark Mass & Flavor Mixing

Naively, we expect a mass term from the fermion bilinear $-m\bar{\psi}\psi$, where ψ is a fermion field. Let the projector be

$$P_{L,R} = \frac{1}{2}(\mathbb{1} \mp \gamma^5). \quad (2.39)$$

These satisfy the usual projection operator properties

$$(P_{L,R})^2 = P_{L,R}, \quad P_L + P_R = \mathbb{1}, \quad P_L P_R = P_R P_L = 0. \quad (2.40)$$

We can use these to decompose the fermion fields into their chiral states

$$\psi_{L/R} = P_{L,R}\psi \quad \text{and} \quad \bar{\psi}_{L/R} = \bar{\psi}P_{R,L} \quad (2.41)$$

and rewrite the mass term as

$$-m\bar{\psi}\psi = -m(\bar{\psi}_R\psi_L + \bar{\psi}_L\psi_R). \quad (2.42)$$

Now, the problem is made manifest: since the left-handed fermions are isospin doublets while the right-handed fermions are isospin singlets, they transform differently under $SU(2)_L \times U(1)_Y$:

$$\begin{aligned} \psi_L &\rightarrow \psi'_L = \psi_L e^{i\mathbf{W}\cdot\mathbf{T} + i\alpha Y}, \\ \psi_R &\rightarrow \psi'_R = \psi_R e^{i\alpha Y}. \end{aligned} \quad (2.43)$$

Thus, the Lagrangian will not be $SU(2)_L \times U(1)_Y$ invariant in the presence of an explicit mass term. In the context of quark masses, let

$$\begin{aligned} Q_L^i &= \begin{pmatrix} u^i \\ d^j \end{pmatrix}_L = \left(\begin{pmatrix} u \\ d \end{pmatrix}_L, \begin{pmatrix} c \\ s \end{pmatrix}_L, \begin{pmatrix} t \\ b \end{pmatrix}_L \right) \\ u_R^i &= (u_R, c_R, t_R), \\ d_R^i &= (d_R, s_R, b_R). \end{aligned} \quad (2.44)$$

The way out is to introduce a fermion-Higgs interaction term in the Lagrangian:

$$-\mathcal{L} = Y_d^{ij} \bar{Q}_L^i \phi d_R^j + Y_u^{ij} \bar{Q}_L^i \tilde{\phi} u_R^j, \quad (2.45)$$

where $Y_{u,d}^{ij}$ is the fermion-Higgs Yukawa coupling, with flavor indices i, j , ϕ is the complex scalar field defined in Equation(2.19) and

$$\tilde{\phi} = -i\sigma_2 \phi^* = (-i) \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix}^* = \begin{pmatrix} \phi^0 \\ \phi^- \end{pmatrix}. \quad (2.46)$$

When the scalar field acquires a non-zero vacuum expectation value, we have

$$\begin{aligned} -\mathcal{L} &= Y_d^{ij} \bar{Q}_L^i \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v+h \end{pmatrix} d_R^j + Y_u^{ij} \bar{Q}_L^i \frac{1}{\sqrt{2}} \begin{pmatrix} v+h \\ 0 \end{pmatrix} u_R^j \\ &= M_d^{ij} \bar{d}_L^i d_R^j + M_u^{ij} \bar{u}_L^i u_R^j + \Lambda_d^{ij} \bar{d}_L^i d_R^j h + \Lambda_u^{ij} \bar{u}_L^i u_R^j h. \end{aligned} \quad (2.47)$$

When $i = j$, this gives us mass terms of the form $M_{u,d} \propto vY_{u,d}$ as well as the quark-Higgs interaction term of strength $\Lambda_{u,d} \propto Y_{u,d}$. For the case when $i \neq j$, however, there are ‘mass’ terms involving different quark flavors, *e.g.* $\bar{d}_L^1 d_R^2 = \bar{d}_L s_R$. This is the result of working in the flavor basis. To properly interpret quark masses, we need to work in the mass basis. To do so, we diagonalise $M_{u,d}$ via

$$D_{u,d} = V_L^{u,d} M_{u,d} V_R^{u,d\dagger}, \quad (2.48)$$

where $D_{u,d}$ is a diagonal matrix in the mass basis and $V_{L,R}^{u,d}$ are unitary matrices. Working with the mass terms in Equation (2.47) in vector notation,

$$\begin{aligned} -\mathcal{L} &= \bar{d}_L M_d d_R + \bar{u}_L M_u u_R, \\ &= \bar{d}_L V_L^{d\dagger} V_R^d M_d V_L^{d\dagger} V_R^d d_R + \bar{u}_L V_L^{u\dagger} V_R^u M_u V_L^{u\dagger} V_R^u u_R, \\ &= \bar{d}'_L D_d d'_R + \bar{u}'_L D_u u'_R, \end{aligned} \quad (2.49)$$

where the primed quark fields are in the mass basis, $q_R \rightarrow q'_R = V_R^q q_R$, $\bar{q}_L \rightarrow \bar{q}'_L = \bar{q}_L V_L^{q\dagger}$, for $q = u, d$. This is to distinguish from the quark fields in flavor basis q , *i.e.* no prime.

Let us see how this transformation into the mass basis affects the other terms in the full Lagrangian. The covariant derivative for the left-handed fermions is

$$\begin{aligned} i\bar{Q}_L \gamma^\mu \left(\partial_\mu + \frac{i}{2} g \mathbf{W}_\mu \cdot \boldsymbol{\tau} + \frac{i}{2} g' Y B_\mu \right) Q_L \\ = i\bar{u}\not{\partial}u + i\bar{d}\not{\partial}d - \frac{g}{\sqrt{2}} (\bar{d}_L \gamma^\mu W_\mu^+ u_L + \bar{u}_L \gamma^\mu W_\mu^- d_L) + \dots \end{aligned} \quad (2.50)$$

where ellipses denote the rest of the expansion that are irrelevant to our current study. Now, expressing the quark fields in the mass basis, we have

$$\mathcal{L} = \frac{g}{\sqrt{2}} \left(\bar{d}_L (V_L^{d\dagger} V_L^u) \gamma^\mu W_\mu^+ u_L + \bar{u}_L (V_L^{u\dagger} V_L^d) \gamma^\mu W_\mu^- d_L \right). \quad (2.51)$$

This product of matrices $V_L^{u\dagger} V_L^d$ is a 3×3 unitary matrix known as the Cabibbo-Kobayashi-Maskawa (CKM) matrix [14, 15]. By convention, one chooses the u -type quark fields to be the same in the mass and flavor basis, that is

$$u_i = u'_i, \quad (2.52)$$

$$d_i = V_{\text{CKM}}^{ij} d'_j, \quad (2.53)$$

where i indexes the flavor generation and

$$V_{\text{CKM}} = \begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix}. \quad (2.54)$$

The unitarity of the matrix allows us to make the following constraints

$$\sum_i V_{ij} V_{ik}^* = \delta_{jk}, \quad \sum_j V_{ij} V_{kj}^* = \delta_{ik}, \quad (2.55)$$

where i, j, k indexes the quark flavors. The CKM matrix elements are free parameters in the Standard Model. Thus, their precise determination is crucial for the search of BSM physics. For example, a constraint on the first row ($i = k = u$)

takes the following form

$$|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2 = 1. \quad (2.56)$$

Should the determination of these matrix elements yield statistically-significant departures from unity, it may signal hitherto unknown interaction from the BSM sector. From the recent PDG review [4], this was found to be

$$|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2 = 0.9985 \pm 0.0007, \quad (2.57)$$

where a 2.2σ tension to unity exists. To resolve or raise the tension, one must provide more precise determinations of these matrix elements. An avenue of active research is to improve the precision on hadronic quantities involved in determining V_{ud} and V_{us} . We will return to this point later.

2.2.2 Quantum Chromodynamics

The Running Coupling

Quantum Chromodynamics (QCD for short) is a non-Abelian gauge theory. Its Lagrangian is packaged similarly to QED, that is,

$$\mathcal{L} = \sum_f i\bar{\psi}^f \not{D}\psi^f - \frac{1}{4}F_{\mu\nu}^a F^{\mu\nu a}, \quad (2.58)$$

where f is the flavor index, $a = 1, \dots, 8$ is the color index and the covariant derivative is

$$D_\mu = \partial_\mu + igA_\mu^a T^a, \quad (2.59)$$

with g the strong coupling, T^a the SU(3) generators in the fundamental representation and the field strength tensor is

$$F_{\mu\nu}^a = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a - gf^{abc}A_\mu^b A_\nu^c \quad (2.60)$$

with f^{abc} the structure constant from $[T^a, T^b] = if^{abc}T^c$. Compared to Equation (2.8), an additional feature in the QCD Lagrangian is the gluon self interaction in the field strength tensor. Together with the interactions from the covariant derivative, these are illustrated in Figure 2.2.

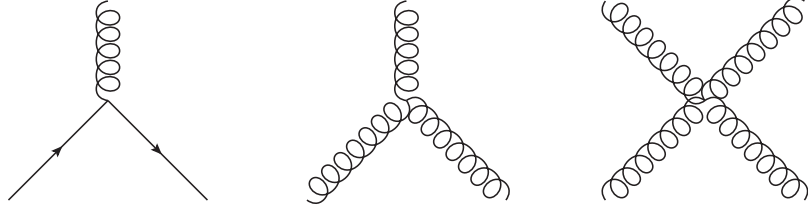


Figure 2.2 *Schematic Feynman diagrams showing the different interactions in permitted by the QCD Lagrangian. Solid lines represent fermions and squiggly lines represent gluons. The cubic and quartic gluon self interactions are shown in the centre and right diagrams.*

In quantum field theory, coupling constants are not actually constant but ‘run’ with the energy scale μ . By studying the renormalisation group equation of the coupling g ,

$$\beta(g) = \mu \frac{\partial g}{\partial \mu}, \quad (2.61)$$

where $\beta(g) = b_0 g^3$ at 1-loop, we obtain

$$g^2(\mu^2) = \frac{g^2(\mu_0^2)}{1 - g(\mu_0^2)b_0 \log \frac{\mu^2}{\mu_0^2}} \quad (2.62)$$

for some reference scale μ_0 . For QED,

$$b_0 = \frac{1}{12\pi^2}. \quad (2.63)$$

Then, using $\alpha = g^2/4\pi$, the electromagnetic coupling becomes

$$\alpha(\mu^2) = \frac{\alpha(\mu_0^2)}{1 - \frac{\alpha(\mu_0^2)}{3\pi} \log \frac{\mu^2}{\mu_0^2}}. \quad (2.64)$$

At $\mu_0 \sim 1\text{MeV}$, the electric charge can be measured to a high degree of precision, a recent report from CODATA [16] gives

$$\alpha(1\text{MeV}) = \frac{e^2}{4\pi} = 7.2973525693(11) \times 10^{-3}. \quad (2.65)$$

From Equation (2.64), we see that α grows slowly with energy scale μ , *e.g.* $\alpha(M_Z^2) \approx \frac{1}{128}$ [17].

Similarly, we can study the running of the QCD coupling, known as the ‘strong’ coupling g_s , through its β -function. Indeed, Gross, Wilczek [18] and Politzer [19]

calculated the simple³ 1-loop contribution to be

$$\beta(g) = -\frac{g_s^3(\mu_0)}{(4\pi)^2} \left(11 - \frac{2}{3}N_f \right). \quad (2.66)$$

Note the minus sign that was not present in the QED β -function (see Equation (2.63)). Expressing the strong coupling in like manner to electromagnetism, *i.e.* $\alpha_s = g_s^2/4\pi$, it runs as

$$\alpha_s(\mu^2) = \frac{\alpha_s(\mu_0^2)}{1 + (11 - \frac{2}{3}N_f) \frac{\alpha_s(\mu_0^2)}{4\pi} \log \frac{\mu^2}{\mu_0^2}}. \quad (2.67)$$

Several remarks can be made here. Consider the β -function in Equation (2.66): the factor ‘11’ comes from the gluon self interactions. This distinctive feature originates from the non-Abelian properties of the gauge group. The number of quark flavors N_f is a free parameter in this function. Up to $N_f = 16$, $\beta(g) < 0$. To this day, experimental constraints have set $N_f = 6^4$. Given this, the β -function of QCD with 3 quark generations is negative. Now, there exists an energy scale $\mu = \Lambda_{\text{QCD}}$ such that

$$\left(11 - \frac{2}{3}N_f \right) \frac{\alpha_s(\mu_0^2)}{4\pi} \log \frac{\Lambda_{\text{QCD}}^2}{\mu_0^2} = 1. \quad (2.68)$$

Solving for $\alpha(\mu_0^2)$, we can rewrite Equation (2.67) as

$$\alpha_s(\mu^2) = \frac{4\pi}{(11 - \frac{2}{3}N_f) \log \frac{\mu^2}{\Lambda_{\text{QCD}}^2}}. \quad (2.69)$$

For $\mu > \Lambda_{\text{QCD}}$, the coupling strength becomes weaker in the high energy limit while the coupling diverges and enters the non-perturbative regime as $\mu \rightarrow \Lambda_{\text{QCD}}$ from above. This phenomenon is called *asymptotic freedom* and its discovery earned Gross, Wilczek and Politzer their Nobel Prize in 2004. Figure 2.3 shows the running of the strong coupling.

³single coupling, *i.e.* ignoring quark masses

⁴*e.g.* see 2019 analysis summary by CMS.

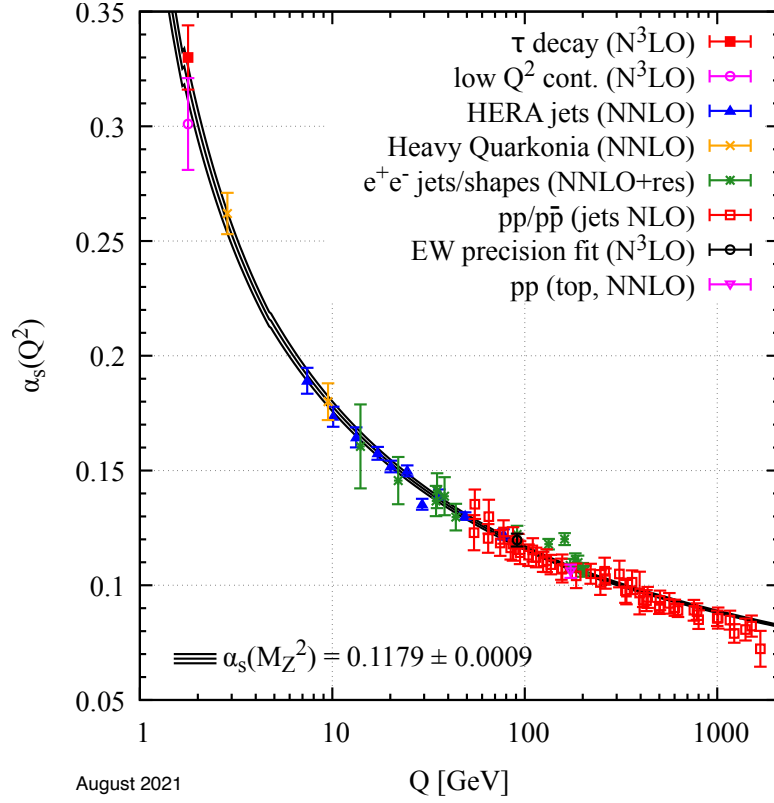


Figure 2.3 *The running of the QCD coupling $\alpha(Q^2) = g_s^2/4\pi$ as a function of the 4-momentum transfer Q , and the various experimental determinations, taken from [4].*

Chiral Symmetries

Let us return to the QCD Lagrangian in Equation (2.58). For this section, we do not restrict the number of flavors N_f . For convenience, we recast it here

$$\mathcal{L} = \sum_f i\bar{\psi}^f \not{D}\psi^f - \frac{1}{4}F_{\mu\nu}^a F^{\mu\nu a}.$$

This Lagrangian is invariant under *vector transformations*, *i.e.*

$$\psi^f \rightarrow e^{i\alpha T_j} \psi^f, \quad \bar{\psi}^f \rightarrow \bar{\psi}^f e^{i\alpha T_j}, \quad (2.70)$$

$$\psi^f \rightarrow e^{i\alpha \mathbf{1}} \psi^f, \quad \bar{\psi}^f \rightarrow \bar{\psi}^f e^{i\alpha \mathbf{1}}, \quad (2.71)$$

where α is a constant and $T_j, j = 1, \dots, N_f^2 - 1$ are the generators of $SU(3)$ acting in flavor space. One can always decompose these fermion fields into its left- and right-handed components using projectors (see Equation (2.39)). One can then

show that, under *chiral* or *axial-vector* transformations, *i.e.*

$$\psi^f \rightarrow e^{i\alpha\gamma^5 T_j} \psi^f, \quad \bar{\psi}^f \rightarrow \bar{\psi}^f e^{i\alpha\gamma^5 T_j}, \quad (2.72)$$

$$\psi^f \rightarrow e^{i\alpha\gamma^5 \mathbb{1}} \psi^f, \quad \bar{\psi}^f \rightarrow \bar{\psi}^f e^{i\alpha\gamma^5 \mathbb{1}}, \quad (2.73)$$

the left- and right-handed quark fields of different flavors mix while leaving the Lagrangian above invariant.

Thus, the massless Lagrangian respects the $SU(N_f)_L \times SU(N_f)_R \times U(1)_V \times U(1)_A$ symmetry. However, when the theory is fully quantised, the fermion determinant is not invariant under the axial-vector transformation in Equation (2.73), *i.e.* the $U(1)_A$ symmetry is broken explicitly by the fermion integration measure. Additionally, the ground state is not invariant under chiral rotations. Consider the *chiral condensate*,

$$\langle 0 | \bar{\psi} \psi | 0 \rangle = \langle 0 | \bar{\psi}_L \psi_R + \bar{\psi}_R \psi_L | 0 \rangle \neq 0. \quad (2.74)$$

Much like an explicit mass term in the Lagrangian (see Equation (2.42)), this term is not invariant under $SU(N_f)_L \times SU(N_f)_R$. As a result, chiral symmetry is spontaneously broken by the QCD vacuum into $SU(N_f)$ by the presence of N_f degenerate masses. In the case where the masses are non-degenerate, this is further broken to $U(1) \times \cdots \times U(1)$ (N_f times).

To summarise, for N_f flavors the $SU(N_f)_L \times SU(N_f)_R \times U(1)_V \times U(1)_A$ undergoes

1. explicit breaking of $U(1)_A$ due to non-invariance of the fermion determinant (known as axial anomaly);
2. spontaneous breaking of chiral symmetry by QCD vacuum, *i.e.* $SU(N_f)_L \times SU(N_f)_R$ into $SU(N_f) \times U(1)$ and
3. further breaking into $U(1) \times \cdots \times U(1)$ due to non-degenerate quark masses.

Thus, beginning with $(N_f^2 - 1) + 1$ generators, after spontaneous symmetry breaking one has 1 generator leftover. By Goldstone's theorem, we expect to have $(N_f^2 - 1) + 1 - 1 = N_f^2 - 1$ massless Goldstone bosons. For $SU(2)$, these are the $\pi^\pm$ and π^0 . Extending to $SU(3)$, we have additionally the $K^\pm, K^0, \bar{K}$ and the η .

2.3 Decays in the Weak Sector

2.3.1 Leptonic Decay Rates: Derivation

We would like to answer the question: given a period of measurement time T , what is the probability of an initial state i becoming a final state f ? We begin with the normalised transition probability $P(i \rightarrow f)$, which is defined as

$$P(i \rightarrow f) = \frac{|\langle f|S - \mathbb{1}|i\rangle|^2}{\langle f|f\rangle \langle i|i\rangle}, \quad (2.75)$$

where S is the usual S -matrix and the denominators are given by

$$\langle i|i\rangle = 2p_i^0(2\pi)^3\delta^3(0) = 2p_i^0V, \quad (2.76)$$

$$\langle f|f\rangle = \prod_f (2p_f^0V). \quad (2.77)$$

In the above, the volume factors come from working in a finite box⁵ of size V , where

$$\begin{aligned} \delta^3(\mathbf{p} - \mathbf{q}) &= \frac{1}{(2\pi)^3} \int_V d^3x e^{-i(\mathbf{p}-\mathbf{q})\cdot\mathbf{x}}, \\ &= \frac{V}{(2\pi)^3} \delta_{\mathbf{p}\mathbf{q}}. \end{aligned} \quad (2.78)$$

In the numerator, the matrix element can be expressed in terms of the invariant decay amplitude $\mathcal{M}_{fi}$ as

$$\langle f|S - \mathbb{1}|i\rangle = (2\pi)^4\delta^4\left(p_i - \sum_{r \in f} p_r\right) \mathcal{M}_{fi}. \quad (2.79)$$

Our transition probability is thus

$$P(i \rightarrow f) = \frac{|\mathcal{M}_{fi}|^2}{2m_i} T(2\pi)^4\delta^4\left(p_i - \sum_{r \in f} p_r\right) \prod_f \left(\frac{1}{2p_f^0V}\right), \quad (2.80)$$

where, compared to Equations (2.75)-(2.77), we have exchanged one of the δ -functions for a 4-volume factor VT and we have replaced p_i^0 with its rest mass m_i since one can always Lorentz boost into the rest frame of the initial particle.

⁵Just as in an experimental situation.

In experiments, it is difficult to measure the final state momenta with infinite precision. The two ways around this are 1) integrating over all momentum or 2) integrating over some region corresponding to the detector precision. Opting for the latter, we note that the momentum of a 1-particle states in a finite (momentum-space) volume is $V d^3 p_r / (2\pi)^3$ for each $r \in f$, so the volume factors from the integration measure cancels with those in Equation (2.80). Thus, let the Lorentz invariant phase space integral be

$$d\rho_f = (2\pi)^4 \delta^4 \left(p_i - \sum_{r \in f} p_r \right) \prod_{r \in f} \left[\frac{d^3 p_r}{(2\pi)^3} \frac{1}{2p_r^0} \right]. \quad (2.81)$$

When we divide the transition amplitude by the total time, we get the expression we want. Let

$$\begin{aligned} \Gamma(i \rightarrow f) &= \frac{1}{T} \int \prod_{r \in f} \left[\frac{d^3 p_r}{(2\pi)^3} V \right] P(i \rightarrow f), \\ &= \frac{1}{2m_i} (2\pi)^4 \delta^4 \left(p_i - \sum_{r \in f} p_r \right) \int \prod_{r \in f} \left[\frac{d^3 p_r}{(2\pi)^3} \frac{1}{2p_r^0} \right] |\mathcal{M}_{fi}|^2, \\ &= \frac{1}{2m_i} \int d^3 \rho_f |\mathcal{M}_{fi}|^2. \end{aligned} \quad (2.82)$$

Of particular interest is the two-body decay $i \rightarrow f_1 f_2$. It can be shown that the Lorentz-invariant phase space integral reduces to [17]

$$(2\pi)^4 \delta^4 \left(p_i - \sum_{r \in f} p_r \right) \int \prod_{r \in f} \left[\frac{d^3 p_r}{(2\pi)^3} \frac{1}{2p_r^0} \right] = \int \frac{d\Omega_{\text{cm}}}{4\pi} \frac{1}{8\pi} \frac{2|\mathbf{p}|}{E_{\text{cm}}} = \frac{|\mathbf{p}|}{4\pi m_i} \quad (2.83)$$

where $\mathbf{p}$ is the 3-momentum of one of the final state particles E_{cm} is the centre-of-mass energy and $d\Omega_{\text{cm}}$ is the volume integral in spherical coordinates.

2.3.2 Leptonic Decay Rate: A Study of Light Pseudoscalars

Now that we have developed the necessary tools in the previous section, let us study the muonic decay of a π^+ meson, $\pi^+ \rightarrow \mu^+ \nu$. A similar procedure can be applied to the other pseudoscalar of interest, the K^+ meson.

First, the kinematics⁶. From conservation of 4-momentum,

$$\begin{aligned} p_\pi^2 &= (p_\mu + p_\nu)^2, \\ M_{\pi^+}^2 &= m_{\mu^+}^2 + 2E_\mu |\mathbf{p}_\mu| + 2|\mathbf{p}_\mu|^2, \end{aligned} \quad (2.84)$$

where in the second line we work in the rest frame of the π^+ meson and we have swapped the neutrino 3-momenta for the lepton's. Solving this for the lepton momentum gives

$$|\mathbf{p}_\mu| = \frac{M_{\pi^+}}{2} \left(1 - \frac{m_{\mu^+}^2}{M_{\pi^+}^2} \right). \quad (2.85)$$

Next, note that since $M_{\pi^+}, M_{K^+} \ll m_W$, this process takes place well below the electroweak scale. We are thus in the appropriate regime to use the effective Lagrangian

$$\mathcal{L}_{\text{eff}}(x) = \frac{G_F}{\sqrt{2}} J_{\text{lep}\tau}(x) J_{\text{had}}^\tau(x), \quad (2.86)$$

where G_F is the Fermi constant. The leptonic current is

$$J_{\text{lep}}^\tau(x) = \bar{\nu}(x) \Gamma_L^\tau \mu(x) \quad (2.87)$$

and the hadronic current can be decomposed into

$$J_{\text{had}}^\tau(x) = V^\tau(x) - A^\tau(x) = \sum_{q_1, q_2} V_{q_1 q_2} \bar{q}_1(x) \Gamma_L^\tau q_2(x), \quad (2.88)$$

with

$$V^\tau(x) = \sum_{q_1, q_2} V_{q_1 q_2} \bar{q}_1(x) \gamma^\tau q_2(x), \quad (2.89)$$

$$A^\tau(x) = \sum_{q_1, q_2} V_{q_1 q_2} \bar{q}_1(x) \gamma^\tau \gamma^5 q_2(x), \quad (2.90)$$

where $V_{q_1 q_2}$ is the CKM matrix element between quark flavors $q_1 = u, c$ and $q_2 = d, s, b$ and $\Gamma_L^\tau = \gamma^\tau(1 - \gamma^5)$ is the $V - A$ current. The S -matrix is thus

$$S = \mathcal{T} \exp i \int d^4x J_{\text{lep}\tau}(x) J_{\text{had}}^\tau(x). \quad (2.91)$$

Since the spacetime integral will yield a δ -function, we consider the invariant

⁶We use lower case ' m ' for masses of fundamental particles and upper case ' M ' for masses of composite particles.

amplitude below. Suppressing function arguments from here on, we have

$$\begin{aligned}\mathcal{M}^{r,s} &= \langle \mu^+, r; \nu, s | \mathcal{L}_{\text{eff}} | \pi^+ \rangle, \\ &= \frac{G_F}{\sqrt{2}} \langle \mu^+, r; \nu, s | J_{\text{lep}\tau} | 0 \rangle \langle 0 | J_{\text{had}}^\tau | \pi^+ \rangle.\end{aligned}\quad (2.92)$$

Let us evaluate these two matrix elements in order. First, the hadronic piece

$$\begin{aligned}\langle 0 | J_{\text{had}}^\tau | \pi^+ \rangle &= \sum_{q_1, q_2} V_{q_1 q_2} [\langle 0 | \bar{q}_1 \gamma^\tau q_2 | \pi^+ \rangle - \langle 0 | \bar{q}_1 \gamma^\tau \gamma^5 q_2 | \pi^+ \rangle], \\ &= V_{ud} A_\pi^\tau,\end{aligned}\quad (2.93)$$

where we have packaged the non-perturbative QCD matrix element into A_π^τ . Under parity transformations, the initial state $|\pi^+\rangle$ is odd while the vector and axial matrix elements transform as an axial-vector and vector, respectively. Since the only Lorentz variable is the momentum 4-vector, p_π , only the axial matrix element has a non-zero contribution. Additionally, one can perform a Lorentz boost into the rest frame of the π^+ meson, where only $\tau = 0$ component contributes in the 4-momentum. Thus, let

$$A_\pi = \langle 0 | \bar{q}_1 \gamma^0 \gamma^5 q_2 | \pi^+ \rangle = i f_\pi M_{\pi^+}, \quad (2.94)$$

where we packaged all the non-perturbative effects of the QCD matrix element in the pion decay constant, f_π . Now, for the leptonic piece. Let

$$L^{r,s}(\mathbf{p}_\mu) \equiv \langle \mu^+, r; \nu, s | \bar{\nu} \Gamma_L^0 \ell | 0 \rangle = \bar{u}^s(\mathbf{p}_\nu) \Gamma_L^0 v^r(\mathbf{p}_\mu), \quad (2.95)$$

where u and v are the Dirac spinors and $\mathbf{p}_\nu = -\mathbf{p}_\mu$. The only Lorentz index to contribute is $\tau = 0$ due to the axial matrix element. At this stage, the invariant amplitude is

$$\mathcal{M}^{r,s} = i V_{ud} f_\pi M_{\pi^+} \frac{G_F}{\sqrt{2}} \bar{u}^s(\mathbf{p}_\nu) \Gamma_L^0 v^r(\mathbf{p}_\mu). \quad (2.96)$$

We square the amplitude and take the spin-sum average, giving

$$\begin{aligned}|\mathcal{M}|^2 &= \sum_{r,s} |\mathcal{M}^{r,s}|^2, \\ &= \frac{G_F^2}{2} |V_{ud}|^2 f_\pi^2 M_{\pi^+}^2 \sum_{r,s} \bar{u}^s(\mathbf{p}_\nu) \Gamma_L^0 v^r(\mathbf{p}_\mu) \bar{v}^r(\mathbf{p}_\mu) \Gamma_L^0 u^s(\mathbf{p}_\nu), \\ &= \frac{G_F^2}{2} |V_{ud}|^2 f_\pi^2 M_{\pi^+}^2 \text{Tr} \left[\not{p}_\nu \Gamma_L^0 (\not{p}_\mu - m_{\mu^+}) \Gamma_L^0 \right].\end{aligned}\quad (2.97)$$

One can show that the trace gives

$$\text{Tr} \left[\not{p}_\nu \Gamma_L^0 (\not{p}_\mu - m_{\mu^+}) \Gamma_L^0 \right] = 8 |\mathbf{p}_\mu| (E_\mu - |\mathbf{p}_\mu|). \quad (2.98)$$

Using Equation (2.85) in Equation (2.98),

$$\text{Tr} \left[\not{p}_\nu \Gamma_L^0 (\not{p}_\mu - m_{\mu^+}) \Gamma_L^0 \right] = 4 m_{\mu^+}^2 \left(1 - \frac{m_{\mu^+}^2}{M_{\pi^+}^2} \right). \quad (2.99)$$

Now, we assemble the decay rate following the formula in Equation (2.82), giving

$$\begin{aligned} \Gamma_\pi^{\text{tree}} \equiv \Gamma(\pi^+ \rightarrow \mu^+ \nu) &= \frac{1}{2M_{\pi^+}} \int d^3\rho |\mathcal{M}|^2, \\ &= \frac{G_F^2}{4\pi} |V_{ud}|^2 f_\pi^2 M_{\pi^+}^2 m_{\mu^+}^2 \left(1 - \frac{m_{\mu^+}^2}{M_{\pi^+}^2} \right)^2, \end{aligned} \quad (2.100)$$

where we have used Equation (2.83) to evaluate the phase space integral. This is the tree-level expression for the leptonic decay of a π^+ meson. An identical expression for the K^+ meson can be obtained by swapping $\pi^+ \rightarrow K^+$.

2.4 Isospin-breaking Effects in Flavor Physics

The determination of CKM matrix elements requires the joint effort of precise experimental measurements and predictions from theory. One of the experimental avenues of interest is the leptonic decay channels. In the previous section, the tree-level decay rate was

$$\Gamma_P^{\text{tree}} = \frac{G_F^2}{8\pi} M_P m_\ell^2 \left(1 - \frac{m_\ell^2}{M_P^2} \right)^2 |f_P|^2 |V_{q_1 q_2}|^2 \quad (2.101)$$

for a general pseudoscalar P and lepton ℓ . The pseudoscalar decay constant f_P was defined in Equation (2.94), which was

$$A_P = \langle 0 | \bar{q}_1 \gamma^0 \gamma^5 q_2 | P \rangle = i V_{q_1 q_2} f_P M_P.$$

As noted previously, since the decay constant encapsulates the non-perturbative effects of QCD, it is evaluated numerically using lattice QCD methods, which we will introduce in the following chapter. Traditionally, these calculations were

performed in the $\alpha = 0, \delta m = 0$ regime⁷, known as the *isospin-symmetric* QCD theory⁸. However, since recent lattice determinations of f_K and f_π have attained percent-level precision [20], further progress will necessitate the inclusion of *isospin-breaking* effects since $\alpha \sim \frac{\delta m}{\Lambda_{\text{QCD}}} \sim 1\%$.

Moreover, for the case of light charged pseudoscalars, $P = K^\pm, \pi^\pm$, it is the inclusive decay rate that is measured, *i.e.* the decay rate of a pseudoscalar into a lepton, its neutrino partner with and without an external final state photon. This is due to the experimental difficulty in distinguishing between final states with or without a soft photon. To use the inclusive rate for the extraction of $V_{q_1 q_2}$, first we express the inclusive rate as

$$\begin{aligned}
\Gamma(P \rightarrow \ell \nu [\gamma]) &= \mathcal{K}_P \sum_{r,s} |\mathcal{M}_P^{r,s}|^2 \\
&= \mathcal{K}_P \sum_{r,s} |\mathcal{M}_{P,0}^{r,s} + \delta \mathcal{M}_P^{r,s}|^2, \\
&= \mathcal{K}_P \sum_{r,s} \left[|\mathcal{M}_{P,0}^{r,s}|^2 + \mathcal{M}_{P,0}^{r,s} \delta \mathcal{M}_P^{r,s\dagger} + \mathcal{M}_{P,0}^{r,s\dagger} \delta \mathcal{M}_P^{r,s} + |\delta \mathcal{M}_P^{r,s}|^2 \right], \\
&= \Gamma_P^{\text{tree}} (1 + \delta R_P) + \mathcal{O}(\alpha^2, \delta m^2),
\end{aligned} \tag{2.102}$$

where r and s are spinor indices. By conservation of 4-momentum, $p_P = p_\ell + p_\nu$, the lepton and neutrino have equal and opposite 3-momenta, so we can write the kinematic factor as

$$\mathcal{K}_P = \frac{G_F^2}{16\pi} |V_{q_1 q_2}|^2 \frac{1}{2M_P} \left(1 - \frac{m_\ell^2}{M_P^2} \right). \tag{2.103}$$

If we identify $\mathcal{M}_0^{r,s}$ as the tree-level amplitude (see Equation (2.101)), then

$$\delta R_P = \frac{2 \sum_{r,s} \text{Re} \left[\delta \mathcal{M}_P^{r,s} \mathcal{M}_{P,0}^{r,s\dagger} \right]}{\sum_{r,s} |\mathcal{M}_{P,0}^{r,s}|^2} \tag{2.104}$$

denotes the isospin-breaking correction to the tree-level amplitude. In this thesis, our objective is to determine the ratio of CKM matrix elements $\frac{|V_{us}|}{|V_{ud}|}$ which can

⁷To work in this unphysical theory, a separation scheme must be defined beforehand and we relegate this discussion to §4.1.

⁸Note that there is isospin symmetry within QED, arising from the different quark charges. Here, our isosymmetric theory is degenerate in quark mass and charge.

be extracted from a ratio of inclusive rates via

$$\frac{|V_{us}|^2}{|V_{ud}|^2} = \frac{\Gamma(K^+ \rightarrow \mu^+ \nu_\mu [\gamma])}{\Gamma(\pi^+ \rightarrow \mu^+ \nu_\mu [\gamma])} \frac{M_{K^+}}{M_{\pi^+}} \frac{M_{\pi^+}^2 - m_{\mu^+}^2}{M_{K^+}^2 - m_{\mu^+}^2} \mathcal{F}^{-2}, \quad (2.105)$$

where

$$\mathcal{F} = \frac{f_K}{f_\pi} \sqrt{1 + \delta R_{K\pi}} \quad (2.106)$$

and $\delta R_{K\pi} \equiv \delta R_K - \delta R_\pi$. By using experimental measurements of the inclusive rate (*i.e.* branching ratios and mean lifetimes) and masses, the term $\delta R_{K\pi}$ encapsulates the ratio of isospin-breaking correction to the hadronic decay amplitudes. The lattice determination of $\delta R_{K\pi}$ is thus the main focus of this thesis.

Chapter 3

Quantum Field Theory on the Lattice

In this chapter we introduce the methodology for calculating non-perturbative QCD effects with discretised, finite-volume quantum field theories in numerical simulations. One of the highly practical approach to study low energy/strongly-coupled physics was first proposed by K. Wilson in 1974 [21] and is called *Lattice Quantum Chromodynamics*, or Lattice QCD for short. Note that this chapter is not intended as an exhaustive review, but presenting only what is necessary and sufficient for the calculation in this thesis. Most of the results from this chapter and further discussions can be found in [22].

Of central importance to our work is the notion that physical information may be extracted from the vacuum expectation value of time-ordered quantum fields. For simplicity, consider scalar fields ϕ . The n -point correlation function is defined by

$$C(x_1, \dots, x_n) = \langle \Omega | T \{ \phi(x_1) \dots \phi(x_n) \} | \Omega \rangle, \quad (3.1)$$

where $|\Omega\rangle$ is the vacuum state and $T\{\dots\}$ is the time-ordering operator. This object can be generated via the path integral formalism,

$$C(x_1, \dots, x_n) = \frac{1}{Z} \int D\phi \phi(x_1) \dots \phi(x_n) e^{-iS[\phi]}, \quad (3.2)$$

where $S[\phi] = \int d^4x \mathcal{L}(x)$ is the action of the theory and

$$Z = \int D\phi e^{iS[\phi]} \quad (3.3)$$

is the normalisation. The physical information of the correlation function can be obtained by studying the RHS of Equation (3.1). First, we need the complete set of states

$$\mathbb{1} = |\Omega\rangle \langle \Omega| + \sum_n \int \frac{d^3p}{(2\pi)^3} \frac{|n, \mathbf{p}\rangle \langle n, \mathbf{p}|}{\omega_n(\mathbf{p})} \quad (3.4)$$

where the summation index n represents all relevant quantum numbers of a given state and $|n, \mathbf{p}\rangle$ is a simultaneous eigenstate of the Hamiltonian and 3-momentum operator. Here, the normalisation is

$$\omega_n(\mathbf{p}) = \begin{cases} 1 & \text{if } n = \Omega, \\ 2E_n(\mathbf{p}) & \text{if } n \geq 0, \end{cases} \quad (3.5)$$

with $E_n^2(\mathbf{p}) = E_n^2(\mathbf{0}) + |\mathbf{p}|^2$ is the continuum dispersion relation.

As an example, consider a 2-point function $C(x) = \langle \Omega | \phi(x) \phi(0) | n, \mathbf{p} \rangle$. Inserting a complete set of states gives

$$\langle \Omega | \phi(x) \phi(0) | \Omega \rangle = \sum_n \int \frac{d^3p}{(2\pi)^3} \frac{|Z_n|^2}{\omega_n(\mathbf{p})} e^{-i\mathbf{p} \cdot \mathbf{x}} e^{-i\omega_n t}, \quad (3.6)$$

where $Z_n = \langle \Omega | \phi(0) | \Omega \rangle$ and we have used the translation property, $\phi(x) = e^{iP \cdot x} \phi(0) e^{-iP \cdot x}$ with $P = (H, \mathbf{P})$ being a 4-vector containing the Hamiltonian and 3-momentum operator. Projecting onto a specific momentum $\mathbf{k}$,

$$C(\mathbf{k}, t) \equiv \int d^3x C(x) e^{i\mathbf{k} \cdot \mathbf{x}} = \sum_n \frac{|Z_n|^2}{\omega_n(\mathbf{k})} e^{-i\omega_n t}. \quad (3.7)$$

We will return to Equations (3.2) and (3.7) shortly. First, let us migrate our discussion to Euclidean spacetime.

3.1 Analytic Continuation from Minkowski to Euclidean

Dynamic Variables

The analytic continuation from Minkowski to Euclidean spacetime proceeds as

$$x^0 \rightarrow x^4 = ix^0, \quad (3.8)$$

$$p^0 \rightarrow p^4 = ip^0 \quad (3.9)$$

such that

$$\begin{aligned} (k \cdot x) &= \eta_{\mu\nu} k^\mu x^\nu, \\ &= -k^4 x^4 - \mathbf{k} \cdot \mathbf{x}, \\ &= -\delta_{\mu\nu} k_E^\mu x_E^\nu, \\ &= -(k_E \cdot x_E), \end{aligned} \quad (3.10)$$

where $\delta_{\mu\nu} = \text{diag}(1, 1, 1, 1)$ and

$$p^2 = \eta_{\mu\nu} p^\mu p^\nu = (p^0)^2 - \mathbf{p} \cdot \mathbf{p} = (-ip^4)^2 - \mathbf{p} \cdot \mathbf{p} = -m^2. \quad (3.11)$$

In Euclidean space, the Lorentz indices run as $\mu = 1, 2, 3, 4$ and there is no distinction between upper and lower indices.

γ -matrices

The γ -matrices in Minkowski space must satisfy the anticommutation relation

$$\{\gamma^\mu, \gamma^\nu\} = 2\mathbb{1}\eta^{\mu\nu}, \quad (3.12)$$

where $\eta = \text{diag}(1, -1, -1, -1)$. In Euclidean space, this becomes

$$\{\gamma^\mu, \gamma^\nu\} = 2\mathbb{1}\delta^{\mu\nu}. \quad (3.13)$$

This implies

$$\gamma^0 = \gamma_E^4, \quad (3.14)$$

$$\gamma^j = i\gamma_E^j, \quad j = 1, 2, 3. \quad (3.15)$$

The Feynman slash notation becomes

$$\not{p} = \gamma^0 p_0 - \gamma^j p_j = \eta_{\mu\nu} \gamma^\mu p^\nu = -i (\gamma_E^4 p_E^4 + \gamma_E^j p_E^j) = -i \not{p}_E. \quad (3.16)$$

Dirac Equation & Spinors

With the above, we can construct the Dirac equation in Euclidean space. From Equation (3.16),

$$\not{\partial} = \gamma^0 \frac{\partial}{\partial x^0} - \gamma^j \frac{\partial}{\partial x^j} = i \left(\gamma_E^4 \frac{\partial}{\partial x^4} + \gamma_E^j \frac{\partial}{\partial x^j} \right) = i \not{\partial}_E. \quad (3.17)$$

The Euclidean Dirac equation for a fermion ψ follows as

$$(\not{\partial}_E + m)\psi = 0. \quad (3.18)$$

For the positive/negative frequency solutions to the Dirac equation, the outer product of the spinors are

$$\sum_{r,s} u^r(p_E) \bar{u}^s(p_E) = -i \not{p}_E + m \quad \text{and} \quad (3.19)$$

$$\sum_{r,s} v^r(p_E) \bar{v}^s(p_E) = -i(\not{p}_E + m) \quad (3.20)$$

respectively.

Correlation Functions in Euclidean Space

Let us now review the consequences of the analytic continuation into Euclidean space. Returning to the n -point correlation functions, the path integral formalism is now

$$C(x_1, \dots, x_n) = \int D\phi \phi(x_1) \dots \phi(x_n) e^{-S[\phi]}, \quad (3.21)$$

i.e. we can now interpret e^{-S} as a Boltzmann weight factor and $D\phi e^{-S}$ as a probability density. This integration can now be understood as averaging over

$\phi(x_1) \dots \phi(x_n)$ by drawing on random fields $D\phi e^{-S[\phi]}$.

Next, the functional form of the correlation function in Equation (3.7) is also modified:

$$C(\mathbf{k}, t) = \sum_n \frac{|Z_n|^2}{\omega_n(\mathbf{k})} e^{-\omega_n t}. \quad (3.22)$$

We see then that it is built from a sum of states with different quantum numbers. We order the tower of states such that $w_0 < w_1 < \dots$. Then, at large t , only the ground state $\omega_0(\mathbf{0}) = 2M$ remains. Relabelling the zero momentum correlation function as $C(t)$, we have

$$\lim_{t \rightarrow \infty} C(t) = \frac{|Z_0|^2}{2M} e^{-Mt}. \quad (3.23)$$

Often, one is interested in the ground state mass. Looking at Equation (3.23), we can define the effective mass as

$$M_{\text{eff}}(t) = \log \frac{C(t)}{C(t+1)}. \quad (3.24)$$

Thus, at large t , $M_{\text{eff}} \rightarrow M$.

3.2 Discretising Quantum Field Theory

Consider a 4-dimensional lattice Λ ,

$$\Lambda = \{n = (n_1, n_2, n_3, n_4) \in \mathbb{Z}_4\}, \quad (3.25)$$

where $n_j = 0, 1, \dots, N_j - 1$ for $j = 1, 2, 3$ and $n_4 = 0, 1, \dots, N_4 - 1$ are the spatial and temporal extent, respectively. Typically, $N_1 = N_2 = N_3 = N_L$ and $N_4 = N_T$. This lattice is said to have a (finite) volume of $V = L^3 \times T$, where $L = aN_L$ and $T = aN_T$.

Now we replace continuous spacetime by its discretised version, *i.e.* $x = an$. Since the lattice spacing a gives the notion of physical distances between the lattice sites, we can understand the fermion fields as living on the sites of Λ , *i.e.* $\psi(x) \rightarrow \psi(an)$ ¹. In this formulation, the partial derivative is discretised in the following

¹For function arguments, we will alternate between $f(x)$ and $f(n)$ based on whether the emphasis is on the spacetime or lattice coordinate.

symmetric manner

$$\partial_\mu \psi(n) = \frac{1}{2a} (\psi(n + \hat{\mu}) - \psi(n - \hat{\mu})), \quad (3.26)$$

where $\hat{\mu}$ is a unit vector in the μ -direction.

Next, we impose upon a function f on this lattice to have *toroidal* boundary conditions, *i.e.*

$$f(n + \hat{\mu}N_\mu) = e^{i2\pi\theta_\mu} f(n), \quad (3.27)$$

where $\theta_\mu \in \mathbb{Z}$ for periodic boundary conditions and $\theta_\mu \in \mathbb{Z} + \frac{1}{2}$ for anti-periodic boundary conditions. The corresponding momentum space $\tilde{\Lambda}$ is

$$\tilde{\Lambda} = \left\{ p = \frac{2\pi}{aN_\mu} (k_\mu + \theta_\mu) \right\} \quad k_\mu \in \left(-\frac{N_\mu}{2}, \frac{N_\mu}{2} \right] \quad (3.28)$$

such that plane waves also obey Equation (3.27).

Now, define the Fourier transform of a function f to be

$$\tilde{f}(p) = a^4 \sum_{n \in \Lambda} f(n) e^{-ip \cdot na}. \quad (3.29)$$

Then, the inverse Fourier transform is

$$f(n) = \frac{1}{V} \sum_{k \in \tilde{\Lambda}} \tilde{f}(k) e^{ik \cdot na}, \quad (3.30)$$

using the following result

$$\sum_{k \in \tilde{\Lambda}} e^{ik \cdot (n-n')a} = \prod_{i=1}^4 N_i \delta_{n_i n'_i}. \quad (3.31)$$

Now, the completeness relation in Equation (3.4) becomes

$$\mathbb{1} = |\Omega\rangle \langle \Omega| + \frac{1}{L^3} \sum_{p \in \tilde{\Lambda}, n} \frac{|n, \mathbf{p}\rangle \langle n, \mathbf{p}|}{\omega_n(\mathbf{p})}. \quad (3.32)$$

Together with the external gauge fields U_μ , the naive discretisation of the QCD action is

$$S_F[\psi, \bar{\psi}, U] = a^4 \sum_{n, n' \in \Lambda} \bar{\psi}(n) D(n|n') \psi(n') \quad (3.33)$$

where

$$D(n|n') = \frac{1}{2a} \sum_{\mu=\pm 1}^{\pm 4} \gamma^\mu U_\mu(n) \delta_{n'n+\hat{\mu}} + m \delta_{n'n} \quad (3.34)$$

is the naive Dirac operator with $\gamma^{-\mu} = -\gamma^\mu$, U_μ is the $SU(3)$ gauge field, with $U_{-\mu}(n) = U_\mu^\dagger(n - \hat{\mu})$. One can show that the action is invariant under the following transformation

$$\begin{aligned} \psi(n) &\rightarrow \Omega(n) \psi(n), & \bar{\psi}(n) &\rightarrow \bar{\psi}(n) \Omega(n) & \text{and} \\ U_\mu(n) &\rightarrow \Omega(n) U_\mu(n) \Omega^\dagger(n + \hat{\mu}) \end{aligned} \quad (3.35)$$

where $\Omega \in SU(3)$ at each lattice site n .

Let us exponentiate this action and insert it into the path integral formalism,

$$C(x_1, \dots, x_n) = \frac{1}{Z} \int D\psi D\bar{\psi} DU \prod_{j=1}^n O_j[\psi, \bar{\psi}, U] e^{-S_F[\psi, \bar{\psi}, U]} e^{-S_G[U]}. \quad (3.36)$$

Evaluating the fermionic (Grassmann) integrals will yield the fermion determinant,

$$Z_f[U] = \int D\psi D\bar{\psi} e^{-S_F[\psi, \bar{\psi}, U]} = \det D[U]. \quad (3.37)$$

The integral is now

$$\frac{1}{Z} \int DU \langle O_1 \dots O_n \rangle_f[U] e^{-S_G[U]}, \quad (3.38)$$

where

$$Z = \int DU Z_f[U] e^{-S_G[U]} \quad (3.39)$$

and

$$\langle O_1 \dots O_n \rangle_f[U] = \int D\psi D\bar{\psi} \prod_{j=1}^n (O_j[\psi, \bar{\psi}, U]) e^{-S_F[\psi, \bar{\psi}, U]}. \quad (3.40)$$

Here, we keep the functional dependence on U to remind ourselves that these fermionic expectation values will vary with the input gauge fields.

To summarise, the construction of an n -point correlation function involves two steps: 1) for each gauge field configuration, evaluate the fermionic integral and 2) average over all gauge configuration with Boltzmann factor $e^{-S_G[U]}$.

3.2.1 Chiral Symmetry on the Lattice & the Nielsen-Ninomiya No-Go Theorem

Let us begin with the naively discretised Dirac operator (see Equation (3.34)) and compute the propagator. For simplicity, consider the non-interacting case, where the gauge links $U_\mu = \mathbb{1}$. Looking ahead to discussions about chiral symmetry, we may also set $m = 0$. First, the Fourier transform of D is

$$\tilde{D}(p) = \frac{i}{a} \sum_{\mu=1}^4 \gamma^\mu \sin p_\mu a. \quad (3.41)$$

Inverting this gives

$$\tilde{D}^{-1}(p) = \frac{i \sum_\mu \gamma^\mu \sin(p_\mu a)}{a^{-1} \sum_\mu \sin^2 p_\mu a}. \quad (3.42)$$

Note that the quark propagator is the inverse of the Dirac operator in coordinate space

$$D^{-1}(y|x) = \frac{1}{V} \sum_{p \in \tilde{\Lambda}} \tilde{D}^{-1}(p) e^{-ip \cdot (y-x)}. \quad (3.43)$$

In the continuum limit $a \rightarrow 0$,

$$\tilde{D}^{-1}(p) \rightarrow \frac{i \not{p}}{p^2}. \quad (3.44)$$

Thus, for massless fermions, there is a pole at $p = (0, 0, 0, 0)$. However, on the lattice, momentum is discretised and bounded (see Equation (3.28)). Whenever $p_\mu = 0$ or $p_\mu = \frac{\pi}{a}$, one hits a pole of the form $(\frac{\pi}{a}, 0, 0, 0), (0, \frac{\pi}{a}, 0, 0), \dots, (0, 0, 0, \frac{\pi}{a})$. There are $2^4 - 1 = 15$ unphysical poles, known as *doublers*.

To remove these doublers, Wilson [21] proposed the following (massless) Dirac operator in momentum space

$$\tilde{D}(p) = \frac{i}{a} \sum_{\mu=1}^4 \gamma^\mu \sin p_\mu a + \frac{1}{a} \sum_{\mu=1}^4 (1 - \cos p_\mu a), \quad (3.45)$$

where the new term on the RHS is called the *Wilson term*. For $p_\mu = 0$, this new term vanishes, leaving only the physical pole. For $p_\mu = \frac{\pi}{a}$, this term contributes as $\frac{2}{a}$. When inverted, the Wilson term will contribute to the Dirac propagator like a mass term $\frac{2d}{a}$, where d is the number of momentum components with $p_\mu = \frac{\pi}{a}$. One can check that in the continuum limit, the Wilson term becomes heavy and

decouples from the theory.

The (massless) Wilson Dirac operator reads

$$D(n|m) = \frac{1}{2a} \sum_{\mu=\pm 1}^{\pm 4} (\mathbb{1} - \gamma^\mu) U_\mu(n) \delta_{m, n+\hat{\mu}} + \frac{4}{a} \delta_{m, n}. \quad (3.46)$$

One of the crucial features of QCD in the continuum is the spontaneous breaking of chiral symmetry. On the lattice, the removal of doublers necessitates a mass-like term in the Lagrangian, which in turn breaks chiral symmetry explicitly rather than spontaneously. This Catch-22 is the *Nielsen-Ninomya No-Go Theorem*[23].

We see that discretised Dirac operators do not satisfy $\{D, \gamma^5\} = 0$ without the cost of generating doublers. To work around this, let us modify chiral symmetry on the lattice in a way which is compatible with its continuum version. This will take the form of the Ginsparg-Wilson equation [24]

$$\{\gamma^5, D\} = aD\gamma^5D. \quad (3.47)$$

In the limit where $a \rightarrow 0$, one recovers the continuum version. By the same spirit, the continuum chiral rotations (see Equation (2.73)) must be re-defined as

$$\psi \rightarrow \exp i\alpha\gamma^5 \left(\mathbb{1} - \frac{a}{2}D \right) \cdot \psi, \quad \text{and} \quad \bar{\psi} \rightarrow \bar{\psi} \cdot \exp i\alpha\gamma^5 \left(\mathbb{1} - \frac{a}{2}D \right), \quad (3.48)$$

where D in the above must satisfy the Ginsparg-Wilson equation. Recall that, on the lattice, with explicit spin (greek) and color (roman) indices,

$$(D\psi)_{\alpha b}(x) = a^4 \sum_{x' \in a\Lambda} \sum_{\beta, c} D_{\alpha\beta, bc}(x|x') \psi_{\beta c}(x'), \quad (3.49)$$

i.e. the Dirac operator connects fermions on neighbouring sites. One can show that $\bar{\psi}D\psi$ is invariant under chiral rotations on the lattice, provided D satisfies the Ginsparg-Wilson equation.

Before presenting a candidate Dirac operator that satisfies Equation (3.47), we make several remarks. In the continuum, chiral rotations are strictly local transformations (see Equation (2.73)). By contrast, imposing chiral symmetry on the lattice connects fermions on neighbouring sites. This is a consequence of discretising the covariant derivative term in the Dirac operator. As a result,

chirality of lattice fermions is determined by the gauge fields on the neighbouring lattice sites.

3.2.2 Domain Wall Fermions

Now, we introduce a discretised Dirac operator which satisfies the Ginsparg-Wilson equation. One such solution is called *Domain Wall Fermions*, or DWF for short. First introduced by Kaplan in 1992 [25], these are chiral fermions that live on the 4D surface of a 5D lattice. Let Λ_5 be the 5-dimensional lattice with volume $V_5 = L_s \times L^3 \times T$, where $L_s = aN_5$ is the extent of the 5th dimension, with N_5 the number of 5D slices on Λ_5 . The fermion fields that live in Λ_5 are noted by $\Psi_{ab}(x, s)$ and $\bar{\Psi}_{\beta c}(y, r)$, *i.e.* they carry identical copies of spin and color indices for the additional degree of freedom, $s, r = 0, \dots, N_5 - 1$.

The DWF action has the following form

$$S[\Psi, \bar{\Psi}, U] = a^4 \sum_{s,r=0}^{N_5-1} \sum_{n,n' \in \Lambda} \bar{\Psi}(n, r) D^{\text{dw}}(n, r | n', s) \Psi(n', s), \quad (3.50)$$

where the Dirac operator has two pieces:

$$D^{\text{dw}}(n, r | n', s) = \delta_{s,r} D(n | n') + \delta_{n,n'} D_5(r | s). \quad (3.51)$$

In the first term, the 4D fermions propagate across Λ on a given 5D *surface*. This can be built with the Wilson Dirac operator (see Equation (3.46)),

$$D(n | n') = (4 - M_5) \delta_{n,n'} - \frac{1}{2} \sum_{\mu=\pm 1}^{\pm 4} (\mathbb{1} - \gamma^4) U_\mu(n) \delta_{n+\hat{\mu}, n'}, \quad (3.52)$$

where M_5 is a new mass parameter, constrained to $0 < M_5 < 1$ to ensure that the theory is doubler-free and possesses a positive transfer matrix. Note that U_μ are the usual 4D QCD gauge fields. This means that copies of the gauge field may be re-used on each 5D slice in the simulation.

The other term in Equation (3.51) propagates through the *bulk* of Λ_5 for a fixed point in Λ . It is given by

$$\begin{aligned} D_5(r | s) = & \delta_{s,r} - (\mathbb{1} - \delta_{r, N_5-1}) P_- \delta_{r+1, s} - (\mathbb{1} - \delta_{r, 0}) P_+ \delta_{r-1, s} \\ & + m(P_- \delta_{r, N_5-1} \delta_{0, s} + P_+ \delta_{r, 0} \delta_{N_5-1, s}) \end{aligned} \quad (3.53)$$

where $P_{\pm} = \frac{1}{2}(\mathbb{1} \pm \gamma^5)$ is the usual chiral projector in the continuum.

The 4D physical fermion fields is defined in terms of the 5D fields as

$$\begin{aligned}\psi(x) &= P_- \Psi(x, 0) + P_+ \Psi(x, L_s - 1) \\ \bar{\psi}(x) &= \bar{\Psi}(x, L_s - 1) P_+ + \bar{\Psi}(x, 0) P_-.\end{aligned}\tag{3.54}$$

Taken together, the term

$$\bar{\psi}(x)\psi(x) = \bar{\Psi}(x, L_s - 1) P_- \Psi(x, 0) + \bar{\Psi}(x, 0) P_+ \Psi(x, L_s - 1)\tag{3.55}$$

is exactly the coefficient multiplying m in Equation (3.53). Thus, m in this theory can indeed be identified as the usual mass parameter in the 4D QCD Lagrangian.

In this formulation, one can show that Equation (3.51) satisfies the Ginsparg-Wilson equation, making this a Dirac operator of chiral fermions on the lattice.

3.3 Lattice Quantum Chromodynamics - A Practical Tour

3.3.1 Fermionic Correlation Functions

The fermionic integral in Equation (3.40) was

$$\langle O_1 \dots O_n \rangle_f[U] = \int D\psi D\bar{\psi} \prod_{j=1}^n (O_j[\psi, \bar{\psi}, U]) e^{-S_f[\psi, \bar{\psi}, U]}.$$

This can be evaluated using *Wick's theorem*, which will reveal the propagators we need to generate in our lattice simulations.

As an example, let these fermionic operators be the creation/annihilation interpolators of the π meson,

$$O_{\pi}(x) = \bar{d}(x)\gamma^5 u(x)\tag{3.56}$$

and consider its 2-point function. Suppressing the functional dependence on U

and writing out the spin-color indices explicitly,

$$\begin{aligned}
\langle O_\pi(y) O_\pi^\dagger(x) \rangle_f &= \left\langle \bar{d}_b^\alpha(y) \gamma_{\alpha\beta}^5 u_{\beta_c}(y) \bar{u}_e^\sigma(x) \gamma_{\sigma\tau}^5 d_f^\tau(x) \right\rangle_f \\
&= - \left\langle d_f^\tau(x) \bar{d}_b^\alpha(y) \gamma_{\alpha\beta}^5 u_{\beta_c}(y) \bar{u}_e^\sigma(x) \gamma_{\sigma\tau}^5 \right\rangle_f \\
&= -\text{Tr} [S^d(x|y) \gamma^5 S^u(y|x) \gamma^5] \det D \\
&= -\text{Tr} [S^{d\dagger}(y|x) S^u(y|x)] \det D
\end{aligned} \tag{3.57}$$

where $S^q(y|x) = q(x)\bar{q}(x)$ is the quark propagator going from x to y and $\det D$ is the fermionic determinant of the Dirac operator. Here, the overall (-1) arises from anticommuting odd number of Grassmann fields. In the final line, we used γ^5 -hermiticity,

$$S^{q\dagger}(x|y) = \gamma^5 S^q(y|x) \gamma^5, \tag{3.58}$$

which is a symmetry of most lattice implementations of the Dirac operator, including this work's. We will see below that this property is vital in reducing computational costs. Figure 3.1 shows a representation of Equation (3.57).

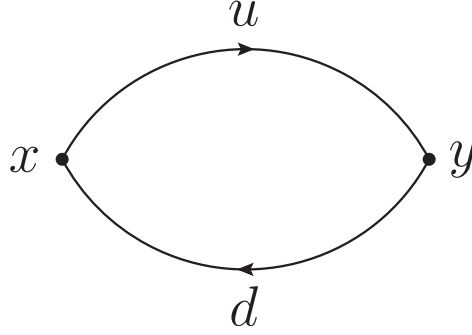


Figure 3.1 *A schematic diagram of a 2-point function, where the ‘ π ’ meson propagates from x to y , with $t_y > t_x$. With γ^5 -hermiticity, the backward propagating d quark can be re-interpreted as a forward propagating $\bar{d}$ quark.*

The quark propagator S is the solution to the Dirac equation for a given source η . That is, for a Dirac operator D , one solves the equation

$$DS = \eta \tag{3.59}$$

to obtain

$$S = D^{-1}\eta. \tag{3.60}$$

This amounts to inverting the Dirac operator D . Recall that in QCD, D contains

spin and color indices. For a lattice of size N , this is a square matrix of size $12N$. Even for a modest lattice size, *e.g.* $N = 16^3 \times 24$, this matrix has $\mathcal{O}(10^{12})$ complex entries. Thus, inverting the full matrix is a prohibitively expensive task. In the following, we will examine some candidates for the source η . Here, we note that most lattice calculations make use of Krylov subspace methods, *e.g.* the conjugate gradient (CG) algorithm[26], to solve for S . The rate of convergence of the CG algorithm is related to the condition number of the Dirac matrix,

$$\kappa = \left(\frac{\lambda_{\min}}{\lambda_{\max}} \right) \propto (am_q)^{-1}, \quad (3.61)$$

where λ are the extremal eigenvalues of the Dirac matrix. This relation tells us that inverse proportionality to the quark mass poses a challenge to lattice simulations: lighter quark masses lead to larger condition number and hence greater computational burden to obtain the propagator. On the other hand, where γ^5 -hermiticity is available (*e.g.* this work), one obtains the reverse propagator for free by Hermitian-conjugating the propagator matrix (see Equation (3.58)).

Point Sources

By exploiting translation invariance, one can extract the relevant physical information by considering the propagation from one site to all the others. For a fixed spin β_0 and color c_0 , this amounts to solving

$$S_{\alpha\beta_0}_{bc_0}(n'|n_0) = \sum_{n \in \Lambda} D_{\alpha\beta}_{bc}^{-1}(n'|n) \eta_{\beta\beta_0}_{cc_0}(n, n_0). \quad (3.62)$$

For all 12 spin-color combinations from site n_0 , we must evaluate the above for 12 η 's. This η is called the *point source* and its explicit form is

$$\eta_{\beta\beta_0}_{cc_0}(n, n_0) = \delta_{nn_0} \delta_{\beta\beta_0} \delta_{cc_0}, \quad (3.63)$$

which gives the intuitive understanding of Equation (3.62) as a propagation from site n_0 to all other sites n , for a given spin-color combination.

Gauge-fixed Wall Sources

Recall from Equation (3.24), the 2-point correlation function is a sum of exponentials of different states. Optimising the interpolators at the source may lead to greater overlap with the state one is interested in, and hence stronger correlation signal. This can be achieved by ‘smearing’ the source, thereby mimicking a more realistic spatial wave function.

A smeared source that is used in this work is the *wall source* [22], defined as

$$\eta_{\beta\beta_0}^w(\mathbf{n}, \mathbf{n}_0, \mathbf{p}) = \delta_{n^4 n_0^4} \delta_{\beta\beta_0} \delta_{cc_0} e^{i\mathbf{p}\cdot\mathbf{x}}, \quad (3.64)$$

i.e. for a fixed timeslice n^4 , we sum over all (spatial) point sources. The sink may be smeared as well, but this operation is performed after inverting the Dirac operator and so does not contribute much to the computational cost.

Note that the choice in Equation (3.64) is not gauge-invariant. In this work, we use the Coulomb gauge,

$$\sum_{j=1}^3 \partial_j A_j = 0. \quad (3.65)$$

Sequential Sources

To extract matrix elements from correlation functions, the quark propagators must include current insertions, *e.g.* the E.M. vector current. Since each new quark propagator requires an inversion of the Dirac matrix, one aims to minimise the number of matrix inversion in a lattice simulation where possible.

To do this, we use the *sequential-source method*. The strategy is as follows: 1) generate a propagator from a given source η to all lattice sites,

$$S(n|0) = \sum_{u \in \Lambda} D^{-1}(n, u) \eta(u, 0), \quad (3.66)$$

then 2) generate another propagator from the current insertion site n to m , using the first propagator as part of the source, *i.e.*

$$\Xi(m|0) = \sum_{n \in \Lambda} D^{-1}(m, n) J(n) S(n|0), \quad (3.67)$$

where J is the current operator. Note that successive current insertions can be sequentially inserted with the above equation. The propagators $S(n|0)$ and $\Xi(m|0)$, together with their Hermitian conjugate are the basic building blocks of a meson correlation function with current insertion. The correlation function

$$C(x) = \text{Tr} [S(0|x)\Gamma_{\text{snk}}\Xi(x|0)\Gamma_{\text{src}}] \quad (3.68)$$

corresponds to a diagram like Figure 3.2, where $\Gamma_{\text{src/snk}}$ are the γ -structures of the source and sink interpolators, respectively. Note that in Equation (3.67) the current is summed over all lattice sites in Λ . In the case where the matrix element of the current is of interest, the temporal component may be kept free and we generate a 3-point correlation function instead.

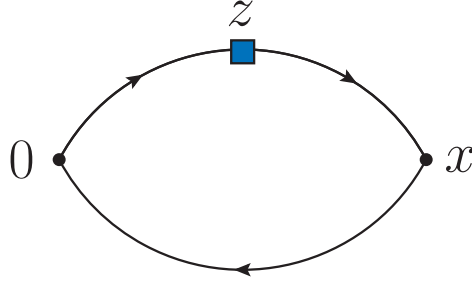


Figure 3.2 *A schematic diagram of a correlation function with sequential insertion, denoted by the blue box. Integrating over $z \in a\Lambda$ gives a 2-point correlation function, whereas integrating over spatial coordinates gives a 3-point correlation function.*

3.3.2 Evaluating the Gauge Field Path Integral

For lattices of large volumes, Equation (3.38) cannot be evaluated analytically. Instead, we may approximate the gauge field integral with the average of an observable evaluated over N_{cfg} gauge configurations, distributed with a probability proportional to $e^{-S_G[U]}$, *i.e.*

$$\frac{1}{Z} \int DU O[U] e^{-S_G[U]} \approx \frac{1}{N_{\text{cfg}}} \sum_{n=1}^{N_{\text{cfg}}} O[U_n], \quad (3.69)$$

where the shorthand $O = \langle O_1 \dots O_n \rangle_f$ was used for the fermionic vacuum expectation value. To generate the gauge configurations U_n , we apply Markov Chain Monte Carlo algorithms. In this work, the gauge configurations are generated by the RBC/UKQCD collaboration using Hybrid Monte Carlo algorithm [27].

Details about the lattice setup of this work are presented in §5.1.

3.4 Quantum Electrodynamics in a Finite Box

In the full theory, the presence of electromagnetism modifies the action. The gauge fields U_μ are now endowed with a $U(1)$ phase

$$U_\mu(x) \rightarrow e^{-ie_j A_\mu(x)} U_\mu(x), \quad (3.70)$$

where $e_j = q_j e$ is the fractional charge of the j 'th quark, *i.e.* $e_j \in \{e_u, e_d, e_s\} = \{2/3, -1/3, -1/3\}$ in units of positron charge e .

We now study the effects of introducing a photon in a finite lattice as reviewed in [28]. First, let us impose periodic boundary conditions in the spatial and temporal directions. Taken together, the lattice is a 4-torus $\mathbb{T}$. The Euclidean Maxwell action in a given gauge ξ is

$$S_\gamma[A] = \sum_x \left[\frac{1}{4} \sum_{\mu, \nu} F_{\mu\nu}(x) F_{\mu\nu}(x) + \frac{1}{2\xi} \sum_\rho (\partial_\rho A_\rho(x))^2 \right], \quad (3.71)$$

where $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ is the usual field strength tensor and, on the lattice, we have the forward derivative, defined with some test function f as

$$\partial_\mu f(x) = f(x + \mu) - f(x). \quad (3.72)$$

Working in Feynman gauge ($\xi = 1$) and integrating by parts, Equation (3.71) becomes

$$S_\gamma[A] = -\frac{1}{2} \sum_x \sum_\mu A_\mu(x) \partial^2 A_\mu(x). \quad (3.73)$$

The photon propagator is thus

$$\begin{aligned}
\Delta_{\mu\nu}(x-y) &\equiv \langle A_\mu(x)A_\nu(y) \rangle = -\delta_{\mu\nu}(\partial^2)^{-1}\delta_{xy}, \\
&= \frac{\delta_{\mu\nu}}{V} \sum_{k \in \tilde{\Lambda}} (\partial^2)^{-1} e^{-ik \cdot (x-y)}, \\
&= \frac{\delta_{\mu\nu}}{V} \sum_{k \in \tilde{\Lambda}} \frac{e^{-ik \cdot (x-y)}}{|k|^2}.
\end{aligned} \tag{3.74}$$

This propagator is ill-defined due to the singular $k = 0$ term in the summation. Consider a shift transformation on the photon field

$$A_\mu(x) \rightarrow A'_\mu(x) = A_\mu(x) + \frac{c_\mu}{V}, \tag{3.75}$$

where c_μ is some constant 4-vector. Since this transformation amounts to a constant shift, the action is invariant under this shift symmetry. The Fourier transform of this new field is

$$\frac{1}{V} \sum_{k \in \tilde{\Lambda}} A'_\mu(k) e^{ik \cdot x} = \frac{1}{V} \sum_{k \in \tilde{\Lambda}} [A_\mu(k) + c_\mu \delta_{k0}] e^{ik \cdot x}, \tag{3.76}$$

$$\Rightarrow A'_\mu(k) = A_\mu(k) + c_\mu \delta_{k0}, \tag{3.77}$$

i.e., this shift symmetry exhibited by the transformation in Equation (3.75) generates a redundancy in the zero mode. Indeed, if we write $c_\mu = \partial_\mu C(x)$ for some scalar function C , this is reminiscent of the redundancy problem one encounters in gauge fixing. One can similarly employ the trick by Fadeev and Popov [29] to count each physical field configuration only once.

First, we write the identity as

$$1 = \int dc_\mu \delta \left(\sum_{x \in \mathbb{T}} A'_\mu(x) \right). \tag{3.78}$$

Inserting this into the path integral formalism

$$\begin{aligned}\langle O \rangle &= \frac{1}{Z} \int DA \, O[A] e^{-S_\gamma[A]}, \\ &= \frac{1}{Z} \int DA \int dc_\mu \delta \left(\sum_{x \in \mathbb{T}} A'_\mu(x) \right) O[A] e^{-S_\gamma[A]}.\end{aligned}\tag{3.79}$$

Next, we make the change of variable $A_\mu(x) \rightarrow A'_\mu(x)$. Since this is a shift, it leaves the integration measure, $O[A]$ and the action unchanged. Relabelling the dummy variable A'_μ back to A_μ , we get

$$\langle O \rangle = \frac{1}{Z_{TL}} \int DA \int dc_\mu \delta \left(\sum_{x \in \mathbb{T}} A_\mu(x) \right) O[A] e^{-S_\gamma[A]},\tag{3.80}$$

where Z_{TL} is the modified normalisation

$$Z_{TL} = \int DA \int dc_\mu \delta \left(\sum_{x \in \mathbb{T}} A_\mu(x) \right) e^{-S_\gamma[A]}.\tag{3.81}$$

Thus, the c_μ integral measure in Equation (3.80) will cancel with that in Z . In [30], this is called QED_{TL} . The δ -function ensures that only physically inequivalent gauge configurations contribute to $\langle O \rangle$.

Consider including an interaction term to the photon action with some source $J_\mu(x)$. To keep this term invariant under the shift transformation, one can check that the interaction term must take the form

$$S_{\gamma,int}[A, J] = \sum_{x \in \mathbb{T}} A_\mu(x) \left[J_\mu(x) - \frac{1}{V} \sum_{y \in \mathbb{T}} J_\mu(y) \right].\tag{3.82}$$

Thus, we see that the QED_{TL} prescription of removing redundant zero modes introduces non-locality in the spatial and temporal coordinates since $A_\mu(x)$ now couples to the source $J_\mu(y)$ at all spacetime points. In particular, non-locality in time renders the definition of a bounded transfer matrix impossible for fermionic matter fields [28].

A related prescription that preserves locality in time is the QED_{L} formulation,

first introduced in [31], where Equation (3.80) is modified to

$$\langle O \rangle = \frac{1}{Z_L} \int DA \int dc_\mu \delta \left(\sum_{\mathbf{x} \in \mathbb{T}^3} A_\mu(t, \mathbf{x}) \right) O[A] e^{-S_\gamma[A]}. \quad (3.83)$$

The interaction term is modified into

$$S_{\gamma,int}[A, J] = \sum_{x \in \mathbb{T}} A_\mu(x) \left[J_\mu(x) - \frac{1}{L^3} \sum_{\mathbf{y} \in \mathbb{T}^3} J_\mu(t, \mathbf{y}) \right]. \quad (3.84)$$

A photon propagator generated with the above interaction term will remain local in time, thereby avoiding issues with the transfer matrix, but it nevertheless suffers from non-local contributions in the spatial component. Our naive expectation is that these finite-volume effects (FVE) will vanish in the infinite volume limit. We relegate further discussions to [28]. Here, we simply note that once a hadronic mass and its electromagnetic correction are determined with the QED_L prescription on $\mathbb{T}$, we can determine its mass in the infinite volume via [30]

$$M(T, L) = M \left[1 - q^2 \alpha \frac{\kappa}{2ML} \left(1 + \frac{2}{ML} \right) + \mathcal{O} \left(\frac{\alpha}{L^3} \right) \right], \quad (3.85)$$

where $M(T, L)$ is the QCD+QED mass from the lattice, M is the infinite volume mass we are solving for, q is the charge of the pseudoscalar and $\kappa = 2.837297(1)$ is determined from evaluating an integral over Jacobi theta functions [30]. Equation (3.85) will be needed for the tuning procedure (see §5.5.1).

Chapter 4

Isospin-Breaking Corrections on the Lattice

In Chapter 2, we showed how the CKM matrix element can be extracted from leptonic decays. To control the uncertainties coming from non-perturbative hadronic quantities such as f_P , we proposed to evaluate them by means of lattice QCD, whose foundations we laid in Chapter 3. In context of a lattice simulation, then, we now discuss the procedure of defining an isospin-symmetric point where we calculate the corrections to the physical prediction from. Then, we present the strategy to remove infrared-divergences coming from virtual $\mathcal{O}(\alpha)$ corrections to the matrix element. Finally, we will discuss the strategy to extract the isospin-breaking corrections from the generated correlators and from analytic calculations.

From this chapter onward, to lighten the notation, all dimensionful quantities (*e.g.* quark/hadron masses) are in lattice units. The lattice spacing will be made explicit when comparisons with physical results are made. Unless stated otherwise, all parameters from this chapter onward are bare.

4.1 Calculations with a Near-Physical Theory

In the Standard Model, we assume that low energy observables can be predicted to a high degree of precision with a theory of QCD+QED. Yet, already within the context of leptonic decays, we encounter observables such as the axial matrix

element A_P (see Equation (2.94)) only in the theory of (isospin-symmetric) QCD. Such unphysical definitions arise from the practical limitations of calculating the observable in the full QCD+QED theory. In the context of the lattice community, growing availability of computing resources allows us to compute the observable of interest in a near-physical theory of QCD(+QED) and correct for the mismatch via perturbations of the physical inputs.

The discussion in this section is divided into two: first, we will discuss the procedure of predicting a physical observable from a near-physical theory. Then, we will define the isospin limit and present a similar perturbative correction method to apply to our near-physical simulation. This latter discussion will be useful for calculating isospin-breaking corrections to the leptonic decay width.

4.1.1 Predicting Physical (QCD+QED) Observables

For a 3-flavor theory of quarks, the strong coupling constant g_s , the electric charge e , and the up-, down- and strange-quark masses are the parameters of the QCD+QED Lagrangian. In the following, it is useful to perform a change of basis into the isospin basis, *i.e.* $(m_u, m_d, m_s) \rightarrow (m_{ud}, \delta m, m_s)$, where

$$m_{ud} = \frac{1}{2}(m_u + m_d) \quad \text{and} \quad \delta m = m_u - m_d. \quad (4.1)$$

In this basis, an isospin-symmetric QCD theory is clear where $\alpha = 0$, $m_{ud} = m_l$ and $\delta m = 0$. Let $\mathbf{g}^\phi = (g_s, \alpha, m_{ud}, \delta m, m_s)$ be the vector denoting the physical values of the bare parameters of the Lagrangian. Note that, since we are only working to $\mathcal{O}(\alpha)$, we may safely fix the electromagnetic coupling to its Thomson limit, *i.e.* $e = \sqrt{4\pi\alpha}$, with $\alpha = 7.2973525693(11) \times 10^{-3}$ [16], without the need to impose a renormalisation condition.

For the same g_s , let $\hat{\mathbf{g}} = (\hat{g}_s, 0, \hat{m}_l, 0, \hat{m}_s)$ be the vector that denotes an arbitrary point in the theory subspace where $\alpha = 0$, $\delta m = 0$, where $\hat{m}_u = \hat{m}_d = \hat{m}_l$. In the context of lattice QCD calculations, such a point corresponds to the simulation input choices, where $\hat{m}_l$ is set by hand. We call it the *near-physical* point since the observables (*e.g.* hadronic masses) predicted by these bare parameters are close to their physical values. Due to the fact that there is a small mismatch between the near-physical inputs and the physical parameters, we need to correct for this discrepancy by tuning the bare quark masses such that a set of experimental observables are reproduced by our near-physical setup. Since our near-physical

inputs $\hat{\mathbf{g}}$ are very nearly physical, we may perform a linear expansion of an observable X in the full theory in terms of each coupling

$$X(\mathbf{g}^\phi) = X(\hat{\mathbf{g}}) + \alpha \left. \frac{\partial X}{\partial \alpha} \right|_{\mathbf{g}=\hat{\mathbf{g}}} + \sum_q (m_q - \hat{m}_q) \left. \frac{\partial X}{\partial m_q} \right|_{\mathbf{g}=\hat{\mathbf{g}}} + \dots \quad (4.2)$$

where the ellipses denote higher order terms. The tuning procedure amounts to quantifying the mismatch with $(m_q - \hat{m}_q)$ for $q = l, s$. These are determined by solving a set of linear equations, *e.g.* using a dimensionless ratio of masses

$$\frac{M_P(\mathbf{g}^\phi)}{M_{\Omega^-}(\mathbf{g}^\phi)} = \frac{M_P^{\text{exp.}}}{M_{\Omega^-}^{\text{exp.}}} \quad (4.3)$$

for $X(g^\phi)$, where the superscript ‘exp.’ denote their value from experimental measurements. For three flavors, $q = u, d, s$, we require three hadronic observables, which we choose to be $P = \pi^+, K^+, K^0$.

4.1.2 Defining the Isospin-symmetric Theory of QCD

The calculation of isospin-breaking correction from an isospin-symmetric QCD setup necessitates an unphysical separation of QCD and QED since there are no physical processes which partake exclusively in strong interactions. This ambiguity must be dealt with consistently and in this section we explain the procedure we have adopted in our calculation.

We consider the following mesonic quantities, first introduced by BMW in [32, 33]

$$\begin{aligned} M_{ud}^2 &= \frac{M_{\bar{u}u}^2 + M_{\bar{d}d}^2}{2}, & \Delta M^2 &= M_{\bar{u}u}^2 - M_{\bar{d}d}^2, \\ M_{K\chi}^2 &= \frac{M_{K^+}^2 + M_{K^0}^2 - M_{\pi^+}^2}{2}, \end{aligned} \quad (4.4)$$

where $\bar{q}q$ are the neutral pseudoscalars built from connected-only quark propagators. At leading order in partially-quenched Chiral Perturbation Theory (PQ χ PT) [32, 34],

$$M_{ij}^2 = 2B_0(m_i^R + m_j^R) + \frac{2Ce^2}{F_0^2}(q_i - q_j)^2, \quad (4.5)$$

where $m_{i,j}^R$ is the renormalised quark mass, $q_{i,j}$ is the fractional charge of $m_{i,j}$, C

is a low energy constant and

$$B_0 = \frac{\Sigma_0}{F_0^2} \Big|_{m_u, m_d, m_s \rightarrow 0} \quad (4.6)$$

is related to the quark condensate with

$$\Sigma_0 = -\langle \bar{u}u \rangle|_{m_u, m_d, m_s \rightarrow 0} \quad \text{and} \quad F_0 = \sqrt{2}f_\pi. \quad (4.7)$$

First, note that

$$\begin{aligned} M_{\pi^+}^2 &= 2B_0 \left(m_{ud} + \frac{1}{2}\delta m \right) + e^2 \frac{2C}{F_0^2}, & M_{\pi^0}^2 &= 2B_0 \left(m_{ud} - \frac{1}{2}\delta m \right), \\ M_{K^+}^2 &= B_0 \left(m_{ud} + \frac{1}{2}\delta m + m_s \right) + e^2 \frac{2C}{F_0^2}(1 + \epsilon), & M_{K^0}^2 &= B_0 \left(m_{ud} - \frac{1}{2}\delta m + m_s \right), \end{aligned} \quad (4.8)$$

where, with foresight, we have included the correction to Dashen's theorem [35] ϵ in our PQ χ PT formula such that

$$\frac{(M_{K^+}^2 - M_{K^0}^2)^\gamma}{(M_{\pi^+}^2 - M_{\pi^0}^2)^\gamma} = 1 + \epsilon, \quad (4.9)$$

where the superscript γ denotes the electromagnetic contribution to the meson mass-squared splittings. In the limit $\epsilon \rightarrow 0$, we recover Dashen's theorem. Applying these to Equation (4.4), we find

$$\begin{aligned} M_{ud}^2 &= 2B_0 m_{ud}^R + \dots & \Delta M^2 &= 2B_0(m_u^R - m_d^R) + \dots \\ M_{K\chi}^2 &= 2B_0 m_s^R + \frac{2Ce^2}{F_0^2}\epsilon \dots, \end{aligned} \quad (4.10)$$

where the ellipses denote higher order terms. We see that these pseudoscalar squared masses are directly proportional to the quark masses we are interested in. Due to this relation, we can define the isospin limit of QCD as follows.

Let $\bar{\mathbf{g}} = (\hat{g}_s, 0, \bar{m}_l, 0, \bar{m}_s)$ be the vector of bare coupling in this theory, *i.e.* bare parameters in the isospin limit are denoted with an overhead bar. We may expand these masses in the isospin limit with respect to each coupling

$$M^2(\bar{\mathbf{g}}) = M^2(\hat{\mathbf{g}}) + \sum_q (\bar{m}_q - \hat{m}_q) \frac{\partial M^2}{\partial m_q} \Big|_{\mathbf{g}=\hat{\mathbf{g}}} + \dots, \quad (4.11)$$

for $M^2 \in \{M_{ud}^2, \Delta M^2, M_{K\chi}^2\}$. Here, we assume that our near-physical inputs are also close to the isospin limit. Although the isospin limit is itself arbitrary, we choose a point in the theory subspace such that we produce the experimental value of the neutral pion mass. In §5.5.1, this assumption is verified numerically. After obtaining the set $(m_q - \hat{m}_q)$ from the procedure described in §4.1.1, we fix the LHS of these pseudoscalars to the following constraints

$$\begin{aligned} M_{ud}^2(\bar{\mathbf{g}}) &= M_{ud}^2(\mathbf{g}^\phi), \\ \Delta M^2(\bar{\mathbf{g}}) &= 0, \\ M_{K\chi}^2(\bar{\mathbf{g}}) &= M_{K\chi}^2(\mathbf{g}^\phi). \end{aligned} \tag{4.12}$$

Most notably, by fixing $\Delta M^2(\bar{\mathbf{g}})$ to zero, we have the analogous constraint of $m_u - m_d = 0$. This procedure will yield another set of bare quark mass shifts $(\bar{m} - \hat{m})$ for all quark flavors that corrects for the discrepancy between our near-physical inputs and the isospin limit we wish to calculate the isospin-breaking correction from. Now, because isospin-breaking corrections appear as percent level contributions to the physical theory, we can modify Equation (4.2) in context of the isospin limit to

$$X(\mathbf{g}^\phi) = X(\bar{\mathbf{g}}) + \alpha \frac{\partial X}{\partial \alpha} \Big|_{\mathbf{g}=\bar{\mathbf{g}}} + \sum_q (m_q - \bar{m}_q) \frac{\partial X}{\partial m_q} \Big|_{\mathbf{g}=\bar{\mathbf{g}}} + \dots \tag{4.13}$$

Now, the quark mass shifts can be obtained trivially from

$$(m_q - \bar{m}_q) = (m_q - \hat{m}_q) - (\bar{m}_q - \hat{m}_q) \tag{4.14}$$

for each quark flavor q .

4.1.3 Defining the Isospin-broken Theory of QCD

It may be of phenomenological interest to make a further separation of the isospin-breaking effects into its electromagnetic and $m_u \neq m_d$ contribution. For example, this is useful for predicting the electromagnetic part of the kaon mass squared splitting, which is essential for calculating the corrections to Dashen's theorem (see §5.5.1). Following the discussion in FLAG [20], we may express the physical observable X as

$$X^\phi = \bar{X} + \delta X^{\text{EM}} + \delta X^{\text{QCD}}, \tag{4.15}$$

where the terms on the RHS are the observable in the isospin limit, the electromagnetic and isospin-broken QCD corrections to $\bar{X}$, respectively. The latter corresponds to the $m_u \neq m_d$ theory of QCD with $\alpha = 0$ and in the following we denote the couplings for this theory as $\mathbf{g}^{\text{QCD}} = (\hat{g}_s, 0, m_{ud}^{\text{QCD}}, \delta m^{\text{QCD}}, \bar{m}_s)$. Analogous to the procedure of defining the isospin limit in the above, we can obtain another set of bare quark mass shifts ($m^{\text{QCD}} - \hat{m}$) by solving the following set of constraints:

$$\begin{aligned} M_{ud}^2(\mathbf{g}^{\text{QCD}}) &= M_{ud}^2(\mathbf{g}^\phi), \\ \Delta M^2(\mathbf{g}^{\text{QCD}}) &= \Delta M^2(\mathbf{g}^\phi), \\ M_{K\chi}^2(\mathbf{g}^{\text{QCD}}) &= M_{K\chi}^2(\mathbf{g}^\phi), \end{aligned} \tag{4.16}$$

where the new constraint on ΔM^2 now reflects the $m_u \neq m_d$ feature of this theory. Using the linear expansion formula in Equation (4.2), we make the following identification for Equation (4.15):

$$\begin{aligned} \bar{X} &= \hat{X} + \sum_q (\bar{m}_q - \hat{m}_q) \frac{\partial X}{\partial m_q} \Big|_{\mathbf{g}=\hat{\mathbf{g}}}, \\ \delta X^{\text{QCD}} &= \sum_q (m_q^{\text{QCD}} - \bar{m}_q) \frac{\partial X}{\partial m_q} \Big|_{\mathbf{g}=\bar{\mathbf{g}}}. \end{aligned} \tag{4.17}$$

Then, the electromagnetic contribution is then simply

$$\delta X^{\text{EM}} = X^\phi - (\bar{X} + \delta X^{\text{QCD}}). \tag{4.18}$$

4.2 Isospin-breaking Correction in Leptonic Decays

When including isospin-breaking corrections, we will need to remove the infrared (IR) divergences coming from $\mathcal{O}(\alpha)$ QED corrections to the amplitude. This is achieved by combining together contributions from virtual and real photon interactions. The former must be evaluated non-perturbatively, since all momentum modes of the photon are involved in the interaction with the initial hadron. For final state photons that are sufficiently soft such that they do not resolve the internal structure of the hadron, the latter term may be evaluated analytically. For the case of $K_{\mu 2[\gamma]}$ and $\pi_{\mu 2[\gamma]}$, χPT predicts the structure-dependent (SD) QED contribution to be negligible [36]. Indeed, this has been shown to be the case in [37].

The methodology of separating the calculation of real and virtual isospin-breaking corrections, along with the regulating and removal of IR divergences from the amplitudes computed on the lattice, was developed in [38] and applied in the successive papers (see [39, 40]). Here we will adopt the same strategy and write the inclusive rate for a generic pseudoscalar P^+ and lepton ℓ^+ as

$$\begin{aligned}\Gamma(P^+ \rightarrow \ell^+ \nu_\ell [\gamma]) &= \Gamma_0 + \Gamma_1, \\ &= \lim_{L \rightarrow \infty} (\Gamma_0(L) - \Gamma_0^{\text{uni}}(L)) + \lim_{\lambda \rightarrow 0} (\Gamma_0^{\text{uni}}(\lambda) + \Gamma_1(\lambda, \Delta E_\gamma)),\end{aligned}\quad (4.19)$$

where the subscript integers denote the number of real photons in the final state and ΔE_γ is the energy threshold of the final state real photons [41]. Since the virtual corrections in Γ_0 are evaluated with numerical simulations, the lattice box size L is a natural choice of IR regulator. While it is feasible to compute the real photon contribution on the lattice [37], for now we will implement the analytic approach as in [38]. Here, we use a fictitious photon mass λ to regulate the IR divergence. Additionally, an intermediate term Γ_0^{uni} with the same IR divergence as $\Gamma_{0,1}$ is introduced and calculated in the point-like approximation, *i.e.* the initial hadron is treated as a point-like particle. Here ‘uni’ stands for *universal*, as the finite-volume decay rate up to $\mathcal{O}(1/L)$ is independent of the internal structure of the decaying meson. This ensures the IR divergences cancel numerically. The first bracketed term, then, removes the universal $\mathcal{O}(1/L)$ finite volume effects (FVE) [42, 43]. In [40], the $\mathcal{O}(1/L^2)$ SD terms have been removed by fitting lattice ensembles of different volumes to an $SU(2)$ -inspired fit function. Meanwhile, in recent progress [44] the $\mathcal{O}(1/L^2)$ SD terms have been calculated explicitly. Thus, we can update Equation (4.19) to

$$\Gamma(P^+ \rightarrow \ell^+ \nu_\ell [\gamma]) = \lim_{L \rightarrow \infty} (\Gamma_0(L) - \Gamma_0^{(2)}(L)) + \lim_{\lambda \rightarrow 0} (\Gamma_0^{\text{uni}}(\lambda) + \Gamma_1(\lambda, \Delta E_\gamma)), \quad (4.20)$$

where

$$\Gamma_0^{(n)}(L) = \Gamma_0^{\text{uni}}(L) + \Delta \Gamma_0^{(n)}(L). \quad (4.21)$$

The term $\Gamma_0^{(n)}(L)$ will be discussed in §4.6. Here, we only note that the residual FVE now begins at $\Gamma_0(L) - \Gamma_0^{(2)}(L) \sim \mathcal{O}(1/L^3)$. The second bracketed term in Equation (4.20) has been calculated analytically in [38], which we will adopt for our calculation of $K_{\mu 2}[\gamma]/\pi_{\mu 2}[\gamma]$ (see §4.7).

In Chapter 2, we introduced an effective 4-fermion operator for the weak interaction. As a result, an additional procedure is needed to match this local operator to the SM. Typically, this is done through the W-regularisation scheme

[45]. On the lattice, we propose the following effective weak Hamiltonian

$$\mathcal{H}_W = \frac{G_F}{\sqrt{2}} V_{q_1 q_2} \left[1 + \frac{\alpha}{4\pi} \delta Z^W \right] Z_V O_W, \quad (4.22)$$

where $V_{q_1 q_2}$ is the CKM matrix element associated to the $q_1 \rightarrow q_2$ flavor transition, G_F is Fermi's constant, Z_V is the QCD renormalisation constant and

$$O_W = (\bar{\nu} \Gamma_L^\mu \ell) (\bar{q}_2 \Gamma_L^\mu q_1), \quad (4.23)$$

where $\Gamma_L^\mu = \gamma^\mu (\mathbb{1} - \gamma^5)$ is the $V - A$ current. The renormalisation term

$$\mathcal{Z}(\alpha) = \left[1 + \frac{\alpha}{4\pi} \delta Z^W \right] Z_V \quad (4.24)$$

is twofold: 1) the matching between the effective weak Hamiltonian and the SM and 2) the renormalisation of the lattice operator to the W-regularised version. In a discretised action where chiral symmetry is preserved (*e.g.* DWF), the lattice operator is renormalised multiplicatively. If chiral symmetry is explicitly broken by the lattice action, then there will be an additional additive constant. Note that, if a mass-independent renormalisation scheme is chosen, then $\mathcal{Z}$ will be the same for different pseudoscalars.

With the 4-fermion operator defined, let us begin by evaluating the isosymmetric QCD matrix element. This is

$$\bar{\mathcal{M}}_P^{r,s} = \mathcal{Z}_0 \langle \ell^+, r; \nu, s | O_W | P \rangle, \quad (4.25)$$

where r, s are spinor indices and $\mathcal{Z}_0 \equiv \mathcal{Z}(0) = Z_V$. Using Equation 4.23,

$$\begin{aligned} \langle \ell^+, r; \nu, s | O_W | P \rangle &= \langle \ell^+, r; \nu, s | (\bar{\nu} \Gamma_L^\mu \ell) (\bar{q}_2 \Gamma_L^\mu q_1) | P \rangle. \\ &= \langle \ell^+, r; \nu, s | \bar{\nu} \Gamma_L^\mu \ell | 0 \rangle \langle 0 | \bar{q}_2 \Gamma_L^\mu q_1 | P \rangle \end{aligned} \quad (4.26)$$

where, in Euclidean space, the hadronic piece of the axial matrix element is

$$\bar{\mathcal{A}}_P^0 = \langle 0 | \bar{q}_2 \Gamma^0 q_1 | P \rangle = \frac{\bar{M}_P f_P}{\mathcal{Z}_0}, \quad (4.27)$$

where $\bar{M}_P$ is the pseudoscalar mass in the isosymmetric QCD theory. Now, let $\bar{\mathbf{p}}_\ell$ be the lepton 3-momentum determined from the isosymmetric QCD pseudoscalar mass $\bar{M}_P$, and $\bar{\mathbf{p}}_\nu = -\bar{\mathbf{p}}_\ell$ as per 3-momentum conservation. Evaluating the spin-

sum average, we obtain

$$\begin{aligned}
|L(\bar{\mathbf{p}}_\ell)|^2 &= \sum_{r,s} \bar{u}(\bar{\mathbf{p}}_\nu) \Gamma_L^0 v(\bar{\mathbf{p}}_\ell) \bar{v}(\bar{\mathbf{p}}_\ell) \Gamma_L^0 u(\bar{\mathbf{p}}_\nu), \\
&= 8|\bar{\mathbf{p}}_\ell|^2 (E_\ell^2(\bar{\mathbf{p}}_\ell) - E_\nu^2(\bar{\mathbf{p}}_\ell)), \\
&= 4m_{\ell^+}^2 \left(1 - \frac{m_{\ell^+}^2}{\bar{M}_P^2}\right),
\end{aligned} \tag{4.28}$$

where in the final line we substituted the results from Equation (2.85). The isosymmetric QCD decay amplitude squared is thus

$$|\bar{\mathcal{M}}_P|^2 = \sum_{r,s} |\bar{\mathcal{M}}_P^{r,s}|^2 = 4|f_P|^2 \bar{M}_P^2 m_{\ell^+}^2 \left(1 - \frac{m_{\ell^+}^2}{\bar{M}_P^2}\right). \tag{4.29}$$

Note that the lepton trace in Equation (4.28) is only dependent on the 3-momentum of the outgoing charged lepton. We can use this property to define the full QCD+QED amplitude via

$$\frac{|\mathcal{M}_P|^2}{|L|^2} = |\mathcal{Z}\mathcal{A}_P|^2. \tag{4.30}$$

The PDG definition of the tree-level decay rate may be expressed as

$$\Gamma^{\text{tree}} = \mathcal{K} |\mathcal{Z}_0|^2 |\bar{\mathcal{A}}_P|^2 |L|^2 \left(\frac{M_{P^+}^2}{\bar{M}_P^2}\right), \tag{4.31}$$

where $\mathcal{K}_P$ is the kinematic factor defined in Equations (2.103). Using Equations (4.30) and (4.31), we rewrite the isospin-breaking correction in Equation (2.102) as

$$\begin{aligned}
\delta R_P &= \frac{\Gamma(P^+ \rightarrow \ell^+ \nu_\ell [\gamma]) - \Gamma^{\text{tree}}}{\Gamma^{\text{tree}}}, \\
&= \frac{|\mathcal{Z}|^2 |\mathcal{A}_P|^2}{|\mathcal{Z}_0|^2 |\bar{\mathcal{A}}_P|^2} - \left(\frac{M_{P^+}}{\bar{M}_P}\right)^2.
\end{aligned} \tag{4.32}$$

Let $\delta X = \sum_g (g - \bar{g}) \partial_g X$ be a shorthand to denote the leading order expansion of a quantity X about the coupling g . Since the isospin-breaking parameters are small, we can perturbatively expand the QCD+QED quantities $\mathcal{Z}$, $\mathcal{A}_P$ and M_{P^+}

as

$$\begin{aligned}\mathcal{Z} &= \mathcal{Z}_0 + \delta\mathcal{Z} + \mathcal{O}(g^2), \\ \mathcal{A}_{P^+} &= \bar{\mathcal{A}}_P + \delta\mathcal{A}_{P^+} + \mathcal{O}(g^2), \\ M_{P^+} &= \bar{M}_P + \delta M_{P^+}.\end{aligned}\tag{4.33}$$

Inserting this back into Equation (4.32), we obtain

$$\delta R_P = 2 \left(\text{Re} \left[\frac{\delta\mathcal{Z}}{\mathcal{Z}_0} \right] + \text{Re} \left[\frac{\delta\mathcal{A}_{P^+}}{\bar{\mathcal{A}}_P} \right] - \frac{\delta M_{P^+}}{\bar{M}_P} \right).\tag{4.34}$$

Thus, the quantity of interest

$$\begin{aligned}\delta R_{K\pi} &\equiv \delta R_K - \delta R_\pi \\ &= 2 \left(\text{Re} \left[\frac{\delta\mathcal{A}_K}{\bar{\mathcal{A}}_K} \right] - \text{Re} \left[\frac{\delta\mathcal{A}_\pi}{\bar{\mathcal{A}}_\pi} \right] - \left(\frac{\delta M_K}{\bar{M}_K} - \frac{\delta M_\pi}{\bar{M}_\pi} \right) \right).\end{aligned}\tag{4.35}$$

This is what we should expect from using the definition of decay rates in Equation (2.102), *i.e.* in keeping only the decay constant in the isosymmetric QCD theory, the mass correction is subtracted away, given that masses are determined from experimental measurements in this definition. Note that, in this difference, the renormalisation and its $\mathcal{O}(\alpha)$ correction exactly cancel if evaluated in a mass-independent scheme. Thus, there is no need to compute $\delta\mathcal{Z}$ on the lattice for $\delta R_{K\pi}$.

Let e_1 and e_2 be the fractional charge factor of the u -type and d -type quark flavor, respectively, in units of positron charge. Let us also introduce a shorthand for the partial derivatives, where $\partial_g = \frac{\partial}{\partial g}$. In particular, let $\partial_{e_{qq'}}^2 = \partial_{e_q} \partial_{e_{q'}}$. At $\mathcal{O}(\alpha, \delta m)$, the matrix element correction consists of

$$\begin{aligned}\frac{\delta\mathcal{A}_{P^+}}{\bar{\mathcal{A}}_P} &= \sum_{m_q} (m_q - \bar{m}_q) \frac{\partial_{m_q} \mathcal{A}_{P^+}}{\bar{\mathcal{A}}_P} + \sum_{i,j=1}^2 e_i e_j \theta_{ij} \frac{\partial_{e_{ij}}^2 \mathcal{A}_{P^+}}{\bar{\mathcal{A}}_P} \\ &\quad + \sum_{i=1}^2 e_i e_\ell \frac{\partial_{e_{i\ell}}^2 \mathcal{A}_{P^+}}{\bar{\mathcal{A}}_P} + e_\ell^2 \frac{\partial_{e_{\ell\ell}}^2 \mathcal{A}_{P^+}}{\bar{\mathcal{A}}_P},\end{aligned}\tag{4.36}$$

where

$$\theta_{ij} = \begin{cases} \frac{1}{2} & \text{if } i \neq j, \\ 1 & \text{otherwise.} \end{cases}\tag{4.37}$$

Before moving on, some remarks about the above equation are in order. The

$\mathcal{O}(e_\ell^2)$ self-energy correction of the final charged lepton is absorbed in its wavefunction renormalisation. As such, we do not need to compute this diagram on the lattice. Secondly, the $\mathcal{O}(e_j^2, e_j e_k, (m - \bar{m})_q)$ terms, for $j, k = 1, 2$, are corrections to the initial hadron. Such a matrix element may be factorised into its hadronic and leptonic piece. In this thesis, we call these the **factorisable corrections** and these are shown in Figures 4.1 and 4.2(a)-(c). On the other hand, the $\mathcal{O}(e_j e_\ell)$ correction consists of a photon coupling to one of the initial pseudoscalar's quark legs and the final state charged lepton. Electromagnetic corrections of this form cannot be factorised and thus are called **non-factorisable corrections**. These are shown in Figure 4.2(e)-(f).

We extract terms in Equation (4.36) from Euclidean n -point correlation functions, generated with the path integral formalism from Equation (3.36) for 5D fields. Let

$$\langle O \rangle = \frac{1}{Z} \int D[U] D[A] D[\Psi] D[\bar{\Psi}] O[\Psi, \bar{\Psi}, U, A] e^{-S_F[\Psi, \bar{\Psi}, U, A]} e^{-S_g[U]} e^{-S_\gamma[A]} \quad (4.38)$$

be the correlation function in the full QCD+QED theory, where we additionally integrate over the $U(1)$ gauge fields A , weighted by the photon action (see §3.4). Since the isospin-breaking couplings are small (*i.e.* $\alpha \sim \frac{\delta m}{\Lambda_{\text{QCD}}} \sim \mathcal{O}(1\%)$), we adopt the *perturbative method*, first introduced in [46], to generate correlation functions. At leading order,

$$\langle O \rangle = \langle O \rangle_0 + \sum_q (m - \bar{m})_q \frac{\partial}{\partial m_q} \langle O \rangle \Big|_{m_q = \bar{m}_q} + \frac{1}{2!} \sum_{i,j \in \{1,2,\ell\}} e_i e_j \frac{\partial^2}{\partial e_i \partial e_j} \langle O \rangle \Big|_{e_{i,j}=0}, \quad (4.39)$$

where $\langle O \rangle_0$ is the QCD-only correlation function and $\mathcal{O}(\alpha(m - \bar{m})_q)$ cross-terms are neglected. From this equation, a couple of comments are in order. First, we see that isospin-breaking corrections may be extracted from the gradient of the QCD+QED correlation functions. Even if only QCD gauge configurations are available, the gradients can also be generated from insertions of scalar/vector currents in the QCD 2-point correlation function. Secondly, evaluating the Wick contraction in the above equation will generate diagrams where disconnected fermion loops couple to the fermion line via gluons or photons. Some lattice calculations (such as this) neglect disconnected QCD contributions. Additionally, *electro-quenched approximation* is usually applied, where sea quarks are electrically neutral and do not partake in electromagnetic interactions.

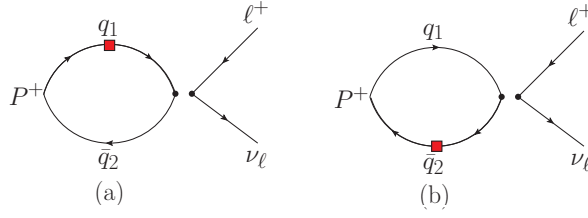


Figure 4.1 *Correlation functions with scalar insertions on quark legs (marked with red boxes).*

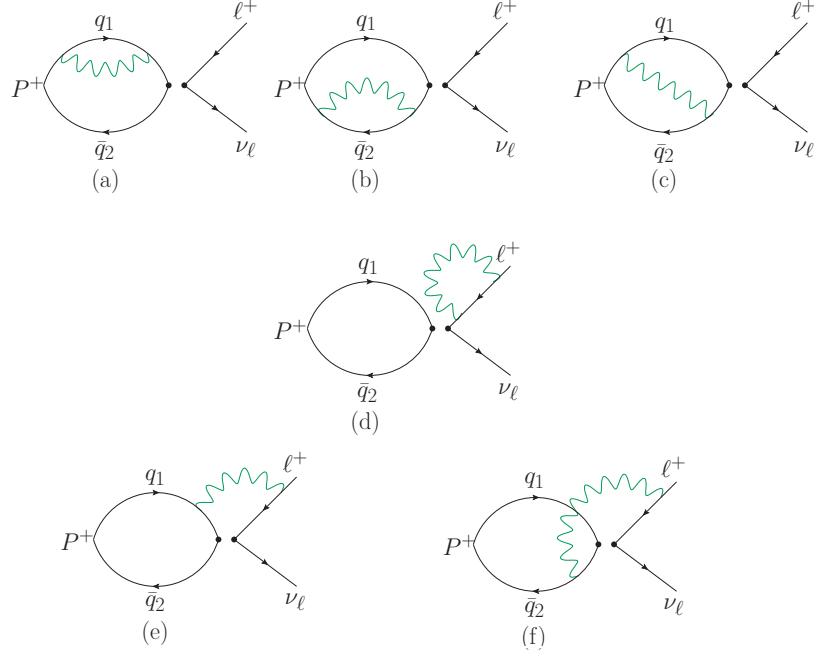


Figure 4.2 *Correlation functions with all possible insertions of the electromagnetic current (marked with green squiggle lines) at $\mathcal{O}(e^2)$. Electromagnetic interactions with sea quarks are currently neglected.*

4.3 Construction of Lattice Time Correlators with Isospin-breaking Effects

4.3.1 Hadronic Correlators

The hadronic tree-level time correlator for a light pseudoscalar P has the usual form

$$C_{P,0}^{pj}(t) \equiv \langle \phi_j(x) \phi_p^\dagger(0) \rangle = \sum_{\mathbf{x}} \text{Tr} \left[\gamma^5 S^{q_2}(0|x) \Gamma_{\text{snk}}^j S^{q_1}(x|0) \right], \quad (4.40)$$

where $\phi = \bar{q}_2 \Gamma q_1$, with $q_1 = l, q_2 = l, s$, $S^q(y|x)$ is the q -quark propagator from the 4-vector x to y and

$$\Gamma_{\text{snk}}^j = \begin{cases} \gamma^5 & \text{if } j = p, \\ \gamma^0 \gamma^5 & \text{if } j = a \end{cases} \quad (4.41)$$

is the pseudoscalar (p) or axial-pseudoscalar (a) interpolator at the sink. Now, let

$$\mathcal{S}_q(x) = \bar{q}(x) \mathbb{1} q(x) \quad (4.42)$$

be the scalar density for quark flavors, $q \in \{l, s\}$, and

$$S^{q,m}(y|0) = \sum_x S^q(y|x) \mathbb{1} S^q(x|0) \quad (4.43)$$

be the sequential propagator with the scalar insertion. Then, let

$$\begin{aligned} \partial_{m_{q_1}} C_P^{pj}(t) &\equiv \sum_{x,y} \langle \phi_j(y) \mathcal{S}_{q_1}(x) \phi_p^\dagger(0) \rangle, \\ &= \sum_y \text{Tr} [\gamma^5 S^{q_2}(0|y) \Gamma_{\text{snk}}^j S^{q_1,m}(y|0)] \end{aligned} \quad (4.44)$$

and similarly for q_2 . Let

$$\mathcal{J}_{em}(x) = Z_V \sum_{q \in \{l,s\}} \bar{q}(x) \gamma^\mu A_\mu(x) q(x) \quad (4.45)$$

be the local implementation of the electromagnetic current (renormalised by Z_V),

$$S^{q,e}(y|0) = i \sum_x S^q(y|x) \gamma^\mu A_\mu(x) S^q(x|0) \quad (4.46)$$

be the fermion propagator with a single $\not{A}$ insertion and

$$S^{q,ee}(y|0) = \sum_{x_1, x_2} S^q(y, x_2) \gamma^\mu S^q(x_2, x_1) \gamma^\nu S^q(x_1, 0) \Delta_{\mu\nu}(x_1 - x_2) \quad (4.47)$$

be the self energy propagator for the fermion, where

$$\Delta_{\mu\nu}(x_1 - x_2) = \langle A_\mu(x_1) A_\nu(x_2) \rangle_{\text{EM}} \quad (4.48)$$

is the photon propagator. Then,

$$\partial_{e_{11}}^2 C_P^{pj}(t) = \sum_{\mathbf{y}} \text{Tr} [\gamma^5 S^{q_2}(0|y) \Gamma_{\text{snk}}^j S^{q_1, ee}(y|0)] \quad (4.49)$$

is, along with $e_1 \rightarrow e_2$, the correlator corresponding to the self energy diagram and

$$\partial_{e_{12}}^2 C_P^{pj}(t) = \sum_{\mathbf{y}} \text{Tr} [\gamma^5 S^{q_2, e}(0|y) \Gamma_{\text{snk}}^j S^{q_1, e}(y|0)] \quad (4.50)$$

is that of the exchange diagram. Combining Equations (4.49) and (4.50), the $\mathcal{O}(e^2)$ hadronic correlator is

$$\partial_e^2 C_P^{pj}(t) = \frac{4}{9} \partial_{e_{11}}^2 C_P^{pj}(t) + \frac{1}{9} \partial_{e_{22}}^2 C_P^{pj}(t) - \frac{2}{9} \partial_{e_{12}}^2 C_P^{pj}(t). \quad (4.51)$$

4.3.2 Hadron-Leptonic correlators

We begin with a discussion on the implementation of the lepton on the lattice. The neutrino is a spectator particle in this decay, so we choose to omit it in our simulation and add it in the analysis stage. Let

$$\tilde{O}_{W\varepsilon} = (\bar{\ell} \Gamma_L^\tau)_\varepsilon (\bar{q}_2 \Gamma_L^\tau q_1) \quad (4.52)$$

be the weak decay operator we construct on the lattice. The omission of the neutrino operator leaves an open spinor index ε .

To construct the correlators corresponding to this decay process, note that there are 3 unique times: the insertion time of 1) the pseudoscalar interpolator t_P , 2) the weak operator t_H , and 3) the lepton source t_ℓ . We build the non-factorisable correlator by first fixing the lepton source-sink separation $\Delta t_\ell = t_\ell - t_H$, thereby treating the weak operator insertion as the sink time. The tree-level correlator is

$$\begin{aligned} \tilde{C}_{P\ell,0}(t_P, t_H, \Delta t_\ell)_{\varepsilon_1 \varepsilon_2} &\equiv \left\langle \ell_{\varepsilon_1}(x_\ell) \tilde{O}_{W\varepsilon_2}(x_H) \phi_p^\dagger(x_P) \right\rangle e^{ip_\nu x_H}, \\ &= \sum_{\mathbf{x}_P, \mathbf{x}_H, \mathbf{x}_\ell} \text{Tr} [\gamma^5 S^{q_2}(x_P, x_H) \Gamma_L^\tau S^{q_1}(x_H, x_P)] (\Gamma_L^\tau S^\ell(x_H, x_\ell))_{\varepsilon_1 \varepsilon_2} e^{i\mathbf{p}_\nu \cdot \mathbf{x}_H} \end{aligned} \quad (4.53)$$

and at $\mathcal{O}(\alpha)$,

$$\begin{aligned}
\partial_{e_{1\ell}}^2 \tilde{C}_{P\ell}(t_P, t_H, \Delta t_\ell)_{\varepsilon_1 \varepsilon_2} &\equiv \sum_{z_1, z_2} \left\langle \ell(x_\ell) \mathcal{J}_{em}(z_1) \tilde{O}_W(x_H) \mathcal{J}_{em}(z_2) \phi_p^\dagger(x_P) \right\rangle_{\varepsilon_1 \varepsilon_2} e^{ip_\nu x_H}, \\
&= \sum_{\mathbf{x}_P, \mathbf{x}_H, \mathbf{x}_\ell} \text{Tr} \left[\gamma^5 S^{q_2}(x_P, x_H) \Gamma_L^\tau S^{q_1, e}(x_H, x_P) \right] \left(\Gamma_L^\tau S^{\ell, e}(x_H, x_\ell) \right)_{\varepsilon_1 \varepsilon_2} e^{i\mathbf{p}_\nu \cdot \mathbf{x}_H}
\end{aligned} \tag{4.54}$$

and similarly for $q_1 \rightarrow q_2$, $e_{1\ell} \rightarrow e_{2\ell}$. In the above, we added a phase for the neutrino to conserve the 4-momentum of this process. We saturate the spinor indices to obtain

$$C_{P\ell\nu,0}(t_P, t_H, \Delta t_\ell) = \text{Tr} \left[\not{p}_\nu \tilde{C}_{P\ell,0}(t_P, t_H, \Delta t_\ell) \Gamma_L^0 \right] \tag{4.55}$$

and

$$\begin{aligned}
\partial_e^2 C_{P\ell\nu}(t_P, t_H, \Delta t_\ell) &= \frac{2}{3} \text{Tr} \left[\not{p}_\nu \partial_{e_{1\ell}}^2 \tilde{C}_{P\ell}(t_P, t_H, \Delta t_\ell) \Gamma_L^0 \right] \\
&\quad - \frac{1}{3} \text{Tr} \left[\not{p}_\nu \partial_{e_{2\ell}}^2 \tilde{C}_{P\ell}(t_P, t_H, \Delta t_\ell) \Gamma_L^0 \right].
\end{aligned} \tag{4.56}$$

4.4 Functional Form of Time Correlators

Let us now study the functional form of the finite time correlators obtained from the simulation in this section.

4.4.1 Factorisable Analysis

To begin, consider the following QCD+QED time pp correlator for a P meson with some arbitrary momentum, $\mathbf{k}$:

$$\begin{aligned}
C_P^{pp}(\mathbf{k}, t, t_0) &= \sum_{\mathbf{x}} \langle \phi_p(\mathbf{x}, t) \phi_p^\dagger(\mathbf{0}, t_0) \rangle e^{-i\mathbf{k} \cdot \mathbf{x}}, \\
&= \sum_{\mathbf{x}} \sum_{n, \mathbf{p}} \frac{1}{\omega_n(\mathbf{p})} \langle n, \mathbf{p} | e^{-HT} \phi_p(\mathbf{x}, t) \phi_p^\dagger(\mathbf{0}, t_0) | n, \mathbf{p} \rangle e^{-i\mathbf{k} \cdot \mathbf{x}}.
\end{aligned} \tag{4.57}$$

On the RHS of Equation (4.57), this is a finite T expression of the operator trace. We see that as $T \rightarrow \infty$, we recover the infinite time expression where $n = 0$. For

the moment, consider the case where $n = 0$. To evaluate this, we insert a complete set of states (Equation (3.32)) and noting that, under (Euclidean) translation, an operator O transforms as

$$O(\mathbf{x}, t) = e^{i\mathbf{P}\cdot\mathbf{x}+Ht} O e^{-i\mathbf{P}\cdot\mathbf{x}-Ht}, \quad (4.58)$$

where $\mathbf{P}$ is the translation operator H is the Hamiltonian. Thus, Equation (4.57) becomes

$$\begin{aligned} \sum_{\mathbf{x}} \langle \Omega | e^{-HT} \phi_p(t) \phi_p^\dagger(t_0) | \Omega \rangle \\ = \frac{1}{L^3} \sum_{\mathbf{x}} \sum_{n, \mathbf{p}} \frac{1}{\omega_n(\mathbf{p})} \langle \Omega | e^{-HT} \phi_p(\mathbf{x}, t) | n, \mathbf{p} \rangle \langle n, \mathbf{p} | \phi_p^\dagger(\mathbf{0}, t_0) | \Omega \rangle, \quad (4.59) \\ = \frac{1}{L^3} \sum_{\mathbf{x}} \sum_{n, \mathbf{p}} \frac{\langle \Omega | \phi_p | n, \mathbf{p} \rangle \langle n, \mathbf{p} | \phi_p^\dagger | \Omega \rangle}{\omega_n(\mathbf{p})} e^{-\omega_n(t-t_0)} e^{-i(\mathbf{k}-\mathbf{p})\cdot\mathbf{x}}, \end{aligned}$$

where the shorthand $|\Omega\rangle = |0, \mathbf{0}\rangle$. As before, the energy eigenstates ω_n are ordered such that $0 < \omega_0 \leq \omega_1 \leq \dots \leq \omega_n$. For $t - t_0 \gg 0$, the dominant contribution is the ground state $\omega_0 = 2M_P$. Now we evaluate the summation over $\mathbf{x}$ and project to zero momentum ($\mathbf{k} = \mathbf{0}$) to obtain

$$C_P^{pp}(t, t_0) \equiv C_P^{pp}(\mathbf{0}, t, t_0) = \frac{|Z_P|^2}{2M_P} e^{-M_P(t-t_0)}, \quad (4.60)$$

where $|Z_P|^2 = |\langle P, \mathbf{0} | \phi_p^\dagger | \Omega \rangle|^2$ represents the probability of creating a $|P\rangle$ state with zero momentum from the vacuum.

Now, consider the case where $n \neq \Omega$ in Equation (4.57), Equation (4.60) is modified with

$$\begin{aligned} \sum_{\mathbf{x}} \sum_{n, \mathbf{p}} \frac{1}{\omega_n(\mathbf{p})} \langle n, \mathbf{p} | e^{-HT} \phi_p(\mathbf{x}, t) \phi_p^\dagger(\mathbf{0}, t_0) | n, \mathbf{p} \rangle e^{-i\mathbf{k}\cdot\mathbf{x}} \\ = \frac{1}{L^3} \sum_{\mathbf{x}} \sum_{n, \mathbf{p}} \frac{\langle n, \mathbf{p} | \phi_p | \Omega \rangle \langle \Omega | \phi_p^\dagger | n, \mathbf{p} \rangle}{\omega_n(\mathbf{p})} e^{-\frac{1}{2}\omega_n(T-(t-t_0))} e^{-i(\mathbf{k}-\mathbf{p})\cdot\mathbf{x}}. \quad (4.61) \end{aligned}$$

After projecting to zero momentum, we see that as the source-sink separation grows, this term begins to contribute as

$$C_P^{pp}(t, t_0) \stackrel{(t-t_0) \sim T}{\sim} \frac{|Z_P|^2}{2M_P} e^{-M_P(T-(t-t_0))}. \quad (4.62)$$

Combining Equations (4.60) and (4.62) together, the pp correlator in finite T is

$$C_P^{pp}(t, t_0) = c_P^{pp} \left(e^{-M_P(t-t_0)} + e^{-M_P(T-(t-t_0))} \right), \quad (4.63)$$

where the coefficient is $c_P^{pp} = \frac{|Z_P|^2}{2M_P}$. The periodicity of this finite T correlator is made manifest when re-structured as

$$C_P^{pp}(t, t_0) = 2c_P^{pp} e^{-M_P \frac{T}{2}} \cosh M_P \left(\frac{T}{2} - (t - t_0) \right). \quad (4.64)$$

One can repeat the same exercise with the axial-pseudoscalar interpolator $\phi_a = \bar{q}_2 \gamma^0 \gamma^5 q_1$ at the sink:

$$C_P^{pa}(t, t_0) = \sum_{\mathbf{x}} \sum_{n, \mathbf{p}} \frac{1}{\omega_n(\mathbf{p})} \langle n | e^{-TH} \phi_a(t) \phi_p^\dagger(t_0) | n \rangle \quad (4.65)$$

and obtain

$$C_P^{pa}(t, t_0) = 2c_P^{pa} e^{-M_P \frac{T}{2}} \sinh M_P \left(\frac{T}{2} - (t - t_0) \right), \quad (4.66)$$

where $c_P^{pa} = \frac{A_P Z_P^\dagger}{2M_P}$ and $A_P = \langle \Omega | \phi_a | P, \mathbf{0} \rangle$ is the axial matrix element. Note that we obtain a sinh function for the pa correlator because A_P is odd under time reversal. In practice, due to invariance in time translation, we shift all $t_0 \in [0, T - 1]$ to the origin and drop the label t_0 from here on. Thus, t is to be interpreted as the distance away from the pseudoscalar source.

Having considered the full QCD+QED pp/pa correlators, we now discuss how corrections to the masses and matrix elements may be extracted from finite T correlators with current insertions. The above derivations may be summarised as

$$C_P^{pj}(t) = 2c_P^{pj} e^{-M_P \frac{T}{2}} f^{pj} (M_P \tilde{t}), \quad (4.67)$$

where $\tilde{t} = \frac{T}{2} - t$ and

$$f^{pj} (M_P \tilde{t}) = \begin{cases} \cosh M_P \tilde{t} & \text{if } j = p, \\ \sinh M_P \tilde{t} & \text{if } j = a. \end{cases} \quad (4.68)$$

Let $g \in \{e^2, m_{ud}, \delta m, m_s\}$ be the coupling of interest. We can express them as an

expansion about the point of simulation

$$\begin{aligned} M_P &= \hat{M}_P + \delta_g M_P + \dots, \\ c_P^{pj} &= \hat{c}_P^{pj} + \delta_g c_P^{pj} + \dots, \end{aligned} \quad (4.69)$$

where $\delta_g Y = (g - \hat{g})\partial_g Y$. For $(g - \hat{g}) \ll 1$, we can insert Equation (4.69) into Equation (4.67) to obtain

$$\begin{aligned} c_P^{pj} e^{-M_P \frac{T}{2}} &= (\hat{c}_P^{pj} + \delta_g c_P^{pj} + \dots) \left(1 - \delta_g M_P \frac{T}{2} + \dots \right) e^{-\hat{M}_P \frac{T}{2}}, \\ &= e^{-\hat{M}_P \frac{T}{2}} \hat{c}_P^{pj} \left(1 + \frac{\delta_g c_P^{pj}}{\hat{c}_P^{pj}} - \delta_g M_P \frac{T}{2} \right) \end{aligned} \quad (4.70)$$

and

$$f^{pj}(M_P \tilde{t}) = f^{pj}(\hat{M}_P \tilde{t}) + \delta_g M_P \tilde{t} f^{pj'}(\hat{M}_P \tilde{t}) + \dots, \quad (4.71)$$

where $f^{pj'}$ indicates a derivative in g . Together, these give

$$\begin{aligned} C_P^{pj}(t) &= 2e^{-\hat{M}_P \frac{T}{2}} \hat{c}_P^{pj} f^{pj}(\hat{M}_P \tilde{t}) \\ &\times \left[1 + (g - \hat{g}) \left(\frac{\partial_g c_P^{pj}}{\hat{c}_P^{pj}} - \partial_g M_P \frac{T}{2} + \partial_g M_P \tilde{t} F^{pj}(\hat{M}_P \tilde{t}) \right) \right], \end{aligned} \quad (4.72)$$

where

$$F^{pj}(\hat{M}_P \tilde{t}) \equiv \frac{f^{pj'}(\hat{M}_P \tilde{t})}{f^{pj}(\hat{M}_P \tilde{t})} = \begin{cases} \tanh \hat{M}_P \tilde{t} & \text{if } j = p, \\ \coth \hat{M}_P \tilde{t} & \text{if } j = a. \end{cases} \quad (4.73)$$

From a path integral standpoint, the full QCD+QED correlator may be expressed as a sum of the QCD-only correlator and correlators with insertion of currents associated to expansion parameter g , that is

$$\begin{aligned} C_P^{pj}(t) &= C_{P,0}^{pj}(t) + \delta_g C_P^{pj}(t) + \dots, \\ &= C_{P,0}^{pj}(t) \left[1 + (g - \hat{g}) \left(\frac{\partial_g C_P^{pj}(t)}{C_{P,0}^{pj}(t)} \right) \right] + \dots \end{aligned} \quad (4.74)$$

By matching Equations (4.72) and (4.74), we find that

$$C_{P,0}^{pj}(t) = 2e^{-\hat{M}_P \frac{T}{2}} \hat{c}_P^{pj} f^{pj} \left(\hat{M}_P \tilde{t} \right) \quad (4.75)$$

$$R_{P,g}^{pj}(t) \equiv \frac{\partial_g C_P^{pj}(t)}{C_{P,0}^{pj}(t)} = \frac{\partial_g \hat{c}_P^{pj}}{\hat{c}_P^{pj}} - \partial_g M_P \frac{T}{2} + \partial_g M_P \tilde{t} F^{pj} \left(\hat{M}_P \tilde{t} \right). \quad (4.76)$$

From Equation (4.75), we can extract the decay constant via

$$f_P = \hat{c}_P^{pa} \sqrt{\frac{2}{\hat{M}_P \hat{c}_P^{pp}}}. \quad (4.77)$$

From the functional form of the correlator ratio in Equation (4.76), we can extract mass and matrix element corrections associated with the parameter g . This result is the functional form of correlator ratios in finite T . We find that, for $T \rightarrow \infty$,

$$\begin{aligned} R_{P,g}^{pj}(t) &= \frac{\partial_g \hat{c}_P^{pj}}{\hat{c}_P^{pj}} - \partial_g M_P \frac{T}{2} + \partial_g M_P \tilde{t} F^{pj} \left(\hat{M}_P \tilde{t} \right), \\ &\stackrel{T \rightarrow \infty}{=} \frac{\partial_g \hat{c}_P^{pj}}{\hat{c}_P^{pj}} - \partial_g M_P t, \end{aligned} \quad (4.78)$$

i.e. we recover the infinite volume linear dependence since $\tanh x, \coth x \rightarrow 1$ in the large x limit.

In the infinite volume limit, we see that the mass correction may be extracted directly from the finite difference of the ratios:

$$\partial_g M_P = \lim_{T \rightarrow \infty} \left[R_{P,g}^{pj}(t) - R_{P,g}^{pj}(t+1) \right]. \quad (4.79)$$

However, in the finite time limit, the (anti-)periodic effects contribute as $t \rightarrow \frac{T}{2}$. One can extract the mass derivative with

$$\partial_g M_P = \frac{R_{P,g}^{pj}(t) - R_{P,g}^{pj}(t+1)}{\tilde{t} F^{pj} \left(\hat{M}_P \tilde{t} \right) - (\tilde{t} - 1) F^{pj} \left(\hat{M}_P \tilde{t} \right)}. \quad (4.80)$$

Strong Isospin-breaking Correction

For tuning the setup and calculating strong isospin-breaking corrections, we need correlators with scalar densities. From Equation (4.76), the functional form of

their ratio is

$$\begin{aligned} R_{P,m_q}^{pp}(t) &\equiv \frac{\partial_{m_q} C_P^{pp}(t)}{C_{P,0}^{pp}(t)} = \frac{\partial_{m_q} \hat{C}_P^{pp}}{\hat{C}_P^{pp}} - \partial_{m_q} M_P \frac{T}{2} + \partial_{m_q} M_P \left(\frac{T}{2} - t \right) \tanh \hat{M}_P \left(\frac{T}{2} - t \right), \\ R_{P,m_q}^{pa}(t) &\equiv \frac{\partial_{m_q} C_P^{pa}(t)}{C_{P,0}^{pa}(t)} = \frac{\partial_{m_q} \hat{C}_P^{pa}}{\hat{C}_P^{pa}} - \partial_{m_q} M_P \frac{T}{2} + \partial_{m_q} M_P \left(\frac{T}{2} - t \right) \coth \hat{M}_P \left(\frac{T}{2} - t \right). \end{aligned} \quad (4.81)$$

The quark mass derivatives in the isospin basis $(m_{ud}, \delta m, m_s)$ are

$$\frac{\partial}{\partial m_{ud}} = \begin{cases} \frac{\partial}{\partial m_u} + \frac{\partial}{\partial m_d} = 2 \frac{\partial}{\partial m_l} & \text{if } P = \pi^+, \\ \frac{\partial}{\partial m_{u/d}} = \frac{\partial}{\partial m_l} & \text{if } P = K^+, K^0, \end{cases} \quad (4.82)$$

$$\frac{\partial}{\partial \delta m} = \frac{\partial}{\partial m_u} - \frac{\partial}{\partial m_d} = \begin{cases} 0 & \text{if } P = \pi^+, \\ \pm \frac{\partial}{\partial m_l} & \text{if } P = K^+(K^0) \end{cases} \quad (4.83)$$

where in the second equalities we use the fact that $m_u = m_d = m_l$ in this setup (see §5.1). Thus, the relevant ratios are

$$\begin{aligned} R_{\pi^+, m_{ud}}^{pj}(t) &= 2R_{\pi^+, m_l}^{pj}(t), \\ R_{K^+, m_{ud}}^{pj}(t) &= R_{K^+, m_l}^{pj}(t), \\ R_{K^+, \delta m}^{pj}(t) &= R_{K^+, m_l}^{pj}(t), \\ R_{K^0, \delta m}^{pj}(t) &= -R_{K^0, m_l}^{pj}(t), \end{aligned}$$

and $R_{K^+, m_s}^{pp}(t)$.

Electromagnetic Correction

From Equation (4.76), we have

$$\begin{aligned} &= \frac{\partial_{e_{ij}}^2 C_P^{pp}}{\hat{C}_P^{pp}} - \partial_{e_{ij}}^2 M_P \frac{T}{2} R_{P, e_{ij}}^{pp}(t) \equiv \frac{\partial_{e_{ij}}^2 C_P^{pp}(t)}{C_{P,0}^{pp}(t)} + \partial_{e_{ij}}^2 M_P \left(\frac{T}{2} - t \right) \tanh \hat{M}_P \left(\frac{T}{2} - t \right), \\ &= \frac{\partial_{e_{ij}}^2 C_P^{pa}}{\hat{C}_P^{pa}} - \partial_{e_{ij}}^2 M_P \frac{T}{2} R_{P, e_{ij}}^{pa}(t) \equiv \frac{\partial_{e_{ij}}^2 C_P^{pa}(t)}{C_{P,0}^{pa}(t)} + \partial_{e_{ij}}^2 M_P \left(\frac{T}{2} - t \right) \coth \hat{M}_P \left(\frac{T}{2} - t \right). \end{aligned} \quad (4.84)$$

Thus, for $P = \pi^+, K^+$,

$$\begin{aligned} R_{P,e^2}^{pp} &= \frac{4}{9} \cdot R_{P,e_{11}}^{pp}(t) + \frac{1}{9} \cdot R_{P,e_{22}}^{pp}(t) - \frac{2}{9} \cdot R_{P,e_{12}}^{pp}(t), \\ R_{P,e^2}^{pa} &= \frac{4}{9} \cdot R_{P,e_{11}}^{pa}(t) + \frac{1}{9} \cdot R_{P,e_{22}}^{pa}(t) - \frac{2}{9} \cdot R_{P,e_{12}}^{pa}(t). \end{aligned} \quad (4.85)$$

For $P = K^0, d\bar{d}$,

$$\begin{aligned} R_{P,e^2}^{pp} &= \frac{1}{9} \cdot (R_{P,e_{11}}^{pp}(t) + R_{P,e_{22}}^{pp}(t) + R_{P,e_{12}}^{pp}(t)), \\ R_{P,e^2}^{pa} &= \frac{1}{9} \cdot (R_{P,e_{11}}^{pa}(t) + R_{P,e_{22}}^{pa}(t) + R_{P,e_{12}}^{pa}(t)). \end{aligned} \quad (4.86)$$

For $P = u\bar{u}$,

$$\begin{aligned} R_{P,e^2}^{pp} &= \frac{4}{9} \cdot (R_{P,e_{11}}^{pp}(t) + R_{P,e_{22}}^{pp}(t) + R_{P,e_{12}}^{pp}(t)), \\ R_{P,e^2}^{pa} &= \frac{4}{9} \cdot (R_{P,e_{11}}^{pa}(t) + R_{P,e_{22}}^{pa}(t) + R_{P,e_{12}}^{pa}(t)). \end{aligned} \quad (4.87)$$

4.4.2 Non-Factorisable Analysis

To make the non-factorisable time correlators more physically intuitive, let us first introduce an additional time variable - the neutrino sink position t_ν . Then, consider the time ordering, where $t_\ell, t_\nu > t_H > t_P$,

$$\begin{aligned} C_{P\ell\nu}(t_\nu, t_\ell, t_H, t_P) \\ = \sum_{\{\mathbf{x}\}} \sum_{n, \mathbf{p}} \frac{1}{\omega_n(\mathbf{p})} \langle n, \mathbf{p} | e^{-HT} \bar{\ell}(\mathbf{x}_\ell, t_\ell) \Gamma_L^0 \nu(\mathbf{x}_\nu, t_\nu) O_W(\mathbf{x}_H, t_H) \phi_p^\dagger(\mathbf{0}, t_P) | n, \mathbf{p} \rangle \end{aligned} \quad (4.88)$$

where $\{\mathbf{x}\}$ is a shorthand for all spatial coordinates. Here, we have implicitly projected to zero 3-momentum since the decay is conventionally treated in the meson rest frame. Inserting complete sets of states, the forward propagating

term, denoted by the superscript ‘ f ’, gives

$$\begin{aligned}
C_{P\ell\nu}^f(t_\nu, t_\ell, t_H, t_P) &= \sum_{\{\mathbf{x}\}} \langle \Omega | \bar{\ell}(\mathbf{x}_\ell, t_\ell) \Gamma_L^0 \nu(\mathbf{x}_\nu, t_\nu) O_W(\mathbf{x}_H, t_H) \phi_p^\dagger(\mathbf{0}, t_P) | \Omega \rangle, \\
&= \sum_{\{\mathbf{x}\}} \sum_{\{n\}, \{\mathbf{p}\}} \prod_{i=1}^3 \left[\frac{1}{\omega_{n_i}(\mathbf{p}_i)} \right] \langle \Omega | \bar{\ell}(\mathbf{x}_\ell, t_\ell) | n_1, \mathbf{p}_1 \rangle \Gamma_L^0 \langle n_1, \mathbf{p}_1 | \nu(\mathbf{x}_\nu, t_\nu) | n_2, \mathbf{p}_2 \rangle \\
&\quad \times \langle n_2, \mathbf{p}_2 | O_W(\mathbf{x}_H, t_H) | n_3, \mathbf{p}_3 \rangle \\
&\quad \times \langle n_3, \mathbf{p}_3 | \phi_p^\dagger(\mathbf{0}, t_P) | \Omega \rangle \\
&= \sum_{\substack{\{\mathbf{x}\}, \{\mathbf{p}\} \\ \{n\}}} \frac{Z_{n_1, n_2} \mathcal{M}_{n_2, n_3} Z_{n_3}^\dagger}{\omega_{n_1}(\mathbf{p}_1) \omega_{n_2}(\mathbf{p}_2) \omega_{n_3}(\mathbf{p}_3)} e^{-\frac{1}{2} \omega_{n_1}(t_\ell - t_\nu)} e^{-\frac{1}{2} \omega_{n_2}(t_\nu - t_H)} e^{-\frac{1}{2} \omega_{n_3}(t_H - t_P)} \\
&\quad \times e^{-i \mathbf{p}_1 \cdot \mathbf{x}_\ell} e^{-i(\mathbf{p}_2 - \mathbf{p}_1) \cdot \mathbf{x}_\nu} e^{-i(\mathbf{p}_3 - \mathbf{p}_2) \cdot \mathbf{x}_H}.
\end{aligned} \tag{4.89}$$

By doing all spatial sums, the lowest lying energy states in this configuration are $n_1 = (\ell; s)$, $n_2 = (\ell\nu; s, r)$, $n_3 = P$ with momenta $\mathbf{p}_\ell = \mathbf{p}_1$, $\mathbf{p}_\nu = \mathbf{p}_2 - \mathbf{p}_1$, $\mathbf{p}_P = \mathbf{p}_3 = \mathbf{0}$. Now, we evaluate these overlap factors and matrix elements

$$Z_{n_1, n_2} \equiv \langle \Omega | \bar{\ell} | \ell; s, \mathbf{p}_\ell \rangle \Gamma_L^0 \langle \ell; s, \mathbf{p}_\ell | \nu | \ell\nu; s, r, \mathbf{0} \rangle = Z_{\ell\nu} \bar{v}^s(\mathbf{p}_\ell) \Gamma_L^0 u^r(\mathbf{p}_\nu) \tag{4.90}$$

$$\mathcal{M}_{n_2, n_3} \equiv \langle \ell\nu; s, r, \mathbf{0} | O_W | P, \mathbf{0} \rangle = \bar{u}^r(\mathbf{p}_\nu) \mathcal{A}_P v^s(\mathbf{p}_\ell), \tag{4.91}$$

and $Z_P^\dagger = \langle P, \mathbf{0} | \phi_p^\dagger | \Omega \rangle$. Now we have

$$\begin{aligned}
C_{P\ell\nu}^f(t_\nu, t_\ell, t_H, t_P) &= Z_{\ell\nu} \Gamma_L^0 \frac{\sum_s v^s(\mathbf{p}_\ell) \bar{v}^s(\mathbf{p}_\ell)}{2E_\ell(\mathbf{p}_\ell)} \frac{\sum_r u^r(\mathbf{p}_\nu) \bar{u}^r(\mathbf{p}_\nu)}{2E_{\ell\nu}(\mathbf{p}_\ell + \mathbf{p}_\nu)} \frac{\mathcal{A}_P Z_P^\dagger}{2M_P} \\
&\quad \times e^{-E_\ell(t_\ell - t_\nu)} e^{-E_{\ell\nu}(t_\nu - t_H)} e^{-M_P(t_H - t_P)}.
\end{aligned} \tag{4.92}$$

Using the spin-sum average formula in Equations (3.19) and (3.20), this gives us the forward term

$$\begin{aligned}
C_{P\ell\nu}^f(t_\nu, t_\ell, t_H, t_P) &= \frac{Z_{\ell\nu} Z_P^\dagger}{8M_P E_{\ell\nu} E_\nu} \text{Tr} \left[(i \not{p}_\ell + m_\ell) \Gamma_L^0 i \not{p}_\nu \mathcal{A}_P \right] \\
&\quad \times e^{-E_\ell(t_\ell - t_\nu)} e^{-E_{\ell\nu}(t_\nu - t_H)} e^{-M_P(t_H - t_P)}.
\end{aligned} \tag{4.93}$$

For the backward contribution, denoted by superscript ‘ b ’, the procedure is similar for $t_\ell, t_\nu > t_H > t_P$. We begin with

$$C_{P\ell\nu}^b(t_\nu, t_\ell, t_H, t_P) = \sum_{\{\mathbf{x}\}} \sum_{\substack{n \neq 0 \\ \mathbf{p}}} \frac{1}{\omega_n(\mathbf{p})} \langle n, \mathbf{p} | e^{-HT} \bar{\ell}(\mathbf{x}_\ell, t_\ell) \Gamma_L^0 \nu(\mathbf{x}_\nu, t_\nu) O_W(\mathbf{x}_H, t_H) \phi_p^\dagger(\mathbf{0}, t_P) | n, \mathbf{p} \rangle. \quad (4.94)$$

We insert a complete set of states and translate the operators, which gives

$$\begin{aligned} &= \sum_{\{\mathbf{x}\}} \sum_{\{n\}, \{\mathbf{p}\}} \prod_{i=1}^4 \left[\frac{1}{\omega_{n_i}(\mathbf{p}_i)} \right] \langle n_4, \mathbf{p}_4 | e^{-HT} \bar{\ell}(\mathbf{x}_\ell, t_\ell) | n_1, \mathbf{p}_1 \rangle \Gamma_L^0 \langle n_1, \mathbf{p}_1 | \nu(\mathbf{x}_\nu, t_\nu) | n_2, \mathbf{p}_2 \rangle \\ &\quad \times \langle n_2, \mathbf{p}_2 | O_W(\mathbf{x}_H, t_H) | n_3, \mathbf{p}_3 \rangle \\ &\quad \times \langle n_3, \mathbf{p}_3 | \phi_p^\dagger(\mathbf{0}, t_P) | n_4, \mathbf{p}_4 \rangle \\ &= \sum_{\substack{\{\mathbf{x}\}, \{\mathbf{p}\} \\ \{n\}}} \frac{Z_{n_1, n_2, n_4} \mathcal{M}_{n_2, n_3} Z_{n_3, n_4}^\dagger}{\omega_{n_1}(\mathbf{p}_1) \omega_{n_2}(\mathbf{p}_2) \omega_{n_3}(\mathbf{p}_3) \omega_{n_4}(\mathbf{p}_4)} \\ &\quad \times e^{-\frac{1}{2}\omega_{n_4}(T-(t_\ell-t_P))} e^{-\frac{1}{2}\omega_{n_1}(t_\ell-t_\nu)} e^{-\frac{1}{2}\omega_{n_2}(t_\nu-t_H)} e^{-\frac{1}{2}\omega_{n_3}(t_H-t_P)} \\ &\quad \times e^{-i(\mathbf{p}_1-\mathbf{p}_4)\cdot\mathbf{x}_\ell} e^{-i(\mathbf{p}_2-\mathbf{p}_1)\cdot\mathbf{x}_\nu} e^{-i(\mathbf{p}_3-\mathbf{p}_2)\cdot\mathbf{x}_H} \end{aligned} \quad (4.95)$$

We identify the lowest lying energy states to be $n_1 = 0$, $n_2 = (\nu; r)$, $n_3 = (P\bar{\ell}; s)$ and $n_4 = (\bar{\ell}; s)$, where we denote $\bar{\ell}$ as the charge conjugate of ℓ . These imply the momenta are

$$\mathbf{p}_1 = \mathbf{0}, \quad \mathbf{p}_2 = \mathbf{p}_\nu, \quad \mathbf{p}_3 = \mathbf{p}_\nu + \mathbf{p}_P = \mathbf{p}_\nu, \quad \mathbf{p}_4 = -\mathbf{p}_\ell, \quad (4.96)$$

Now we perform the summations to impose 3-momentum conservation and evaluate the overlap operators

$$Z_{n_1, n_2, n_4} \equiv \langle \bar{\ell}; s, -\mathbf{p}_\ell | \bar{\ell} | \Omega \rangle \Gamma_L^0 \langle \Omega | \nu | \nu; r, \mathbf{p}_\nu \rangle = Z'_{\ell\nu} \bar{u}^s(-\mathbf{p}_\ell) \Gamma_L^0 u^r(\mathbf{p}_\nu), \quad (4.97)$$

$$\mathcal{M}_{n_2, n_3} \equiv \langle \nu; r, \mathbf{p}_\nu | O_W | P\bar{\ell}; s, -\mathbf{p}_\ell \rangle = \bar{u}^r(\mathbf{p}_\nu) \mathcal{A}'_P u^s(-\mathbf{p}_\ell), \quad (4.98)$$

$$Z_{n_3, n_4}^\dagger \equiv \langle P\bar{\ell}; s, -\mathbf{p}_\ell | \phi_p^\dagger | \bar{\ell}; s, -\mathbf{p}_\ell \rangle = Z_{P\bar{\ell}}^\dagger. \quad (4.99)$$

Now, we have

$$\begin{aligned}
C_{P\ell\nu}^b(t_\nu, t_\ell, t_H, t_P) &= Z'_{\ell\nu} \Gamma_L^0 \frac{\sum_s u^s(-\mathbf{p}_\ell) \bar{u}^s(-\mathbf{p}_\ell)}{2E_\ell(-\mathbf{p}_\ell)} \frac{\sum_r u^r(\mathbf{p}_\nu) \bar{u}^r(\mathbf{p}_\nu)}{2E_\nu(\mathbf{p}_\nu)} \frac{\mathcal{M}'_P Z_{P\ell}^\dagger}{2E_{P\ell}} \\
&\times e^{-E_\ell(T-(t_\ell-t_P))} e^{-E_\nu(t_\nu-t_H)} e^{-E_{P\ell}(t_H-t_P)}.
\end{aligned} \tag{4.100}$$

Performing the spin-sum average, we find

$$\begin{aligned}
C_{P\ell\nu}^b(t_\nu, t_\ell, t_H, t_P) &= \frac{Z'_{\ell\nu} Z_{P\ell}^\dagger}{8E_\ell E_{P\ell} E_\nu} \text{Tr} \left[\gamma^0(-i\not{p}_\ell + m_\ell) \gamma^0 \Gamma_L^0(-i\not{p}_\nu) \mathcal{A}'_P \right] \\
&\times e^{-E_\ell(T-(t_\ell-t_P))} e^{-E_\nu(t_\nu-t_H)} e^{-E_{P\ell}(t_H-t_P)}.
\end{aligned} \tag{4.101}$$

Comparing Equations (4.93) and (4.101), we see that the backward propagating matrix element is a different contribution.

On the lattice, there are several differences: 1) since the neutrino is a spectator, we do not include an interpolator for the neutrino, 2) we shift the pseudoscalar interpolator to the origin and 3) the lepton sink t_ℓ is fixed at some distance relative to the weak Hamiltonian insertion time t_H , *i.e.* $\Delta t_\ell = \text{const.}$ That is, we consider

$$\begin{aligned}
\tilde{C}_{P\ell}(t_H, \Delta t_\ell)_{\sigma_1 \sigma_2} &= \sum_{\{\mathbf{x}\}} \sum_{n, \mathbf{p}} e^{-i\mathbf{p}_\nu \cdot \mathbf{x}_\nu} \langle n, \mathbf{p} | e^{-HT} \bar{\ell}_{\sigma_1}(\mathbf{x}_\ell, t_\ell) \tilde{O}_{W, \sigma_2}(\mathbf{x}_H, t_H) \phi_p^\dagger(0) | n, \mathbf{p} \rangle,
\end{aligned} \tag{4.102}$$

where the tilde denotes an amputation of the neutrino leg and $\sigma_{1,2}$ are the leftover spinor indices. A neutrino phase is also added by hand to ensure 3-momentum conservation is preserved. Removing the neutrino contribution in Equations (4.92) and (4.100), we have

$$\begin{aligned}
\tilde{C}_{P\ell}(t_H, \Delta t_\ell)_{\sigma_1 \sigma_2} &= \tilde{C}_{P\ell}^f(\Delta t_\ell, t_H)_{\sigma_1 \sigma_2} + \tilde{C}_{P\ell}^b(\Delta t_\ell, t_H)_{\sigma_1 \sigma_2} \\
&= \frac{[\mathcal{A}_P \sum_s v^s(\mathbf{p}_\ell) \bar{v}^s(\mathbf{p}_\ell)]_{\sigma_1 \sigma_2}}{2E_\ell(\mathbf{p}_\ell)} \frac{Z_\ell Z_P^\dagger}{2M_P} e^{-E_\ell(t_\ell-t_H)} e^{-M_P t_H} \\
&+ \frac{[\mathcal{A}'_P \sum_s u^s(-\mathbf{p}_\ell) \bar{u}^s(-\mathbf{p}_\ell)]_{\sigma_1 \sigma_2}}{2E_\ell(-\mathbf{p}_\ell)} \frac{Z'_\ell Z_{P\ell}^\dagger}{2E_{P\ell}} e^{-E_\ell(T-(\Delta t_\ell+t_H))} e^{-E_{P\ell} t_H},
\end{aligned} \tag{4.103}$$

where we have used $t_\ell = \Delta t_\ell + t_H$ to modify the time-dependence of the backward contribution. To recover the matrix elements in Equations (4.93) and (4.101), one

simply left multiply the above with Γ_L^0 and the neutrino spin-sum $(-i\not{p}_\nu)$, giving

$$C_{P\ell\nu}(t_H, \Delta t_\ell) = -i \text{Tr} \left[\Gamma_L^0 \not{p}_\nu \tilde{C}_{P\ell}(t_H, \Delta t_\ell) \right]. \quad (4.104)$$

Projectors

From Equation (4.103), we see that the signal for the matrix element we desire is contaminated by a different backward contribution. To that end, we construct a set of projectors $\mathcal{P}$ such that

$$\tilde{C}_{P\ell}(t_H, \Delta t_\ell)_{\sigma_1\sigma_2} \mathcal{P}_{v(\mathbf{p}_\ell)} = \tilde{C}_{P\ell}^f(t_H, \Delta t_\ell)_{\sigma_1\sigma_2}, \quad (4.105)$$

$$\tilde{C}_{P\ell}(t_H, \Delta t_\ell)_{\sigma_1\sigma_2} \mathcal{P}_{u(-\mathbf{p}_\ell)} = \tilde{C}_{P\ell}^b(t_H, \Delta t_\ell)_{\sigma_1\sigma_2}. \quad (4.106)$$

The form of these projectors can be deduced as

$$\mathcal{P}_{u(-\mathbf{p})} = \frac{1}{2E_\ell} \gamma^0 \sum_r [u^r(-\mathbf{p}_\ell) \bar{u}^r(-\mathbf{p}_\ell)] \quad \text{and} \quad (4.107)$$

$$\mathcal{P}_{v(\mathbf{p})} = -\frac{1}{2E_\ell} \gamma^0 \sum_r [v^r(\mathbf{p}_\ell) \bar{v}^r(\mathbf{p}_\ell)] \quad (4.108)$$

since

$$\begin{aligned} u^{r\dagger}(-\mathbf{p}_\ell) v^s(\mathbf{p}_\ell) &= v^{r\dagger}(\mathbf{p}_\ell) u^s(-\mathbf{p}_\ell) = 0, \\ u^{r\dagger}(-\mathbf{p}_\ell) u^s(-\mathbf{p}_\ell) &= v^{r\dagger}(\mathbf{p}_\ell) v^s(\mathbf{p}_\ell) = 2E_\ell \delta^{r,s} \end{aligned} \quad (4.109)$$

and the minus sign in Equation (4.108) comes from the Euclidean spin-sum average (see Equation (3.20)).

Thus, we can express the forward propagating piece with respect to the full correlator using this projector;

$$C_{P\ell\nu}^f(t_H, \Delta t_\ell) = \text{Tr} \left[\left(\tilde{C}_{P\ell}(t_H, \Delta t_\ell) \mathcal{P}_{v(\mathbf{p}_\ell)} \right) \Gamma_L^0 \not{p}_\nu \right]. \quad (4.110)$$

In Figures 5.8 and 5.12, we compare the effects of applying this projector to the lattice data.

Non-factorisable electromagnetic correction

The unique electromagnetic correction coming from this topology of correlator is when a photon couples to one of the quarks and the final state charged lepton. This generates an electromagnetic correction to the matrix amplitude $\mathcal{A}_P$ as seen in the above. Expanding about the simulation point, we have

$$\mathcal{A}_P = \hat{\mathcal{A}}_P + e_1 e_\ell \partial_{e_{1\ell}}^2 \mathcal{A}_P + e_2 e_\ell \partial_{e_{2\ell}}^2 \mathcal{A}_P + \mathcal{O}(e^4), \quad (4.111)$$

where e_j and e_ℓ are the j 'th quark and lepton electric charges, respectively, in units of positron. At leading order, $\hat{\mathcal{A}}_P = \langle \Omega | \phi_a | P, \mathbf{0} \rangle = \hat{M}_P \hat{f}_P / \mathcal{Z}_0$ is related to the decay constant. We can obtain the $\mathcal{O}(e^2)$ coefficients in the usual manner of considering a perturbative expansion of the QCD+QED time correlators. Working with the forward-projected correlators, we have

$$C_{P\ell\nu}^f(t_H, \Delta t_\ell) = C_{P\ell\nu,0}^f(t_H, \Delta t_\ell) + \sum_{j=1,2} e_j e_\ell \partial_{e_{j\ell}} C_{P\ell\nu}^f(t_H, \Delta t_\ell) + \mathcal{O}(e^4). \quad (4.112)$$

Matching Equations (4.111) and (4.112) order by order, we find

$$R_{P\ell\nu}^f(t_H, \Delta t_\ell) \equiv \sum_{j=1,2} e_j e_\ell \frac{\partial_{e_{j\ell}}^2 C_{P\ell\nu}^f(t_H, \Delta t_\ell)}{C_{P\ell\nu,0}^f(t_H, \Delta t_\ell)} = \sum_{j=1,2} e_{q_j} e_\ell \frac{\partial_{e_{j\ell}}^2 \mathcal{A}_P}{\hat{\mathcal{A}}_P}, \quad (4.113)$$

i.e. due to the projector, we expect to extract the electromagnetic correction from a plateau in the t_H and Δt_ℓ plane.

4.4.3 Omega Analysis

Although the primary hadrons studied in this thesis are the K and π mesons, we require the Ω^- baryon for scale setting (see 4.1.1) when we convert our lattice results to physical predictions. In the following, the vacuum state $|\Omega\rangle$ is not to be confused with the baryon Ω^- .

Tree

The Ω^- baryon is a spin- $\frac{3}{2}$ fermion. Let $\psi = \sum_{a,b,c} \epsilon_{abc} s_a^T C \gamma_\mu s_b s_c$ be a spin- $\frac{3}{2}$ interpolator and $\bar{\psi} = \psi^\dagger \gamma^0$ its conjugate. Here, s is the strange quark field; a, b, c are the color indices; $C = \gamma^0 \gamma^2$ is the charge conjugation operator and ϵ is the

Levi-Civita symbol. The omega baryon time correlator in full QCD+QED is

$$C_\Omega(\mathbf{k}, t, t_0) = \sum_{\mathbf{x}} \sum_{n, \mathbf{p}, s} \langle n, \mathbf{p}, s | e^{-HT} \psi(\mathbf{x}, t) \bar{\psi}(\mathbf{0}, t_0) | n, \mathbf{p}, s \rangle e^{-i\mathbf{k} \cdot \mathbf{x}}, \quad (4.114)$$

where we write explicitly the spin quantum number s . The procedure is similar to the pseudoscalar time correlator: insert a complete set of states, translate the operators and project to definite momentum. An additional feature of the spin- $\frac{3}{2}$ baryon is that the interpolators couple to both parity channels:

$$\begin{aligned} C_\Omega(t, t_0) \equiv C_\Omega(\mathbf{0}, t, t_0) = \sum_s \left[\frac{e^{-M_{\Omega^-}^+(t-t_0)}}{2M_{\Omega^-}^+} \langle \Omega | \psi | n^+, \mathbf{0}, s \rangle \langle n^+, \mathbf{0}, s | \bar{\psi} | \Omega \rangle \right. \\ + \frac{e^{-M_{\Omega^-}^-(t-t_0)}}{2M_{\Omega^-}^-} \langle \Omega | \psi | n^-, \mathbf{0}, s \rangle \langle n^-, \mathbf{0}, s | \bar{\psi} | \Omega \rangle \\ + \frac{e^{-M_{\Omega^-}^+(T-(t-t_0))}}{2M_{\Omega^-}^+} \langle n^+, \mathbf{0}, s | \psi | \Omega \rangle \langle \Omega | \bar{\psi} | n^+, \mathbf{0}, s \rangle \\ \left. + \frac{e^{-M_{\Omega^-}^-(T-(t-t_0))}}{2M_{\Omega^-}^-} \langle n^-, \mathbf{0}, s | \psi | \Omega \rangle \langle \Omega | \bar{\psi} | n^-, \mathbf{0}, s \rangle \right], \end{aligned} \quad (4.115)$$

where $M_{\Omega^\pm}^\pm$ are the lowest lying energy state with quantum numbers $n^\pm$ in the $\pm$ parity channel. Using the following definitions of the overlap factor

$$\langle \Omega | \psi | n^+, \mathbf{0}, s \rangle = Z^+ u_s(p^+), \quad (4.116)$$

$$\langle \Omega | \psi | n^-, \mathbf{0}, s \rangle = Z^- \gamma^5 u_s(p^-), \quad (4.117)$$

$$\langle \Omega | \bar{\psi} | n^+, \mathbf{0}, s \rangle = Z^+ \bar{v}_s(p^+), \quad (4.118)$$

$$\langle \Omega | \bar{\psi} | n^-, \mathbf{0}, s \rangle = Z^- \gamma^5 \bar{v}_s(p^-) \quad (4.119)$$

and with the Euclidean spin-sum average from Equations (3.19) and (3.20) and $\gamma^5 \not{p} \gamma^5 = -\not{p}$, we obtain

$$\begin{aligned} C_\Omega(t, t_0) = |Z^+|^2 P^+ e^{-M_{\Omega^-}^+(t-t_0)} + |Z^-|^2 P^- e^{-M_{\Omega^-}^-(t-t_0)} \\ + |Z^+|^2 P^- e^{-M_{\Omega^-}^+(T-(t-t_0))} + |Z^-|^2 P^+ e^{-M_{\Omega^-}^-(T-(t-t_0))}, \end{aligned} \quad (4.120)$$

where the projectors $P^\pm = \frac{1}{2}(1 \pm \gamma^0)$ appear in this final expression. Since we are only interested in the parity-positive channel, we use the fact that the projector is idempotent and orthonormal and define

$$C_\Omega^+(t, t_0) \equiv \text{Tr} [P^+ C_\Omega(t, t_0)] = |Z^+|^2 e^{-M_{\Omega^-}^+(t-t_0)} + |Z^-|^2 e^{-M_{\Omega^-}^-(T-(t-t_0))}, \quad (4.121)$$

where the trace acts on the parity operators. Similar to the non-factorisable study, we see now that the backward propagating state is not the one we want. Thus, we have to restrict to $0 \leq t_0 < t < \frac{T}{2}$. As before, shifting all source positions t_0 to zero, we have

$$C_{\Omega}^{+}(t) = |Z^{+}|^2 e^{-M_{\Omega}^{+} t}. \quad (4.122)$$

As before, we may expand each term in Equation (4.122) about the simulation point

$$\begin{aligned} C_{\Omega}^{+}(t) &= (c_{\Omega,0} + \delta_g c_{\Omega-}) (1 - \delta_g M_{\Omega-} t) e^{-\hat{M}_{\Omega} t}, \\ &= c_{\Omega,0} e^{-\hat{M}_{\Omega} t} \left(1 + \frac{\delta_g c_{\Omega-}}{c_{\Omega,0}} - \delta_g M_{\Omega-} t \right) + \mathcal{O}(g^2), \end{aligned} \quad (4.123)$$

where $c_{\Omega-}$ is the correlator overlap factor. Expanding LHS up to $\mathcal{O}(g^2)$, we can match the following

$$C_{\Omega,0}^{+}(t) = c_{\Omega,0} e^{-\hat{M}_{\Omega} t}, \quad (4.124)$$

$$\frac{\partial_g C_{\Omega}^{+}(t)}{C_{\Omega,0}^{+}(t)} = \frac{\partial_g c_{\Omega-}}{c_{\Omega,0}} - \partial_g M_{\Omega-} t \quad (4.125)$$

for an expansion parameter g . More specifically, the QED correlator ratio is

$$R_{\Omega, e_{22}}(t) \equiv Z_V^2 \frac{1}{9} \cdot \frac{\partial_{e_{22}}^2 C_{\Omega}(t)}{C_{\Omega,0}(t)} = \frac{\partial_{e_{22}}^2 c_{\Omega-}}{c_{\Omega,0}} - \partial_{e_{22}}^2 M_{\Omega-} t \quad (4.126)$$

and the strange quark scalar insertion correlator ratio is

$$R_{\Omega, m_s}(t) \equiv \frac{\partial_{m_s} C_{\Omega}(t)}{C_{\Omega,0}(t)} = \frac{\partial_{m_s} c_{\Omega-}}{c_{\Omega,0}} - \partial_{m_s} M_{\Omega-} t, \quad (4.127)$$

i.e. for $0 < t \ll \frac{T}{2}$, the mass correction can be obtained from the gradient of a linear fit.

4.5 Strategy for Lattice Data Analysis

The isospin-breaking correction to the ratio of inclusive rates as defined in Equation (4.35) is built from the result of multiple correlator fit analyses. In this section, the strategy for extracting the relevant quantities from lattice time

correlators is discussed. Due to the various classes of correlators involved in this calculation, we adopt a data-driven approach to standardise the fitting criteria, which we explain below.

For a given analysis, if multiple time correlators share one or more common parameters, these correlators are fitted simultaneously. Let the number of time correlators to be fitted simultaneously be N_{corr} . Further, let $\tau_k^j = [t_{min}^{(j)}, t_{max}^{(j)}]$ be the k 'th candidate fit interval on the j 'th time correlator, bounded by $t_{min}^{(j)} \leq t \leq t_{max}^{(j)}$. In an analysis where $N_{corr} = 1$, the j index is dropped. For $N_{corr} > 1$, let $\boldsymbol{\tau}_k = (\tau_k^1, \dots, \tau_k^{N_{corr}})$ denote the full set of fit intervals in a fit. To determine the optimum τ (or $\boldsymbol{\tau}$) that best fits the data - and hence the best fit parameters for determining $\delta R_{K\pi}$ - let $F^{(n)}(\boldsymbol{\tau})$ be the result of the n 'th model parameter for a given $\boldsymbol{\tau}$, with $n = 1, \dots, N_{par}$, where N_{par} is the number of parameters in a fit model and let N_{fit} be the number of t_{min}/t_{max} combinations in τ (or $\boldsymbol{\tau}$). Then, our data-driven approach is as follows:

1. fit the data N_{fit} times using the functional forms derived in previous section to obtain a range of fit interval candidates $\boldsymbol{\tau}_k$, where $k = 1, \dots, N_{fit}$.
2. Associate each $\boldsymbol{\tau}_k$ with a weight w_k .
3. Rank each $\boldsymbol{\tau}_k$ by w_k .
4. Select the $\boldsymbol{\tau}_k$ associated with the optimum weight and use $F^{(n)}(\boldsymbol{\tau}_k)$ to determine $\delta R_{K\pi}$.

Before proceeding further, some comments are in order. First, the N_{fit} associated with each analysis varies. In general, for an analysis involving N_{corr} correlators, one has

$$N_{fit} = \prod_{j=1}^{N_{corr}} \sum_{\Delta t^{(j)}=1}^{\frac{T}{2}} \Delta t^{(j)} = \left(\frac{(T/2)(T/2+1)}{2} \right)^{N_{corr}}, \quad (4.128)$$

where $\Delta t^{(j)} = t_{max}^{(j)} - t_{min}^{(j)}$. In the above, the summation is bounded by half the lattice temporal extent $T/2$ because the correlators are either folded, *i.e.*

$$C(t) = \frac{1}{2}(C(t) + sC((T-t) \bmod T)), \quad (4.129)$$

where $s = \pm 1$ depending on the periodicity of the correlator, or the information is irrelevant to our calculation at $t > T/2$. Depending on the size of N_{fit} , different strategies are employed to obtain a large sample of τ in Step 1. Let a *fit scan* refer to some iterative procedure where one obtains a range of τ and the weights w associated to them. The specifics of the fit scan procedure will be discussed in the following subsections.

Second, a well-defined weight should be used in Step 2 of this procedure. Classic candidates include the chi-squared test χ^2 or the p -value. However, for large N_{corr} , one runs the risk of obtaining a large multiplicity of τ with ‘good’ p -values, some that sample only a limited region of the statistical information available¹. Instead, for this project, we choose to use the Akaike Information Criterion [47], or AIC for short. This criterion has appeared in recent lattice calculations as a means to assess model selection (*e.g.* see BMW [30, 33]). It is defined as

$$\exp \left[-\frac{1}{2} (\chi^2 + 2N_{\text{par}}) \right]. \quad (4.130)$$

This weight function rewards low χ^2 but penalises overfitting (large N_{par}). However, in an analysis where the fit functions are known, this may also be used for data subset selection, as shown by Jay and Neil [48]. Let the total number of data points in a correlator be $N = N_{inc.} + N_{exc.}$, where $N_{inc./exc.}$ are the data points one include/exclude in a given fit interval τ . The exponent of the AIC weight is modified to be

$$\exp \left[-\frac{1}{2} (\chi^2 + 2N_{\text{par}} + 2N_{exc.}) \right]. \quad (4.131)$$

This was first given in [30] and modified from $2N_{exc} \rightarrow N_{exc}$ in [33]. Similar to Equation (4.130), this function punishes a choice τ that is limited to a small region, *i.e.* large $N_{exc.}$. With $N_{inc.} = N_{\text{par}} + N_{\text{dof}}$, Equation (4.131) can be re-

¹We find that this is the case in practice for the factorisable analyses.

parametrised as

$$\begin{aligned}
& \exp \left[-\frac{1}{2} (\chi^2 + 2N_{\text{par}} + 2(N - N_{\text{inc}})) \right] \\
& = \exp \left[-\frac{1}{2} (\chi^2 - 2N_{\text{dof}} + 2N) \right], \\
& \Rightarrow w = \exp \left[-\frac{1}{2} (\chi^2 - 2N_{\text{dof}}) \right],
\end{aligned} \tag{4.132}$$

where N is dropped in the definition of w in the last line. N is a constant in all correlators and thus contributes as a multiplicative constant to w . With this definition, Step 3 and 4 in the strategy involves finding the maximum weight, *i.e.* when χ^2 is minimised with the largest N_{dof} possible.

Below, we divide the discussion about the choice of fit scan procedures into two classes. In Case 1, we will examine the fit scan procedure for analyses that have manageable N_{fit} . In Case 2, we will introduce a method to approach analyses with prohibitively large N_{fit} .

4.5.1 Case 1: Small N_{fit}

In analyses where N_{fit} is small, we can afford to determine all possible $F^{(n)}(\tau)$ on a personal laptop or remote machine. We will call this method the *brute force scan* in later discussions.

4.5.2 Case 2: Large N_{fit}

For analyses where N_{fit} is so large that it is not feasible to evaluate all τ , we employ the *genetic algorithm* (GA). Introduced by John Holland [49] in the 1960s, this iterative search algorithm is inspired by biological evolution. A typical GA cycle has 5 stages as presented below:

1. **Initialisation** : initialise with population size $P_0 > 1$ of chromosomes
2. **Crossover** : offspring chromosomes produced from parent chromosomes
3. **Mutation** : population chromosomes may be subjected to random variations

4. **Fitness selection** : the fitness of entire population is evaluated and ranked
5. **Re-initialisation/termination**: GA cycle repeats/terminates based on termination condition

The aim of the GA is to move one population of ‘chromosomes’ to a new and fitter population by means of natural selection via genetics-inspired operators called *crossover* and *mutation* [50]. The crossover combines the ‘genes’² between two chromosomes to promote genetic diversity in a population; mutation introduces a stochastic element, in which a mutated chromosome may gain a competitive edge against the crossover population during the fitness selection phase. Lastly, the fitness criteria is a user-defined metric that determines whether the algorithm enters another ‘generation’ or terminates.

In the context of this analysis, the fit intervals $\tau^{(j)}$ are the genes and the vector $\boldsymbol{\tau}$ is the chromosome. Our fitness metric-of-choice is the AIC weight and our termination condition is when the average of the top 5 AIC weights remain unchanged for 1000 generation. This choice is arbitrary. We sought for a ‘sweet spot’, where the algorithm does not terminate prematurely, nor does it take an unreasonable duration, rendering repetitions impossible. The modified recipe is:

1. In each generation, begin with an initial population of $\boldsymbol{\tau}_k, k = 1, \dots, P_0$
2. Evolve $\boldsymbol{\tau}_k, \forall k$ with genetic operators to produce $N_{\text{offspr.}}$ number of offspring.
3. Fit all $\boldsymbol{\tau}_{k'}, k' = 1, \dots, P_0 + N_{\text{offspr.}}$.
4. Choose top P_0 $\boldsymbol{\tau}_k$ with largest AIC weights for next generation.
5. Repeat Step 2-4 until termination condition is satisfied.

Details of the GA runs are discussed in Appendix C. Here, we remark that the GA not only finds the fittest $\boldsymbol{\tau}$ from an initial population pool, the mutation feature introduces, with a small but non-zero probability, completely new variation on $\boldsymbol{\tau}$. These features make the GA an efficient way of exploring the $\boldsymbol{\tau}$ -space without getting immediately stuck in a ‘local minimum’³.

²For the purpose of this illustration, it is sufficient to think of genes as constituents of the chromosome.

³The concept of a ‘minimum’ is, at best, illustrative since the $\boldsymbol{\tau}$ is a discretised space of integers.

4.6 Corrections to Virtual Contribution in Finite Volume

The virtual corrections contain photons that are able to probe the internal structure of the initial hadron. As such, they must be evaluated in lattice simulations in a finite-sized box. Due to the infinite range of the electromagnetic interaction, these will come with power-law finite volume effects. The two ways to remove these FVE are 1) by numerically fitting to simulation results obtained from multiple volumes or 2) by studying analytically the volume-scaling and subtracting these effects from the simulation result. Given that the work in [44] is also done with the QED_L formalism, we opt for the latter approach. In Equation (4.20), that which removes FVE's from the lattice result may be expressed in terms of the tree-level rate and a dimensionless function $Y^{(n)}(L)$

$$\Gamma_0^{(n)}(L) = \Gamma^{\text{tree}} \left[1 + \frac{\alpha}{4\pi} Y^{(n)}(L) \right] + \mathcal{O} \left(\frac{1}{L^{n+1}} \right). \quad (4.133)$$

In this form, $\Gamma_0^{(n)}(L)$ is a truncated series expansion in inverse powers of L , the lattice spatial extent. The dimensionless function may be further decomposed into the infinite and finite volume piece using a fictitious photon mass λ as an IR regulator [44],

$$Y^{(n)}(L) = Y^{\text{IV}}(\lambda) + Y_{\log} \log \frac{L\lambda}{2\pi} + Y_0 + \sum_{j=1}^n \frac{M_\pi^j}{(M_\pi L)^j} Y_j \quad (4.134)$$

where, up to $n = 2$,

$$Y^{\text{IV}}(\lambda) = -\frac{5}{4} + 2 \log \frac{m_\ell^2}{m_W^2} + \log \frac{m_W^2}{\lambda^2} - A_1(\mathbf{v}_\ell) \left[\log \frac{m_\ell^2}{\lambda^2} + \log \frac{M_P^2}{\lambda^2} - 2 \right], \quad (4.135)$$

$$Y_{\log} = 2(1 - 2A_1(\mathbf{v}_\ell)), \quad (4.136)$$

$$Y_0 = \frac{c_3 - 2(c_3(\mathbf{v}_\ell) - B_1(\mathbf{v}_\ell))}{2\pi} + 2(1 - \log 2), \quad (4.137)$$

$$Y_1 = -\frac{(1 + r_\ell^2)^2 c_2 - 4r_\ell^2 c_2(\mathbf{v}_\ell)}{M_P(1 - r_\ell^4)}, \quad (4.138)$$

$$Y_2 = -\frac{F_A^P}{f_P} \frac{4\pi [(1 + r_\ell^2)^2 c_1 - 4r_\ell^2 c_1(\mathbf{v}_\ell)]}{M_P(1 - r_\ell^4)} + \frac{8\pi [(1 + r_\ell^2) c_1 - 2c_1(\mathbf{v}_\ell)]}{M_P^2(1 - r_\ell^4)}, \quad (4.139)$$

where $r_\ell = m_\ell/M_P$, F_A^P is the axial form factor, c_j and $c_j(\mathbf{v}_\ell)$ are the finite volume coefficients for $j = 1, 2, 3$ and

$$|\mathbf{v}_\ell| = \frac{1 - r_\ell^2}{1 + r_\ell^2}, \quad (4.140)$$

$$A_1(\mathbf{v}_\ell) = -\frac{1}{2} \frac{1 + r_\ell^2}{1 - r_\ell^2} \log r_\ell^2, \quad (4.141)$$

$$B_1(\mathbf{v}_\ell) = \frac{\pi}{|\mathbf{v}_\ell|} \left[\text{Li}_2 \frac{2|\mathbf{v}_\ell|}{|\mathbf{v}_\ell| - 1} - \text{Li}_2 \frac{2\mathbf{v}_\ell}{|\mathbf{v}_\ell| + 1} + 4\mathbf{v}_\ell A_1(\mathbf{v}_\ell) \log 2 \right]. \quad (4.142)$$

Given these definitions, we see that the $\mathcal{O}(\log \lambda)$ terms of Equation (4.134) cancel and $Y^{(n)}(L)$ depends only on L . Additionally, the appearance of the structure-dependent F_A^P at $n = 2$ indicates that $Y^{(1)}(L)$ is a universal contribution that matches exactly the result in [42]. As such, $Y^{(n)}(L)$ for $n > 1$ is a generalisation of the work accomplished in [42, 43]. When we substitute Equations (4.135)-(4.139) into Equation (4.134), we find that, for $n = 2$,

$$\begin{aligned} Y_P^{(2)}(L) = & \frac{3}{4} + 4 \log \left(\frac{m_\ell}{m_W} \right) + 2 \log \left(\frac{m_W L}{4\pi} \right) + \frac{c_3 - 2(c_3(\mathbf{v}_\ell) - B_1(\mathbf{v}_\ell))}{2\pi} \\ & - 2A_1(\mathbf{v}_\ell) \left[\log \frac{M_P L}{2\pi} + \log \frac{m_\ell L}{4\pi} - 1 \right] - \frac{1}{M_P L} \left[\frac{(1 + r_\ell^2)^2 c_2 - 4r_\ell^2 c_2(\mathbf{v}_\ell)}{1 - r_\ell^4} \right] \\ & + \frac{1}{(M_P L)^2} \left[-\frac{F_A^P}{f_P} \frac{4\pi M_P [(1 + r_\ell)^2 c_1 - 4r_\ell^2 c_1(\mathbf{v}_\ell)]}{1 - r_\ell^4} \right. \\ & \quad \left. + \frac{8\pi [(1 + r_\ell^2) c_1 - 2c_1(\mathbf{v}_\ell)]}{(1 - r_\ell^4)} \right]. \end{aligned} \quad (4.143)$$

This expression will be needed in the next chapter when we remove the FVEs from our lattice calculation.

4.7 Contribution from Real Photon Emission

To keep the electromagnetic corrections to the matrix element IR-finite, we must include the contribution from a real photon, $P^+ \rightarrow \ell^+ \nu \gamma$. The strategy outlined in Equation (4.20) contains the term

$$\Gamma_{1,P}^{\text{pt}}(\Delta E_\gamma) = \lim_{\lambda \rightarrow 0} (\Gamma_0^{\text{uni}}(\lambda) + \Gamma_1(\lambda, \Delta E_\gamma)), \quad (4.144)$$

where we remind the reader here that λ is the fictitious photon mass acting as an IR regulator. The Feynman diagrams associated to the pseudoscalar-lepton vertex correction are shown in Figure 4.3(a)-(c). These contribute to Γ_0^{uni} . The contribution from real photon emission diagrams are shown in Figure 4.3(d)-(f). They contribute to Γ_1 instead. Up to the D_s meson, the final state photon is sufficiently soft such that it cannot resolve the internal hadronic structure. Thus, we can treat the initial pseudoscalar in the point-like approximation and calculate these contributions with perturbation theory in QED [38].

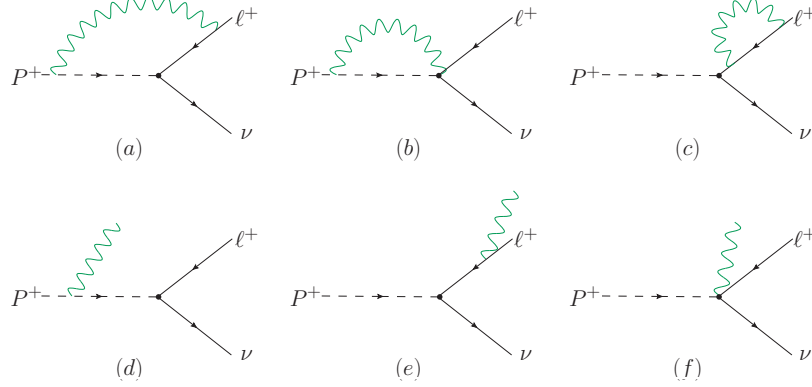


Figure 4.3 *The Feynman diagrams associated to the $\mathcal{O}(e^2)$ contributions in $\Gamma_{1,P}^{\text{pt}}$. Here, the P^+ meson is represented by a single scalar line since it is treated in the point-like approximation in this calculation.*

If we separate the $\mathcal{O}(e^2)$ contribution as

$$\Gamma_{1,P}^{\text{pt}}(\Delta E_\gamma) = \Gamma^{\text{tree}} \left(1 + \frac{\alpha}{4\pi} \delta\Gamma_{1,P}^{\text{pt}}(\Delta E_\gamma) \right), \quad (4.145)$$

then the contribution to $\delta R_{K\pi}$ is [38]

$$\begin{aligned} \delta\Gamma_{1,P}^{\text{pt}}(\Delta E_\gamma) = & 3 \log \left(\frac{M_P^2}{m_W^2} \right) - 8 \log(1 - r_\ell^2) - \frac{3r_\ell^4}{(1 - r_\ell^2)^2} \log r_\ell^2 \\ & - 8 \frac{1 + r_\ell^2}{1 - r_\ell^2} \text{Li}_2(1 - r_\ell^2) + \frac{13 - 19r_\ell^2}{2(1 - r_\ell^2)}, \\ & + \frac{6 - 14r_\ell^2 - 4(1 - r_\ell^2) \log(1 - r_\ell^2)}{1 - r_\ell^2} \log r_\ell^2, \end{aligned} \quad (4.146)$$

where

$$\text{Li}_2(z) = \int_z^0 dt \frac{1}{t} \log(1 - t) \quad (4.147)$$

is the dilogarithm. When we apply Equation (4.146) to Equation (4.20), we see that the term involving the weak boson will cancel exactly in the difference

between each meson's contribution.

Chapter 5

Results

The assembly of $\delta R_{K\pi}$ proceeds in four stages:

1. extraction of the virtual IB corrections from a range of time correlators generated from lattice simulations,
2. tuning of simulation results to the appropriate isospin-symmetric theory via a chosen scheme,
3. removal of finite volume effects (FVE's) and
4. combination with $\mathcal{O}(e^2)$ radiative correction.

In the preceding chapter, we explored the choices of fit scan procedure based on the size of N_{fit} . Now, for our ensemble which we detail in §5.1, we apply these fit scans to our lattice data and present the result of each fit analysis. These simulation observables are then tuned to the isospin-symmetric point based on the plan laid out in §5.5.1. In the process, we also compute the corrections to Dashen's theorem and the quark mass ratio as a validity check of our isospin-symmetric point. Finally, we combine our tuned observables with the analytic results to determine $\delta R_{K\pi}$. The impact of our theoretical prediction of $\delta R_{K\pi}$ on $\frac{|V_{us}|}{|V_{ud}|}$ is relegated to the last section.

5.1 Setup

For this calculation, we generate correlators in a $48^3 \times 96$ lattice using near-physical Möbius Domain Wall Fermions. The Domain wall mass is $M_5 = 1.8$ and the length of the fifth dimension is $L_s = 24$. See [51] for more details. The QCD gauge configurations are generated by the RBC/UKQCD collaboration using the Iwasaki gauge action [52]. The sea quark masses are $am_l^{sea} = 0.00078$, $am_s^{sea} = 0.0362$, where a is the lattice spacing. We choose the valence up- and down-quark masses to have the same value as the sea $am_u = am_d = am_l^{sea}$ and similarly for the valence strange quarks $am_s = am_s^{sea}$. In this setup, the lattice spacing has been determined (without QED) to be $a^{-1} = 1.7295(38)\text{GeV}$ [51]. The simulated pion mass of this ensemble is $\hat{M}_\pi = 139.15(36)\text{ MeV}$.

For the interpolators, we use Coulomb gauge-fixed wall sources. As such, we will need to generate correlators with both wall and point sinks in order to extract the axial matrix element. To facilitate with the computational demands of inverting the Dirac operator for near-physical light quarks, we employ ZMöbius fermions (see [53] and references therein) together with the deflation eigenvectors generated by the RBC/UKQCD collaboration for this $48^3 \times 96$ ensemble. Light quark propagators can then be obtained with a smaller L_s , thereby reducing the simulation cost. This rational approximation of the Möbius DWF action must be corrected for, and we discuss this below and in detail in Appendix B. We share propagators between the pion and kaon in order to reduce the calculation and I/O storage demands of these deflation eigenvectors. On the other hand, since the lepton does not participate in strong interactions, its propagator is generated using a free DWF action, where its input mass is chosen such that the pole mass reproduces the experimentally-measured value. The lepton propagators are also given twist angles to ensure that 3-momentum is conserved in lattice simulations [54]. We also note that, in this calculation, disconnected QCD contributions are neglected.

The implementation of QED in our lattice simulation is as follows: we remove the photon's spatial zero mode with the QED_L formalism [31]. At the time of this work, we do not have a conserved E.M. current implemented for Domain Wall fermions. Instead, we sequentially insert a local E.M. current in Feynman gauge to obtain a sequential propagator with an $\mathcal{A}$ insertion. The correlators built from these propagators are renormalised by a factor of $Z_V = 0.71081$ [55] for each insertion. On a smaller lattice volume, we compared observables that

are sensitive to the E.M. current implementation and found that the difference between them are comparable with $\mathcal{O}(a^2)$ discretisation effects (see Appendix D). In this work, we have also used the electro-quenched approximation of QED, *i.e.* treating the sea quarks as electrically-neutral.

The correlation functions used in this calculation are generated from a set of 60 QCD configurations, which are then resampled with the bootstrap method (see Appendix A). To improve the statistics of the factorisable correlators, we insert the source interpolator on each timeslice (96 in total for this ensemble) for each QCD configuration. Using translation invariance, these sources are shifted back to the origin and averaged. Similarly, for the omega correlators, we insert the source interpolator on every other timeslice. We find that the precision is comparable with the factorisable correlators in spite of the $2\times$ difference in statistics. As for the non-factorisable correlators, we generate 8 different lepton source-sink separations, $\Delta t_\ell = 12, 16, \dots, 40$. Analogous to the factorisable case, we average over all 96 source positions for each QCD configuration to boost our statistics for each Δt_ℓ correlator. These additional source positions are binned such that we have 60 measurements for each analysis.

ZMöbius-to-Möbius Correction

The ZMöbius formulation for the DWF action allows us to compute light quark propagators with a smaller L_s and is therefore cheaper than a direct calculation of light propagators using the Möbius formalism. This is thanks to the availability of eigenvectors for deflation mentioned previously. However, we must now comment on the potential issue concerning unitarity, arising from hadronic correlators where the valence and sea light quarks are generated with different actions. To that end, we propose a correction to the ZMöbius data, analogous to the all-mode averaging (AMA) method first proposed in [56]. Let $O[S_A^l(t_{\text{src}})]$ be an observable computed with a light quark propagator S_A^l whose source is inserted at t_{src} , generated from a particular lattice-regularised action A . Then, analogous to the AMA strategy, we identify the ZMöbius observable $O[S_{ZM}^l]$ to be the approximation of our target observable $O[S_M^l]$. We can obtain a ‘corrected’ expectation value of O with the following correction

$$\langle O \rangle_M = \langle O \rangle_{ZM} + \langle \tilde{O} \rangle_M - \langle \tilde{O} \rangle_{ZM} \quad (5.1)$$

where, on the RHS,

$$\begin{aligned}\langle O \rangle_{ZM} &= \frac{1}{N_{cfg}} \sum_i \frac{1}{T} \sum_{t_{src}=0}^{T-1} O_i[S_{ZM}^l(t_{src})], \\ \langle \tilde{O} \rangle_{(Z)M} &= \frac{1}{N_{cfg}} \sum_i \frac{1}{2} (O_i[S_{(Z)M}^l(0)] + O_i[S_{(Z)M}^l(T/2)]),\end{aligned}\tag{5.2}$$

and N_{cfg} is the number of QCD gauge configurations. In our study, $N_{cfg} = 60$ and $\langle \tilde{O} \rangle_{(Z)M}$ is generated with $O[S_{(Z)M}^l]$ on two source positions: $t_{src} = 0, T/2$. In Figure 5.1, we compare the signal magnitude of the Möbius correction to the statistical precision on the pure ZMöbius wall-point pp data.

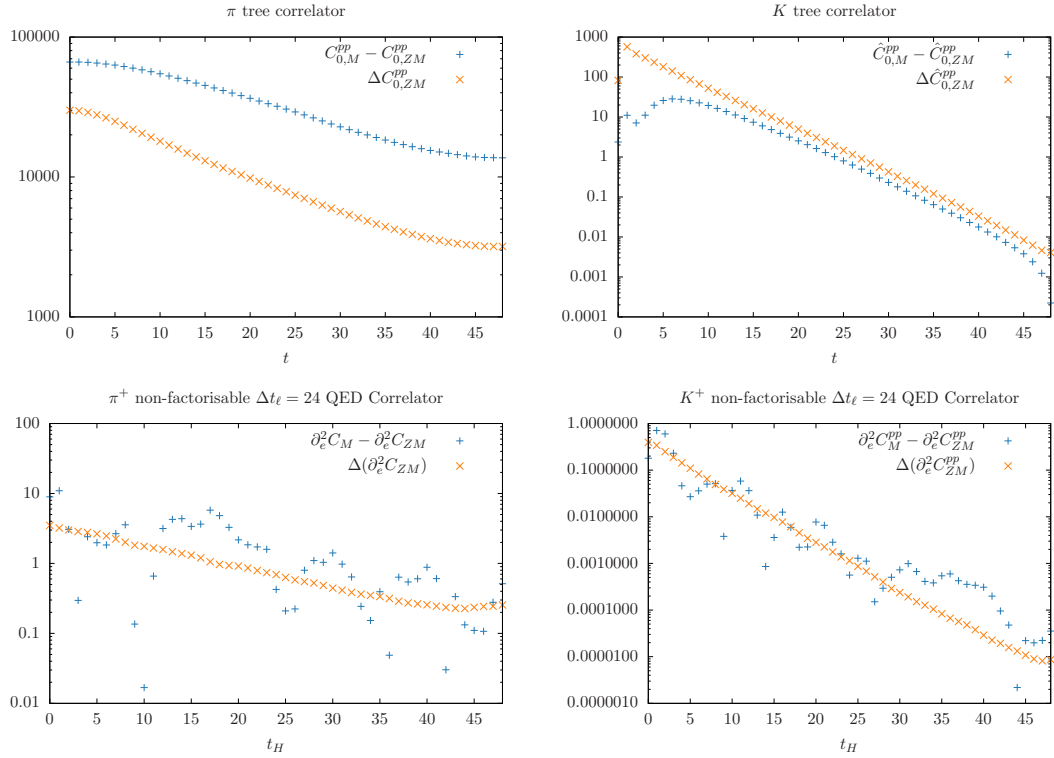


Figure 5.1 Comparison of the Möbius correction central value (blue) to the statistical error of the ZMöbius correlators (orange) for the π and K meson. Both sets are wall-pt pp correlators.

There are notable hierarchies in both meson correlators. In the pion case, the Möbius correction signal for the 2-point correlator is distinguishable from statistical precision, illustrated by the fact that the blue data points are always larger in magnitude than the orange. This hierarchy is exactly inverted in the case of kaons, where we see that the Möbius correction is, at best, comparable with statistical precision. Apart from the exception in the non-factorisable QED

correlator, where the Möbius signal is comparable with the statistical precision, this hierarchy is what we should expect. The pion is built with two light quark propagators generated by the ZMöbius action and thus receives a relatively larger correction than the kaon, where only one of its quark propagator is generated with the ZMöbius action. In both pion and kaon cases, the correlators of the other factorisable diagrams exhibit the respective hierarchy. These, along other comparisons, are shown in Appendix B.

5.2 Omega Analysis

When we consider Equations (4.124), (4.126) and (4.127), there are no common fit parameters between each correlators. Hence, there are three independent analyses to extract the QCD-only mass, the electromagnetic and strong isospin-breaking mass correction. These consist of finding a 1-dimensional fit interval τ that maximises the AIC weight. For a lattice of temporal extent $T = 96$, we would naively expect

$$N_{fit} = \frac{48(48 + 1)}{2} = 1172. \quad (5.3)$$

However, due to the Signal-to-Noise Ratio (StNR) problem that is intrinsic to baryon correlators[57, 58], the number of meaningful fits to consider is actually lower since we do not allow t_{max} to approach the middle of the lattice. Thus, we are in the ‘small N_{fit} ’ case and the brute force scan is applied.

The top result from the brute force scan is shown in Figures 5.2, 5.4 and 5.6 for the tree-level correlator, the QED and m_s scalar insertion correlator ratio, respectively. For the tree-level correlator, we present the effective mass plot using Equation (3.24). To ensure that the fit intervals are safe from excited states and backward propagating contribution, we perturb the boundaries of a chosen τ , $\tau' = [t_{min} \pm s, t_{max} \pm s]$ up to some small integer s , and compute the correlated difference of the fit result $F^{(n)}(\tau) - F^{(n)}(\tau')$. The chosen fit interval τ is in a stable region if the correlated difference is consistent with zero within the statistical error. Figures 5.3, 5.5 and 5.7 show the evolution of fit parameters with respect to t_{min} and t_{max} . As we approach the choice t_{min}/t_{max} from below/above, we see that the correlated difference begins to plateau at the zero line.

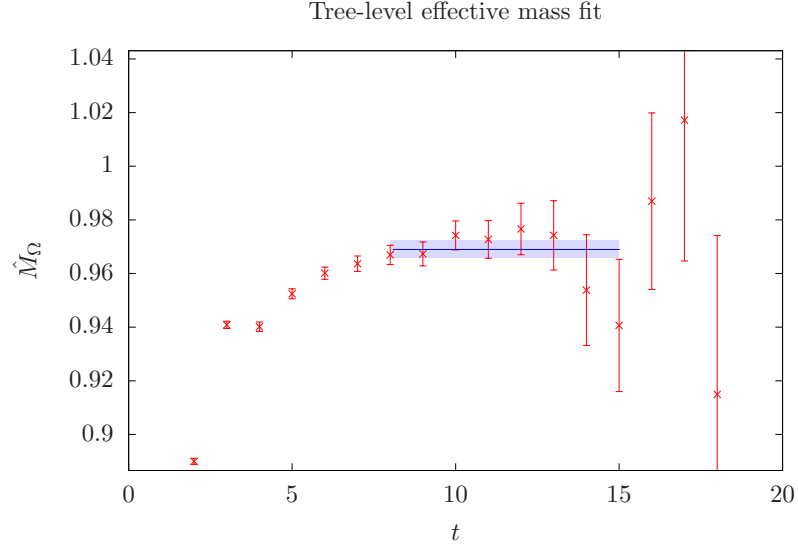


Figure 5.2 *The effective mass plot of Ω^- baryon obtained by applying Equation (3.24) to the QCD-only time correlator. The navy blue line is the fit curve and the blue band is the error.*

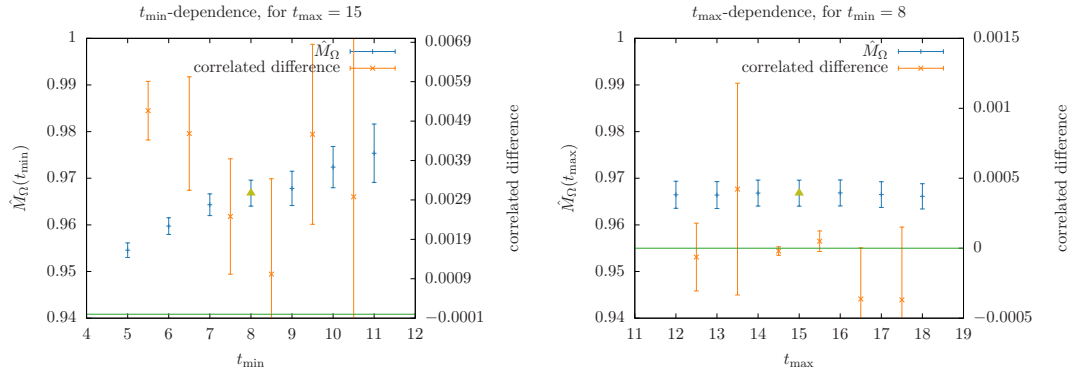


Figure 5.3 *The left y-axis is the Ω^- baryon mass (blue) as a function of $t_{\min}$ (left) and $t_{\max}$ (right). The right y-axis is the correlated difference between neighbouring $t_{\min}$ (left)/ $t_{\max}$ (right) values (orange). The green line indicates zero on the correlated difference. The olive triangle indicates the $t_{\min}/t_{\max}$ of choice.*

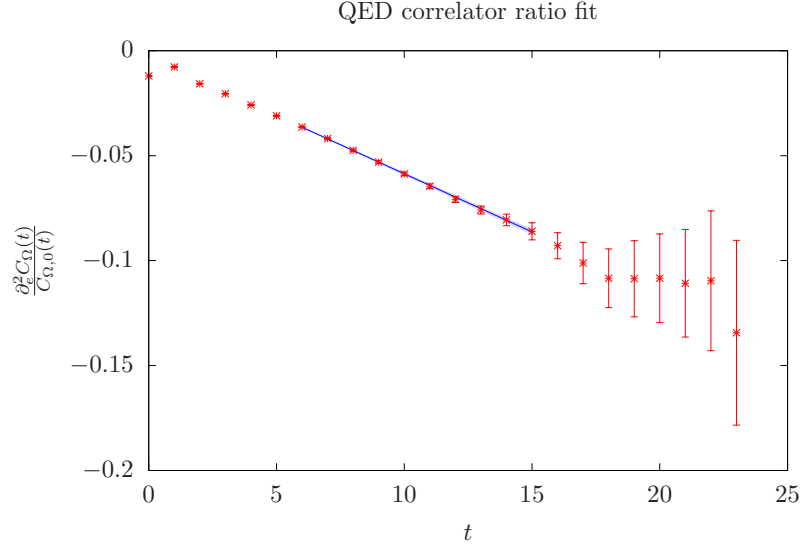


Figure 5.4 *A linear fit to the QED ratio of the Ω^- baryon. The blue line is the fit and the gradient of this line is the (negative of the) electromagnetic correction to the Ω^- .*

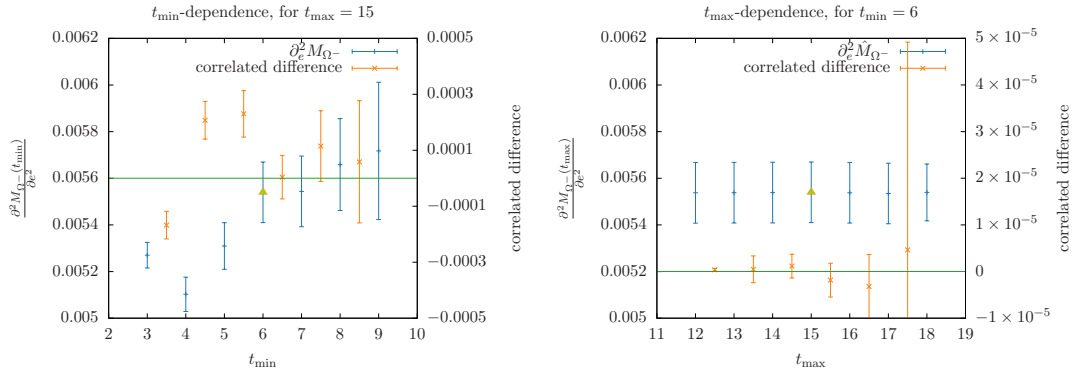


Figure 5.5 *The left y-axis is the Ω^- baryon mass derivative w.r.t e (blue) as a function of t_{min} (**left**) and t_{max} (**right**). The right y-axis is the correlated difference between neighbouring t_{min} (**left**)/ t_{max} (**right**) values (orange). The green line indicates zero on the correlated difference. The olive triangle indicates the t_{min}/t_{max} of choice.*

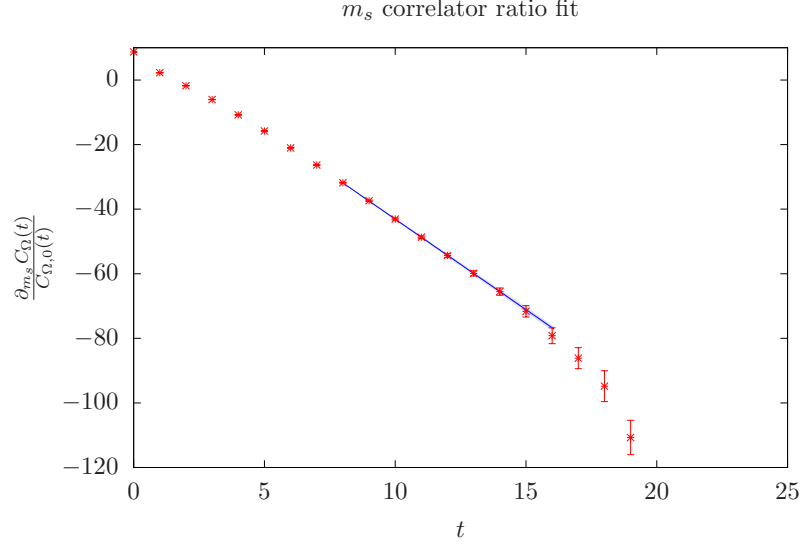


Figure 5.6 A linear fit to the m_s ratio of the Ω^- baryon. The blue line is the fit and the gradient of this line is the (negative of the) Ω^- mass correction due to m_s scalar insertion.

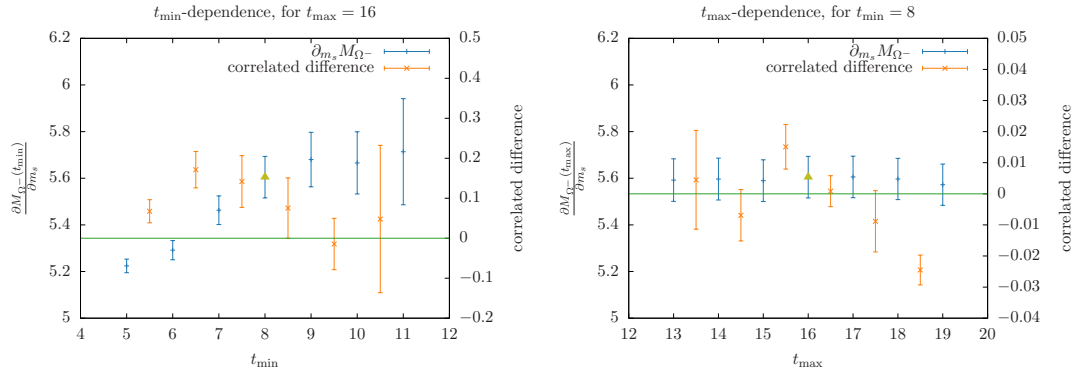


Figure 5.7 The left y-axis is the Ω^- baryon mass derivative w.r.t m_s (blue) as a function of t_{min} (left) and t_{max} (right). The right y-axis is the correlated difference between neighbouring t_{min} (left)/ t_{max} (right) values (orange). The green line indicates zero on the correlated difference. The olive triangle indicates the t_{min}/t_{max} of choice.

5.3 Non-Factorisable Analysis

In §4.4.2, we introduced the spinor projectors as a means to remove unwanted backward contribution. The relevant projector was presented in Equation (4.108),

which we recast here for convenience:

$$\mathcal{P}_{v(\mathbf{p})} = -\frac{1}{2E_\ell} \gamma^0 \sum_r [v^r(\mathbf{p}_\ell) \bar{v}^r(\mathbf{p}_\ell)].$$

Note that this projector is constructed with continuum dispersion relation, *i.e.* $E_\ell = \sqrt{m_\ell^2 + |\mathbf{p}_\ell|^2}$. In principle, one should construct a project using the discretised, action-specific dispersion relation, but a numerical comparison between projectors implemented with the continuum and lattice dispersion relations indicate the difference between the two in this near-physical setup is $\mathcal{O}(10^{-5})$ [1]. Thus, in this analysis, we apply the above projector to our lattice data.

In Figures 5.8 and 5.9, we present the effects of using the projector defined in Equation (4.108) on the π^+ and K^+ non-factorisable correlator ratio, respectively. In the left panels, we see that the correlator ratios suffer from Δt_ℓ -dependent backward propagating effects (see Equations (4.101) and (4.103)). Once the projector is applied, the plateaux converge for all Δt_ℓ , which is an encouraging sign that the dominant backward propagating effects are removed.

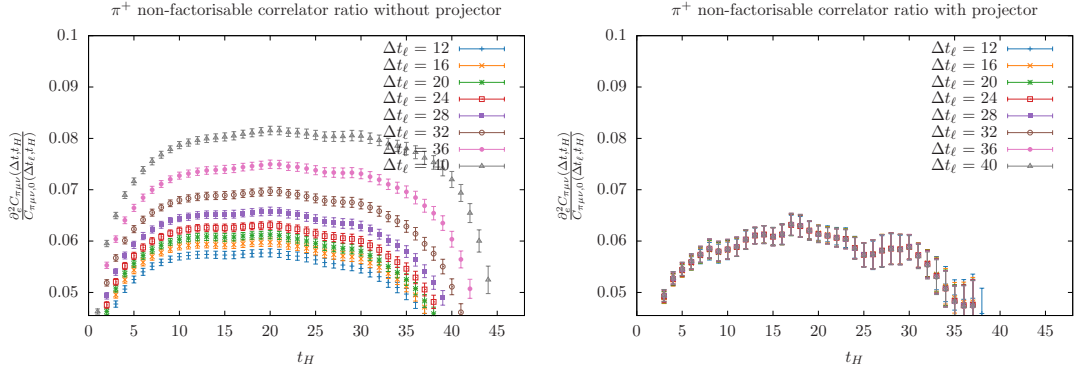


Figure 5.8 Comparison of π^+ non-factorisable ratio without (*left*) and with (*right*) spinor projection for all lepton source-sink separation, Δt_ℓ .

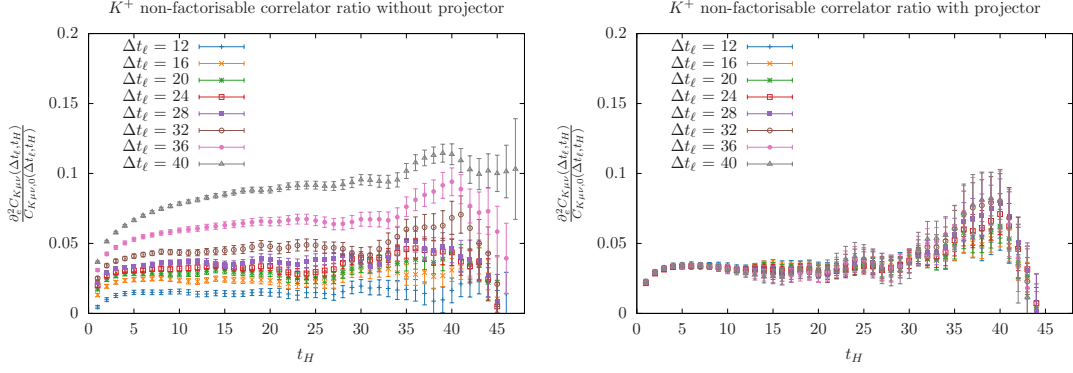


Figure 5.9 Comparison of K^+ non-factorisable ratio without (**left**) and with (**right**) spinor projection for all lepton source-sink separation, Δt_ℓ .

For this analysis, there are two time ranges to consider: 1) the weak Hamiltonian insertion t_H and 2) the lepton source-sink separation Δt_ℓ . For each $\Delta t_\ell = 12, 16, \dots, 40$, a correlator as a function of t_H is generated. We found that it is simpler and sufficient to consider the same τ for each Δt_ℓ correlator we include in a fit. Thus, in total there are

$$N_{fit} = \frac{48(48+1)}{2} \times \frac{8(8+1)}{2} = 42336 \quad (5.4)$$

fits. We consider only the first half of the temporal extent $T = 96$ since the latter half has a different matrix element. For this analysis, a brute force scan in the 2D plane can be applied.

An example of a good fit in the π^+ and K^+ sector with the projectors applied are shown in Figures 5.10 and 5.12, respectively. To check the stability of the candidate fit intervals, we compute the t_{min} -/ t_{max} -dependence of the amplitude correction and evaluate the neighbouring correlated difference. This is shown in Figures 5.11 and 5.13. This check is particular important in the kaon case, where the scan suggests a t_{max} that extends beyond the plateau region. According to Figure 5.13, the fit is stable.

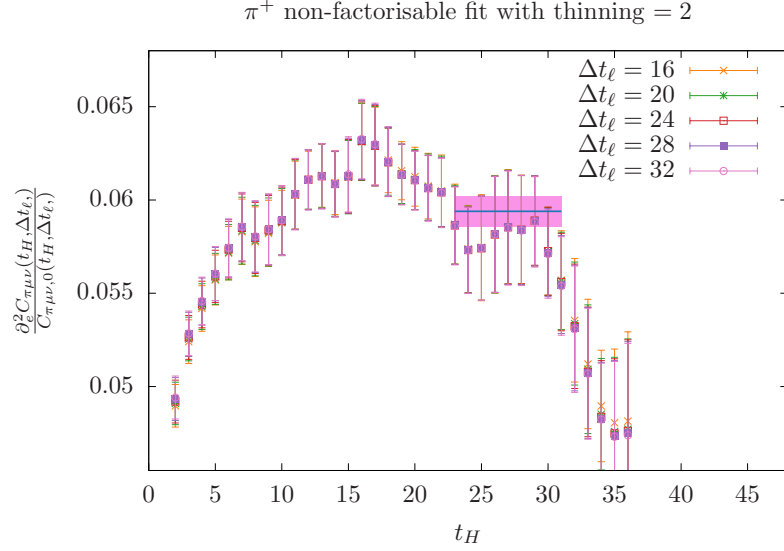


Figure 5.10 *A constant fit to the plateau of the π^+ non-factorisable correlator ratio. With thinning = 2, only the dataset containing odd-numbered timeslices is considered in this fit. The blue line is the fit and the pink band is the statistical error.*

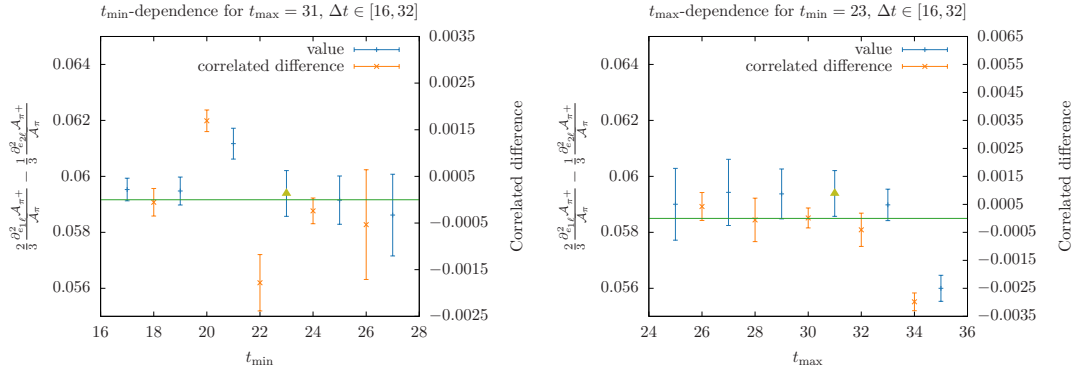


Figure 5.11 *The left y-axis is the electromagnetic correction to the non-factorisable π^+ amplitude as a function of $t_{\min}$ (left) and $t_{\max}$ (right) (blue). The right y-axis is the correlated difference between neighbouring $t_{\min}$ (left)/ $t_{\max}$ (right) values (orange). The green line indicates zero on the correlated difference. The olive triangle indicates the $t_{\min}/t_{\max}$ of choice.*

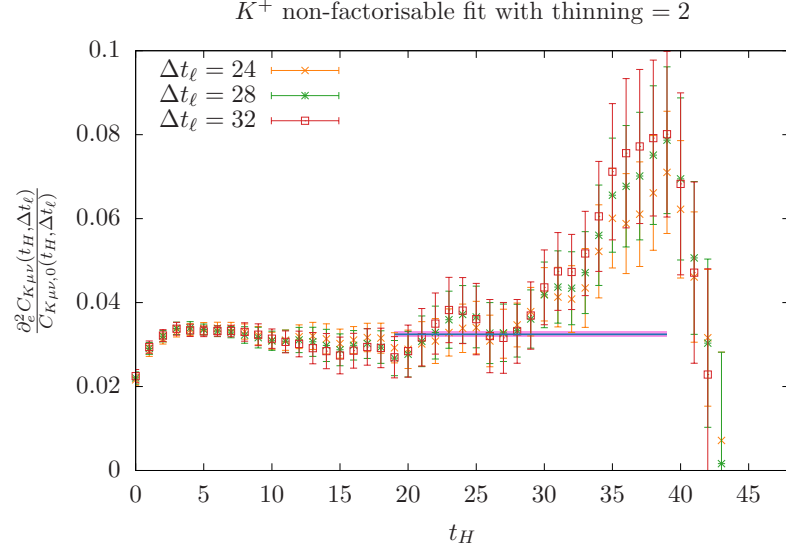


Figure 5.12 *A constant fit to the plateau of the K^+ non-factorisable correlator ratio. With thinning = 2, only the dataset containing odd-numbered timeslices is considered in this fit. The blue line is the fit and the pink band is the statistical error.*

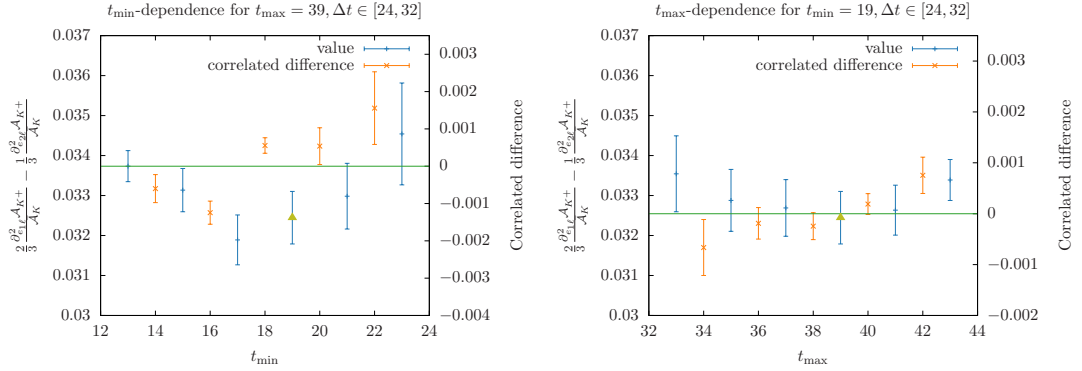


Figure 5.13 *The left y-axis is the electromagnetic correction to the non-factorisable K^+ amplitude as a function of t_{min} (left) and t_{max} (right) (blue). The right y-axis is the correlated difference between neighbouring t_{min} (left)/ t_{max} (right) values (orange). The green line indicates zero on the correlated difference. The olive triangle indicates the t_{min}/t_{max} of choice.*

5.4 Factorisable Analysis

When we consider Equations (4.75)-(4.84), we see that there is a common parameter between the six fit functions - the QCD-only simulation mass $\hat{M}_P$. Since we want a unique determination of each parameter $F^{(n)}(\tau)$, we do a

simultaneous fit of all correlators and correlator ratios. For each meson P , there are in total

$$\begin{aligned} N_{corr}^{\pi} &= (\# \text{ diagrams}) \times 2 = 8, \\ N_{corr}^K &= (\# \text{ diagrams}) \times 2 = 12, \end{aligned} \tag{5.5}$$

where the factor of 2 accounts for the two γ -structure at the sink. Suppose, then, for each correlator, the fit interval is bounded by $0 \leq t_{min} < t_{max} \leq 47$, then

$$\begin{aligned} N_{fit}^{\pi} &= \left(\frac{(48+1)48}{2} \right)^8 \sim 3 \times 10^{24}, \\ N_{fit}^K &= \left(\frac{(48+1)48}{2} \right)^{12} \sim 7 \times 10^{36}. \end{aligned} \tag{5.6}$$

We see that the space of possible fit intervals is prohibitively large to explore with a brute force scan. As an amusing back-of-the-envelope calculation, assuming the program completes a fit every second, it would take $\sim 3 \times 10^6$ times the current age of the Universe to accomplish this brute force scan¹. Thus, we apply the GA to search the $\boldsymbol{\tau}$ -space.

To capture as much statistical information in a correlator as possible, we make two adjustments. First, we allow for thinning of data into odd and even sets. That is, for a given t_{min}, t_{max} , fit only timeslices t , where

$$t_{min} \leq t \leq t_{max} \quad \text{and} \quad (t_{min} - t) \bmod 2 = 0. \tag{5.7}$$

Secondly, we also set a requirement of fitting *at least* 4 timeslices per correlator. This is another arbitrary choice, but it prevents the GA from promoting some $\boldsymbol{\tau}$ that has good AIC weight, but with one or more correlator fitting only one data point. These two combined together helps the GA to include as much statistical information per correlator as possible. In the opposite direction, however, we also fix a maximum *fiducial volume* of $5 \leq t_{min}^{(j)} < t_{max}^{(j)} \leq 40, \forall j$. This exclusion zone in the $\dim N_{corr}$ $\boldsymbol{\tau}$ -space assists the GA in avoiding $\tau^{(j)}$ that are prone to excited states (early t) or in a noisy region about ($t \sim T/2$).

Since the GA is a heuristic approach for searching the $\boldsymbol{\tau}$ -space, we run the GA multiple times to gather statistics. With an initial population of $P_0 = 25$ and

¹ $10^{24} \text{fits } s^{-1} / 60 \text{smin}^{-1} / 60 \text{minhr}^{-1} / 24 \text{hrd}^{-1} / 365 \text{dyr}^{-1} / 10^9 \text{yr} / T_{uni} = 3170979$, where $T_{uni} \sim 10^{10} \text{yrs}$.

a unique random number generator (rng) seed for the genetic operators, a GA run will terminate with P_0 fittest τ 's. We began with 80 independent rng seeds, generating a total of $80 \times 25 = 2000$ fittest τ candidates. We later boosted the statistics by a factor of 2.5, and with $200 \times 25 = 5000$ fittest τ we found no change in the order of magnitude of the top candidates' AIC weights. This indicates that the GA has converged (see Appendix C).

We chose τ 's with the maximum AIC weight to show in Figures 5.14-5.19 for the π and K meson. In each plot, there are two sets of data: a wall-wall pp and wall-pt pa correlator or correlator ratio. These are fitted to their functional form discussed in §4.4. The π^+ meson combined fit has $N_{\text{dof}} \sim 80$ while the K^+ meson has $N_{\text{dof}} \sim 90$. As such, the error band on the fit curve is not visible on the figures.

In Figures 5.16 and 5.18, the K^+ wall-wall pp signal appears to be noisier than its π^+ counterpart. This does not appear to hamper the quality of the AIC weight associated to this fit.

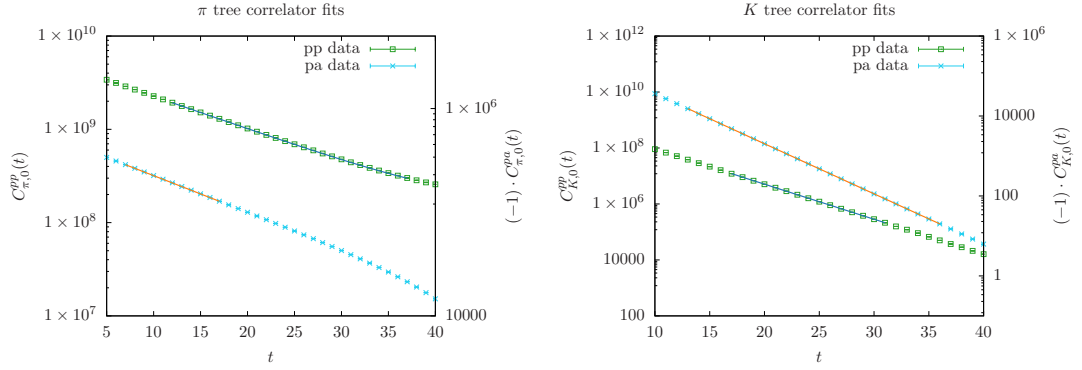


Figure 5.14 A cosh / sinh fit of the wall-wall pp /wall-pt pa QCD-only correlator for π (**left**) and K (**right**). The fit curves are navy and orange, respectively. The error bands on the fits are not visible at this scale. Note that the large values on the y-axes are due to the volume factors present in the time correlators. The wall-pt pa correlators are multiplied by (-1) because $C_{P_0}^{pa}(t < \frac{T}{2}) < 0$.

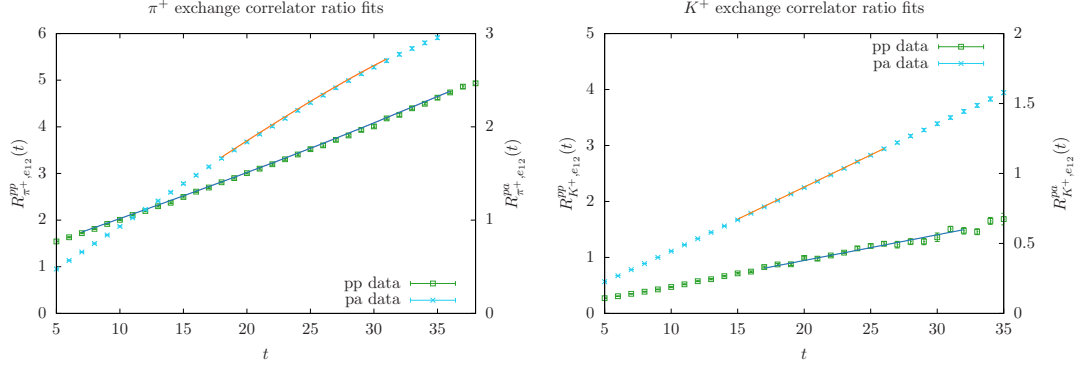


Figure 5.15 A tanh / coth fit of the wall-wall pp/wall-pt pa exchange correlator ratio for π^+ (**left**) and K^+ (**right**). The fit curves are navy and orange, respectively. The error bands on the fits are not visible at this scale.

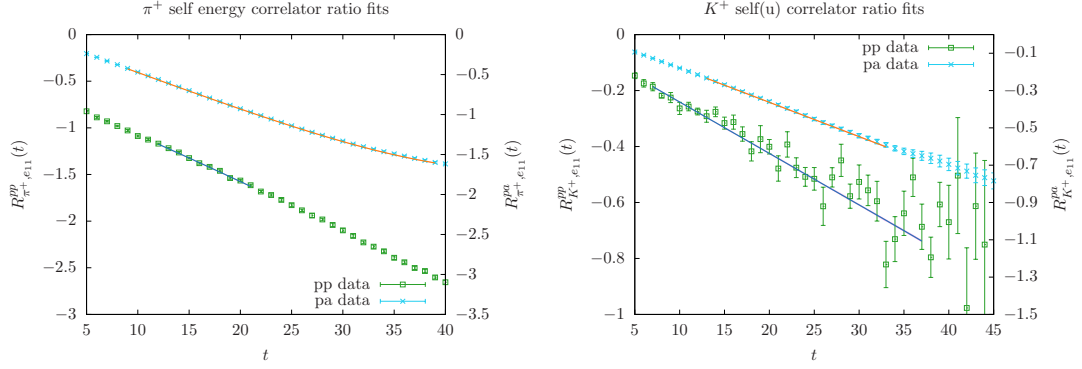


Figure 5.16 A tanh / coth fit of the wall-wall pp/wall-pt pa u-type quark self energy correlator ratio for π^+ (**left**) and K^+ (**right**). The fit curves are navy and orange, respectively. The error bands on the fits are not visible at this scale. Although the K^+ pp fit appears to be fitting into a noisy region, this has not diminished the quality of the AIC weight.

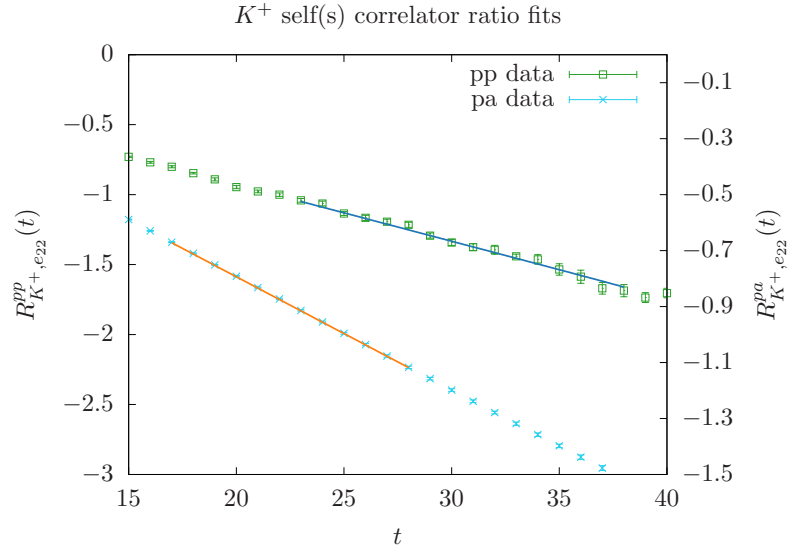


Figure 5.17 *A tanh / coth fit of the wall-wall pp/wall-pt pa d-type quark self energy correlator ratio for K^+ . The fit curves are navy and orange, respectively. The error bands on the fits are not visible at this scale.*

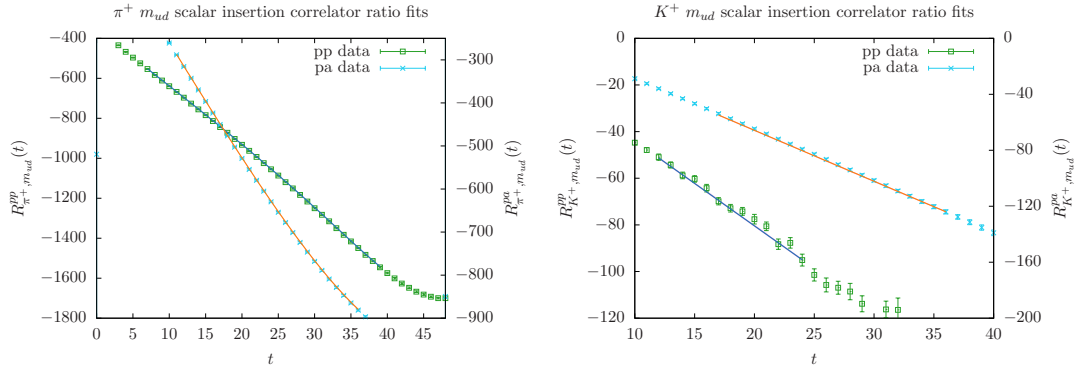


Figure 5.18 *A tanh / coth fit of the wall-wall pp/wall-pt pa m_{ud} scalar insertion correlator ratio for π^+ (left) and K^+ (right). The fit curves are navy and orange, respectively. The error bands on the fits are not visible at this scale. Although the K^+ pp fit appears to be fitting into a noisy region, this has not diminished the quality of the AIC weight.*

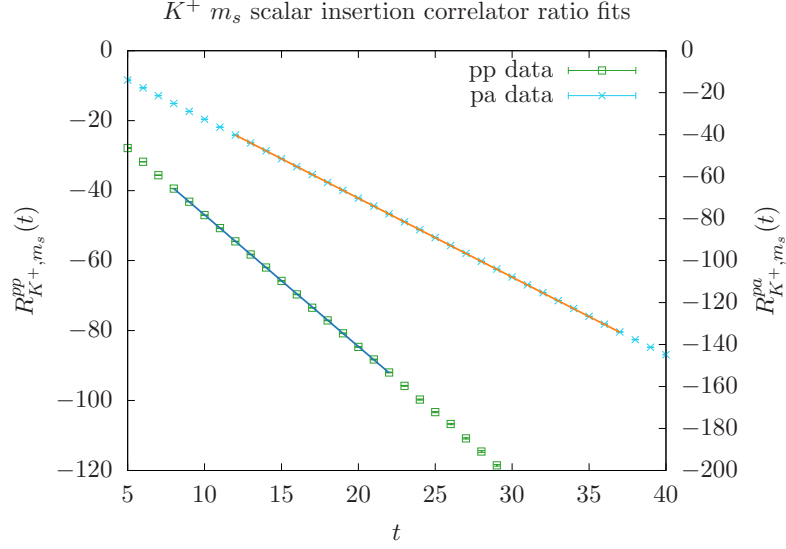


Figure 5.19 *A tanh / coth fit of the wall-wall pp/wall-pt pa m_s scalar insertion correlator ratio for K^+ . The fit curves are navy and orange, respectively. The error bands on the fits are not visible at this scale.*

5.5 Determination of $\delta R_{K\pi}$

In the above, we performed 7 analyses: the omega tree level, QED and m_s fit; the π^+ and K^+ non-factorisable combined fit; the π^+ and K^+ factorisable combined fit. Now that we have obtained fit results from each of them, we are in the position to determine $\delta R_{K\pi}$. First, we will present results from our procedure of tuning the lattice results to the isosymmetric QCD point of our choice before calculating the lattice contribution $\delta R_{K\pi}^{\text{latt.}}$. Then, we evaluate numerically the analytic formulas discussed in §4.6-4.7. We combine the lattice and analytic contributions to obtain

$$\delta R_{K\pi} = \delta R_{K\pi}^{\text{latt.}} + \frac{\alpha}{4\pi} \left(\delta \Gamma_{1,K\pi}^{\text{pt}}(\Delta E_\gamma) - 2 \cdot Y_{K\pi}^{(2)}(48) \right). \quad (5.8)$$

Finally, we will discuss how the statistical and the full systematic error budget are estimated and present the result with its error budget in §5.5.3.

5.5.1 Tuning to the Isosymmetric QCD Point

With the factorisable and omega analyses completed, we are in the position to tune our simulated results to the desired isosymmetric QCD point before calculating $\delta R_{K\pi}$. Our strategy proceeds as in §4.1. We also compute some observables of interest to compare the results from our lattice setup with currently published results.

To the Physical Point

For the physical point, our proxy of choice are:

$$\begin{aligned} \alpha^{\text{exp.}} &= 7.2973525693(11) \times 10^{-3}, & \left(\frac{M_{\pi^+}^{\text{exp.}}}{M_{\Omega^-}^{\text{exp.}}}\right)^2 &= 0.0069643(24), \\ \left(\frac{M_{K^+}^{\text{exp.}}}{M_{\Omega^-}^{\text{exp.}}}\right)^2 &= 0.087132(31), & \left(\frac{M_{K^0}^{\text{exp.}}}{M_{\Omega^-}^{\text{exp.}}}\right)^2 &= 0.088527(31), \end{aligned} \quad (5.9)$$

where the PDG[4] values are quoted. Let the vector

$$\Sigma^\phi = \left(\alpha^{\text{exp.}}, \left(\frac{M_{\pi^+}^{\text{exp.}}}{M_{\Omega^-}^{\text{exp.}}}\right)^2, \left(\frac{M_{K^+}^{\text{exp.}}}{M_{\Omega^-}^{\text{exp.}}}\right)^2, \left(\frac{M_{K^0}^{\text{exp.}}}{M_{\Omega^-}^{\text{exp.}}}\right)^2 \right) \quad (5.10)$$

and the bare quark mass shift from the simulation to the physical point be $\Delta m = m^\phi - \hat{m}$, where $m \in \{m_{ud}, \delta m, m_s\}$. These physical observables can be expressed in terms of our simulated observable in the following expansion:

$$\Sigma_i^\phi = \hat{\Sigma}_i + \alpha \frac{\partial \Sigma_i}{\partial \alpha} + \Delta m_{ud} \frac{\partial \Sigma_i}{\partial \hat{m}_{ud}} + \Delta \delta m \frac{\partial \Sigma_i}{\partial \delta \hat{m}} + \Delta m_s \frac{\partial \Sigma_i}{\partial \hat{m}_s}, \quad (5.11)$$

where the index $i = 0, \dots, 3$ iterates through the components in Equation (5.10). Here, we are reminded that the hat (*e.g.* $\hat{m}_{ud}$) denotes a quantity at the simulation point. For $i = 1, 2, 3$, we apply Leibniz rule:

$$\begin{aligned} \frac{\partial \Sigma_i}{\partial g_j} &= \frac{\partial}{\partial g_j} \left(\frac{M_i}{M_{\Omega^-}} \right)^2, \\ &= \left(\frac{\partial_{g_j} M_i^2}{\hat{M}_{\Omega^-}^2} - 2 \left(\frac{\hat{M}_i}{\hat{M}_{\Omega^-}} \right)^2 \cdot \frac{\partial_{g_j} M_{\Omega^-}}{\hat{M}_{\Omega^-}} \right), \end{aligned} \quad (5.12)$$

for $g = (\alpha, \hat{m}_{ud}, \delta \hat{m}, \hat{m}_s)$. Here, M_i indexes the hadronic masses in Equation (5.10). In vector notation, the tuning parameters $\Delta \mathbf{g} = (\Delta \alpha, \Delta m_{ud}, \Delta \delta m, \Delta m_s)$

can be obtained via

$$\Delta \mathbf{g} = G^{-1} \left(\mathbf{\Sigma}^\phi - \hat{\mathbf{\Sigma}} \right), \quad (5.13)$$

where the matrix element $G_{ij} = \frac{\partial \Sigma_i}{\partial g_j}$. For the mass derivatives determined in §5.4, we obtained

$$\begin{aligned} \Delta \hat{m}_{ud} &= -0.000105(15), \\ \Delta \delta \hat{m} &= -0.0009608(54), \\ \Delta \hat{m}_u &= -0.000585(14), \\ \Delta \hat{m}_d &= 0.000375(17), \\ \Delta \hat{m}_s &= -0.00103(39) \end{aligned} \quad (5.14)$$

and $\Delta \alpha = (\alpha^\phi - \hat{\alpha}) = \alpha^{\text{exp.}}$ since $\frac{\partial \Sigma_0}{\partial g_j} = \delta_{j0}$. One may also determine the lattice spacing by using the following relation:

$$a = \frac{(aM_{\Omega^-})^\phi}{M_{\Omega^-}^{\text{exp}}}, \quad (5.15)$$

where

$$(aM_{\Omega^-})^\phi = \hat{M}_{\Omega^-} + \alpha \frac{\partial M_{\Omega^-}}{\partial \alpha} + \Delta m_s \frac{\partial M_{\Omega^-}}{\partial \hat{m}_s}, \quad (5.16)$$

with $M_{\Omega^-}^{\text{exp.}} = 1672.45 \text{ MeV}$ [4]. The QCD+QED inverse lattice spacing of this setup is

$$a^{-1} = 1739(9) \text{ MeV}. \quad (5.17)$$

To the Isosymmetric QCD Point

To define the isosymmetric QCD point, we use the BMW mesonic scheme discussed in §4.1.2 (see Equation (4.4)). For convenience, they are

$$\begin{aligned} M_{ud}^2 &= \frac{M_{\bar{u}u}^2 + M_{\bar{d}d}^2}{2} \approx 2B_0 m_{ud}^R, & \Delta M^2 &= M_{\bar{u}u}^2 - M_{\bar{d}d}^2 \approx 2B_0 \delta m^R, \\ M_{K\chi}^2 &= \frac{M_{K^+}^2 + M_{K^0}^2 - M_{\pi^+}^2}{2} \approx 2B_0 m_s + e^2 \frac{2C}{F_0^2} \epsilon. \end{aligned}$$

Thus, our proxy for the isosymmetric QCD point is

$$\mathbf{\Sigma} = (\alpha, M_{ud}^2, \Delta M^2, M_{K\chi}^2). \quad (5.18)$$

For the isosymmetric QCD point, where $\delta m = \alpha = 0$, we fix the proxy to the

following values:

$$\begin{aligned}
\bar{\Sigma} &= (0, (M_{ud}^2)^\phi, 0, (M_{K\chi}^2)^\phi), \\
&= (0, 0.006034(68), 0, 0.07798(83)), \\
&= (0, 18251(206), 0, 235872(2512)) \text{ MeV}^2,
\end{aligned} \tag{5.19}$$

where $(M_{ud}^2)^\phi$ and $(M_{K\chi}^2)^\phi$ are obtained using the simulation-to-physical point bare quark mass shifts in the previous determination (see Equation (5.14)). In the final line of Equation (5.19), the results have been converted to physical units using Equation (5.17) and one can compare it with experimental values from the PDG:

$$(M_{ud}^2)^{\text{exp.}} = 18218.74(14)\text{MeV}^2 \quad \text{and} \quad (M_{K\chi}^2)^{\text{exp.}} = 235926.9(9.3)\text{MeV}^2, \tag{5.20}$$

where $(M_{ud}^2)^{\text{exp.}}$ is interpreted as the physical neutral pion mass squared. As before, let $\Delta\bar{m} = \bar{m}_q - \hat{m}$ be the bare quark mass shift from the simulation to the isosymmetric QCD point. Using $\bar{\Sigma}$ as input for Equation (5.13), we obtain

$$\begin{aligned}
\Delta\bar{\alpha} &= 0, \\
\Delta\bar{m}_{ud} &= -0.000104(15), \\
\Delta\delta\bar{m} &= 0, \\
\Delta\bar{m}_s &= -0.00094(39).
\end{aligned} \tag{5.21}$$

The matrix of derivatives $\bar{G}$ is shown in Table 5.1. This can be compared with its prediction in PQ χ PT. We take the numerical values of the quark condensate Σ_0 and the decay constant in $\overline{\text{MS}}$ at $\mu = 2\text{GeV}$ from the most recently-published result from MILC09A [59] in FLAG [20], which are

$$\Sigma_0 = 1.47(14) \times 10^7 \text{MeV}^3 \quad \text{and} \quad F \equiv \sqrt{2}f_\pi = 78.3(3.2)\text{MeV}. \tag{5.22}$$

This gives

$$B_0 = \frac{\Sigma_0}{F_0^2} = 2.40(31) \times 10^3 \text{MeV}. \tag{5.23}$$

Together with $C = 4.2 \times 10^7 \text{MeV}^5$ [60] and the FLAG $(2+1)$ flavor average of $\epsilon = 0.73(17)$ [20], the leading order PQ χ PT predictions are shown in Table 5.2.

Lattice results				
	$\frac{\partial}{\partial\alpha}$	$\frac{\partial}{\partial m_{ud}}$	$\frac{\partial}{\partial\delta m}$	$\frac{\partial}{\partial m_s}$
α	1	0	0	0
M_{ud}^2	$2.32(37) \times 10^{-5}$	4.5198(49)	0	0
ΔM^2	$1.39(22) \times 10^{-5}$	0	4.5198(49)	0
$M_{K\chi}^2$	$2.097(12) \times 10^{-3}$	-0.1589(73)	0	2.17103(94)

Table 5.1 *The derivatives of the isosymmetric QCD proxy (i.e. BMW meson mass and electric charge) w.r.t various couplings in lattice units. The quoted error is statistical only.*

PQ χ PT predictions				
	$\frac{\partial}{\partial\alpha}$	$\frac{\partial}{\partial m_{ud}}$	$\frac{\partial}{\partial\delta m}$	$\frac{\partial}{\partial m_s}$
α	1	0	0	0
M_{ud}^2	0	4.1319	0	0
ΔM^2	0	0	4.1319	0
$M_{K\chi}^2$	1.671×10^{-3}	0	0	2.06593

Table 5.2 *The LO PQ χ PT predictions of the BMW mesons in lattice units, quoted to the same significant figures as the lattice results. Analytic formula can be found in Equation (4.4).*

A couple of remarks are in order. First, where LO PQ χ PT predicted zero E.M. contribution to the neutral pseudoscalars, we have a small but non-zero E.M. signal from the self-energy and exchange correlator fits with the appropriate charge factors (see Figures 5.15 and 5.16). This signal is thus a NLO contribution in PQ χ PT. Secondly, the derivative of $M_{K\chi}^2$ w.r.t the electric charge is directly proportional to the violation of Dashen's theorem, parametrised by ϵ in Equation 4.4. The fact that the lattice determination of these pseudoscalar derivatives are in the same ballpark as the LO PQ χ PT predictions is an encouraging sign that this isosymmetric scheme is consistent with well-established theoretical frameworks.

Isosymmetric QCD to Physical Point

Let $\Delta m'_q = (m^\phi - \bar{m})$ be the bare quark mass shift between the isosymmetric QCD and the physical point. Once Δm and $\Delta \bar{m}$ have been determined, we can

take the difference to obtain

$$\Delta m'_q = m_q^\phi - \bar{m}_q = \Delta m_q - \Delta \bar{m}_q. \quad (5.24)$$

Using the results in Equations (5.14) and (5.21), we obtain

$$\begin{aligned} \Delta m'_{ud} &= -4.71(74) \times 10^{-7}, \\ \Delta \delta m' &= -9.608(53) \times 10^{-4}, \\ \Delta m'_s &= -8.862(52) \times 10^{-5}. \end{aligned} \quad (5.25)$$

Using this prescription to define the isosymmetric QCD point, we compute two observables of interest below as a sanity check: 1) the correction to Dashen's theorem ϵ and 2) the ratio of light quark masses m_u^R/m_d^R . Both are compared with the current values reported in FLAG.

Correction to Dashen's Theorem

Originally introduced in 1969 [35], R. Dashen set out to prove that, up to $\mathcal{O}(e^2)$,

$$M_{K^+}^2 - M_{K^0}^2 = M_{\pi^+}^2 - M_{\pi^0}^2 \quad (5.26)$$

when one ignores strong isospin breaking effect. That this is in direct contradiction to experimental results led to the formulation of the correction parameter ϵ , defined as

$$\epsilon = \frac{(\Delta M_K^2 - \Delta M_\pi^2)^\gamma}{\Delta M_\pi^2}, \quad (5.27)$$

where $\Delta M_P^2 = M_{P^+}^2 - M_{P^0}^2$ is the squared mass difference and the superscript γ denotes the contribution arising from electromagnetic corrections only. Due to G-parity, ΔM_π^2 does not receive $\mathcal{O}(\delta m)$ contributions, thus

$$\Delta M_\pi^2 = (\Delta M_\pi^2)^\gamma, \quad (5.28)$$

which modifies Equation (5.27) to

$$\epsilon = \frac{(\Delta M_{K^+}^2 - \Delta M_{K^0}^2)^\gamma}{\Delta M_\pi^2} - 1. \quad (5.29)$$

If Dashen's theorem holds true, then the above would return zero. Thus, ϵ quantifies the violation to the theorem.

To proceed, we need the kaon mass squared splitting due to electromagnetic corrections. This quantity requires an unphysical separation of QED and QCD. To that end, let $\Delta m_q^{QCD} = (m_q^{QCD} - \hat{m}_q)$ be the bare quark mass shift from the simulation to the $(m_u \neq m_d, \alpha = 0)$ QCD point. Once again, the BMW mesons in Equation (4.4) are used. To reflect this $\delta m \neq 0$ QCD theory, we fix $(\Delta M^2)^\phi$ to its ‘physical’ value. Numerically, we have

$$\begin{aligned}\Sigma^{QCD} &= (0, (M_{ud}^2)^\phi, (\Delta M^2)^\phi, (M_{K\chi}^2)^\phi), \\ &= (0, 0.006034(68), -0.004340(25), 0.07798(83)), \\ &= (0, 18251(206), -13127(76), 235872(2512)) \text{ MeV}^2,\end{aligned}\tag{5.30}$$

in lattice and physical units, respectively. Using this as input to Equation (5.13), we obtain

$$\begin{aligned}\Delta m_{ud}^{QCD} &= -0.000104(15), \\ \Delta \delta m^{QCD} &= -0.0009602(53), \\ \Delta m_s^{QCD} &= -0.00094(39).\end{aligned}\tag{5.31}$$

Following the notation from FLAG[20], the electromagnetic contributions to K^+ are

$$\begin{aligned}(M_{K^+}^2)^\gamma &= (M_{K^+}^2)^\phi - (M_{K^+}^2)^{QCD}, \\ &= \hat{M}_{K^+}^2 + \alpha \frac{\partial M_{K^+}^2}{\partial \alpha} + \sum_{m_q} \Delta m_q \frac{\partial M_{K^+}^2}{\partial \hat{m}_q} - \left(\hat{M}_{K^+}^2 + \sum_{m_{q'}} \Delta m_{q'}^{QCD} \frac{\partial M_{K^+}^2}{\partial \hat{m}_{q'}} \right), \\ &= \alpha \frac{\partial M_{K^+}^2}{\partial \alpha} + \sum_q (\Delta m_q - \Delta m_q^{QCD}) \frac{\partial M_{K^+}^2}{\partial \hat{m}_q},\end{aligned}\tag{5.32}$$

where from the second line onward we expand the squared masses in terms of QCD-only lattice quantities, their derivatives and Δm_q and Δm_q^{QCD} . This is identical for K^0 . Thus, the electromagnetic contribution to the kaon squared masses are

$$\begin{aligned}(M_{K^+}^2)^\gamma - (M_{K^0}^2)^\gamma &= 0.0007141(76), \\ &= 2160(23) \text{ MeV}^2.\end{aligned}\tag{5.33}$$

As for the denominator of Equation (5.29), it suffices to use $\Delta M_\pi^2 = (139.57039(18))^2 -$

$134.9768(5)^2)\text{MeV}^2$ from the PDG[4]. Then, assembling the fraction, we obtain

$$\epsilon = 0.713(18), \quad (5.34)$$

where error is statistical only. For reference, the current FLAG value in $N_f = 2+1$ theory is

$$(\text{FLAG}) \quad \epsilon = 0.73(17). \quad (5.35)$$

We see that our lattice determination of ϵ is in good agreement with currently published results. We remind the reader that Equation (5.34) is not a prediction of ϵ since it is the result from one lattice spacing. However, it is encouraging that the near-physical ensemble produces comparable results. Figure 5.20 shows a comparison with the other values of ϵ in FLAG [20].

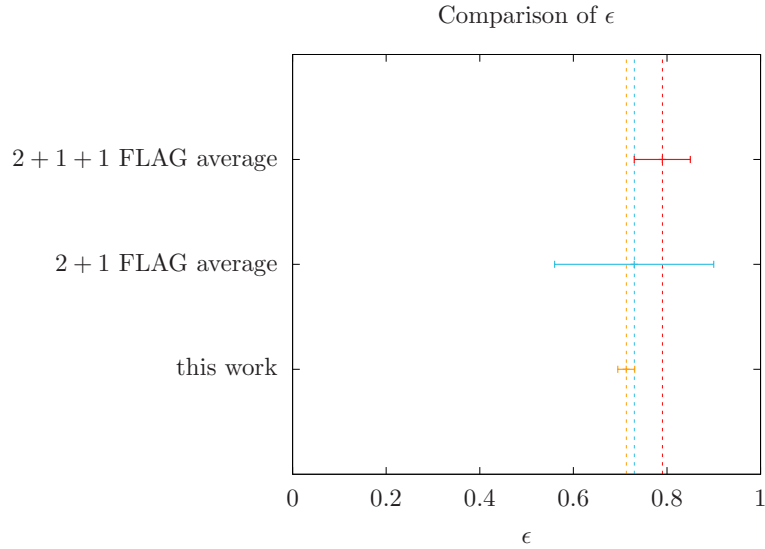


Figure 5.20 *A comparison of the correction to Dashen's theorem ϵ between this work and currently published FLAG averages. For reference, Dashen's theorem predicts $\epsilon = 0$. The error of 'this work' (orange) is statistical only.*

Renormalised Light Quark Mass Ratio

We are interested in computing the ratio m_u^R/m_d^R as a cross-check. Although we have been working with bare quark masses in this tuning procedure, in the ratio any multiplicative renormalisation constant will cancel up to $\mathcal{O}(\alpha)$ corrections. To that end, we plan to predict δm^R from our setup and use the FLAG value for m_{ud}^R to determine the ratio. Let us collect some results from the previous set of

calculations. Recall from Equations (4.4) and (5.30),

$$\Delta M^2 = 2B_0\delta m^R + \dots \approx -13127(76)\text{MeV}^2. \quad (5.36)$$

To compute δm^R , we use B_0 as quoted above (Equation (5.23)). Applying this to $(\Delta M^2)^\phi$ in Equation (5.30), we obtain

$$\delta m^R = -2.74(34) \text{ MeV}. \quad (5.37)$$

Using the $2 + 1$ average from FLAG

$$m_{ud}^R = 3.381(40) \text{ MeV}, \quad (5.38)$$

and with the relation $m_{u/d} = m_{ud} \pm \frac{\delta m}{2}$, we obtain

$$m_u^R = 2.01(17) \text{ MeV}, \quad (5.39)$$

$$m_d^R = 4.75(17) \text{ MeV}, \quad (5.40)$$

$$\text{(this work)} \quad \frac{m_u^R}{m_d^R} = 0.423(51), \quad (5.41)$$

$$\text{(FLAG)} \quad \frac{m_u^R}{m_d^R} = 0.485(19) \quad (5.42)$$

where the $N_f = 2 + 1$ average of m_u/m_d from FLAG[20] has been included for reference. Regarding this $\sim 1\sigma$ discrepancy between this work and the FLAG average, we must be reminded that only the LO PQ χ PT term is included in our determination of δm^R and discretisation effects were not studied. For a precise determination, we must calculate the renormalisation constants on the lattice instead. Nevertheless, this exercise demonstrates that our tuning procedure - namely, the definition of isosymmetric QCD using unphysical BMW mesons - is capable of producing estimation which is consistent with predictions from first principle calculations.

5.5.2 Assembling $\delta R_{K\pi}$

Contribution from Double Derivatives

From §5.5.1, the expansion of a physical observable X about its isosymmetric point is given by Equation (4.13), which we recast here for convenience:

$$X(\mathbf{g}^\phi) = X(\bar{\mathbf{g}}) + \alpha \frac{\partial X}{\partial \alpha} \Big|_{\alpha=0} + \sum_q (m_q - \bar{m}_q) \frac{\partial X}{\partial m_q} \Big|_{m_q=\bar{m}_q} + \dots$$

Since our simulation point is not the desired isosymmetric point, we extract $\partial_{m_q} X|_{m_q=\hat{m}_q}$ from time correlators, not $\partial_{m_q} X|_{m_q=\bar{m}_q}$. Nevertheless, we can expand the latter about the simulation point, given their proximity (see Equations (5.21)):

$$\frac{\partial X(\bar{g})}{\partial m_q} = \frac{\partial X(\hat{g})}{\partial m_q} + \sum_{g'} (g' - \hat{g}) \frac{\partial^2 X}{\partial m_q \partial g'} \Big|_{g'=\hat{g}} + \dots, \quad (5.43)$$

i.e. we pick up $\mathcal{O}((m_q - \bar{m}_q)(m_q - \hat{m}_q), \alpha(m_q - \bar{m}_q))$ cross terms. The double derivative coefficients can be extracted from correlators with two insertions of the appropriate currents. Due to the cost of generating correlation functions with two current insertions, we studied the $\mathcal{O}(e_{q\ell}(m_q - \bar{m}_q))$ contributions at limited statistics and found that their contribution cannot be resolved with the current statistical precision.

Thus, we defer the inclusion of cross terms to future work.

Contribution from Lattice Calculation

Given a fit scan procedure we obtain a set fit ranges and their associated AIC weights from each analysis. We now discuss the procedure of fit range selection. Naively, we could choose the fit range with the highest AIC weights and compute $\delta R_{K\pi}$ with just 7 fits. However, the fit scans show that there is still a large multiplicity of good fit results. In order to incorporate this multiplicity in the results, we choose N_i fits from each analysis and generate $N_{\text{pred}} = \prod_{i=1}^7 N_i$ predictions of $\delta R_{K\pi}$.

Due to the product operator, N_{pred} grows multiplicatively with increasing N_i . To visualise this distribution, we propose to build a histogram of N_{pred} $\delta R_{K\pi}$'s. We

also re-weigh the histogram entries with the total AIC

$$\begin{aligned}
w_{tot} &= \prod_{i=1}^7 w_i, \\
&= \exp \left[-\frac{1}{2} \sum_{i=1}^7 (\chi_i^2 - 2N_{\text{dof},i}) \right],
\end{aligned} \tag{5.44}$$

where the index i denotes the χ^2 and N_{dof} from each of the 7 analyses. Here, the summation applies because the analyses are independent. While the absolute value of w_{tot} has no intrinsic meaning, the *relative* size between the N_{pred} different weights informs us which prediction is preferable to the others. With this weighting procedure, we do not need to include every fit scan result since the exponential will suppress the relatively inferior fit results. For practical reasons, we impose a cut-off by selecting only the fit ranges associated to the top 5 AIC weights in each analysis. This gives us a total of $N_{\text{pred}} = 5^7 = 78125$. To determine the value of $\delta R_{K\pi}^{\text{latt.}}$, then, we opted for the median of the histogram. In determining $\delta R_{K\pi}^{\text{latt.}}$ through this histogram procedure, its value will no longer be solely from a unique set of fits. Instead, it is the 50th percentile of the distribution. This removes the bias of cherry-picking specific fit ranges to determine $\delta R_{K\pi}^{\text{latt.}}$. Moreover, by opting for the histogram median as the definitive value of $\delta R_{K\pi}$, our result will not be subjected to as drastic a variation due to outlier predictions compared to, say, the mean.

The result of this procedure is shown in Figure 5.21. To generate this histogram, we determine the mass and amplitude corrections of each analysis from their respective choice fits, tune the setup to the desired isosymmetric QCD point, and predict $\delta R_{K\pi}^{\text{latt.}}$ as in Equation (4.35) using only the central value of the fit results. For each of the $N_{\text{pred}} = 5^7$, then, we distribute them across b bins and weigh each bin entry by their combined AIC weight as defined in Equation (5.44). For this work, we found $b = 20$ to be optimal for a distribution of this size. The error bars on the bin are determined by generating a histogram for each bin for all of the bootstrap samples and taking the interval between the 2.28th and the 97.72nd percentile, *i.e.* the $\pm 2\sigma$ confidence interval. The median here is indicated in purple, its statistical error and fit systematics are in navy blue and magenta, respectively (see below). Its central value is

$$\delta R_{K\pi}^{\text{latt.}} = -0.0101268. \tag{5.45}$$

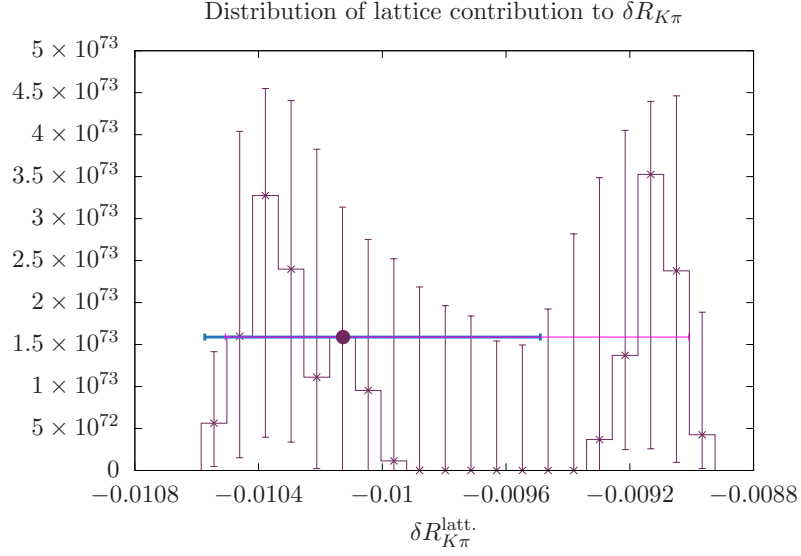


Figure 5.21 *Histogram displaying distribution of $\delta R_{K\pi}^{\text{latt.}}$. The blue and magenta band are the statistical and fit systematic errors, respectively. The double peak structure suggests that there are two sets of fit intervals with statistically distinct fit results with comparably good AIC weights.*

Contribution from Analytic Results

What remains to evaluate are the finite volume corrections and contributions from the real photon emission diagram. For these quantities, it suffices to use the PDG mass as inputs (see §5.5.3).

First, the $\mathcal{O}(\alpha)$ finite volume effects (FVE) to be subtracted from $\delta R_{K\pi}^{\text{latt.}}$. For convenience, we recall the formula here:

$$\begin{aligned}
Y_P^{(2)}(L) = & \frac{3}{4} + 4 \log \left(\frac{m_\ell}{m_W} \right) + 2 \log \left(\frac{m_W L}{4\pi} \right) + \frac{c_3 - 2(c_3(\mathbf{v}_\ell) - B_1(\mathbf{v}_\ell))}{2\pi} \\
& - 2A_1(\mathbf{v}_\ell) \left[\log \frac{M_P L}{2\pi} + \log \frac{m_\ell L}{4\pi} - 1 \right] - \frac{1}{M_P L} \left[\frac{(1 + r_\ell^2)^2 c_2 - 4r_\ell^2 c_2(\mathbf{v}_\ell)}{1 - r_\ell^4} \right] \\
& + \frac{1}{(M_P L)^2} \left[-\frac{F_A^P}{f_P} \frac{4\pi M_P [(1 + r_\ell^2)^2 c_1 - 4r_\ell^2 c_1(\mathbf{v}_\ell)]}{1 - r_\ell^4} \right. \\
& \quad \left. + \frac{8\pi [(1 + r_\ell^2) c_1 - 2c_1(\mathbf{v}_\ell)]}{(1 - r_\ell^4)} \right],
\end{aligned}$$

where $r_\ell^2 = (m_\ell/M_P)^2$. Using $L = 48a$, $F_A^\pi = 0.0119(1)$ and $F_A^K = 0.0060(177)$

from the PDG [4] and FV coefficients from [44], we obtain

$$Y_{K\pi}^{(2)}(48) = Y_K^{(2)}(48) - Y_\pi^{(2)}(48) = -6.204720. \quad (5.46)$$

Next, the contributions from the real photon emission diagram, introduced in Equation (4.146), has the following analytic form:

$$\begin{aligned} \delta\Gamma_{1,P}^{\text{pt}}(\Delta E_\gamma) = & 3 \log\left(\frac{M_P^2}{m_W^2}\right) - 8 \log(1 - r_\ell^2) - \frac{3r_\ell^4}{(1 - r_\ell^2)^2} \log r_\ell^2 \\ & - 8 \frac{1 + r_\ell^2}{1 - r_\ell^2} \text{Li}_2(1 - r_\ell^2) + \frac{13 - 19r_\ell^2}{2(1 - r_\ell^2)}, \\ & + \frac{6 - 14r_\ell^2 - 4(1 - r_\ell^2) \log(1 - r_\ell^2)}{1 - r_\ell^2} \log r_\ell^2. \end{aligned}$$

Its numerical value is

$$\delta\Gamma_{1,K\pi}^{\text{pt}}(\Delta E_\gamma) = \delta\Gamma_{1,K}^{\text{pt}}(\Delta E_\gamma) - \delta\Gamma_{1,\pi}^{\text{pt}}(\Delta E_\gamma) = -10.04443. \quad (5.47)$$

In this next section, we will discuss the error budget.

Prediction of $\delta R_{K\pi}$

Using the values in Equations (5.45), (5.46) and (5.47), we evaluate Equation 5.8 and get a central value of

$$\delta R_{K\pi} = \delta R_{K\pi}^{\text{latt.}} + \frac{\alpha}{4\pi} \left(\delta\Gamma_{1,K\pi}^{\text{pt}}(\Delta E_\gamma) - 2Y_{K\pi}^{(2)}(48) \right) = -0.008753426. \quad (5.48)$$

5.5.3 Estimating Statistical & Systematic Uncertainties

Statistical Error

The median in Figure 5.21 is generated using the central value of the fit results. To obtain the statistical error on the median, we generate the remaining 2000 histograms, one for each bootstrap sample, and determine their median. A histogram of these 2001 medians is generated and we take the $\pm 2\sigma$ interval as the statistical error on the median. We find that, from the weighted histogram,

$$\delta R_{K\pi} = -0.00875(^{+64}_{-45})_{\text{stat.}}. \quad (5.49)$$

The asymmetry on this error is less pronounced if we opt for 1σ interval. However, we chose 2σ to be conservative in our estimate.

Fit Systematics

In Figure 5.21, the histogram contains two significant peaks. We trace this multi-peak structure to the kaon factorisable analysis, where the variation of the top 5 fit intervals are responsible for these two clusters of $\delta R_{K\pi}^{\text{latt.}}$ distribution. Based on our data-driven approach to the correlator analyses, the fit intervals contributing to this AIC-weighted histogram are all equally valid. Nevertheless, we will estimate the systematics associated to our fit strategy.

On the histogram of the central samples, we once again take $\pm 2\sigma$ interval and quote that as our fit systematics. According to Figure 5.21, the $\pm 2\sigma$ interval (in magenta) accounts for both histogram peaks. This gives us

$$\delta R_{K\pi} = -0.00875({}_{-38}^{+112})_{\text{fit}}. \quad (5.50)$$

$\mathcal{O}(a^2)$ Discretisation Error

With only a single lattice spacing on this ensemble, no continuum extrapolation is available at the time of writing. Thus, we expect discretisation effects in our determination of $\delta R_{K\pi}^{\text{latt.}}$ to appear at $\mathcal{O}(a^2)$. We take as the discretisation error budget $(a\Lambda_{\text{QCD}})^2$ of our lattice calculation $\delta R_{K\pi}^{\text{latt.}}$, where the QCD scale Λ_{QCD} is the only relevant scale to make this dimensionless. From the physical point tuning step, we determined $a^{-1} = 1730\text{MeV}$, which is consistent with [61]. For the physical scale, we take a conservative estimate $\Lambda_{\text{QCD}} = 400\text{MeV}$ [62]². This gives us $(a\Lambda_{\text{QCD}})^2 \sim 5\%$ of $\delta R_{K\pi}^{\text{latt.}}$, resulting in

$$\delta R_{K\pi} = -0.00875(54)_{a^2}. \quad (5.51)$$

Electro-quenched QED

As noted in §5.1, we treat the sea quarks as electrically-neutral in this calculation. Thus, their electromagnetic interactions with the charged fermions on the lattice are neglected. To quantify this electro-quenching effect, we first separate $\delta R_{K\pi}^{\text{latt.}}$

²Other estimations such as $\Lambda_{\text{QCD}}(\overline{\text{MS}}) = 300\text{MeV}$ [63] give $(a\Lambda)^2 \sim 3\%$

into its electromagnetic and strong isospin-breaking contributions $\delta_{\text{EM}}^{\text{latt.}}$ and $\delta_{\text{SU}(2)}^{\text{latt.}}$, respectively, by an appropriate separation scheme outlined in §4.1.3. Then, we take 10% of δ_{EM} as the electro-quenching error. In practice, for each $\delta R_{K\pi}^{\text{latt.}}$ prediction, we apply the separation scheme to obtain $\delta_{\text{EM}}^{\text{latt.}}$ and generate a histogram. We take the median of this histogram as the central value of $\delta_{\text{EM}}^{\text{latt.}}$. This is shown in Figure 5.22. The central value is

$$\delta_{\text{EM}}^{\text{latt.}} = -0.00474383. \quad (5.52)$$

Taking 10% of it as the error, we have

$$\delta R_{K\pi} = -0.00875(47)_{\text{qQED}}. \quad (5.53)$$

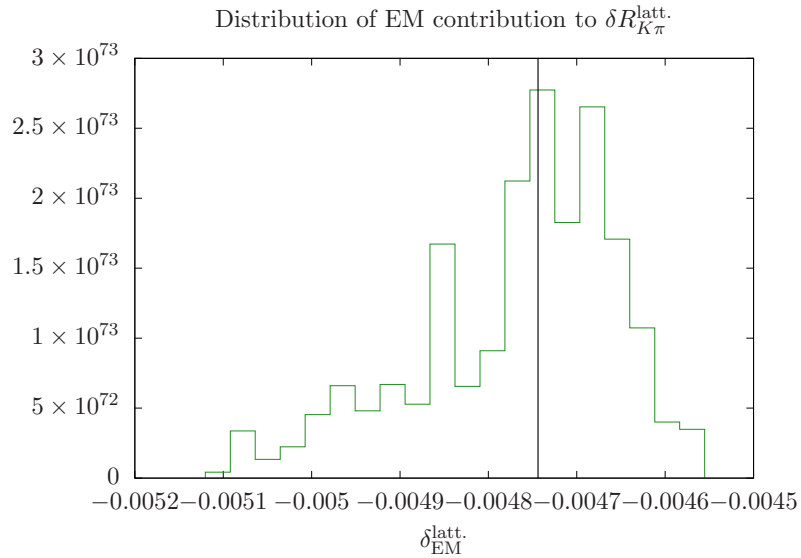


Figure 5.22 *Histogram displaying distribution of $\delta_{\text{EM}}^{\text{latt.}}$. The black vertical line indicates where the median is.*

Analytic vs. Lattice Masses

To obtain $\delta R_{K\pi}$, we need to include finite volume corrections and the point-like radiative term. These two are analytic contributions, depending only on the pseudoscalar mass³. Our near-physical point setup allows us to calculate these contributions directly using PDG inputs and hence do not contribute to the error budget on our lattice calculation.

³additionally, the decay constants in the FV correction piece.

However, we note that in this ensemble,

$$\begin{aligned}\hat{M}_{\pi^+} &\approx 139.5 \text{ MeV}, \\ \hat{M}_{K^+} &\approx 499.2 \text{ MeV},\end{aligned}\tag{5.54}$$

i.e the physical charged kaon mass is about 5MeV off from the experimental value. We can quantify this violation of energy conservation for the meson P with the following dimensionless parameter

$$\epsilon_P = \frac{\omega_{\text{in}} - \omega_{\text{out}}}{\omega_{\text{in}} + \omega_{\text{out}}},\tag{5.55}$$

where $\omega_{\text{in}} = \hat{M}_P$ is our simulated pseudoscalar mass and $\omega_{\text{out}} = E_\ell + |\mathbf{p}_\nu| = M_P^{\text{exp}}$ is the total energy of the outgoing states. For the analytic terms, this equals the experimentally measured mass. We find that

$$\begin{aligned}\epsilon_{\pi^+} &= -0.00037, \\ \epsilon_{K^+} &= 0.0055.\end{aligned}\tag{5.56}$$

This violation is a sub-percent level effect at best. As we will see in the following section, this systematic effect can be safely neglected.

Finite Volume Effects (FVE)

The finite volume effects (FV) are subtracted from $\delta R_{K\pi}^{\text{latt.}}$ via

$$Y_P^{(n)}(L) = Y^{\text{IV}}(\lambda) + Y_{\log} \log \frac{L\lambda}{2\pi} + Y_0 + \sum_{j=1}^n \frac{M_\pi^j}{(M_\pi L)^j} Y_j.\tag{5.57}$$

Structure-dependent (SD) terms first appear at $\mathcal{O}(1/L^2)$ such that one may write

$$Y_{j \geq 2} = Y_j^{\text{uni}} + Y_j^{\text{SD}},\tag{5.58}$$

Let

$$Y_{K\pi}^{(n)}(L) = Y_K^{(n)}(L) - Y_\pi^{(n)}(L).\tag{5.59}$$

At $\mathcal{O}(1/L)$, we have

$$Y_{K\pi}^{(1)}(48) = -3.958.\tag{5.60}$$

Up to $\mathcal{O}(1/L^2)$, we have

$$\begin{aligned}
Y_{K\pi}^{(2)}(48) &= Y_{K\pi}^{(1)}(48) + \frac{M_\pi^2}{(M_\pi L)^2} (Y_2^K - Y_2^\pi), \\
&= -3.958 + \frac{1}{(M_\pi L)^2} (17.3197 - 51.0118) \\
&= -6.20472.
\end{aligned} \tag{5.61}$$

At $\mathcal{O}(1/L^3)$, in addition to the universal and structure-dependent contributions, there is an additional branch cut contribution that is specific to the QED_L prescription, the latter two of which are currently under study. Adding to our $\mathcal{O}(1/L^2)$ result the universal contribution in the next order, we have

$$\begin{aligned}
Y_{K\pi}^{(3),\text{uni}}(48) &= Y_{K\pi}^{(2)}(48) + \frac{M_\pi^3}{(M_\pi L)^3} (Y_3^{K,\text{uni}} - Y_3^{\pi,\text{uni}}) \\
&= -6.20472 + \frac{1}{(M_\pi L)^3} (-12.7647 - (-208.759)) \\
&= -2.8298.
\end{aligned} \tag{5.62}$$

Let us compare the second line of Equations (5.61) and (5.62). We observe that $M_\pi^2 Y_2^P = -M_\pi^3 Y_3^{P,\text{uni}}$ for $P = K, \pi$. Together with an enhanced $Y_3^{\pi,\text{uni}}$ value, including the universal $\mathcal{O}(1/L^3)$ term drives total contribution towards the $Y_{K\pi}^{(1)}$ value. Taking the following ratio,

$$\frac{Y_{K\pi}^{(3),\text{pt}}(48) - Y_{K\pi}^{(2)}(48)}{Y_{K\pi}^{(2)}(48)} \approx -0.54, \tag{5.63}$$

we find $\sim 50\%$ shift when we include the $\mathcal{O}(1/L^3)$ universal term. Since we have incomplete knowledge of the full $\mathcal{O}(1/L^3)$ contribution, we restrict the finite volume corrections to $\mathcal{O}(1/L^2)$ and assign as systematic uncertainty 50% on the central value (Equation 5.61):

$$Y_{K\pi}^{(2)} = -6.20(3.10). \tag{5.64}$$

Propagating this through Equation (5.8), we obtain

$$\delta R_{K\pi} = -0.00875(367)_{\text{FVE}}. \tag{5.65}$$

Total Error Budget

The above error budget estimations are summarised in Table 5.3. The statistical and systematic contributions may be added in quadrature to produce the total error, which is shown in the bottom two rows of the table.

We observe that the dominant contribution by far comes from the finite volume systematics. This conservative estimation is due to the fact that there is currently insufficient information about the structure-dependent and branch cut piece at $\mathcal{O}(1/L^3)$. From comparing the total error with and without the finite volume systematics, we see that there is an average factor of 3 between them. Hence, further investigations into the structure-dependent terms is a highly attractive prospect. Additionally, the discretisation effects may be better controlled when data from a second set of lattice spacing becomes available. At the time of writing, data with electromagnetic current insertion on the sea quarks are becoming available, which will remove the systematics from a electro-quenched QED setup and instead modify the statistical and fit systematics.

$\delta R_{K\pi}$	
central value	−0.00875
statistical	$\left(\begin{smallmatrix} +64 \\ -45 \end{smallmatrix}\right)$
QED quenching	(± 47)
fit	$\left(\begin{smallmatrix} +112 \\ -38 \end{smallmatrix}\right)$
discretisation	(± 54)
FVE	(± 367)
total	$\left(\begin{smallmatrix} +395 \\ -378 \end{smallmatrix}\right)$
total (w/o FVE)	$\left(\begin{smallmatrix} +147 \\ -93 \end{smallmatrix}\right)$

Table 5.3 *Error budget of $\delta R_{K\pi}$. The total error is obtained by adding each contribution in quadrature.*

Table 5.4 compares this calculation with currently published results. The only other lattice calculation was published by the RM123-Soton collaboration. Using the formula

$$N = \frac{|y_1 - y_2|}{\sqrt{\sigma_1^2 + \sigma_2^2}} \quad (5.66)$$

to calculate the number of σ 's for measurements $y_{1,2}$ with standard deviations $\sigma_{1,2}$, we find that, neglecting our conservative FVE estimation, there is $\sim 2.1\sigma$ tension between this work and RM123-Soton's. For our work, we have

symmetrised the error using $\sigma = \frac{1}{2}(\sigma_+ + \sigma_-)$, where $\sigma_{\pm}$ are the upper/lower bound. Interestingly, both lattice results (RM123-Soton and this work) are consistent with χ PT predictions [64], owing to its large uncertainty. Figure 5.23 summarises the results in Table 5.4.

	$\delta R_{K\pi}$
RM123-Soton[41, 65, 66]	$-0.0126(14)$,
χ PT [64]	$-0.0112(42)$
this work	$-0.00875(^{+395}_{-378})$
this work w/o FVE	$-0.00875(^{+147}_{-93})$

Table 5.4 *Comparison of $\delta R_{K\pi}$ from currently published results. Error quoted in this table is the total error.*

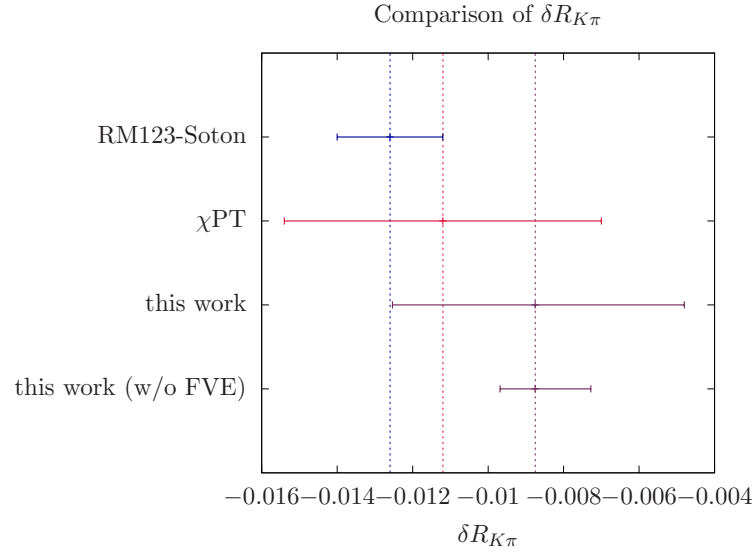


Figure 5.23 *Comparison of currently published results for $\delta R_{K\pi}$ with this work.*

5.6 Determination of $\frac{|V_{us}|}{|V_{ud}|}$

With the isospin-breaking corrections computed, we are finally in the position to determine the CKM matrix element ratio $\frac{|V_{us}|}{|V_{ud}|}$. Recall that this is related to the ratio of inclusive decay rates via the master formula

$$\frac{|V_{us}|^2}{|V_{ud}|^2} = \frac{\Gamma(K^+ \rightarrow \mu^+ \nu_\mu [\gamma])}{\Gamma(\pi^+ \rightarrow \mu^+ \nu_\mu [\gamma])} \frac{M_{K^+}^3}{M_{\pi^+}^3} \frac{(M_{\pi^+}^2 - m_{\mu^+}^2)^2}{(M_{K^+}^2 - m_{\mu^+}^2)^2} \mathcal{F}^{-1}, \quad (5.67)$$

where

$$\mathcal{F} = \frac{|f_K|^2}{|f_\pi|^2} (1 + \delta R_{K\pi}) \quad (5.68)$$

and f_K/f_π is the ratio of decay constants determined in the isosymmetric QCD theory of choice. As mentioned in §2.4, the terms on the RHS of Equation (5.67) that multiply $\mathcal{F}^{-1}$ may be evaluated using inputs from the PDG [4]. These are tabulated in Table 5.5. To obtain the inclusive rate, we require experimental measurements of the branching ratio $\mathcal{B}$ and mean lifetime τ of the pseudoscalar to evaluate the following relation:

$$\Gamma(P \rightarrow \mu^+ \nu_\mu [\gamma]) = \frac{\mathcal{B}(P \rightarrow \mu^+ \nu_\mu [\gamma])}{\tau_P}, \quad (5.69)$$

for $P = \pi^+, K^+$. This is especially crucial for the charged kaon, which decays into a muon lepton-neutrino pair $\sim 63\%$ of the time. Thus, Equation (5.67) is modified into

$$\frac{V_{us}}{V_{ud}} = \left[\frac{\mathcal{B}(K^+ \rightarrow \mu^+ \nu_\mu [\gamma])}{\mathcal{B}(\pi^+ \rightarrow \mu^+ \nu_\mu [\gamma])} \frac{\tau_{\pi^+}}{\tau_{K^+}} \frac{M_{K^+}^3}{M_{\pi^+}^3} \frac{(M_{\pi^+}^2 - m_{\mu^+}^2)^2}{(M_{K^+}^2 - m_{\mu^+}^2)^2} \mathcal{F}^{-1} \right]^{\frac{1}{2}}. \quad (5.70)$$

P	π	K
$\mathcal{B}(P^+ \rightarrow \mu^+ \nu_\mu [\gamma])$	0.9998770(4)	0.6356(11)
τ_{P^+}	$2.6033(5) \times 10^{-8} \text{ s}$	$1.2380(20) \times 10^{-8} \text{ s}$
M_{P^+}	139.57039(18) MeV	493.677(16) MeV
m_{μ^+}	105.6583745(24) MeV	

Table 5.5 *The branching ratio, mean lifetime and the mass for the light pseudoscalars π^+ and K^+ and the μ^+ mass, as reported in the 2020 edition of the PDG.*

Using this work's $\delta R_{K\pi}$ and $\frac{f_K}{f_\pi}$, we obtain

$$(\text{this work}) \quad \frac{|V_{us}|}{|V_{ud}|} = 0.23166(45)_{\delta R_{K\pi}} (1176)_{\frac{f_K}{f_\pi}} (28)_{\text{exp.}}, \quad (5.71)$$

where the errors are factorised into the $\delta R_{K\pi}$, decay constant ratio and experimental precision, respectively. The significant uncertainty on the ratio

of decay constants comes from an additional discretisation error since this is the result from a single lattice spacing. For reference, we also show a prediction where the FV estimation in the error budget of $\delta R_{K\pi}$ is neglected:

$$(\text{this work w/o FVE}) \quad \frac{|V_{us}|}{|V_{ud}|} = 0.23166(14)_{\delta R_{K\pi}} (1176)_{\frac{f_K}{f_\pi}} (28)_{\text{exp.}}, \quad (5.72)$$

i.e. the precision of $\delta R_{K\pi}$ is now better than the experiment's. This is a strong motivation for further analytic studies to better control the $\mathcal{O}(1/L^3)$ FV uncertainties.

We could repeat the exercise for the other two published results. First, Cirigliano and Neufeld calculated $\delta R_{K\pi}$ from χ PT [64] and used the FLAG 2 + 1 average of $\frac{f_K}{f_\pi}$ and experimental inputs from the Flavia Working group on Kaon decays [67] and the PDG2010[68]. Using their result of $\delta R_{K\pi} = -0.0112(42)$, we update their determination of the CKM matrix element ratio with the new 2 + 1 FLAG average and PDG inputs, giving

$$(\chi\text{PT}) \quad \frac{|V_{us}|}{|V_{ud}|} = 0.23184(24)_{\delta R_{K\pi}} (65)_{\frac{f_K}{f_\pi}} (28)_{\text{exp.}}. \quad (5.73)$$

The first lattice calculation of $\delta R_{K\pi}$ was done by RM123-Soton (see [40] and reference therein). For $\frac{|V_{us}|}{|V_{ud}|}$, they used the 2 + 1 + 1 FLAG average for $\frac{f_K}{f_\pi}$. Together with $\delta R_{K\pi} = -0.0126(14)$, this gives

$$(\text{RM123-Soton}) \quad \frac{|V_{us}|}{|V_{ud}|} = 0.23131(17)_{\delta R_{K\pi}} (35)_{\frac{f_K}{f_\pi}} (28)_{\text{exp.}}. \quad (5.74)$$

In all three cases, there is good control over the precision of $\delta R_{K\pi}$. Interestingly, although initially motivated by the sub-percent level precision of $\frac{f_K}{f_\pi}$, we find that this is the dominant source of error. Indeed, in Table 5.6, we determine $\frac{|V_{us}|}{|V_{ud}|}$ using our value of $\delta R_{K\pi}$ (excluding FV error) and experimental inputs from the PDG, varying only the inputs for the decay constant ratio. Note that for the entries labelled ‘FLAG 2 + 1(+1) average’, we calculate the weighted average and variance using the FLAG prescription [20]. Since we do not have information on the correlations of results between collaborations, we set $C_{i,j} = 0$ for $i \neq j$. Thus, we to believe these two errors are underestimated. We remind the reader that the $\frac{|V_{us}|}{|V_{ud}|}$ predicted in Table 5.6 are not strictly speaking scheme-independent, since the $\delta R_{K\pi}$ and $\frac{f_K}{f_\pi}$ are determined in different tuning prescriptions. The general conclusion is nevertheless clear - even with the state-of-the-art $\frac{f_K}{f_\pi}$ determination

(*i.e.* see results from RBC/UKQCD[61] and FNAL/MILC[69]), it remains the dominant source of error in our efforts to obtain a precise determination of the CKM matrix element ratio. This also implies that the experimental contributions are sufficiently precise at the current standard of $\frac{|V_{us}|}{|V_{ud}|}$. Now that $\delta R_{K\pi}$ is under control, this incentivises us to re-invest our efforts in pursuing greater precision on $\frac{f_K}{f_\pi}$.

	$\frac{f_K}{f_\pi}$	$\frac{ V_{us} }{ V_{ud} }$
this work	1.1925(596)	0.23166(14)(1176)(28)
FLAG 2+1 best (RBC/UKQCD14 48I)	1.1945(45)	0.23127(14)(87)(28)
FLAG 2+1 average	1.1930(33)	0.23155(14)(65)(28)
FLAG 2+1+1 best (FNAL/MILC 17)	1.1980(15)	0.2306(14)(28)(28)
FLAG 2+1+1 average	1.1966(12)	0.23087(14)(24)(28)

Table 5.6 *Error breakdown of $\frac{|V_{us}|}{|V_{ud}|}$ based on this work’s determination of $\delta R_{K\pi}$ (without FV errors), experimental inputs from the PDG and different inputs of decay constant ratios $\frac{f_K}{f_\pi}$. The first, second and third parentheses of the $\frac{|V_{us}|}{|V_{ud}|}$ column are the $\delta R_{K\pi}$, $\frac{f_K}{f_\pi}$ and experimental errors, respectively.*

Chapter 6

Conclusion & Outlook

In this thesis, we provide an update to the ratio of CKM matrix element $\frac{|V_{us}|}{|V_{ud}|}$. This is extracted from a ratio leptonic decay rates, which comes with non-perturbative hadronic matrix elements. To date, lattice determinations of relevant hadronic quantities, such as the decay constants, have reached percent-level precision. Further improvements necessitates the inclusion of isospin-breaking effects.

In context of this work, we calculated the isospin-breaking correction to the decay amplitude $\delta R_{K\pi}$ on the lattice. This was done using near-physical chiral fermions in the Domain Wall Fermion setup. The isospin-breaking effects were introduced via the perturbative method, where scalar currents and local $\mathcal{A}$ electromagnetic currents were sequentially inserted into quark propagators. By studying the functional form of these finite-time correlators, we performed a series of fits to extract all the components required to build $\delta R_{K\pi}$. We adopted a data-driven approach for this stage of the work, allowing the Akaike Information Criteria (AIC) to decide the best fits for each analysis. For analyses with prohibitively large number of fits, we employed the genetic algorithm (GA) as a means to explore a subset of the search space. While there is no guarantee for a heuristic algorithm to find the best fit of the whole search space, the GA is a much more practical approach than the brute force computation of each fit. Due to the data-driven ethos, we chose five fits with the highest AIC weight from each analysis to generate a distribution of $\delta R_{K\pi}$. Then, its central value and statistical error were determined from the histograms associated to this distribution. Upon estimating the error budget, the finite volume correction turned out to be the dominant source of error, owing to an incomplete knowledge of the $\mathcal{O}(1/L^3)$ term. Further

analytical studies of the structure-dependent and branch cut contributions at $\mathcal{O}(1/L^3)$ are thus highly desirable. Once $\delta R_{K\pi}$ and $\frac{f_K}{f_\pi}$ were determined, we combined it with experimental measurements to obtain a prediction of the CKM matrix element ratio,

$$\begin{aligned} \text{(this work)} \quad \frac{|V_{us}|}{|V_{ud}|} &= 0.23166(45)_{\delta R_{K\pi}} (1176)_{\frac{f_K}{f_\pi}} (28)_{\text{exp.}}, \\ \text{(this work w/o FVE)} \quad \frac{|V_{us}|}{|V_{ud}|} &= 0.23166(14)_{\delta R_{K\pi}} (1176)_{\frac{f_K}{f_\pi}} (28)_{\text{exp.}}, \end{aligned}$$

where the different sources of errors are separated by parentheses. We found that the dominant source of error is coming from the ratio of decay constants. In a comparison exercise, the state-of-the-art $\frac{f_K}{f_\pi}$ was, at best, comparable with the experimental precision. This should revive efforts to provide even more precise determinations of $\frac{f_K}{f_\pi}$ among the lattice community.

Besides the ongoing effort to control the finite volume systematics, there are several short-term projects that can further improve our results. Since $\delta R_{K\pi}$ was computed on a single lattice spacing, continuum extrapolation to the physical point ($a \rightarrow 0$) is not available. Although our current setup produces near-physical hadronic masses, at least two more predictions of $\delta R_{K\pi}$ from setups with different lattice spacing should be prioritised for better control of the $a \rightarrow 0$ extrapolation. Additionally, we remind the reader that this calculation neglects disconnected QCD contributions and QED effects from the sea quarks. At the time of writing, data corresponding to disconnected quark loop contributions for this setup are becoming readily available. Analysing them will give us a more realistic estimation of statistical error. Finally, recall that we circumvented the need to renormalise the effective weak Hamiltonian by computing a ratio of CKM matrix elements. However, to provide a prediction of V_{ud} and V_{us} separately, we need to renormalise the weak operator by calculating $\delta\mathcal{Z}/\mathcal{Z}$ on the lattice.

As we close, let us consider the middle- and long-term prospects. The theoretical formulation presented in this thesis was applied to π and K mesons though, in principle, one can use this to calculate the isospin-breaking correction to the decay amplitude of heavier pseudoscalars. An example application would be the leptonic decays of charmed mesons, *e.g.* D or D_s , where V_{cd} and V_{cs} can be predicted instead. Another avenue of investigation is the semi-leptonic decays of kaons, *e.g.* $K^+ \rightarrow \pi^0 \ell^+ \nu_\ell$ and $K^0 \rightarrow \pi^+ \ell^- \bar{\nu}_\ell$ and their charge conjugate modes, or $K_{\ell 3}$ for short. These will provide another constraint on V_{us} . Isospin-breaking

corrections for these decay amplitudes are currently estimated using χ PT. A first principle calculation of the isospin-breaking corrections on the lattice would be a very attractive prospect.

Appendix A

Bootstrap Resampling

The expectation value of an observable O may be estimated by the average over N independent measurements , *i.e.*

$$\langle O \rangle \approx \bar{O} = \frac{1}{N} \sum_{i=1}^N O_i. \quad (\text{A.1})$$

For an observable that follows a Gaussian distribution, this estimation comes with a variance

$$\sigma^2 = \frac{1}{N-1} \sum_{i=1}^N (\bar{O} - O_i)^2. \quad (\text{A.2})$$

According to the Central Limit Theorem, we expect to recover the ‘true’ expectation value in the limit where $N \rightarrow \infty$.

In the context of lattice simulations, the large N limit is computationally expensive to achieve. Since gauge fields are generated using Markov chain methods, the measurements are not completely independent either since they suffer from autocorrelation. To work around this, we either take measurements which are sufficiently far apart in the Markov chain such that autocorrelations are suppressed, or we bin clusters of measurements and treat the binned data as independent. Both approaches are expensive since the former requires more computer time while the latter more measurements to compensate for statistics.

To resolve this no-win scenario, we apply the *bootstrap resampling* method on our finite measurements. This resampling technique improves the statistics with ‘fake’ data. Let S_0 be a vector containing the original N measurements we have

made:

$$S_0 = (C_1, C_2, \dots, C_N), \quad (\text{A.3})$$

where C_i denotes the i 'th measurement. We call S_0 the *original sample*. We can generate k new samples of size N by randomly selecting from the set of measurements available in S_0 . We call these the *bootstrap samples*. That is,

$$\begin{aligned} S_1 &= (\dots), \\ &\vdots \\ S_k &= (\dots), \quad \text{where } k > N, \end{aligned} \quad (\text{A.4})$$

where $k > N$ and the ellipses represent the N measurements for each sample S_k . Note that measurements of the original sample may be selected repeatedly in each of these generated samples, *i.e.* a sample such as $(\dots, C_4, C_{17}, C_4, C_4, \dots)$ is allowed. Let $\hat{\theta}$ be the mean of the original sample,

$$\hat{\theta} = \frac{1}{N} \sum_{i=1}^N S_{0,i}, \quad (\text{A.5})$$

where an additional subscript i denotes the i 'th measurement in S_0 . The variance takes the following form:

$$\sigma^2 = \frac{1}{k} \sum_{j=0}^k (\theta_j - \hat{\theta})^2, \quad \text{for } k \geq 1, \quad (\text{A.6})$$

where

$$\theta_j = \frac{1}{N} \sum_{i=0}^N S_{j,i} \quad (\text{A.7})$$

is the average of the j 'th bootstrap sample.

Then, for N measurements of an n -point time correlator with N_T number of timeslices, the central value of each timeslice t is determined by $\hat{\theta}(t)$ in Equation (A.5) and its variance $\sigma^2(t)$ by Equation (A.6).

Appendix B

ZMöbius-to-Möbius Correction

In Figures B.1-B.5, we compare the magnitude of the Möbius correction with the statistical precision of each ZMöbius time correlator. These show the consistent hierarchy mentioned in the main text. Namely, the Möbius correction signal is visible in the π^+ correlators while in the K^+ correlators, the correction is, at best, comparable with the statistical precision. The only exception is the non-factorisable correlator, where the Möbius correction is on average comparable with the statistical precision of the ZMöbius correlators.

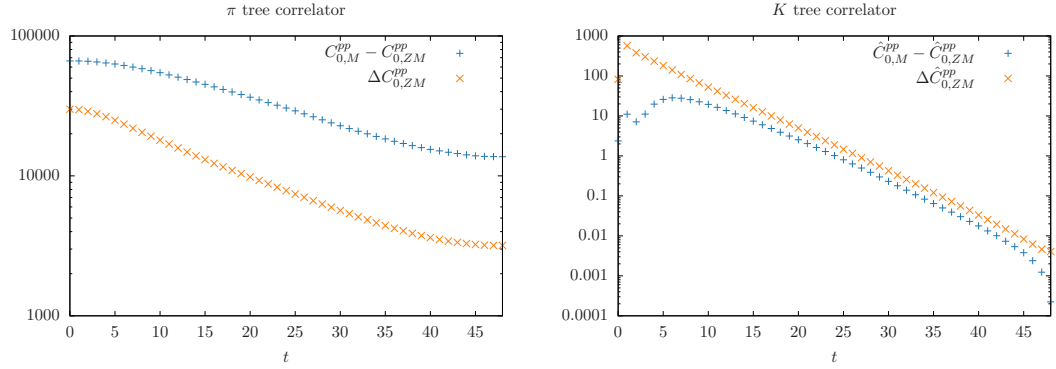


Figure B.1 *Comparison of the Möbius correction central value (blue) to the statistical error of the ZMöbius correlators (orange) for the π^+ and K^+ meson. Both sets are wall-pt pp QCD-only correlators.*

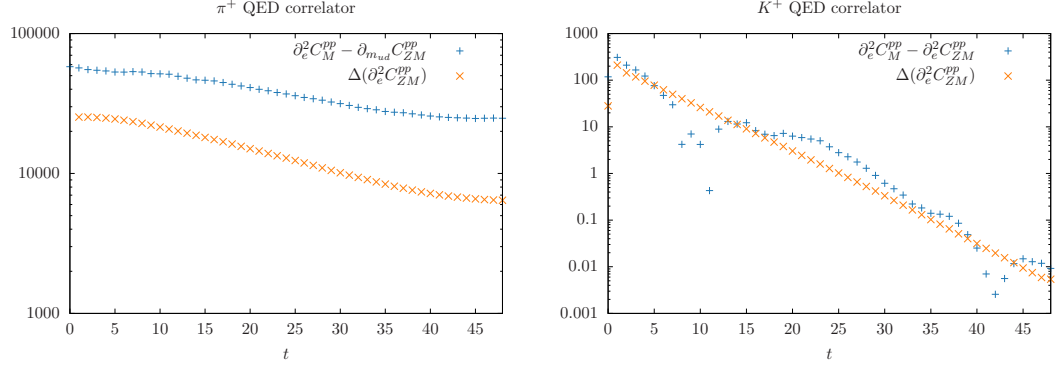


Figure B.2 Comparison of the Möbius correction central value (blue) to the statistical error of the ZMöbius correlators (orange) for the π^+ and K^+ meson. Both sets are wall-pt pp correlators with local E.M. current insertions.

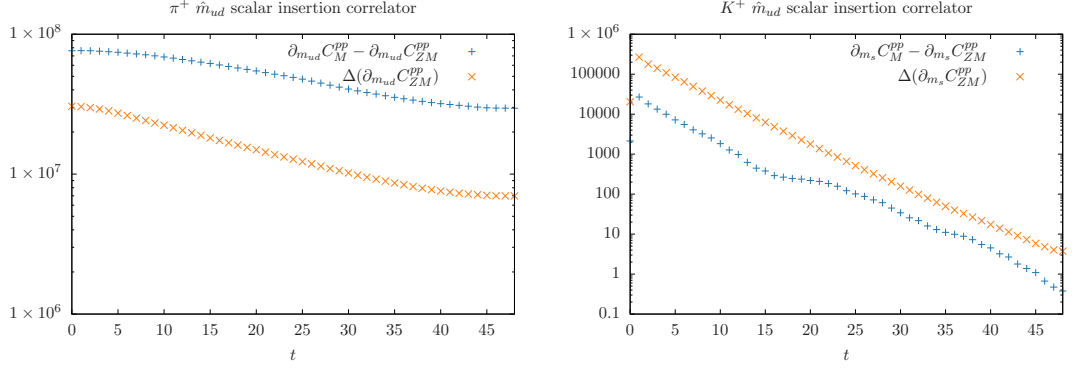


Figure B.3 Comparison of the Möbius correction central value (blue) to the statistical error of the ZMöbius correlators (orange) for the π^+ and K^+ meson. Both sets are wall-pt pp correlators with light quark scalar current insertions.

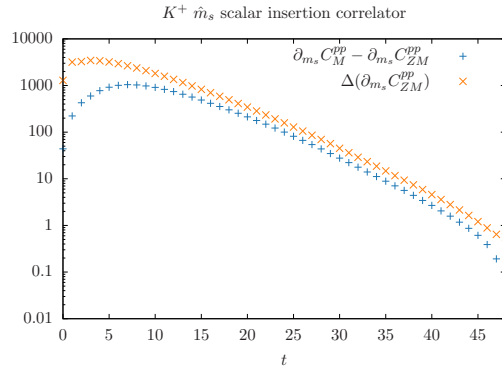


Figure B.4 Comparison of the Möbius correction central value (blue) to the statistical error of the ZMöbius correlators (orange) for the K^+ meson. These correspond to the wall-pt pp correlators with strange quark scalar current insertions.

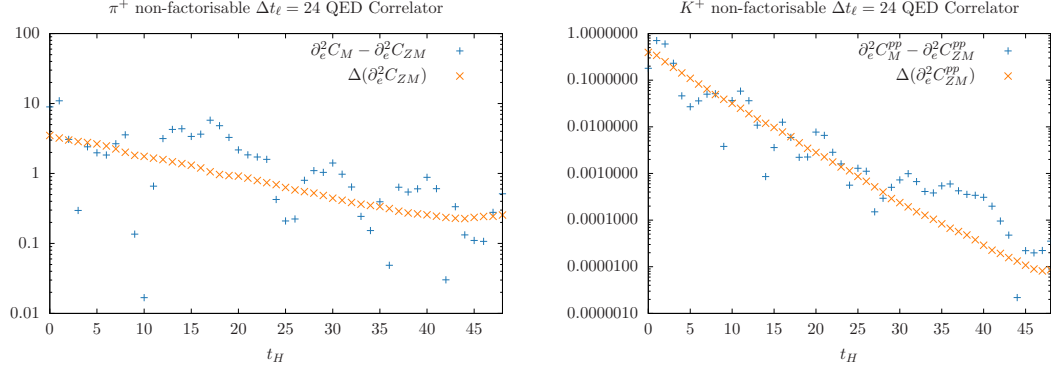


Figure B.5 Comparison of the Möbius correction central value (blue) to the statistical error of the ZMöbius correlators (orange) for the π^+ and K^+ meson. Both sets are non-factorisable wall-pt pa correlators with local E.M. current insertions.

Tables B.1 and B.2 show a comparison of the factorisable fit results from the ZMöbius and Möbius-corrected correlators. Besides the presence of Möbius correction, the only difference is the fit choice, which is directly related to the signal quality of the data with/without said correction. In the O^{ZM} and O^M columns, we find that there is a consistent but slight decrease in statistical precision, where the worst is by a factor of ~ 6 . Additionally, there is a statistically significant discrepancy in the correlated difference between the ZMöbius and Möbius results, with the exception of $\frac{\partial_e^2 \mathcal{A}_{\pi^+}}{\hat{\mathcal{A}}_\pi}$ and $\partial_e^2 M_K$. The correlated ratio shows that this Möbius correction can contribute up to $\sim \mathcal{O}(1\%)$ in the case of $\partial_{m_{ud}} M_{K^+}$ and $\frac{\partial_e^2 \mathcal{A}_{K^+}}{\hat{\mathcal{A}}_K}$.

This comparison shows that it is prudent to include Möbius correction in the time correlators generated from our lattice setup.

	O^{ZM}	O^M	$O^M - O^{ZM}$	O^M / O^{ZM}
$\hat{M}_\pi$	0.080066(18)	0.080658(44)	$5.92(45) \times 10^{-4}$	1.00739(56)
$\partial_{m_{ud}} M_{\pi^+}$	28.199(10)	28.018(30)	$-0.181(30)$	0.9936(11)
$\partial_e^2 M_{\pi^+}$	0.024161(10)	0.024035(67)	$-1.26(68) \times 10^{-4}$	0.9948(28)
$\frac{\partial_{eq}^2 \mathcal{A}_{\pi^+}}{\hat{\mathcal{A}}_\pi}$	0.05914(58)	0.05939(82)	$2.5(8.2) \times 10^{-4}$	1.004(14)

Table B.1 Comparison of π^+ meson factorisable fit results from ZMöbius and Möbius correlators and ratios. The second and third column are the ZMöbius and Möbius fit results, respectively. The fourth and fifth columns are the correlated difference and ratio, respectively.

	O^{ZM}	O^M	$O^M - O^{ZM}$	O^M/O^{ZM}
$\hat{M}_K$	0.288778(17)	0.288541(70)	$-2.38(70) \times 10^{-4}$	0.99918(24)
$\partial_{m_{ud}} M_{K^+}$	3.802(11)	3.641(11)	-0.161(16)	0.9576(40)
$\partial_{m_s} M_{K^+}$	3.7492(14)	3.76209(97)	0.0128(19)	1.00343(50)
$\partial_e^2 M_{K^+}$	0.011543(15)	0.011558(32)	$1.5(3.8) \times 10^{-5}$	1.0013(33)
$\frac{\partial_{eq}^2 \mathcal{A}_{K^+}}{\hat{\mathcal{A}}_K}$	0.03417(42)	0.03245(66)	$-1.72(72) \times 10^{-3}$	0.950(21)

Table B.2 *Comparison of K^+ meson factorisable fit results from ZMöbius and Möbius correlators and ratios. The second and third column are the ZMöbius and Möbius fit results, respectively. The fourth and fifth columns are the correlated difference and ratio, respectively.*

Appendix C

Genetic Algorithm

In this appendix, the GA setup for this calculation will be explained in detail. First, we will consider the genetic operators used. Then, we will present the GA hyperparameters used to produce the factorisable analysis fit results in this work.

Consider two candidate fit intervals, $\boldsymbol{\tau}_k, \boldsymbol{\tau}_{k'} \in P_0$. The crossover operator X generates a new $\boldsymbol{\tau}$ with fit intervals from either of the parent's $\tau^{(j)}$'s, based on a crossover probability p . That is,

$$\boldsymbol{\tau}_{k''} \equiv X(\boldsymbol{\tau}_k, \boldsymbol{\tau}_{k'}) = \left\{ X(\tau_k^{(1)}, \tau_{k'}^{(1)}), \dots, X(\tau_k^{(N_{corr})}, \tau_{k'}^{(N_{corr})}) \right\}, \quad (\text{C.1})$$

where

$$X(\tau_k^j, \tau_{k'}^j) = \begin{cases} \tau_k^j & \text{if } p < 0.5, \\ \tau_{k'}^j & \text{otherwise.} \end{cases} \quad (\text{C.2})$$

This is called *uniform crossover* in literature. Others definitions, such as the single-/multi-point crossover [50], are not considered in this work. We allow the crossover operator to act on the initial P_0 to generate an additional P_c population members.

Once the crossover phase is complete, the population size is now $P \geq P_0$, where the equality is satisfied when the initial population members are sufficiently identical that no distinct offspring can be produced. The mutation operator M then mutates the population $\boldsymbol{\tau}_1, \dots, \boldsymbol{\tau}_P$ at a rate m . That is, for some randomly

drawn $0 \leq p \leq 1$,

$$M(\boldsymbol{\tau}_k) = \begin{cases} \boldsymbol{\tau}_{P+1}, & \text{if } p < m \\ \boldsymbol{\tau}_k & \text{otherwise,} \end{cases} \quad (\text{C.3})$$

where

$$\boldsymbol{\tau}_{P+1} \equiv \left\{ \tau_{P+1}^{(1)}, \dots, M(\tau_{P+1}^{(j)}), \dots, \tau_{P+1}^{(N_{corr})} \right\} \quad (\text{C.4})$$

with $1 \leq j \leq N_{corr}$ also randomly drawn and $M(\tau_{P+1}^{(j)})$ is a fit interval where either t_{min} or t_{max} or both have been modified randomly. The mutation operator defined as in Equation (C.3) ensures that the top P_0 candidates (ranked by AIC weights) are always kept in each generation until a fitter candidate replaces them.

With the operators defined, we can discuss the GA parameters used for this work. To begin, the free parameters in a GA are: the initial population P_0 ; the crossover rate, which is parametrised in this work by the population size after crossover P ; the mutation rate m ; the weight function w to optimise; the maximum number of generations G_{max} and the termination condition. According to a review done by Mitchell [50], there is no one-size-fits-all set of GA parameter inputs. As such, we studied three GA setups to check the validity of our fit conclusions. These are summarised in Table C.1.

First, let

$$\bar{w}_N = \frac{1}{N} \sum_{i=1}^N w_i \quad (\text{C.5})$$

be the average of the top N weights in each generation. In all three setups, we aim to maximise the AIC in each GA run, which terminates when $\bar{w}_5$ does not improve over 1000 successive generations. If this condition cannot be satisfied, we impose a cut-off when a GA run exceeds G_{max} generations. In practice, however, none of the runs hit this cut-off limit. To accelerate the GA in its exploration of the $\boldsymbol{\tau}$ -space, we need to prevent the algorithm returning to the same $\boldsymbol{\tau}$, *i.e.* the GA must have a memory of fits performed in preceding generations. This is achieved by storing previous $\boldsymbol{\tau}$ candidates in an ‘ancestor’ container and checking new offspring against them.

Let the label ‘GAX-Y’ refer to a GA setup with $P_0 = X$ that produces $Y \times 10^3$ fittest candidates across a large number of runs. We first consider ‘GA5-2’ and ‘GA25-2’. The chief differences between these are the initial population P_0 and the number of distinct P_0 inputs, *i.e.* each input has P_0 distinct $\boldsymbol{\tau}$ ’s. To match their statistics, this choice in P_0 will determine the number of seeds required. Here

the seed refers to an integer used to initialise the `std::mt19937` rng required by the genetic operators. For ‘GA5-2’ and ‘GA25-2’, this amounts to running 40 and 80 independently seeded GA runs, respectively. Figure C.1 shows the range of AIC weights of the top 2000 GA winners from each setup, sorted by their weights in descending order. Two features are worth commenting on: 1) that the top weight, indexed by GA candidate #1, in both setups have the same order of magnitude demonstrates that the GA runs with different inputs are converging on τ ’s with similar χ^2 and N_{dof} . 2) the range of AIC weights is narrower in ‘GA25-2’ than ‘GA5-2’ for both pion and kaon. This agrees with intuition since a larger initial population allows greater genetic diversity per generation, and so the likelihood of finding candidates with better AIC weights is improved. For reference, the average number of ancestors per run are shown in Table C.2. Indeed, that searching through a larger volume and converging on the same order of magnitude is an encouragement that the GA, within the allowed runtime, has found a region of optimal τ based on the AIC.

	GA5-2	GA25-2	GA25-5
number of seeds	40	80	200
number of inputs	10	1	1
P_0	5	25	25
P	20	100	100
m	0.3	0.3	0.3
G_{max}	25000	10000	10000
termination con. #1	$\bar{w}_5$ unchanged for 1000 generations		
termination con. #2	GA exceeds G_{max}		
total GA winners	2000	2000	5000

Table C.1 *Table of three different GA setups used in this work. All setups maximise the AIC weight. The average weight $\bar{w}_5$ is defined in the text below Equation (C.5). The total number of GA winners within each run is the product of the first three rows.*

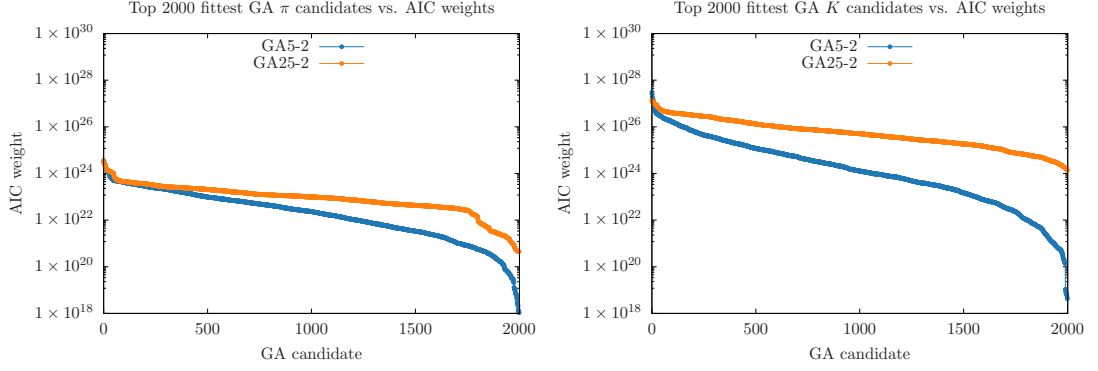


Figure C.1 Comparison of the top 2000 fittest GA τ candidates between two setups, sorted in descending order of AIC weights, for π (left) and K (right) meson.

Since it is not guaranteed *a priori* that the $F^{(n)}$ associated with τ 's of the same weight are consistent, we check this by considering an extension to ‘GA25-2’, where we boosted the statistics by running $\times 2.5$ more GA runs, *i.e.* to obtain 3000 more GA winners, totalling to 5000. This is GA25-5 in Table C.1. We find again that the top weights match in order of magnitude (see Figure C.2). To check whether the $F^{(n)}(\tau)$ of the fittest candidates are stable, we take the top 5 of both setups and generate a histogram of $\delta R_{K\pi}^{\text{latt.}}$ each. This is shown in Figure C.3, along with their median, its statistical error and the fit systematics (see §5.5) superimposed on the histograms. We see that they exhibit similar features, with their medians within each other’s statistical error. The fact that a 150% increase in statistics does not change the median is compelling evidence that the GA is converging on a consistent set of candidates for $F^{(n)}$.

	GA5-2	GA25-2	GA25-5
π	4085.915	32854.5375	33767.365
K	4726.1425	34430.625	33975.085

Table C.2 The average number of ancestors per GA run for each setup and meson.

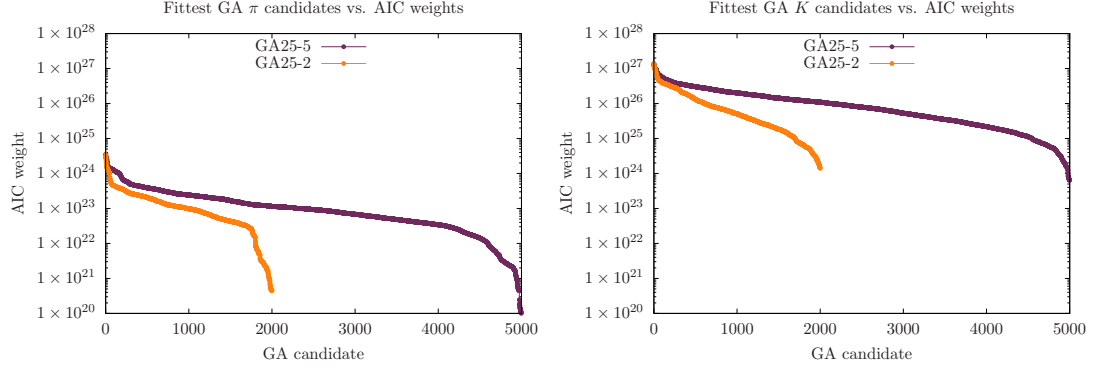


Figure C.2 Comparison of the fittest GA τ candidates between setups ‘GA25-5’ and ‘GA25-2’, sorted in descending order of AIC weights, for the π (left) and K (right) meson.

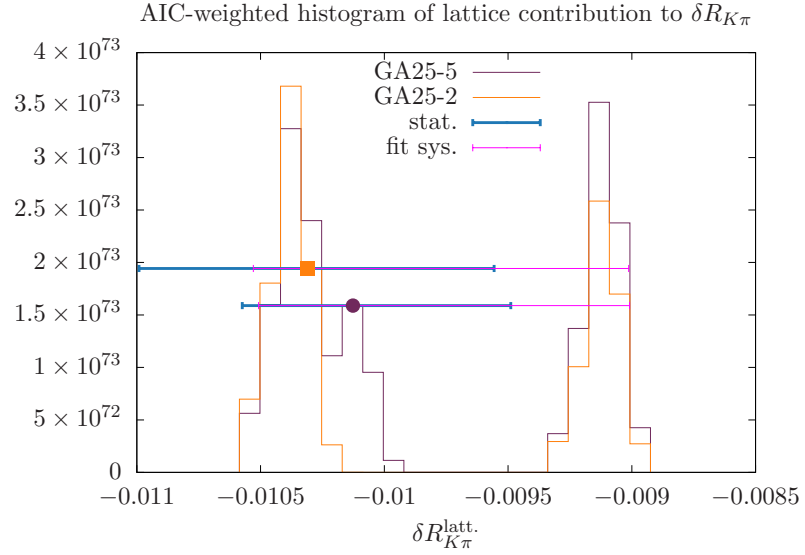


Figure C.3 Histogram generated from top 5 fits of each analysis. Each histogram event is weighted by the total AIC weight. The median of each histogram, along with its statistical error (blue) and the fit systematics (magenta) are superimposed on the histogram.

Appendix D

Local vs. Conserved - a Tale of Two Currents

When this work was conducted, the conserved E.M. implementation for Domain Wall Fermions was not available. Instead, we use a ‘local’ implementation of the E.M. current. When the currents are summed over all lattice sites, an additional tadpole diagram emerges from the conserved implementation whenever the photon legs overlap on the same lattice site. In this appendix, we predict a number of E.M.-sensitive observables using the two current implementations on a smaller lattice to study the differences between them. The specifications of this setup are presented in Table D.1.

action	Shamir Domain Wall Fermions
volume $L^3 \times T \times L_s$	$24^3 \times 64 \times 16$
(inverse) lattice spacing a^{-1}	1730(30)MeV
$\hat{M}_\pi$	339.789(12) MeV
number of QCD config.	10
source positions per config.	32

Table D.1 *Ensemble details.*

In Figure D.1, we provide the effective mass contribution from correlators with E.M. current insertion, computed using Equation (4.80). A fit to the plateaux will give us the diagrammatic contribution to the π^+ meson mass. In Figure D.1(**left**), where both current insertions are on a single quark propagator, the presence of the

tadpole diagram is evident from the approximate factor of 3 difference between the local and conserved plateau. In Figure D.1(**right**), the tapdole diagram is not present since each quark propagator has only a single current insertion. Upon renormalising with $Z_V = 0.71399$ [55], we find that the discrepancy between the local and conserved photon exchange data is up to $\sim 2.5\%$. The K^+ effective masses exhibit a similar trend.

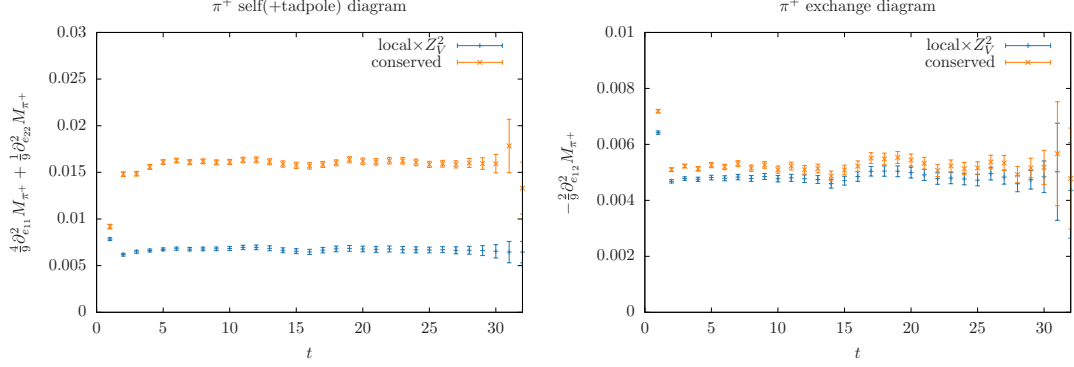


Figure D.1 *left: the self energy (and tadpole) contribution to the π^+ mass. right: the photon exchange contribution to the π^+ mass.*

Table D.2 shows the results of electromagnetic corrections to mass and amplitude, extracted from local and conserved correlator fits. With the exception of the non-factorisable amplitudes, the derivatives computed with local currents are consistently smaller in magnitude to those of conserved currents. In particular, this hierarchy in the mass derivatives will affect the tuning procedure and hence the physical observables we wish to predict.

	local	conserved		local	conserved
$\frac{\partial M_{\pi^+}^2}{\partial e^2}$	0.005476(38)	0.009160(30)	$\frac{\partial_{e_q}^2 \mathcal{A}_{\pi^+}}{\mathcal{A}_{\pi}}$	$5.388(49) \times 10^{-2}$	$1.1743(64) \times 10^{-1}$
$\frac{\partial M_{u\bar{u}}^2}{\partial e^2}$	0.000434(39)	0.005782(29)	$\frac{\partial_{e_q}^2 \mathcal{A}_{K^+}}{\mathcal{A}_K}$	$2.218(48) \times 10^{-2}$	$5.265(57) \times 10^{-2}$
$\frac{\partial M_{K^+}^2}{\partial e^2}$	0.008148(47)	0.012260(54)	$\frac{\partial_{e_{\ell q}}^2 \mathcal{A}_{\pi^+}}{\mathcal{A}_{\pi}}$	$5.374(59) \times 10^{-2}$	$5.287(43) \times 10^{-2}$
$\frac{\partial M_{K^0}^2}{\partial e^2}$	0.0005142(98)	0.002250(13)	$\frac{\partial_{e_{\ell q}}^2 \mathcal{A}_{K^+}}{\mathcal{A}_K}$	$4.493(41) \times 10^{-2}$	$4.494(48) \times 10^{-2}$

Table D.2 *The mass, factorsable (f) and non-factorisable (nf) amplitude derivatives w.r.t e^2 The mass derivatives are in the infinite volume.*

Once the tuning is done, we calculate the E.M. part of the K meson mass-squared difference using the procedure outlined in §5.5.1. Using the central value of $\Delta_{\text{QED}} M_{\pi}^2 = 1261.16 \text{ MeV}^2$ from experimental masses, this allows us to predict

the correction to Dashen's theorem. This is shown in Table D.3.

	local	conserved
$\Delta_{\text{QED}} M_K^2$	2050(73)	2147(75)
ε	0.626(57)	0.702(62)

Table D.3 *The electromagnetic part of the K meson mass squared difference (in MeV^2) and the correction to Dashen's theorem.*

Together with the analytic formulas (Equations (4.143) and (4.146)) evaluated with $M_{K/\pi}$ of this ensemble, we calculated $\delta R_{K\pi}$ and decomposed it into its E.M. and SIB contributions using the procedure outlined in §4.1.3. These are shown in Table D.4.

	local	conserved
$\delta R_{K\pi}$	$-7.04(20) \times 10^{-3}$	$-6.91(20) \times 10^{-3}$
δ_{EM}	$-3.15(12) \times 10^{-3}$	$-2.94(11) \times 10^{-3}$
$\delta_{\text{SU}(2)}$	$-3.89(17) \times 10^{-3}$	$-3.96(17) \times 10^{-3}$

Table D.4 *The correction to $K_{\ell 2}/\pi_{\ell 2}$.*

In Table D.5, we compute the correlated difference and ratio of the observables of interest for this ensemble. We see that $\varepsilon_l - \varepsilon_c$ is consistent with zero. The ratio also shows that there is $\sim 10\%$ decrease in magnitude when using local instead of conserved current. We can trace this back to $\Delta_{\text{QED}} M_K^2$ in Table D.3, where the larger value from the conserved current comes from an interplay between the larger mass squared derivatives and the tuning.

As for $\delta R_{K\pi}$, while $\delta R_{K\pi,l} - \delta R_{K\pi,c}$ is consistent with zero, the result using local current is $\sim 2\%$ larger than the conserved current's. More interestingly, the $\sim 7\%$ relative difference in δ_{EM} is comparable with the estimation of $\mathcal{O}(a^2)$ cut-off effects at $(a\Lambda_{\text{QCD}})^2 \sim 5\%$, using $a^{-1} = 1730\text{MeV}$ and $\Lambda_{\text{QCD}} = 400\text{MeV}$.

O	$O_l - O_c$	O_l/O_c
ε	$-7.7(7.8) \times 10^{-2}$	0.89(11)
$\delta R_{K\pi}$	$-1.3(2.5) \times 10^{-4}$	1.020(36)
δ_{EM}	$-2.1(1.4) \times 10^{-4}$	1.072(49)

Table D.5 *The correlated difference and ratio of observables computed with local (l) and conserved (c) currents.*

While this is not a formal proof, as an empirical statement this numerical exercise indicates that the discrepancy coming from the different E.M. implementations are indeed comparable to $\mathcal{O}(a^2)$ cut-off effects. We believe the use of local current for the main work is appropriate once this discretisation error is included in the error budget of our final result.

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