Pion-pion scattering amplitudes and the timelike pion form factor from $N_f = 2 + 1$

Lattice QCD

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Ben Hörz
Dublin, 10.01.2017
Summary

We study isovector pion-pion scattering and extract the electromagnetic pion form factor in the timelike region from $N_f = 2 + 1$ Lattice QCD ensembles at a single lattice spacing and two pion masses $m_\pi = 200$ MeV and $m_\pi = 280$ MeV, generated through the Coordinated Lattice Simulations (CLS) effort. The spectrum of QCD in a finite box is extracted from temporal correlation functions of suitably chosen single-meson and two-pion interpolating operators. The required correlation functions are efficiently computed using the stochastic LapH method, facilitating the present analysis in large spatial volumes with the bigger of the two spatial extents roughly $L \approx 4.1$ fm. We discuss how the calculation of two-point correlation functions involving the renormalized $O(a)$-improved isovector vector current can be achieved in the stochastic LapH framework.

The finite-volume two-pion spectrum is mapped to the infinite-volume pion-pion scattering amplitude using the Lüscher method, and we extract the Breit-Wigner parameters of the lowest-lying vector resonance, the $\rho$ meson. We implement the variant of the Lellouch-Lüscher method first suggested by Meyer, which enables the extraction of the energy dependence of the electromagnetic pion form factor at a number of discrete points in the timelike region. This form factor shows an enhancement around the mass of the $\rho$ and dominates the QCD contribution to the anomalous magnetic moment of the muon through hadronic vacuum polarization at low energies, and is hence of phenomenological interest.

In the isospin-symmetric setup employed by us, we observe deviations of the extracted form factor from the Gounaris-Sakurai parametrization, but an assessment of cutoff effects and the pion-mass dependence is needed before firm conclusion can be drawn.
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Contents

1. Introduction 1
   1.1. QCD in the Standard Model ................................. 1
   1.2. Regularization of QCD by a Lattice ....................... 5

2. Finite-Volume Spectroscopy Methods 11
   2.1. Observables in Euclidean-time Simulations and Analysis Techniques . 11
   2.2. Probe Operator Construction ................................ 15
   2.3. Practical All-to-All Propagators .......................... 19
      2.3.1. Distillation ........................................... 20
      2.3.2. The Stochastic LapH Method .......................... 24
      2.3.3. Construction of Correlation Functions ................. 29
   2.4. Matrix elements in the Stochastic LapH Framework .......... 32

3. Interpretation of Finite-Volume Observables 39
   3.1. Scattering Amplitudes and Transition Matrix Elements from Finite-
        Volume Spectrum ....................................... 40
      3.1.1. Quantization Condition ............................... 43
      3.1.2. Transition Matrix Elements ......................... 44
   3.2. Workflow for Practical Implementation ..................... 45

4. Numerical Results for Pion-Pion Scattering 49
   4.1. Ensemble Details .......................................... 49
   4.2. Computational Cost ....................................... 53
   4.3. Finite-Volume Spectrum ................................... 55
      4.3.1. Pion Mass and Dispersion Relation ................... 55
      4.3.2. Isovector Two-Pion Spectrum ........................ 58
   4.4. Pion-Pion Scattering Amplitude .......................... 65
   4.5. Timelike Pion Form Factor ................................. 72

5. Concluding Remarks 83
A. \( t_{\text{min}} \)-plots for All Energy Levels \hfill 87

A.1. N200 \hfill 87
   A.1.1. Extraction of the Finite-Volume Spectrum \hfill 87
   A.1.2. Extraction of Current Matrix Elements \hfill 91

A.2. D200 \hfill 97
   A.2.1. Extraction of the Finite-Volume Spectrum \hfill 97
   A.2.2. Extraction of Current Matrix Elements \hfill 101
1. Introduction

1.1. QCD in the Standard Model

In this thesis we present results for scattering amplitudes obtained from numerical simulations of quantum chromodynamics (QCD). QCD is the accepted theory of the strong interaction in the Standard Model of particle physics and it contains a rich phenomenology. Extracting definite predictions however poses great theoretical challenges. While the electroweak sector of the Standard Model lends itself to a treatment in the framework of perturbation theory, such an approach captures the relevant features of QCD only at high energies. This observation (known as asymptotic freedom) goes back to 1973 when the $\beta$-function of QCD, which governs the running of the coupling of the theory with the scale, was shown to be negative \cite{1, 2}. At low energies however a strategy that does not rely on perturbation theory is required. Such a theoretical tool is provided by a discretization of the quantum field theory under consideration on a space-time grid which imposes a momentum cutoff and thus acts as a regulator \cite{3}. While at early stages of its development discretization allowed for theoretical insights to be gained analytically, its modern-day importance derives from the fact that this program renders certain quantum field theories in Euclidean time amenable to numerical simulations. The systematic study of QCD in a discretized form is pursued in the field of lattice QCD, although more general classes of gauge theories are being considered in lattice gauge theory as well.

With the Standard Model of particle physics being tremendously successful at describing experimental data to date, efforts aimed at testing the theory to ever better precision are hoped to reveal hints towards physics beyond the Standard Model. This program comprises vast amounts of ongoing and future experiments in a bid to improve on the precision of a wide range of observables, as well as theoretical work to confront those real-world data. Generally, lattice QCD contributes to this effort in at least two major ways.
1. Introduction

Firstly, the entirety of hadronic states observed in experiment and collected by the Particle Data Group [4] should be described by QCD as the underlying theory. In principle lattice QCD should hence be able to predict the complete QCD spectrum. Among the hadrons observed in experiment, the pseudoscalar pions and kaons stand out due to their small masses compared to the lowest-lying vector mesons. This gap is naturally explained by interpreting the pion and kaon as the Nambu-Goldstone bosons of the spontaneously broken chiral symmetry which QCD exhibits in the limit of massless quarks, with their small masses resulting from the explicit breaking of chiral symmetry by nonzero up, down and strange quark masses [5, 6]. They are stable under the strong interaction, which at low energies is described by Chiral Perturbation Theory (ChPT), the effective low-energy theory of QCD based on the pattern of chiral symmetry breaking. However, most of the experimentally-known hadrons appear as resonances, i.e. enhancements in the scattering cross sections of QCD-stable particles. These unstable particles are not captured by standard ChPT, and other theoretical tools are needed for their investigation, but they are also not readily accessible in Euclidean-time simulations [7]. Fortunately a formalism exists to rigorously relate the spectrum of QCD in a finite box\(^1\) to physically meaningful scattering amplitudes [8, 9, 10, 11], albeit only in a restricted kinematical region. Although the Lüscher formalism was established as a means to treat unstable particles in the context of lattice field theory already in 1990, systematic utilization in dynamical QCD has only begun recently, driven by advancements in the methods used to extract the finite-volume spectrum. In order to map out the spectrum, which includes scattering states of lower-lying stable hadrons, appropriate interpolating operators [12, 13, 14] have to be employed, which in turn requires the evaluation of so-called all-to-all propagators (see for example [15] and references therein). While significant progress has been achieved using distillation [16] to isolate the dominant modes of quark propagation, this approach becomes prohibitively demanding computationally as the box size is increased. Supplementing distillation with a stochastic estimator leads to a more favorable scaling of computational cost with the volume; the stochastic LapH method [17] reduces computational requirements at the expense of a potential decrease in attainable accuracy. A main focus of this thesis is hence to demonstrate that the stochastic LapH method yields sufficiently precise results to allow for an investigation of the lightest known narrow resonance – the \(\rho\)-meson – from lattice QCD.

\(^1\)In contrast to the above use of the term *spectrum*, we here refer to the eigenvalues of the discrete finite-volume Hamiltonian that also includes scattering states. Throughout this thesis we will use the term *spectrum* mainly in this sense, and the meaning will be clarified whenever there is a chance of confusion.
1. Introduction

Secondly, QCD processes contribute to all reactions considered in experiment (although the contribution can be small in practice depending on the process under consideration). Additional theoretical input is then required in order to enable the comparison with otherwise perturbative Standard Model predictions from the electroweak sector. Typically the additional information is encoded in matrix elements of certain operators between hadronic states. For some quantities such as pseudoscalar meson decay constants lattice QCD determinations have matured to a point that they have phenomenological impact as evidenced in their compilation by the Flavor Lattice Averaging Group [18, 19, 20]. Going beyond these ‘gold-plated’ quantities, in this thesis we will present exploratory results for a resonant matrix element, namely the electromagnetic pion form factor in the timelike region. This quantity, which we will define more precisely in a moment, is interesting from a lattice QCD perspective because its determination entails using an extension of the above-mentioned formalism for treating scattering amplitudes [21, 22]. The timelike pion form factor is also relevant phenomenologically as it contributes to the anomalous magnetic moment of the muon \( \alpha_\mu \), for which a discrepancy between theory and experiment of about three standard deviations persists (cf. [23], on which the following short account is based, for a comprehensive review of the status and prospects).

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{muon_a}\caption{Leading-order contribution to the anomalous magnetic moment of the muon \( \alpha_\mu \) from hadronic vacuum polarization (HVP). In the low-energy region the HVP is dominated by the timelike pion form factor as explained in the text.}
\end{figure}

The QCD contribution by hadronic vacuum polarization to the anomalous magnetic moment of the muon at leading-order in the perturbative expansion of electromagnetic interactions is depicted in figure 1.1.\textsuperscript{2} Using analyticity, the corresponding photon self-energy function can be recovered from its imaginary part via a dispersion

\footnotesize
\textsuperscript{2} The other leading-order contribution is the so-called hadronic light-by-light scattering, exploratory lattice investigations of which are currently beginning, see e.g. [24, 25].
1. Introduction

relation. The optical theorem then relates the imaginary part of the hadronic vacuum polarization amplitude to the cross section of the reaction $e^+e^- \rightarrow \text{hadrons}$,

$$\Pi_{\gamma}^\text{had}(q^2) = \frac{\alpha q^2}{3\pi} \int_0^\infty ds \frac{R_{\text{had}}(s)}{s(s - q^2 - i\epsilon)},$$

(1.1)

where

$$R_{\text{had}}(s) = \sigma(e^+e^- \rightarrow \text{hadrons}) \sqrt{\frac{4\pi\alpha_{\text{em}}(s)^2}{3s}},$$

(1.2)

and $\alpha_{\text{em}}(s)$ is the fine-structure constant related to the electromagnetic coupling. At low energies the dominant final state consists of two pions, and the cross section is given by the square of the timelike electromagnetic form factor of the pion $F_\pi(s)$,

$$R_{\text{had}}(s) = \frac{1}{4} \left(1 - \frac{4m_\pi^2}{s}\right)^{\frac{3}{2}} |F_\pi(s)|^2, \quad 4m_\pi^2 < s < 9m_\pi^2,$$

(1.3)

that effectively describes corrections to the coupling of a virtual photon to two pions stemming from their compositeness. The cross section which appears in (1.3) is typically determined from experimental data to rather good precision. Nevertheless a determination from first principles might be desirable, since the interpretation of experimental data typically requires additional model input. For instance, effects from isospin breaking and higher resonances can be disentangled in experimental data only through models [26], while lattice QCD simulations can be carried out with an exact isospin symmetry. From the lattice, the hadronic vacuum polarization is traditionally extracted using current-current correlators, which however suffer from deteriorating signal quality at low momentum transfer as well as potentially sizable finite-volume effects [27, 28]. Extracting the timelike pion form factor in this low-energy region using an extensions of the Lüscher method [22] – which by construction of the formalism only features finite-volume effects which are exponentially suppressed in the box size – could pave the way towards a combined determination of the HVP contribution to the anomalous magnetic moment of the muon with finite-volume effects under control.\(^3\) In this thesis we present such a self-contained extraction of the form factor $F_\pi(s)$ from lattice QCD.

The rest of this thesis is organized as follows: In the remainder of this chapter we give a short overview of lattice QCD. In chapter 2 we describe lattice-specific methods

\(^3\)More generally, finite-volume effects in lattice calculations can be assessed using form factors extracted via the Lüscher formalism in some instances, see e.g. [29] for a related scenario. A thorough understanding of the usage of Lüscher-type analyses might thus be of indirect phenomenological relevance in various ways.
1. Introduction

that we employ. We start by describing the observables required for this work and outlining aspects of their analysis. Then, after reviewing our construction of probe operators and the strategy for computing quark propagators using the stochastic LapH method, we describe how the determination of matrix elements of the electromagnetic current between hadronic states and the vacuum can be accommodated in this framework. The formalism relating observables accessible through lattice QCD simulations to experimentally observable quantities is discussed in chapter 3, where additionally an outline of the practical workflow is given. Chapter 4 starts with an exposition of the gauge ensembles used in this study, followed by the main body of our results. Auxiliary plots detailing our treatment of systematic uncertainties are relegated to appendix A.

1.2. Regularization of QCD by a Lattice

Quantum chromodynamics is a gauge theory based on the gauge group SU(3), whose corresponding charges are conventionally referred to as color. With the quarks transforming according to the fundamental representation, the field theory in Minkowski time is described by the Lagrangian density

$$\mathcal{L} = \sum_{f=u,d,s,...} \bar{q}_f \left( i \gamma^{(M)}_\mu D_\mu - m_f \right) q_f - \frac{1}{4} F_{\mu\nu}^a F_{\mu\nu}^a,$$

where $\gamma^{(M)}_\mu$ are Dirac matrices satisfying the Clifford algebra $\left\{ \gamma^{(M)}_\mu, \gamma^{(M)}_\nu \right\} = 2\eta_{\mu\nu}$, and $D_\mu$ denotes the gauge-covariant derivative

$$D_\mu = \partial_\mu - ig_0 A_\mu,$$

with $A_\mu$ the su(3)-valued vector field and $g_0$ the bare coupling constant. Being an element of the algebra of SU(3), the gauge field $A_\mu$ can be decomposed in terms of the generators of the algebra. In terms of the corresponding coordinates $A^a_\mu$ the gluonic field strength tensor of (1.4) is given by

$$F_{\mu\nu}^a = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu + g_0 f^{abc} A^b_\mu A^c_\nu,$$

where $f^{abc}$ are the structure constants of SU(3). While in the Standard Model the sum in (1.4) extends over all known quark flavors, the charm, bottom and top quark species are irrelevant to the low-energy properties of QCD and can be thought of
1. Introduction

as having been integrated out in an effective field theory sense for our purposes.\(^4\)

In order to define this field theory as a quantum field theory beyond a perturbation approach and to render it numerically tractable at low energies, one employs path-integral quantization of the Euclidean-time theory on a discrete space-time. Under this procedure the quark fields are located at lattice points \(x\), and with each link joining points \(x\) to \(x + a\hat{\mu}\) we associate a \(SU(3)\)-valued matrix \(U_\mu(x)\), where \(\hat{\mu}\) denotes the unit vector in the \(\mu\)-direction. For a given lattice action \(S[\bar{q}, q, U]\), expectation values of observables are given by integrals

\[
\langle \mathcal{O} \rangle = Z^{-1} \int D\bar{q} Dq DU e^{-S[\bar{q}, q, U]} \mathcal{O}.
\]

(1.7)

Here the integration over \(\bar{q}\) and \(q\) is understood as an integral over Grassmann-valued variables at each lattice site, and \(DU\) denotes the product over Haar measures of the \(SU(3)\) link variables. The overall normalization factor \(Z\) is determined by

\[
1 \equiv \langle 1 \rangle = Z^{-1} \int D\bar{q} Dq DU e^{-S[\bar{q}, q, U]}.
\]

(1.8)

The guiding principle in the construction of the lattice action is for it to preserve gauge symmetry exactly at finite lattice spacing and to have the correct continuum limit. As in the continuum, the action consists of a fermionic and a gluonic part,

\[
S[\bar{q}, q, U] = S_f[\bar{q}, q, U] + S_g[U],
\]

(1.9)

and the fermionic part for each quark species can be cast into the form

\[
S_f[\bar{q}, q, U] = \bar{q}M[U]q,
\]

(1.10)

where the Dirac fermion matrix \(M[U]\) is understood to have compound indices encompassing space, time, spin and color. As the action (1.10) is a bilinear in the quark fields, the corresponding integral for fixed \(U\) can be carried out analytically according to the rules of Grassmann integration (see e.g. [31, Chapter 5]). With Grassmann variables \(\bar{\psi}, \psi\) and \(\bar{\xi}, \xi\) Grassmann-valued sources, the central result

\[
\int D\bar{\psi} D\psi \exp \left( -\bar{\psi} M \psi - \bar{\psi} \xi - \bar{\xi} \psi \right) = \det M \exp \left( \bar{\xi} M^{-1} \xi \right),
\]

(1.11)

together with

\[
\frac{\partial}{\partial \xi^a} e^{\mathcal{A} C} = -\xi^b A_{ba} e^{\mathcal{A} C}, \quad \frac{\partial}{\partial \xi^a} e^{\mathcal{A} C} = A_{ab} \xi^b e^{\mathcal{A} C},
\]

(1.12)

\(^4\)See [30] for a quantitative study of the decoupling of heavy quarks.
for a matrix $A$ of ordinary complex numbers, can be used to evaluate integrals of the form

$$
\int D\bar{\psi} D\psi \psi_{a_1} \cdots \psi_{a_n} \bar{\psi}_{b_1} \cdots \bar{\psi}_{b_m} \exp \left( -\bar{\psi}M\psi \right).
$$

(1.13)

For example,

$$
\int D\bar{\psi} D\psi \psi_a \exp \left( -\bar{\psi}M\psi \right)
= -\frac{\partial}{\partial \xi_a} \int D\bar{\psi} D\psi \exp \left( -\bar{\psi}M\psi - \bar{\psi}\xi - \bar{\xi}\psi \right) \bigg|_{\bar{\xi}=0=\xi}
= -\frac{\partial}{\partial \xi_a} \det M \exp \left( \xi M^{-1}\xi \right) \bigg|_{\xi=0=\xi}
= -M^{-1}_{ab} \xi_b \det M \exp \left( \xi M^{-1}\xi \right) \bigg|_{\xi=0=\xi} = 0.
$$

(1.14)

Similarly one finds that all integrals of the form (1.13) vanish unless their integrand consist of an equal number of $ar{\psi}$ and $\psi$ variables. The Feynman propagator is related to the integral

$$
\int D\bar{\psi} D\psi \bar{\psi}_a \psi_b \exp \left( -\bar{\psi}M\psi \right)
= -\frac{\partial}{\partial \xi_a} \frac{\partial}{\partial \xi_b} \int D\bar{\psi} D\psi \exp \left( -\bar{\psi}M\psi - \bar{\psi}\xi - \bar{\xi}\psi \right) \bigg|_{\bar{\xi}=0=\xi}
= -\frac{\partial}{\partial \xi_a} \frac{\partial}{\partial \xi_b} \det M \exp \left( \xi M^{-1}\xi \right) \bigg|_{\xi=0=\xi}
= \frac{\partial}{\partial \xi_a} \left[ \xi_c M^{-1}_{cb} \det M \exp \left( \xi M^{-1}\xi \right) \right] \bigg|_{\xi=0=\xi}
= M^{-1}_{ab} \det M.
$$

(1.15)

Integrals involving a higher but equal number of $\bar{\psi}$ and $\psi$ variables similarly reduce to linear combinations of products of $M^{-1}$ matrix elements according to Wick’s theorem, and one power of the determinant of $M$. In view of the full path integral (1.7), the key point is that the quark fields can be integrated analytically, leaving behind an integral over the gauge fields $U$. The effect of dynamical quarks is encoded in the fermion determinant $\det M$, and we will refer to $M^{-1}[U]$ as the quark propagator in a gauge background $U$. By construction the fermion matrix reduces to $M = \gamma_\mu D_\mu + m$ in the continuum limit, and we define the Euclidean-time gamma
matrices such that they satisfy

$$\gamma^4 = \gamma_4 = \gamma^{(M)}_0 = \gamma^{(M)}_4, \quad \gamma_k = \gamma^k = -i \gamma^k_{(M)} = i \gamma^{(M)}_k,$$  \hspace{1cm} (1.16)

$$\{\gamma_\mu, \gamma_\nu\} = 2 \delta_{\mu\nu}, \quad \gamma_\mu^\dagger = \gamma_\mu, \quad \gamma_5 = \gamma_4 \gamma_1 \gamma_2 \gamma_3.$$  \hspace{1cm} (1.17)

In the continuum, the covariant derivative behaves the same way as an ordinary derivative under Hermitian conjugation, $D_\mu^\dagger = -D_\mu$, and hence, using $\gamma_5^2 = 1$ and $\gamma_5 \gamma_\mu = -\gamma_\mu \gamma_5$,

$$(\gamma_\mu D_\mu + m)^\dagger = D_\mu^\dagger \gamma_\mu^\dagger + m = -\gamma_\mu D_\mu + m$$

$$= -\gamma_5^2 \gamma_\mu D_\mu + \gamma_5^2 m = \gamma_5 (\gamma_\mu D_\mu + m) \gamma_5.$$  \hspace{1cm} (1.18)

The above property is called $\gamma_5$-hermiticity and does also hold for Wilson fermions on a lattice, so that

$$M^\dagger = \gamma_5 M \gamma_5.$$  \hspace{1cm} (1.19)

We will use $\gamma_5$-hermiticity later on to simplify the evaluation of correlation functions, but since $\det(M^\dagger) = (\det M)^*$ and $\det(AB) = \det A \det B$, it also entails the important property that the fermion matrix determinant is real,

$$(\det M)^* = \det(\gamma_5 M \gamma_5) = (\gamma_5)^2 \det M = \det M.$$  \hspace{1cm} (1.20)

Combined with the fact that the gauge action $S_g[U]$ is real, this allows for the path integral (1.7) with quark fields integrated analytically,

$$\langle \mathcal{O} \rangle = Z^{-1} \int D U \ \det M[U] \ e^{-S_g[U]} \ \mathcal{O}'[U],$$  \hspace{1cm} (1.21)

to be estimated using Monte Carlo methods with importance sampling.\(^5\) In the above equation the observable $\mathcal{O}'[U]$ which is obtained from performing the integral over quark fields can depend on the gauge field $U$ both explicitly, for instance for purely gluonic observables, and implicitly via the quark propagator in the given gauge background. While the integral (1.21) is well-defined at finite lattice spacing, it is very high-dimensional. On all but the smallest lattices the integral is therefore usually estimated using Monte Carlo integration with importance sampling, whereby the product of the fermion determinant and the Boltzmann factor is interpreted as

\(^5\)Importance sampling requires the path integral weight to be non-negative. While $\det M$ is not necessarily non-negative for a single species of Wilson fermions, this property is guaranteed when a pair of degenerate quarks is simulated.
1. Introduction

a probability distribution.\(^6\) Approximating the integral (1.21) then proceeds via generating representative gauge fields – in the sense that their contribution to the integral is significant – and evaluating the observables of interest on this collection of gauge backgrounds. Gauge configurations are generated using Markov-chain Monte Carlo methods, usually some variant of the Hybrid Monte Carlo algorithm [32] in simulations with dynamical fermions, which is typically the computationally most expensive part of lattice QCD studies. However, thermalized gauge field configurations can be used to extract a wide range of physical observables, so their generation normally is a collaborative effort.

Ultimately, the preceding formal developments hinge on the availability of a lattice action with the required properties, most essentially one that respects gauge symmetry at finite lattice spacing and has the correct formal continuum limit. Indeed there are a number of viable discretized actions that generally differ by how the continuum limit is approached and their chiral-symmetry properties at finite lattice spacing. The simplest such gauge action is the Wilson gauge action [3] which consists of only \(1 \times 1\) Wilson loops or plaquettes. Several different discretizations for the fermionic part of the action are used in present-day simulations, including Wilson fermions [3], possibly with a twisted mass term [33], staggered fermions [34, 35], Domain Wall fermions [36, 37], and overlap fermions [38, 39]. While the Nielsen-Ninomiya theorem [40] prevents chiral symmetry in its continuum form to be realized by any such fermion discretization, an appropriately defined lattice deformation of chiral symmetry is maintained at finite lattice spacing by fermion discretizations satisfying the Ginsparg-Wilson relation [41]. Finally, the Symanzik program [42] allows for a systematic improvement of the scaling of these discretizations towards the continuum by tuning coefficients of higher–mass-dimension operators in order to remove lattice artifacts at a given power in the lattice spacing.

In this work we employ \(N_f = 2+1\) gauge configurations generated by the Coordinated Lattice Simulations consortium [43] with nonperturbatively \(O(a)\)-improved Wilson fermions [44, 45, 46] and the Lüscher-Weisz action [47] used for the gluons. Wilson fermions are computationally less demanding than fermion discretizations with better chiral-symmetry properties, while still allowing for a rigorous renormalization of quark bilinears and avoiding the theoretical difficulties of the computationally cheaper staggered fermion discretization, making them ideal for this exploratory study. The action and ensemble description is given in section 4.1.

\(^6\)Many physically interesting lattice field theories, e.g. QCD at finite chemical potential and QCD with a \(\theta\)-term, do not satisfy this requirement, giving rise to the so-called sign problem.
2. Finite-Volume Spectroscopy Methods

In this chapter we discuss some basics of the analysis of finite-volume observables, the construction of suitable interpolating operators as well as the computation of correlation functions of said operators. We use the stochastic LapH method [17] to efficiently treat quark propagation in the determination of correlation functions. To extract the isovector electromagnetic pion form factor in the timelike region we require finite-volume matrix elements of the electromagnetic current between hadronic states and the vacuum [22]. The exposition of the stochastic LapH method given in this chapter serves to show how the computation of the required correlation functions involving the electromagnetic current can be accommodated in this framework without spoiling the renormalization properties of the current operator on the lattice.

2.1. Observables in Euclidean-time Simulations and Analysis Techniques

The primary observables relevant to this work are two-point correlation functions of the form

\[ C_{ij}(t) = \langle \Omega | O_i(t + t_0) \bar{O}_j(t_0) | \Omega \rangle \]  

(2.1)

extracted from lattice QCD simulations for a set of operators \( O_i(t + t_0) \) which can annihilate the states of interest at a time \( t_0 + t \), with a corresponding set \( \bar{O}_j(t_0) \) which create these states at an earlier time \( t_0 \). Assuming that the lattice theory in finite volume possesses a Hamiltonian description\(^1\), every such correlation function

\(^1\)In the case of standard Wilson fermions with Wilson parameter \( r = 1 \) the transfer matrix of the theory can be constructed explicitly [48]. From the positive transfer matrix one immediately obtains the Hermitian Hamiltonian of the interacting theory which is related to the transfer
has a spectral representation

\[ C_{ij}(t) = \sum_{n=0}^{\infty} \langle \Omega | e^{H(t+t_0)} O_i(0) e^{-H(t+t_0)} | n \rangle \langle n | e^{H_0} \bar{O}_j(0) e^{-H_0} | \Omega \rangle \]

\[ = \sum_{n=0}^{\infty} e^{E_n(t+t_0)} \langle \Omega | O_i(0) | n \rangle e^{-E_n(t+t_0)} e^{E_n t_0} \langle n | \bar{O}_j(0) | \Omega \rangle e^{-E_\Omega t_0} \]  

in terms of the stationary states – eigenvectors of the Hamiltonian \( H \) – denoted by \(| n \rangle\), which satisfy \( H | n \rangle = E_n | n \rangle \).\(^2\) The finite spatial volume imposes a quantization condition on allowed momenta, rendering all of the stationary-state energies discrete in the spectral decomposition. However, (2.2) receives corrections related to the boundary conditions in the temporal direction. Periodic boundary conditions imply thermal effects (see, for instance, [49]) due to wrapping around the finite temporal extent; open boundary conditions add contributions due to states with vacuum quantum numbers propagating off the temporal boundary [50]. In either case these additional contributions have to be monitored to ensure that they are negligible.

The correlator matrix \( C_{ij} \) in the above form is Hermitian if

\[ \langle \Omega | O_i | n \rangle = \langle n | \bar{O}_i | \Omega \rangle^*, \]

in which case we define the overlap factors by

\[ Z_i^{(n)} = \langle \Omega | O_i | n \rangle, \quad Z_i^{(n)*} = \langle n | \bar{O}_i | \Omega \rangle, \]

and after shifting the energies so that \( E_\Omega = 0 \) we obtain

\[ C_{ij}(t) = \sum_n Z_i^{(n)} Z_j^{(n)*} e^{-E_n t}. \]

We will assume that the energies are ordered such that \( E_0 < E_1 < \ldots \). We postpone the discussion of our construction of suitable interpolating operators \( O_i, \bar{O}_j \) and computation of their correlation functions to section 2.2 and here focus instead on describing our procedure to extract the energies \( E_n \) from Monte Carlo estimates of the correlation matrix \( C_{ij}(t) \).

Such a correlation matrix element is a primary observable, i.e. it has a unique value \( C_{ij}^{[c]}(t) = C_{ij}(t)[U_c] \) on a field configuration \( U_c \), where \( c = 1, \ldots, N_{cfg} \) runs over the available gauge backgrounds and as such corresponds to the integrand of a single

\(^2\) Here we use \( | \Omega \rangle \) to denote the vacuum and \(| n = 0 \rangle\) is an eigenvector of the Hamiltonian. In subsequent sections, where eigenvectors are labeled by a collection of quantum numbers, so that there is no chance of confusion, the vacuum state is simply labeled as \( | 0 \rangle \).
path integral. Let \( d_i^{[c]} \) with \( i = 1, \ldots, N_{\text{data}} \) denote a general collection of \( N_{\text{data}} \) primary observables on some field configuration; the Monte Carlo estimate is given by

\[
E(d_i) = \langle d_i \rangle \equiv \frac{1}{N_{\text{cfg}}} \sum_{c=1}^{N_{\text{cfg}}} d_i^{[c]},
\]

and, assuming autocorrelations are negligible, the Monte Carlo estimate of the covariance between primary observables is

\[
\text{cov}(d_i, d_j) = \frac{1}{N_{\text{cfg}} - 1} \langle (d_i - \langle d_i \rangle)(d_j - \langle d_j \rangle) \rangle = \frac{\langle d_i d_j \rangle - \langle d_i \rangle \langle d_j \rangle}{N_{\text{cfg}} - 1}. \tag{2.7}
\]

Energies and other observables are obtained from the primary observables via a best-fit procedure. The covariance between the data is needed in order to properly treat the correlation between observables measured on the same ensemble of gauge configurations in the construction of the \( \chi^2 \) for the least-squares fit. Let \( \alpha_p \) for \( p = 1, \ldots, N_{\text{param}} \) denote the derived observables of interest, and \( M_i(\alpha, d) \) the model devised to describe the data. We obtain best-fit estimates of the parameters from statistical estimates of the data as the values of \( \alpha \) that minimize

\[
\chi^2 = \sum_{ij} E(d_i - M_i(\alpha, d)) \sigma_{ij}^{-2} E(d_j - M_j(\alpha, d)), \tag{2.8}
\]

where

\[
\sigma_{ij}^2 = \text{cov}(d_i - M_i(\alpha, d), d_j - M_j(\alpha, d)). \tag{2.9}
\]

If the model functions depend only on the parameters \( \alpha \) and not on the data itself, in which case \( \langle M_i(\alpha) \rangle = M_i(\alpha) \), the covariance matrix used in the construction of the correlated \( \chi^2 \) simplifies to the covariance between the data, \( \sigma_{ij}^2 = \text{cov}(d_i, d_j) \).

In principle we could use the decomposition of a correlation function in terms of Hamiltonian eigenstates given in (2.5) and fit to the full correlation matrix for the energies and overlap factors of a number of lowest-lying states directly. In this case the covariance matrix \( \sigma_{ij}^2 \), which has to be estimated from the data, is rather big, \( \dim(\sigma^2) = N_t \cdot N_{\text{op}} \) with \( N_{\text{op}} \) the dimension of the correlation matrix \( C_{ij} \) and \( N_t \) the number of time separations for which it has been computed. In addition to the potentially unwieldy treatment of correlation between the data [51, 52], fits to a
sum of exponentials tend to be unstable absent good initial guesses (see e.g. [53]), rendering this approach difficult in practice.

Fortunately there is an alternative procedure in the form of a variational analysis that exploits the different overlaps of our interpolating operators onto the low-lying states of interest [54]. The different energy levels can be systematically and efficiently extracted by solving the generalized eigenvalue problem (GEVP) [55]

\[ C(t)v_n(t_0, t) = \lambda_n(t_0, t)C(t_0)v_n(t_0, t), \quad (2.10) \]

for each time separation \( t \), where \( t_0 \) denotes a reference time separation, and \( C(t) \) and \( v_n(t_0, t) \) are a \( N_{\text{op}} \times N_{\text{op}} \) matrix and vectors of corresponding dimension, respectively. The eigenvalues \( \lambda_n(t_0, t) \) are then asymptotically given by a single exponential decaying with the energy of interest, with corrections given by

\[ \lambda_n(t_0, t) \propto e^{-E_n t} \left( 1 + \mathcal{O}(e^{-\Delta E_n t}) \right), \quad (2.11) \]

and the energy gap is given by the distance to the nearest neighboring energy in the spectrum. In the above reference it was argued that employing the GEVP leads to earlier ground state saturation compared to solving a standard eigenvalue problem, due to an additional suppression of the coefficients of subleading terms with respect to the leading term. As anticipated in [55] pushing the reference time separation \( t_0 \) out to somewhat large values is desirable to further suppress contamination, and it can be shown [56] that for an \( N_{\text{op}} \)-dimensional correlation matrix with sufficient overlap onto the corresponding number of the low-lying states, the spectral gap is governed by the first energy value in the spectrum above the \( N_{\text{op}} \) lowest states,

\[ \Delta E_n = E_{N_{\text{op}}+1} - E_n, \quad \text{if } t_0 \geq t/2. \quad (2.12) \]

This relation holds provided there are no (accidental) degeneracies in the spectrum, and if the GEVP is solved for each time separation. In this work we instead solve the GEVP for one pair of a reference time separation \( t_0 \), and a single time separation \( t_d \) at which the correlation matrix is diagonalized,

\[ C(t_d)v(t_0, t_d) = \lambda(t_0, t_d)C(t_0)v(t_0, t_d) \quad (2.13) \]

and then define correlation functions between \('optimal' interpolators\)

\[ \hat{C}_{ij}(t) = (v_i(t_0, t_d), C(t)v_j(t_0, t_d)), \quad (2.14) \]
where the outer parenthesis denote an inner product over GEVP indices. Since the Monte Carlo estimate of the correlation matrix, i.e. the mean value using all gauge configurations, is our best estimate, the eigenvectors $v_n(t_0, t_d)$ are obtained from solving the generalized eigenvalue problem on this mean. Performing the diagonalization for every time separation would introduce ambiguities in the level ordering for closely-spaced Hamiltonian eigenstates, which we avoid at the expense of introducing a source of systematic error – resulting from off-diagonal elements of $\hat{C}_{ij}(t)$ not being zero exactly – that must be assessed.

Up to corrections of the form given in (2.11) the diagonal elements of the rotated correlation matrix are hence given by single exponentials, and the spectrum can be obtained from two-parameter correlated-$\chi^2$ fits to a single-exponential ansatz. In this case the model parameters $\alpha_p$ of (2.8) are a real overlap and a real and positive energy eigenvalue. In the present work however our goal is to extract the difference between the energy of a two-pion state and its noninteracting value $2m_\pi$ to high precision. This energy difference can be extracted directly by a fit to the ratio of the two-pion correlation function and the product of correlation functions of its constituent pions. These ratio fits, which are discussed more thoroughly in section 4.3, take the correlation between the two-pion and single-pion correlation functions into account and allow for a more precise extraction of the energy difference.

In order to completely treat all correlations present in the data and consistently propagate uncertainties, the whole analysis is fully bootstrapped [57], where all primary observables are resampled in exactly the same way to preserve beneficial correlation for instance in the ratio fits. The whole analysis from the determination of finite-volume energies to the phase shift extraction to the final fit in order to obtain the resonance parameters is then performed on the average of the original data as well as a collection of resamplings. We use $N_{\text{boot}} = 800$ resamples throughout, and quote $1\sigma$ confidence intervals obtained from the percentiles of the bootstrap distribution. Uncertainties we quote on numerical values assume a symmetric bootstrap distribution, whereas figures show the potentially asymmetric confidence intervals based on the bootstrap distribution percentiles.

### 2.2. Probe Operator Construction

Ultimately the purpose of lattice QCD spectroscopy is to determine the stationary states of the finite-volume Hamiltonian. As in quantum mechanics, exploiting the symmetries of the system under consideration greatly simplifies achieving this goal.
The quantum operator $U_R$ that effects a symmetry transformation $R$ of the system commutes with the Hamiltonian $H$ of the system,

$$[U_R, H] = 0. \quad (2.15)$$

Let $E$ be an $n$-fold degenerate eigenvalue of $H$,

$$H |\phi_k^{(E)}\rangle = E |\phi_k^{(E)}\rangle, \quad k = 1, 2, \ldots, n. \quad (2.16)$$

The eigenvectors then span a subspace in the Hilbert space of states and we have

$$HU_R |\phi_k^{(E)}\rangle = U_R H |\phi_k^{(E)}\rangle = EU_R |\phi_k^{(E)}\rangle, \quad (2.17)$$

so that if $|\phi_k^{(E)}\rangle$ is an eigenstate of $H$ with eigenvalue $E$, so is $U_R |\phi_k^{(E)}\rangle$. The transformed state can therefore be decomposed as

$$U_R |\phi_k^{(E)}\rangle = \sum_{i=1}^{n} |\phi_i^{(E)}\rangle \Gamma_{ik}(R), \quad \Gamma_{ik}(R) = \langle \phi_i^{(E)} | U_R |\phi_k^{(E)}\rangle \quad (2.18)$$

and repeated application gives

$$U_{R_1}U_{R_2} |\phi_k^{(E)}\rangle = \sum_{i=1}^{n} U_{R_1} |\phi_i^{(E)}\rangle \Gamma_{ik}(R_2) = \sum_{i,j=1}^{n} |\phi_j^{(E)}\rangle \Gamma_{ji}(R_1) \Gamma_{ik}(R_2). \quad (2.19)$$

But if the symmetry transformations form a group, we also have

$$U_{R_1R_2} = U_R |\phi_k^{(E)}\rangle = \sum_{j=1}^{n} |\phi_j^{(E)}\rangle \Gamma_{jk}(R_1R_2) \quad (2.20)$$

and hence

$$\Gamma_{jk}(R_1R_2) = \sum_{i=1}^{n} \Gamma_{ji}(R_1) \Gamma_{ik}(R_2), \quad (2.21)$$

that is the $\Gamma_{jk}(R)$ define a unitary representation of the symmetry group. As any representation $\Gamma$ can be characterized by the irreducible representations it contains, we can classify the stationary states of the Hamiltonian by the irreducible representation the eigenvectors of the Hamiltonian belong to. The labels of the irreducible representation are the quantum numbers of the stationary state.

We essentially aim to diagonalize the Hamiltonian of the lattice theory – exploiting symmetries simplifies that task by enforcing a block diagonalization. Creation and annihilation operators should hence transform according to irreducible representa-
tions of the symmetries of the lattice theory. These group-theoretical projections were for example performed in [14] generalizing the construction of extended baryon operators of [12].\(^3\) In the following we enumerate the relevant symmetries. Somewhat trivially we require the operators to be gauge-invariant. In this work we are not concerned with baryons, tetraquarks or objects with even more complicated color structures, but only use mesonic interpolators with color structure given by the singlet part of the coupling of an antiquark and a quark, which in terms of irreducible representations of SU(3)\text{color} is given by

\[ \bar{3} \otimes 3 = 1 \oplus 8. \]  

(2.22)

In the flavor sector there is an exact isospin symmetry since most modern-day lattice QCD simulations are carried out with degenerate up and down quarks\(^4\). In addition to the up and down quark that are taken together to form isospin multiplets, the strange quark content of operators is a separate quantum number. For mesons we also define G-parity,

\[ U_G = C e^{-i\pi T_2}, \]  

(2.23)

as a combination of charge conjugation and a rotation by \(\pi\) in isospin space. This generalization of charge conjugation incorporates the fact that QCD is blind to electric charge, which for instance implies that the strong interaction does not distinguish between \(\pi^+, \pi^-\) and \(\pi^0\).

In contradistinction to the infinite-volume continuum theory, Lorentz rotational symmetry is explicitly broken by both the lattice regularization and the shape of the finite volume used in the simulation. The subgroup left intact on a single time slice in the theory regularized on a hypercubic lattice with finite extent and periodic spatial boundary conditions is the crystallographic space group \(O_{1h}\) that includes translations by lattice vectors, rotations and spatial inversion. The representations of the group of lattice translations are labeled by a total three-momentum \(P = \frac{2\pi}{L^3}d\), \(d \in \mathbb{N}^3\) allowed by the boundary conditions. Next one identifies the subgroup of symmetry transformations that leave \(P\) invariant, known as the little group of \(P\), given in table 2.1. In that table we also show the irreducible representations of the

\(^3\)An alternative way to construct operators which transform irreducibly under the symmetries of the lattice theory while maintaining maximal overlap with the continuum SU(2) group was given in [13].

\(^4\)Isospin-breaking effects due to different up and down quark masses are comparable in size to electromagnetic effects due to their different electric charges, so that both sources of isospin breaking need to be addressed simultaneously in a consistent treatment [58].
Table 2.1: Little groups of $P = \frac{2\pi}{L} d$, the subgroups of $O_h$ that leave $P$ invariant. Creation and annihilation operators with total momentum $P$ are constructed such that they transform irreducibly under the action of the respective little group. The irreducible representations relevant for the $\rho$ resonance are listed in the last column. To improve statistics, correlation functions are constructed for all independent equivalent momenta and averaged over.

<table>
<thead>
<tr>
<th>$d$</th>
<th>Little group of $P$</th>
<th>relevant irreps</th>
</tr>
</thead>
<tbody>
<tr>
<td>$[0, 0, 0]$</td>
<td>$O_h$</td>
<td>$T_{1u}$</td>
</tr>
<tr>
<td>$[0, 0, n]$</td>
<td>$C_{4v}$</td>
<td>$A_1, E$</td>
</tr>
<tr>
<td>$[0, n, n]$</td>
<td>$C_{2v}$</td>
<td>$A_1, B_1, B_2$</td>
</tr>
<tr>
<td>$[n, n, n]$</td>
<td>$C_{3v}$</td>
<td>$A_1, E$</td>
</tr>
</tbody>
</table>

respective little groups relevant to our study of the $\rho$ resonance, which has vector quantum numbers, so the list includes all the little-group irreducible representations containing contributions from the $\ell = 1$ representation of the continuum rotation group. In practice, correlation functions for equivalent momenta, which are connected to the reference momenta in table 2.1 through elements of the little group, are averaged over to increase statistics.

Single-particle mesonic creation and annihilation operators with momentum $P$ are then constructed from an antiquark and a quark field through group-theoretical projections such that they transform irreducibly under the little group of $P$. Note that the reduced rotational symmetry is not related to the lattice regulator alone, but also results from the geometry of the finite box in the spatial directions. Although the breaking of Lorentz symmetry from the lattice regulator vanishes in the continuum limit, the spectrum exhibits the degeneracies expected from restoration of full rotational symmetry only up to finite-volume effects.

To sum up, the bosonic interpolators create states

$$|d, I, I_3, S, \Lambda^{(G)}, \mu\rangle$$

with total momentum $P = \frac{2\pi}{L} d$, total isospin $I$ and isospin projection $I_3$, strangeness $S = \pm 1$, row $\mu$ of irreducible representation $\Lambda$ of the rotation group, and definite G-parity $G \in \{+, -\}$ where applicable. Conventionally we restrict our attention to states of maximal isospin projection $I_3 = I$ and row $\mu = 1$ of the irreducible representations $\Lambda$, which is permissible because by construction all members of these multiplets are degenerate. In the following we will occasionally use the short-hand

\[5\] In the following we will suppress the $I_3$ and $\mu$ labels when it should be understood that they are
notation $\Lambda^{[G]}(d^2)$ to label the irreducible representations.

Finally, apart from $\bar{q}q$-like interpolators constructed as discussed above we also include multi-hadron operators that create states mimicking scattering states of two hadrons.\(^6\) The corresponding states are built from linear combinations of states created by single-particle operators with generalized Clebsch-Gordan coefficients,

\[
|d, I, S, \Lambda^{[G]}\rangle = \sum \left( |d_a, I_a, I_3, S_a, \Lambda_a, \mu_a\rangle \otimes |d - d_a, I_b, I_3, S_b, \Lambda_b, \mu_b\rangle \right) \times |d_a, I_a, I_3, S_a, \Lambda_a, \mu_a\rangle \otimes |d - d_a, I_b, I_3, S_b, \Lambda_b, \mu_b\rangle
\]

where momentum conservation has been included explicitly. The key point to note in (2.25) is that each state created by single-particle operators is projected onto definite momentum individually. A method to treat quark propagation from every lattice point to all other lattice points is required in order to compute correlation functions of such multi-particle operators.

### 2.3. Practical All-to-All Propagators

Propagators from all lattice points on a given time slice to all lattice points are required in the evaluation of correlation functions of multi-particle interpolators. While for correlation functions involving only local single-particle interpolators the spatial summation on the source time slice can be sidestepped using translation invariance, and hence point-to-all quark propagators are sufficient, limiting the summation to the sink time slice does not work for correlation function involving multi-particle interpolators. For present-day lattice QCD simulations, the Dirac fermion matrix $M$ has a dimension of order

\[
\dim(M) = 12 \times N_s^3 \times N_t \sim \mathcal{O}(10^8),
\]

rendering a direct computation of the matrix inverse impossible. However since the action of $M$ on a quark field is known, numerical solutions of the linear system of

---

\(^6\)There is no notion of one-particle and two-particle states in Euclidean time. Strictly speaking the following statements are to be understood through the equivalent statement in terms of interpolating operators for which it is possible to distinguish between single-particle-like and two-particle-like interpolators.

---

\(^6\)Fixed in this way. If the strangeness label $S$ is suppressed, $S = 0$ is understood.
can be computed for a given right-hand side (source vector) $b$ using iterative methods.\(^7\) The exact matrix inverse can in principle be obtained by solving (2.27) for $\dim(M)$ many source vectors, but this approach is, again, unfeasible for realistic lattice sizes. In this section we will discuss how to treat quark propagation efficiently, yielding all-to-all propagators for practical purposes requiring only a relatively small number of solutions of the above equation.

2.3.1. Distillation

The key observation that facilitates the efficient treatment of quark propagation is that the modes of propagation dominating the low-energy behavior of correlation functions are captured by a smaller subspace [16]. Hadron creation operators are built from smoothed fields $\tilde{\psi}, \tilde{\bar{\psi}}$ obtained from applying a low-rank operator $S$ to the quark fields that appear as building blocks in the lattice QCD action,

$$\tilde{\psi}^A_{aa}(x,t), \tilde{\bar{\psi}}^A_{aa}(x,t),$$

with color index $a$, spin index $\alpha$, and quark flavor $A$. Such a smoothing procedure is referred to as smearing in the context of lattice QCD. Smearing techniques are commonly used to enhance the overlap of interpolating operators with the low-lying states relative to higher-lying states, effectively reducing the inadvertent contamination from excited states in correlation functions. An important constraint on possible choices of smearing operators is that they preserve the behavior of the quark fields under the symmetries discussed in the previous section, so as not to spoil the operator construction guided by symmetry. One possible operator to base the construction of the smearing operator $S$ on is the gauge-covariant three-dimensional Laplacian, which in a gauge background $\tilde{U}_k(x)$ is defined by

$$\Delta_{ab}(x,y|\tilde{U}) = \sum_{k=1}^3 \tilde{U}^{ab}_k(x) \delta_{y,x+k} + \tilde{U}^{\dagger ab}_k(x - \hat{k}) \delta_{y,x-k} - 2 \delta_{x,y} \delta^{ab}. \quad (2.29)$$

\(^7\)Solving (2.27), which we will refer to as an inversion in the following, is typically the most computationally expensive part of performing measurements on previously generated gauge configurations. Highly specialized solvers are available exploiting a wide range of physical insights to efficiently solve this equation, see e.g. [59].
In order to suppress UV fluctuations of the gauge field in the definition of the lattice Laplacian, it is beneficial to employ smoothened gauge links $\bar{U}$ obtained from the original gauge fields $U$ through some smearing procedure. A theoretically well-founded smearing algorithm that does not require a re-unitarization is stout smearing [60], which we will employ in this work. The stout-smearing scheme is fully determined by the smearing weight $\rho$ and the number of iterations $n_\rho$, and the level of smearing is essentially governed by their product [60, 61]. These spatially smeared gauge links are used only in the definition of the Laplacian and hence our observables; quark propagation is still computed in the unsmeared gauge background.

The effect of the lattice Laplacian acting on a quark field is to locally average the field in such a way that all the symmetries of the original field are preserved. Since the gauge-covariant Laplacian is Hermitian, its eigenvalues on a single time slice are all real, and the eigenvectors can be chosen to be mutually orthonormal. As in the continuum, the eigenvalues of the Laplacian are all negative. The smearing kernel defined in terms of the Heaviside function

$$S = \Theta(\sigma^2_s + \Delta)$$

then defines a family of smearing schemes as a function of the mass-dimension two cutoff parameter $\sigma^2_s$. The meaning of (2.30) is explained in the eigenbasis of $-\Delta$,

$$S_{ab}(x, y) \approx \delta_{x_4, y_4} \sum_{k=1}^{N_{ev}} v_a^{(k)}(x)v_b^{(k)*}(y),$$

(2.31)

with eigenvectors $v^{(k)}$ and corresponding eigenvalues $\lambda^{(k)} > \lambda^{(k-1)} > \ldots > 0$ on a single time slice such that

$$-\Delta v^{(k)} = \lambda^{(k)} v^{(k)}, \quad \lambda^{(N_{ev}+1)} > \sigma^2_s,$$

(2.32)

which makes it clear that $S$ is an orthogonal projector into the subspace spanned by the $N_{ev}$ low-lying eigenmodes of the three-dimensional Laplacian.\(^8\) In matrix notation with compound indices encompassing space and color, the projector can be written as

$$S = V_s V_s^\dagger,$$

(2.33)

with $V_s^\dagger$ a $N_{ev} \times 3 \cdot N^3_s$ matrix whose rows are the Hermitian conjugates of the $N_{ev}$

\(^8\)We will refer to this subspace as Laplacian-Heaviside subspace, or LapH subspace for short. In the original context it is known as distillation subspace.
eigenvectors. Intuitively, \( V_s^{\dagger} \) acting on a field with space and color indices returns the coefficients of the field expanded in the LapH subspace basis, and \( V_s \) promotes a field with eigenvector indices back to a lattice-wide color vector field. After the projection, an initially perfectly localized quark field is smeared over a finite range that decreases with increasing cutoff \( \sigma^2_s \) and is well described by a Gaussian profile.

For \( N_{ev} = 3 \cdot N_s^3 \) the projection operator becomes the identity.

Little is known analytically about the spectrum of the gauge-covariant Laplacian in a nontrivial gauge background, but numerical studies found that the number of eigenvectors that have to be retained in order to satisfy the cutoff criterion in (2.32) fluctuate very little across time slices and gauge configurations. Therefore we will define our smearing scheme by keeping the number of retained eigenvectors \( N_{ev} \) fixed, rendering (2.31) exact. Furthermore it has been established over a wide range of physical volumes that the density of eigenvalues is proportional to the physical spatial volume of the lattice (at sufficiently high values), which implies

\[
N_{ev} \propto V \equiv (aN_s)^3 \quad \text{for fixed } \sigma^2_s.
\] (2.34)

A value of \( \sigma^2_s \approx (1 \text{ GeV})^2 \) was found to suppress excited-state contamination sufficiently well without oversmearing in numerical tests with nucleon operators [17].

While at the interpolator level the above projection amounts to a smearing, using the smeared quark fields \( \tilde{\psi} \) and \( \tilde{\bar{\psi}} \) as building blocks for interpolators has even more profound consequences at the level of quark propagation. Using Grassmann integration as shown in section 1.2 it will become clear that only a number of inversions proportional to \( 4 \cdot N_{ev} \ll 12 \cdot N_s^3 \) are required in this approach. Correlation functions of many different operators are assembled \textit{a posteriori} using the information about quark propagation in the LapH space, so that the computationally expensive inversions can be re-used for a wide range of observables.

In order to keep this presentation in line with the notation in the literature [17], we perform a change of variables\(^9\) in the path integral of lattice QCD,

\[
\bar{\psi} \to \chi = \bar{\psi} \gamma_4,
\] (2.35)

so that the fermion action is given by

\[
S_F[\chi, \psi, U] = \chi \Omega[U] \psi, \quad \Omega = \gamma_4 M.
\] (2.36)

\(^9\)In [17] this is done to ensure Hermitian baryon correlation functions.
As in (1.15), and using \( \det \gamma_4 = 1 \), integration of the path integral over the Grassmann fields leads to a factor \( \Omega^{-1} \) for each coupling of one \( \psi \) to one \( \chi \) field with compound indices encompassing space, time, color and spin,

\[ \int D\chi D\psi \psi_a \chi_b \exp (-\chi \Omega \psi) = \Omega_{ab}^{-1} \det \Omega, \tag{2.37} \]

which we refer to as a quark line, which can be pictured as starting at the \( \chi \) field and terminating at the \( \psi \) field, based on the index structure of the above result.

If instead smeared fields are taken as basic building blocks of hadron operators, quark lines emerge from factors in the path integral such as

\[ (S \psi)_a (\chi S)_b = S_{ai} \chi_j S_{jb} \tag{2.38} \]

which after integration over the Grassmann fields (for which the complex-number-valued entries of \( S \) are irrelevant) leads to observables of the form

\[ Q_{ab} \equiv S_{ai} \Omega^{-1}_{ij} S_{jb} = (S \Omega^{-1} S)_{ab}. \tag{2.39} \]

Equation (2.39) spells out that the quark propagator \( \Omega^{-1} \) is required only in the LapH subspace,

\[ [S \Omega^{-1} S]_{ab} = [V_s (V_s^\dagger \Omega^{-1} V_s) V_s^\dagger]_{ab} \tag{2.40} \]

as per (2.33), due to the appearance of the corresponding projector on both sides. Effectively, spatial and color indices are replaced by Laplacian eigenmode number, and the matrix elements

\[ \langle t', n', s'| V_s^\dagger \Omega^{-1} V_s | t, n, s \rangle, \tag{2.41} \]

with spin indices \( s, s' = 0, \ldots, 3 \), LapH space basis indices \( n, n' = 0, \ldots, N_{ev} - 1 \), source time \( t \) and sink time \( t' \) are left to be determined through inversions with appropriate sources. Compared to quark propagation schemes that rely on lattice-wide quark fields, LapH smearing results in mild storage requirements as only the relevant matrix elements of (2.41) need to be stored in addition to the spin-blind eigenvectors. For single-hadron correlation functions it is typically sufficient to perform the inversions for a handful of source times \( N_{t0} \). Thus, treating quark propagation in the LapH subspace – which captures the dominant low modes of quark propagation – yields practical all-to-all propagators at a cost proportional to \( N_{ev} \) inversions per gauge configuration. However, in the evaluation of correlation functions of multi-
hadron operators, generally quark propagation on the same time slice is required for each sink time slice, so that the number of necessary inversions ends up near $4 \cdot N_t N_{ev}$ with $N_t$ the time extent of the lattice.

### 2.3.2. The Stochastic LapH Method

Quark propagation in the LapH subspace can be treated exactly with attainable computational cost on lattices up to moderate size and indeed a wide range of state-of-the-art spectroscopy applications are based on this method (see e.g. [62, 63, 64]). Equation (2.34) however illustrates that in order to keep the smearing radius fixed when doubling the linear spatial extent of a lattice, the number of eigenvectors to be retained – and hence the number of required inversions – increases eightfold. The computational cost of performing measurements is dominated by the inversions, which thus scales with the volume as $V^2$, rendering an exact treatment of quark propagation in the LapH subspace impractical on lattices with large physical spatial extent.

Augmenting the approach with a stochastic estimator in the LapH subspace overcomes the volume-squared scaling. The rationale behind this stochastic treatment is that as the Monte Carlo method is used to evaluate the path integral over gauge field configurations, the attainable statistical accuracy of correlation functions is ultimately limited by the finite sampling of the path integral, and it is hence sufficient to obtain estimates of quark lines with an uncertainty comparable to this gauge noise. Such estimates can be reached with far fewer inversions than required for an exact treatment of the quark lines [17].

The matrix inverse of a large matrix $A$ can be estimated stochastically using random noise vectors $\eta$ whose size equals the dimension of $A$, and whose elements have expectation values

$$E(\eta_i) = 0, \quad E(\eta_i \eta_j^*) = \delta_{ij}. \quad (2.42)$$

Assuming that there is a method to solve the equation $AX = \eta$ for a given random source – so that $X = A^{-1} \eta$ – the matrix inverse is given by the expectation value

$$E(X_i \eta_j^*) = E \left( \sum_k A_{ik}^{-1} \eta_k \eta_j^* \right) = \sum_k A_{ik}^{-1} E \left( \eta_k \eta_j^* \right) = \sum_k A_{ik}^{-1} \delta_{kj} = A_{ij}^{-1}, \quad (2.43)$$
which is estimated using the Monte Carlo method. The key idea of the stochastic LapH method is to combine LapH smearing with such a stochastic estimator in the corresponding subspace. Approximations of the quark propagator obtained from Monte Carlo estimates of the expectation value in (2.43) are usually afflicted with variances which are too large to be useful. Variance reduction is achieved by diluting the noise sources [15, 65, 66]. A dilution scheme is defined by specifying a complete set of orthogonal projection operators \( P^{(a)} \), which can be thought of as matrices whose dimension equals that of \( A \), and which satisfy
\[
P^{(a)} P^{(b)} = \delta^{ab} P^{(a)}, \quad P^{(a)\dagger} = P^{(a)}, \quad \sum_{a=0}^{N_{\text{dim}}-1} P^{(a)} = 1.
\] (2.44)

An estimate of the matrix inverse with reduced variance is then given by
\[
A^{-1}_{ij} \approx \frac{1}{N_R} \sum_{r=1}^{N_R} \sum_a X^r[a]_i \eta^r[a]_j,
\] (2.45)
with \( X^r[a] \) the solution of the system of equations for the diluted source \( \eta^r[a] \),
\[
X^r[a] = A^{-1} \eta^r[a], \quad \eta^r[a] = P^{(a)} \eta^r,
\] (2.46)
and noise label \( r \). Some insight into how dilution works can be gained by noting that, as per (2.42) and (2.43), stochastic estimators for the matrix inverse essentially operate by inserting a noisy decomposition of the unit matrix. Considering
\[
\eta_k \eta_j^* = \sum_{ab} P^{(a)}_{kk} \eta_k^a \eta_j^b P^{(b)}_{jj} = \sum_{ab} \eta_k^a \eta_j^b \eta_j^* \eta_k^a, \quad \text{but } E(\eta_k \eta_j^*) = \sum_a E(\eta_k^a \eta_j^a \eta_j^* \eta_k^a).
\] (2.47)
one sees that
\[
\eta_k \eta_j^* \neq \sum_a \eta_k^a \eta_j^a \eta_j^* \eta_k^a.
\] (2.48)
Therefore, while both schemes provide a valid noisy decomposition of the unit matrix, it is plausible that the diluted system produces a lower variance due to the orthogonality between dilution projectors. Additionally, using unit-modulus noise that satisfies \( |\eta^r_r| = 1 \) for each noise index \( r \) exactly instead of only statistically leads to minimal variance in the diagonal elements of the matrix inverse [67].

For the actual task of efficiently estimating quark lines, the noise vectors \( \rho \) are

---

\(^{10}\)This intuitive explanation can be made rigorous by computing the variance for a given noise explicitly, as was done for example in [66]. Any insight into the structure of the matrix to be inverted can readily be exploited to design more efficient dilution schemes.
taken to have spin, time and Laplacian eigenmode number as their indices. Each component is a random $Z_4$ variable so that $E(\rho) = 0$ and $E(\rho \rho^\dagger) = 1$. The quark line of (2.39) written in matrix form is calculated using

\[
Q = S \Omega^{-1} S = S \Omega^{-1} V_s V_s^\dagger \nonumber \\
= \sum_{a=0}^{N_{du}-1} S \Omega^{-1} V_s P(a) P(a) V_s^\dagger \nonumber \\
= \sum_{a=0}^{N_{du}-1} S \Omega^{-1} V_s P(a) E(\rho \rho^\dagger) P(a) V_s^\dagger \nonumber \\
= \sum_{a=0}^{N_{du}-1} E \left( S \Omega^{-1} V_s P(a) \rho (V_s P(a) \rho)^\dagger \right). \tag{2.49}
\]

Defining diluted source and sink vectors,

\[
\varrho^{[a]} = V_s P(a) \rho, \quad \varphi^{[a]} = \Omega^{-1} \varrho^{[a]}, \quad \phi^{[a]} = S \varphi^{[a]}, \tag{2.50}
\]

the Monte Carlo estimate of the quark line with its outer-product form is written succinctly\footnote{Again, a quark line $Q$ is a matrix in space, time, spin and color space. Space and time indices are written as arguments here, but are to be understood just like matrix indices.} as

\[
Q_{a'\alpha';aa} (y, t_F | x, t_0) \approx \frac{1}{N_R} \sum_{r=1}^{N_R} \sum_{b} \varphi^{[b]}_r (y, t_F) \varphi^{[b] \dagger}_r (x, t_0). \tag{2.51}
\]

In practice, when computing the sink vectors, one first obtains the unsmeared sinks $\varrho^{[a]}$ which are subsequently projected back into the LapH subspace to yield the smeared sinks $\phi^{[a]}$. Only the smeared sinks are required to construct correlation functions of LapH-smeared interpolating operators, the unsmeared sinks however will be crucial for the determination of matrix elements of renormalized currents. The construction of correlation functions involving renormalized currents is discussed in section 2.4; here it is only important to note that unsmeared sinks are accessible in the numerical procedure.

In the stochastic LapH method, (2.51) is used directly for forward quark lines for which $t_F > t_0$. The dilution projectors we use for these quark lines are direct products of time dilution, spin dilution and LapH eigenvector dilution projectors. The full projector index $a = (a_T, a_S, a_L)$ is a triplet of indices for time, spin and...
eigenmode dilution respectively. Then the dilution projectors take the form

$$P_{\text{tan};t'\alpha'\alpha n'}^{(a)} = P_{t;\alpha n'}^{(a_T)} P_{\alpha;\alpha'}^{(a_S)} P_{n;n'}^{(a_L)},$$

(2.52)

and the simplest dilutions schemes for these elemental dilution projectors are given by diagonal projectors with some of the diagonal entries set to unity and all other elements vanishing,

$$
\begin{align*}
P_{ij}^{(a)} &= \delta_{ij}, & a = 0, & \text{no dilution} \\
P_{ij}^{(a)} &= \delta_{ij} \delta_{ai}, & a = 0 \ldots N - 1, & \text{full dilution} \\
P_{ij}^{(a)} &= \delta_{ij} \delta_{a,\lfloor J_i/N \rfloor}, & a = 0 \ldots J - 1, & \text{block-}J \\
P_{ij}^{(a)} &= \delta_{ij} \delta_{a, i \mod J}, & a = 0 \ldots J - 1, & \text{interlace-}J
\end{align*}
$$

(2.53)

where $N$ is the dimension of the space of the dilution type: $N = N_t$ the number of time slices on the lattice for time dilution, $N = 4$ for spin dilution, and $N = N_{ev}$ for eigenvector dilution. A dilution scheme is completely specified by a triplet ($T$, $S$, $L$) describing the dilution scheme in time, spin and eigenmode space respectively.

To estimate forward quark lines we employ the dilution scheme ($T_F$, $S_F$, $LI_8$), denoting full time and spin dilution and interlace-8 dilution in eigenmode number.\footnote{In this language, exact distillation as discussed in the previous section corresponds to full dilution ($TF$, $SF$, $LF$), in which case the exact propagator is recovered with $N_R = 1$ noise sources. However this ‘homeopathic limit’ of course entails a number of required inversions proportional to $N_{ev}$.}

Full spin dilution is essential to cleanly extract correlation functions of operators with definite transformation properties under spatial rotations, as mixing among spin components due to the stochastic treatment would corrupt the intended quantum numbers.

Interlacing several eigenvectors in each diluted source is at the heart of overcoming the volume-squared scaling of computational cost of the inversions – in this scheme the required number of inversions per gauge configuration is not proportional to $N_{ev}$, and hence the volume, but a constant. In the parameter space (in lattice spacing, pion mass and physical volume) explored so far the stochastic LapH method generally yields practical results; indeed the calculation of scattering amplitudes as pursued in this work puts rather high demands on the required accuracy of extracted correlation functions that seem to be met by the stochastic LapH method.\footnote{Ultimately the achievable accuracy should be compared to the actual gauge noise to establish the order of the variance due to the stochastic treatment. To date there is no formal comprehensive survey of the so-defined efficacy of the stochastic LapH method in realistic lattice volumes, and no clear physical picture has emerged as to why the method seems to work rather well at all.}

12

13
A potent dilution in time is indispensable for estimating quark lines from \( t_0 \) to \( t_F \neq t_0 \) in order to distill the exponentially-decaying signal from otherwise occurring \( \mathcal{O}(1) \) noise. Usually, inversions are computed for only a small number of source times \( N_{t_0} \ll N_t \) per gauge configuration, because correlation functions extracted using nearby source times tend to be highly correlated.

Since typically quark propagation from \( t_F \) back to \( t_0 \) is also needed to evaluate correlation functions, it is useful to use \( \gamma_5 \)-hermiticity to swap source and sink in our estimate of quark lines to avoid extra inversions. Using \( M = \gamma_5 M \gamma_5 \), so that \( (M^{-1})^\dagger = \gamma_5 M^{-1} \gamma_5 \), and the fact that the LapH projector \( S \) in spin-independent, \( \Phi \neq (\Phi^\dagger)^* \)

\[
Q^\dagger = \left( S M^{-1} \gamma_4 S \right)^\dagger = S \gamma_4 \gamma_5 M^{-1} \gamma_5 S = \gamma_4 \gamma_5 S M^{-1} \gamma_4 S \gamma_5 = -\gamma_5 \gamma_4 Q \gamma_4 \gamma_5,
\]

and a different way to estimate the quark line in (2.51) is

\[
Q_{a\alpha; a'} (y, t_F | x, t_0) = -\left( \gamma_5 \gamma_4 Q \gamma_4 \gamma_5 \right)_{a\alpha; a'} (x, t_0 | y, t_F)^* \\
\approx \frac{1}{N_R} \sum_{r=1}^{N_R} \sum_b \bar{q}^{r[b]} (y, t_F) \bar{\phi}^{r[b]*} (x, t_0), \tag{2.55}
\]

with

\[
\bar{q}^{[b]} = -\gamma_5 \gamma_4 q^{[b]}, \quad \bar{\phi}^{[b]} = \gamma_5 \gamma_4 \varphi^{[b]}, \tag{2.56}
\]

Renaming the indices makes it clear how (2.55) can be used to estimate quark lines starting at arbitrary \( t_F \) and ending at \( t_0 \), given stochastic sources on \( t_0 \) and corresponding sinks on all \( t_F \),

\[
Q_{a\alpha; a'} (x, t_0 | y, t_F) \approx \frac{1}{N_R} \sum_{r=1}^{N_R} \sum_b \bar{q}^{r[b]} (x, t_0) \bar{\phi}^{r[b]*} (y, t). \tag{2.57}
\]

We refer to both quark lines from \( t_0 \) to \( t_F \) and those starting at \( t_F \) and terminating at \( t_0 \) with \( t_0 \neq t_F \) as fixed quark lines and use the dilution scheme described above.

One last additional type of quark propagation, which is needed for the computation of correlation functions of multi-hadron interpolators, is a quark line starting and ending on the same time slice \( t \). Full time dilution is not feasible in that instance.

It is interesting to note that in the context of solving the Dirac equation a similarly obstructive volume-squared scaling is overcome using an inexact deflation method to exploit the properly defined locality of the low-lying quark modes [59]. While probably relevant to the problem at hand here, the exact relation remains to be investigated.
as such a quark line is needed for all sink time slices. Instead we adopt a different dilution scheme (TIn, SF, LI8) with several source times interlaced for these same-time lines or relative quark lines. The additional variance of same-time matrix elements of the quark propagator due to the source being interlaced in time is expected to fall off as least as $e^{-am_\pi n}$ with $an$ the physical interlace distance and $m_\pi$ the lowest-lying hadronic state with the flavor content of the propagator, for instance the pion mass for same-time up or down quark lines. Consequently the time interlace $n$ has to be chosen for each ensemble individually based on its pion mass in lattice units.

Using these dilution schemes the total number of inversions required per gauge configuration and quark mass is

$$N_{\text{inv}} = 4N_{t0}N_{L1}^{t0 \rightarrow tF} \cdot N_{R}^{t0 \rightarrow tF} + 4nN_{L1}^{t \rightarrow t} \cdot N_{R}^{t \rightarrow t},$$

(2.58)

with $N_R$ the number of noises and $N_{LI}$ the Laplacian eigenmode interlace, each for fixed and relative lines respectively.

### 2.3.3. Construction of Correlation Functions

As we will discuss in this section, as a consequence of the outer-product structure of the quark propagators the construction of correlation functions can be divided into two separate stages. After the appropriate objects – meson functions in the stochastic LapH language, which carry dilution and noise indices in addition to the label describing the interpolating operator they come from – have been computed from source and sink vectors and written to disk, the final assembly of correlation functions proceeds via contraction of dilution indices alone, and does not involve any gauge or lattice structures any more.

Each single-site meson interpolator destroying a three-momentum $p$ is a sum of gauge-invariant quark-antiquark elemental operators built from smeared quark fields $\chi$ and $\bar{\psi}$,

$$M_l(t) = c^{(l)}_{\alpha\beta} \Phi_{\alpha\beta}(t), \quad \Phi_{\alpha\beta} = \sum_x e^{-ipx} \chi_{a\alpha}(x, t) \bar{\psi}_{a\beta}(x, t),$$

(2.59)

where $l$ is a label which identifies the interpolating operator, including all the quantum numbers (momentum $p$, symmetry-group irreducible representation $\Lambda$, and row of the irreducible representation $\mu$) and an identifier for each operator in that symmetry channel. The corresponding operator which creates a momentum $p$ takes the
form

$$
\bar{M}(t) = c^{(l)_s}_\alpha \Phi \Phi \alpha = \sum x e^{ipx} \chi\alpha \beta (x, t)\psi\alpha \beta (x, t),
$$

and a meson-to-meson correlation matrix element is given by

$$
C_{ll}(t_F|t_0) = \left\langle M_l(t_F)\bar{M}_l(t_0)\right\rangle = c^{(l)}_\alpha c^{(l)_s}_\alpha \left\langle \Phi \Phi \alpha \beta (t_F)\bar{\Phi} \bar{\Phi}\alpha \beta (t_0)\right\rangle,
$$

where $l$ and $\bar{l}$ have to contain the same quantum numbers, or else the correlation of the respective operators averages to zero. In terms of the smeared quark fields the correlation function reads

$$
C_{ll}(t_F|t_0) = c^{(l)}_\alpha c^{(l)_s}_\alpha \sum x, \bar{x} e^{-ipx} e^{ipx} \left\langle \chi\alpha \beta (x, t_F)\psi\alpha \beta (x, t_F)\bar{\chi}\alpha \beta (\bar{x}, t_0)\psi\alpha \beta (\bar{x}, t_0)\right\rangle,
$$

which, after performing the Grassmann integration in the path integral, leads to the remaining average of two quark lines over gauge configurations

$$
C_{ll}(t_F - t_0) = c^{(l)}_\alpha c^{(l)_s}_\alpha \sum x, \bar{x} e^{-ipx} e^{ipx} \left\langle -Q\alpha\beta (x, t_0|x, t_F) Q_{\alpha\beta} (\bar{x}, t_F|\bar{x}, t_0)\right\rangle_U.
$$

(2.63)

For flavor-singlet operators another combination with each quark line starting and ending at the same space-time point contributes as well, which we do not show here assuming a nonsinglet flavor structure. As explained in the last section it is advantageous to use $\gamma_5$-hermiticity to estimate the first quark line according to (2.57), whereas (2.51) is used to estimate the second quark line. Defining the meson function, which is an object with noise and dilution indices as well as an identifying label for the interpolating operator it comes from,

$$
M_i^{[1, 2]b_1 b_2} (\varphi, \varphi, t) = c^{(l)}_\alpha \sum x e^{-ipx} g_{\alpha\beta}^{[1]} (x, t)\varphi^{[2]}_{\alpha\beta}(x, t),
$$

the meson-to-meson correlation function is written concisely as

$$
C_{ll}(t_F - t_0) = \left\langle -M_i^{[1, 2]b_1 b_2} (\varphi, \varphi, t_F) M_i^{[1, 2]b_1 b_2} (\varphi, \varphi, t_0)\right\rangle_U,
$$

(2.65)

where the sum over dilution indices $b_1, b_2$ is implicit. We refer to the two types of meson functions occurring above as meson sink function and meson source function respectively as they are built exclusively from either quark sinks or quark sources.
In order to ensure an unbiased stochastic estimate of the correlation function, the average over noises $\langle \cdot \rangle_\rho$ must be taken such that ‘parallel quark lines’ whose start and end times coincide are never estimated using the same noise source $\rho$. Therefore at least two independent noise sources are required in the simple meson-to-meson correlator above.

Figure 2.1.: Computation of the correlation function of an isovector two-meson source at time $t_0$ and a single-meson sink at time $t_F$. Each box represents a meson function given by (2.64) with the first quark field located at the top of the box. Lines indicate summation over their dilution indices, and the same noise must be used at both ends of any line. The asterisk denotes complex conjugation.

The key point expressed in this equation is that as a consequence of the outer-product structure of the quark propagator the correlator factorizes into a function associated with the sink time slice $t_F$ and another function associated with the source time slice $t_0$, such that the summations over color, spin and spatial indices are completely separated. Similarly, more complicated correlation functions involving multi-meson operators, which are built from superpositions of single-hadron operators, can be computed by evaluating higher-dimensional sums over dilution indices of the according number of meson functions. The contractions of dilution indices required for a given correlation function are governed by the flavor structure of the interpolators and are inferred from a graphical representation of the involved Wick contractions [17]. As an example figure 2.1 shows the contractions required for an isovector two-meson–to–meson correlation function, which has the same structure as the correlation function of a two-pion interpolator and the isovector current. The corresponding technical machinery is well-established, and we conclude this section by noting that the factorization property (which transforms the task of constructing correlation functions of lattice-wide objects into the equivalent problem of enumerating dilution contractions of meson sink functions) is the key ingredient enabling the extraction of correlators involving renormalized current operators in the stochastic
LapH framework.

### 2.4. Matrix elements in the Stochastic LapH Framework

The electromagnetic pion form factor in the timelike region is an example of an observable whose extraction goes beyond determining the masses of stationary states from the decay of Euclidean correlation functions. The required additional information is encoded in matrix elements of the electromagnetic current between hadronic states and the vacuum,

$$
\langle 0 | j_{\text{em}}^\mu | n \rangle,
$$

where

$$
j_{\text{em}}^\mu = \frac{2}{3} \bar{u} \gamma^\mu u - \frac{1}{3} \bar{d} \gamma^\mu d - \frac{1}{3} \bar{s} \gamma^\mu s + \ldots
$$

(2.66)

Since we work in an isospin-symmetric setup, the light part of the electromagnetic current is decomposed as

$$
j_{\text{em}}^\mu = \frac{1}{6} \left( \bar{u} \gamma^\mu u + \bar{d} \gamma^\mu d \right) + \frac{1}{2} \left( \bar{u} \gamma^\mu u - \bar{d} \gamma^\mu d \right) + \ldots
$$

(2.67)

where the two terms transform as an isoscalar and isovector respectively. We will focus here on the isovector contribution such that disconnected quark lines are absent in correlation functions. The renormalization and $O(a)$ improvement of the vector current for $N_f = 2 + 1$ flavors of Wilson fermions will be discussed more thoroughly in section 4.5, and we only note here that the relevant operator elementals with mass-dimension three and four are [45, 68]

$$
V_\mu^a = \chi \gamma^\mu \tau^a_2 \psi,
$$

$$
\tilde{\partial}_\nu T_{\mu\nu}^a = i \tilde{\partial}_\nu \left[ \chi \gamma^\mu \sigma_{\mu\nu} \tau^a_2 \psi \right],
$$

(2.68)

with flavor index $a$ and $\sigma_{\mu\nu} = \frac{1}{2} [\gamma_\mu, \gamma_\nu]$. The symmetrized lattice derivative acts on color-singlet functions $f(x)$ as

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

(2.69)

The matrix elements of interest are the ones of the vector current with appropriate polarization [69] between hadronic states (created by interpolators which transform
Table 2.2.: Linear combinations of the vector current such that $V^{(d,\Lambda)} = b_{i}^{(d,\Lambda)} V_{i}$ transforms according to the first row of the irreducible representation $\Lambda$ for some representative total momenta. The polarization vectors are matched with the irrep conventions also for various equivalent momenta in moving frames to facilitate an average over these equivalent momenta.

irreducibly under the lattice symmetries) and the vacuum,

$$V^{(d,\Lambda)} = \sum_{\mu} b^{(d,\Lambda)}_{\mu} (V R)^{a}_{\mu}, \quad \sum_{\mu} b^{(d,\Lambda)*}_{\mu} b^{(d,\Lambda)}_{\mu} = 1. \quad (2.70)$$

The polarization vectors $b^{(d,\Lambda)}_{\mu}$ are chosen such that the conventions for irreducible representations match those of our interpolating operators. The linear combinations of current elemental operators for irreducible representations relevant for the isovector contribution to the timelike pion form factor are given in table 2.2 for representative total momenta. Correlation functions in each irreducible representation are averaged over equivalent momenta, for instance $d = [001], [010], [100]$ for $d^2 = 1$, and the polarization vectors $b^{(d,\Lambda)}$ are chosen accordingly. The flavor index $a$ is suppressed with the understanding that the attention is restricted to the isovector part of the electromagnetic current and maximum isospin projection as before. The corresponding matrix elements are obtained from correlation functions of the form

$$D_{j}(t_{F}, t_{0}) = \langle 0 | V^{(d,\Lambda)}(t_{F}) \bar{O}_{j}^{(d,\Lambda)}(t_{0}) | 0 \rangle , \quad (2.71)$$

for each relevant irreducible representation.

The crucial difference to the correlation functions defined earlier is that the annihilation operator at time $t_{F}$ is the external current. LapH quark smearing alters
the renormalization properties of the vector current in a way not accessible by field-theoretic methods.\footnote{Our smearing bears some resemblance to the flow of the quark fields suggested in [70] in the sense that both schemes are based on the Laplacian. The LapH subspace is however spanned by the eigenvectors of the three-dimensional Laplacian, and stout smearing of the gauge links and quark smearing are applied consecutively instead of flowing all fields simultaneously, rendering our smearing scheme unamenable to a field-theoretic analysis.} In order to be able to utilize the renormalization constant, which is known nonperturbatively for the regularization employed in this work, the operators in (2.68) must thus be built from unsmeared quark fields, while the creation operator at time $t_0$ is a linear combination of smeared quark fields as before. In the remainder of this section we demonstrate that such unsmeared current correlators can be computed in the stochastic LapH framework.\footnote{For a similar treatment of external currents in exact distillation see [71].} Indeed, the only necessary modification is that functions similar to the meson sink functions introduced in the previous section, but built from unsmeared solutions to the Dirac equation need to be computed.

Evaluating correlation functions of the form (2.71) in a given gauge background gives rise to a new class of quark lines,

$$\hat{Q}_{ab} = (\Omega^{-1} S)_{ab}$$  \hspace{1cm} (2.72)

with compound indices $a, b$. Quark lines of this type effectively start in the smaller LapH subspace but are not projected back into the LapH subspace after propagation due to the absence of the projector $S$ to the left of $\Omega^{-1}$ in contrast to (2.39). Such a quark line can be estimated stochastically by observing that all the steps in (2.49) go through unchanged even absent the final projection, and the stochastic estimate of the required quark line is

$$\hat{Q}_{a'\alpha';a\alpha} (\mathbf{y}, t_F|\mathbf{x}, t_0) \approx \frac{1}{N_R} \sum_{r=1}^{N_R} \sum_{b} \vartheta^{r[b]} (\mathbf{y}, t_F) g^{r[b]*}_a (\mathbf{x}, t_0)$$  \hspace{1cm} (2.73)

in accordance with (2.51), the key difference being that the unsmeared diluted quark sink $\vartheta^{[b]}$ of (2.50) features in the stochastic estimate. Evidently it is impossible to compute correlation functions with the external current placed at the source time in this framework, as the stochastic LapH method quintessentially relies on the particular way stochastic noise is inserted in the LapH subspace.

As before, quark lines from the sink time $t_F$ back to the source time $t_0$ emerge from the Wick contractions as well. Here they lead to just another class of quark
lines\textsuperscript{16},

\[ \hat{Q}_{ab} = \left( S \Omega^{-1} \right)_{ab} \]  \hspace{1cm} (2.74)

which are projected into the smaller LapH subspace only after propagation. These two more general types of quark lines are related by $\gamma_5$-hermiticity, and (2.54) is generalized to

\[ \hat{Q}^\dagger = \left( M^{-1} \gamma_4 S \right)^\dagger = \gamma_4 \gamma_3 S M^{-1} \gamma_4 \gamma_4 \gamma_5 = -\gamma_5 \gamma_4 \hat{Q} \gamma_4 \gamma_5, \]  \hspace{1cm} (2.75)

or equivalently

\[ \hat{Q} = -\gamma_5 \gamma_4 \hat{Q}^\dagger \gamma_4 \gamma_5, \]  \hspace{1cm} (2.76)

so that, as before, a $t_F$-to-$t_0$ quark line can be estimated using only data from (smeared) sources on $t_0$

\[ \hat{Q}_{ax; a'x'}(x, t_0 | y, t_F) \approx \frac{1}{N_R} \sum_{r=1}^{N_R} \sum_{b} \bar{\varrho}^{[b]}(x, t_0) \bar{\vartheta}^{[b] \ast}(y, t_F). \]  \hspace{1cm} (2.77)

with the smeared source $\bar{\varrho}^{[b]}$ as in (2.56) and the analogous unsmeared sink

\[ \bar{\vartheta}^{[b]} = \gamma_5 \gamma_4 \vartheta^{[b]}. \]  \hspace{1cm} (2.78)

As a last step, it remains to discuss the construction of correlation functions like (2.71) involving external currents from these quark lines, and to define the objects which assume the role of the meson functions in this context. As discussed in the preceding chapter it is sufficient to consider such a correlation function of an isovector single-meson interpolator and the isovector current; the generalization to multi-hadron interpolators is handled through the combinatorics of dilution indices. In our convention the momentum-projected current operator destroying a three-momentum $p$ is given by

\[ J^{(p, \Lambda)}(t) = \sum_{x} e^{-ipx} V^{(p, \Lambda)}(x, t) \]  \hspace{1cm} (2.79)

Up to its renormalization, which is handled a posteriori during the final analysis,
2. Finite-Volume Spectroscopy Methods

the leading-order current operator, with \( p = \frac{2\pi}{L} d \), assumes the form

\[
J^{(d,\Lambda)}(x,t) = \sum_x e^{-ipx} \left( \chi_4 D^{(d,\Lambda)}(x) \cdot \gamma \psi \right)(x,t) \equiv d^{(d,\Lambda)}_{\alpha\beta} \sum_x e^{-ipx} \chi_{aa}(x,t) \psi_{b\beta}(x,t),
\]

(2.80)

with a similar expression for the mass-dimension-four operator governed by the more complicated spin structure of \( \tilde{\partial}_\nu T_{\mu\nu} \) given in (2.68), and which also involves a derivative. The quark line structure emanating from the integration over the quark fields in the correlation function of the external current operator \( J \) and a single-hadron operator \( \bar{M} \),

\[
D_l(t_F|t_0) = d^{(d,\Lambda)}_{\alpha\beta} c^{(i)}_{\alpha\beta} \sum_{x,x} e^{-ipx} e^{ip\bar{x}} \left\langle \chi_{aa}(x,t_F) \psi_{a\beta}(x,t_F) \tilde{\chi}_{\alpha\beta}(\bar{x},t_0) \tilde{\psi}_{\alpha\beta}(\bar{x},t_0) \right\rangle
\]

(2.81)

is the same as in an isovector meson-meson correlator, but with the additional structure indicating the unsmeared quark field insertions. Equation (2.73) is used to estimate the second quark line, (2.77) exploiting \( \gamma_5 \)-hermiticity facilitates an estimate of the first quark line, and by complete analogy with the proceedings in the case of the meson-meson correlator, the current correlation function factorizes into two distinct objects contracted via their dilution indices,

\[
D_l(t_F|t_0) = \left\langle -J^{[b_1b_2]}(\bar{\vartheta}, \vartheta, t_F) \mathcal{M}^{[b_1b_2]}(\bar{\vartheta}, \vartheta, t_0)^* \right\rangle_{U,\rho}.
\]

(2.82)

The meson source function \( \mathcal{M}(\bar{\vartheta}, \vartheta, t_0) \) is the object defined in (2.64) already, and the current sink function

\[
\mathcal{J}^{r_1r_2[b_1b_2]}(\bar{\vartheta}, \vartheta, t) = d^{(d,\Lambda)}_{\alpha\beta} \sum_x e^{-ipx} \bar{\vartheta}_{a\alpha}^{[b_1]}(x,t)^* \tilde{\vartheta}_{\alpha\beta}^{[b_2]}(x,t)
\]

(2.83)

is structurally equivalent to the corresponding meson sink function, but built from the unsmeared quark sinks.

To conclude, we have shown in this section how correlation function involving external currents can be calculated using the stochastic LapH method without spoiling the renormalization properties of the current. In fact – and very much due to the fact that the current operator is a valid interpolator itself – little has to be changed at a fundamental level in the machinery developed for the stochastic LapH framework. For instance the diagrammatic language presented in the original literature to facilitate incorporating all Wick contractions is carried over unaltered. The only
new objects required for the computation of correlation functions of single-hadron or multi-hadron interpolating operators and the external current operator are the current sink functions defined in (2.83). No additional inversions are needed for their construction, and in principle the computational overhead is equivalent to the cost of calculating the corresponding meson sink functions.

In practice it is not feasible to store the unsmeared quark sinks $\varphi$ beyond the runtime of the inversion computations, but it is also unnecessary: after the inversions for all noises and dilutions have been performed, the current sink functions are computed right away, and only the projection of the quark sinks back into the LapH subspace is stored permanently for the standard stochastic LapH workflow. Due to the factorization in the computation of correlation functions, their calculation can proceed off-line for an arbitrary number of interpolating operators with the same quantum numbers.

The only present drawback is that current operators whose correlation functions involve disconnected quark lines – starting and ending at the current insertion point – are not tractable in this framework, hence precluding studies involving flavor-singlet external currents. However one could conceivably devise a scheme where this particular class of diagrams is treated slightly differently to allow for flavor-singlet external currents to be included.
3. Interpretation of Finite-Volume Observables

The ultimate goal of predicting the experimentally observable hadronic states from QCD requires an understanding of how resonances manifest in Euclidean-time simulations in a finite volume. Experimentally, resonances are detected as features in scattering cross sections which are obtained from scattering amplitudes theoretically. Hence ideally one aims to extract scattering amplitudes from lattice QCD simulations. Scattering information is however not directly accessible from Euclidean-time correlation functions at general kinematics [7]. This issue can be overcome by viewing finite volume as a tool rather than an artifact.

Finite-volume correlation functions and physical observables such as masses and energies generally differ from their infinite-volume counterparts by two broad classes of finite-volume effects. Corrections that are exponentially small in $L/r$ with linear box size $L$ and $r$ some length scale of the relevant interactions [8] – for example the inverse pion mass – can typically be ignored for sufficiently large spatial extents satisfying $m_\pi L \gtrsim 4$.\(^1\) The other big class of corrections, which appear at energies above the lowest two-particle threshold\(^2\), falls off as some power of $1/L$ [9]. These corrections encode information on the two-to-two pion scattering amplitude; the precise relation is given in the form of a quantization condition connecting the infinite-volume scattering amplitude and the spectrum of the theory in finite volume with periodic boundary conditions [10, 11]. An extension of this result accommodates non-zero total momentum [72], and more recently various generalizations have been devised to include for example the scattering of non-degenerate particles [73, 74], multiple strongly-coupled two-particle scattering channels [75, 76] and scattering of particles with intrinsic spin [77, 78, 79]. The electromagnetic pion form factor in

\(^1\)In practice, whether these corrections are indeed numerically small depends on the prefactor and hence the observable under consideration. Sufficiently small finite-volume effects for instance in the pion mass are a necessary condition for the following discussion to be applicable.

\(^2\)In QCD the lowest-lying threshold is the two-pion energy.
the timelike region is extracted following the proposal in [22] which is theoretically very similar to earlier work [21] on the weak $K \to \pi\pi$ transition.

Thus, Lüscher-type quantization conditions notably allow for infinite-volume scattering amplitudes and transition matrix elements to be constrained using information accessible through lattice QCD simulations. In this work we are concerned with the simplest case of pion-pion scattering, i.e. scattering of degenerate scalar particles in a kinematic regime where only one scattering channel contributes.

The remainder of this chapter is dedicated to a brief outline of the major steps in the derivation of the quantization condition for this particular scenario in a fully field-theoretic language. Section 3.1 traces the key concepts to derive the quantization condition and the relationship between finite-volume matrix elements and the timelike pion form factor along the lines of [80, 81], and section 3.2 describes the induced practical workflow which allows us to extract the pion-pion scattering amplitude and the timelike pion form factor in the elastic region from lattice QCD data.

### 3.1. Scattering Amplitudes and Transition Matrix Elements from Finite-Volume Spectrum

In this section we follow closely the exposition of [81], sketching only the main points. The key identity – from which both the quantization condition relating pion-pion scattering to the two-pion finite volume spectrum, and the relationship between finite-volume matrix elements and the timelike pion form factor can be derived – expresses the finite-volume correlation function in energy space of interpolating operators $A, B$ coupling to two-pion states,

$$C_L(P) = \int_L d^4x e^{-iPx} \left[ \langle 0|A(x)B^\dagger(0)|0\rangle \right]_L, \quad (3.1)$$

in terms of its infinite-volume counterpart and a finite-volume correction term,

$$C_L(P) = C_\infty(P) - A(P) \frac{1}{F^{-1}(P, L) + \mathcal{M}(P)} B^\dagger(P). \quad (3.2)$$

encompassing the infinite-volume two-to-two scattering amplitude $\mathcal{M}$, infinite-volume matrix elements of $A(0), B^\dagger(0)$, and known finite-volume kinematic functions $F$ which depend only on the details of the finite-volume, such as its geometry and
the spatial boundary conditions imposed. The scattering amplitude $\mathcal{M}$ and finite-volume correction $F$ are naturally thought of as matrices in angular momentum and channel space, and $B^\dagger$ and $A$ as corresponding column and row vectors respectively.\(^3\) While the scattering amplitude is diagonal in angular momentum indices, the underlying rotational symmetry is broken by the finite box with periodic boundary conditions typically used in lattice QCD simulations. This breaking of rotational symmetry leads to a mixing of different partial waves in finite volume which is reflected by the block structure of $F$. Deriving the explicit form of $F$ is rather involved but the final result can be concisely expressed in terms of shifted Lüscher zeta functions introduced in [72]. We will give the formulae relevant to our work in section 3.2.

$$C_L(P) = (A)_{l} (B)_{l}^\dagger + (A)_{l} (\underbrace{B} + \ldots)_{l}^\dagger + \ldots$$

Figure 3.1.: The initial series of ladder diagrams which builds up the two-point correlation function in a finite volume in the range of energies such that only two-particle states can go on-shell. The Bethe-Salpeter kernels (gray blobs) are connected by fully-dressed propagators (lines with a dot), and loop momenta are summed over all allowed finite-volume momenta.

The derivation of (3.2) proceeds in three major steps.

First, the finite-volume correlator $C_L(P)$ is expressed in an infinite diagrammatic series which can be organized in the form of a skeleton expansion, built from two-particle loops with momenta summed – as is adequate in a finite volume with periodic boundary conditions – and Bethe-Salpeter kernels. The skeleton expansion for energies where only two-particle states can go on-shell is shown in figure 3.1. The Bethe-Salpeter kernel depicted by gray blobs in that figure equals the sum of all two-to-two diagrams with no on-shell intermediate states. Crucially, replacing the finite-volume summation with infinite-volume integration of loop momenta generates only corrections which are exponentially suppressed in the spatial extent for diagrams with no on-shell states. Since exponentially suppressed corrections are not controlled in this derivation, the Bethe-Salpeter kernel can hence be taken to have its infinite-volume form. For the same reason the particle propagators appearing in the skeleton expansion can be taken to assume their infinite-volume form, as self-energy diagrams do not contain on-shell intermediate states. The requirement that

\(^3\)The finite-volume correction term, being a scalar with no uncontracted indices, is of course basis-independent as a whole.
the endcap functions $A$ and $B$ do not generate any finite-volume corrections beyond exponentially suppressed ones imposes a restriction on the types of operators feasible for use in this framework which are discussed in [81]. We just note that the local vector current which is the interpolator of interest to us does not generate extra finite-volume corrections. All finite-volume effects in $C_L(P)$ thus arise exclusively from the sums over two-particle loops shown explicitly in figure 3.1.

$$
\begin{align*}
\mathcal{M} &= A + B + \cdots \\
\text{Figure 3.2.}: \text{The finite-volume momentum sum over the two single-particle fully-dressed propagators is written as the sum of the momentum-integrated expression and a correction term, essentially defining } F.
\end{align*}
$$

The second step is to formally write each finite-volume two-particle loop with its momenta summed as its infinite-volume counterpart – where the sum is replaced by an integral over momenta – plus a correction term $F$ which is the difference between the momentum sum and integral. This substitution is performed for each two-particle loop irrespective of whether the loop connects to an interpolator endcap function or the Bethe-Salpeter interaction kernel, so the propagator lines are left dangling in figure 3.2 illustrating the replacement. While the finite-volume residue $F$ of course depends on these endcap functions, it yields a finite-volume matrix $F(P, L)$ in angular-momentum space which is a purely kinematical function with an additional dependence on the spatial box size $L$.

$$
\begin{align*}
\text{Figure 3.3.}: \text{The endcap functions } A \text{ and } B^\dagger \text{ as well as the scattering amplitude } \mathcal{M} \text{ are obtained from summing the geometric series of Bethe-Salpeter kernels. All of these quantities assume their infinite-volume form up to exponentially suppressed corrections, which are neglected throughout.}
\end{align*}
$$

As a last step, the terms in the series are regrouped by the number of finite-volume insertions they contain. The first term with no insertion of the finite-volume residue reproduces the infinite-volume two-point correlation function, and in the other terms
3. Interpretation of Finite-Volume Observables

of the series all infinite-volume diagrams outside and in between factors of $F$ yield geometric series. As shown in figure 3.3, for the infinite-volume terms outside insertions of $F$, the resulting sum is absorbed to give the interpolator endcap functions $A$ and $B^\dagger$ corresponding to the interpolators $A$ and $B^\dagger$ respectively, and the geometric series of interaction Bethe-Salpeter kernels between finite-volume insertions add up to the scattering amplitude $\mathcal{M}$. The difference between the finite-volume and infinite-volume two-point correlation function then is depicted in figure 3.4.

$$C_L(P) - C_\infty(P) = \left( A \frac{1}{F} \right) \left( B^\dagger \right) + \left( A \frac{1}{F^2} \right) \left( B^\dagger \right)$$

Figure 3.4.: The difference between the finite-volume and infinite-volume correlation functions expressed in terms of the endcap functions $A$ and $B^\dagger$, the scattering amplitude $\mathcal{M}$ – all of which are infinite-volume quantities – and finite-volume insertions $F$.

This diagrammatic series is a geometric series in $-\mathcal{M}F$, so that

$$C_L(P) - C_\infty(P) = A(-F) \left( 1 + \mathcal{M}F \right)^{-1} B^\dagger,$$

from which (3.2) is deduced.

3.1.1. Quantization Condition

The relation between the finite-volume spectrum and infinite-volume scattering is established by noting that the poles in $C_L(P)$ are located at the energies of the finite-volume theory. The infinite-volume correlation function $C_\infty(P)$ contains branch-cuts above two-particle thresholds, but does not contain the poles relevant to the finite-volume spectrum. The interpolator endcap functions $A$ and $B^\dagger$ are infinite-volume quantities and may include branch cuts, but do not contain these poles either. Poles in the finite-volume correlation function thus occur for zero eigenvalues of the matrix $F^{-1} + \mathcal{M}$, leading to the quantization condition

$$\det \left( F^{-1} + \mathcal{M} \right) = 0.$$

The extra minus sign is to maintain consistency with [81] where each of our diagrammatic $F$ insertions leads to an algebraic factor of $-F$, cf. figure 2 and (84) in that paper.
For a fixed linear spatial extent \( L \) and known energy dependence of the scattering amplitude \( \mathcal{M} \), the finite-volume spectrum is given by the solutions of this equation. We stress again that this result is valid solely in the kinematical range where only two-particle states can go on-shell, i.e. for energies below the lowest three- or four-particle threshold with the same quantum numbers. For pions in QCD, G-parity prevents mixing between states with even and odd numbers of particles, and the lowest-lying multi-particle threshold relevant to isovector pion-pion scattering is the four-pion threshold.

3.1.2. Transition Matrix Elements

The relationship between finite- and infinite-volume matrix elements of appropriate operators is derived from the correlator

\[
C_L(x_4 - y_4, P) = \int_L \! dx \int_L \! dy \ e^{-iP(x-y)} \left[ \langle 0 | A(x) B^\dagger(y) | 0 \rangle \right]_L ,
\]

which can be evaluated in two ways. In the finite-volume theory, it has the decomposition

\[
C_L(x_4 - y_4, P) = \int_L \! dx \int_L \! dy \sum_n e^{-E_n(x_4 - y_4)} \left[ \langle 0 | A(0) | P, n \rangle \right]_L \left[ \langle P, n | B^\dagger(0) | 0 \rangle \right]_L ,
\]

and on the other hand the finite-volume correlator can also be evaluated using its expression in terms of infinite-volume quantities given in (3.2),

\[
C_L(x_4 - y_4, P) \equiv L^3 \int \! \frac{dP_4}{2\pi} e^{iP_4(x_4 - y_4)} C_L(P) = L^3 \int \! \frac{dP_4}{2\pi} e^{iP_4(x_4 - y_4)} \left( C_\infty(P) - A(P) \frac{1}{F^{-1}(P, L) + \mathcal{M}(P)} B^\dagger(P) \right)
\]

\[
= \sum_n e^{-E_n(x_4 - y_4)} L^3 \langle 0 | A(0) | E_n, P, \text{in} \rangle \left[ R(E_n, P) \langle E_n, P, \text{out} | B^\dagger(0) | 0 \rangle \right] ,
\]

with the residue

\[
R(E_n, P) = \lim_{P_4 \to iE_n} \left[ \frac{-(iP_4 + E_n)}{F^{-1}(P, L) + \mathcal{M}(P)} \right] \]

of the function between \( A(P) \) and \( B^\dagger(P) \) evaluated at the two-particle energy \( E_n \). In (3.7) the integral is closed in the upper half of the complex plane assuming \( x_4 > y_4 \).
as before. The only analytic structure encircled by this contour is the tower of the poles along the imaginary axis corresponding to the finite-volume spectrum, so that the integral is given by the sum of residues at these poles. Equating (3.7), which contains only infinite-volume quantities, and (3.6), one obtains the relation

\[
L \left[ \langle 0 | A(0) | P, n \rangle \right] = L^{-3} \langle 0 | A(0) | E_n, P, \text{in} \rangle \mathcal{R}(E_n, P) \langle E_n, P, \text{out} | B(0) | 0 \rangle
\]

(3.9)
between finite-volume and infinite-volume matrix elements. The amplitude for the vacuum to two-particle transition mediated by a local current is obtained by assigning \( A \) and \( B^\dagger \) to be that current, so that (3.9) relates matrix elements of the current in finite and infinite volume up to exponentially suppressed corrections.

### 3.2. Workflow for Practical Implementation

In the practical use of (3.4) we restrict ourselves to the case of scattering between two identical particles of mass \( m_\pi \). The relevant formulae were first given in [10] and generalized to nonzero total momentum in [72], with a useful summary for instance given in [78].

Denoting by \( E \) an energy eigenvalue in a particular irreducible representation with total momentum \( P = \frac{2\pi}{L} d \) measured in the lattice frame, which is the reference frame where the boundary conditions are imposed, we define the kinematical variables

\[
E^* = \sqrt{E^2 - P^2}, \quad \gamma = \frac{E}{E^*}, \quad q^2 = \frac{1}{4} E^{*2} - m_\pi^2, \quad u^2 = \frac{L^2}{(2\pi)^2} q^2.
\]

(3.10)

In the center-of-mass frame the scattering amplitude is expanded in a partial-wave basis (following the conventions of [80]),

\[
\mathcal{M}_{\ell_1, m_1; \ell_2, m_2} = \delta_{\ell_1 \ell_2} \delta_{m_1 m_2} 16 \pi E^* \exp \left[ \frac{2i\delta_{\ell_1}(q)}{q} \right] \left( \frac{1}{2i} \right),
\]

(3.11)

where \( \delta_\ell \) is the phase shift in the \( \ell \)-th partial wave. The quantization condition (3.4) formally involves a determinant over infinitely many partial waves. In order to put the quantization to practical use, the partial-wave basis has to be truncated and the determinant taken over only a finite number of partial waves. Near threshold this procedure is justified by the partial-wave barrier imposed by angular momentum conservation, but in a general kinematical situation the effect of this truncation has
3. Interpretation of Finite-Volume Observables

<table>
<thead>
<tr>
<th>( \mathbf{d} )</th>
<th>( \text{irrep} \ \Lambda )</th>
<th>( \cot \phi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( [000] )</td>
<td>( T_{1u} )</td>
<td>( w_{00} )</td>
</tr>
<tr>
<td>( [00n] )</td>
<td>( A_1 )</td>
<td>( w_{00} + \frac{2}{\sqrt{5}} w_{20} )</td>
</tr>
<tr>
<td>( )</td>
<td>( E )</td>
<td>( w_{00} - \frac{1}{\sqrt{5}} w_{20} )</td>
</tr>
<tr>
<td>( [0nn] )</td>
<td>( A_1 )</td>
<td>( w_{00} + \frac{1}{2\sqrt{5}} w_{20} + i\sqrt{\frac{6}{5}} w_{21} - \sqrt{\frac{7}{10}} w_{22} )</td>
</tr>
<tr>
<td>( B_1 )</td>
<td>( w_{00} - \frac{1}{\sqrt{5}} w_{20} + \sqrt{\frac{2}{5}} w_{22} )</td>
<td></td>
</tr>
<tr>
<td>( B_2 )</td>
<td>( w_{00} + \frac{1}{2\sqrt{5}} w_{20} - i\sqrt{\frac{6}{5}} w_{21} - \sqrt{\frac{7}{10}} w_{22} )</td>
<td></td>
</tr>
<tr>
<td>( [nnn] )</td>
<td>( A_1 )</td>
<td>( w_{00} - 2i\sqrt{\frac{5}{6}} w_{22} )</td>
</tr>
<tr>
<td>( E )</td>
<td>( w_{00} + i\sqrt{\frac{6}{5}} w_{22} )</td>
<td></td>
</tr>
</tbody>
</table>

Table 3.1.: Linear combinations of Lüscher zeta functions which give the scattering phase shift in each irreducible representation relevant for the \( \ell = 1 \) partial wave in terms of the quantity defined in (3.13).

to be assessed individually. In the case of the \( \rho \) resonance, which appears in the \( \ell = 1 \) partial wave, there is no low-lying resonance in higher partial waves \( \ell = 3, \ldots \) and indeed scattering in higher odd partial waves was shown to be negligible [82]. Neglecting higher partial waves, the quantization conditions reduces to a determinant involving only \( \ell = 1 \) quantities despite \( F \) mixing partial waves in finite volume [80].

The matrix elements of \( F \) are known kinematical functions, which are concisely expressed in terms of shifted Lüscher zeta functions \( Z_{\ell m}(d, \gamma, u^2) \) [72]. Employing group-theoretical projections just as in the construction of interpolating operators allows for a further simplification of the determinant equation by exploiting the block structure of \( F \) dictated by the irreducible representations of the finite-volume rotational symmetry. The quantization condition then takes the particularly simple form

\[
\cot \delta_1(q) = - \cot \phi^{(d,A)}(u), \tag{3.12}
\]

e.g. the negative pseudo-phase \( \phi \), whose cotangent is given by linear combinations of shifted Lüscher zeta functions, coincides with the physical phase shift up to shifts by multiples of \( \pi \). Thus, for every irreducible representation there is a one-to-one mapping between an energy level with center-of-mass energy \( E^* \) and the phase shift \( \delta_1(E^*) \) parametrizing the single-channel scattering amplitude at that energy. The expressions for the irreducible representations relevant to isovector pion-pion...
scattering are given in table 3.1, and we have introduced

\[ w_{\ell m} = -\frac{1}{\gamma \pi^{3/2} u^{\ell+1}} Z_{\ell m} \left( d, \gamma, u^2 \right). \]  

(3.13)

We use the representation of the zeta functions discussed in [78] for their numerical evaluation. The magnitude squared \( u^2 \) of the scattering momentum hence carries all the information about the scattering process. In the noninteracting case it would assume integer values in the \( T_{1u} \) irrep with total zero momentum, and deviations from these noninteracting values encode the interaction strength.

The key formula for the extraction of the pion form factor in the timelike region was first derived for total zero momentum [22] in a conceptually very similar fashion to earlier work on the \( K \rightarrow \pi\pi \) weak transition [21], and then generalized to moving frames [69],

\[ |F_{\pi}(E)^*|^2 = g^{(A)}(\gamma) \left( q \frac{\partial \delta_1(q)}{\partial q} + u \frac{\partial \phi^{(d,A)}(u)}{\partial u} \right) \frac{3\pi E^{*2}}{2q^5 L^3} \left| \langle 0|V^{(d,A)}|d, \Lambda, n \rangle \right|^2, \]  

(3.14)

where

\[ g^{(A)}(\gamma) = \begin{cases} \gamma^{1} & \text{if } \Lambda = A_1^+, \\ \gamma & \text{otherwise}, \end{cases} \]  

(3.15)

and the derivatives stem from the residue \( R \) in (3.9).\(^5\) We will refer to the conversion factor between the finite-volume and infinite-volume matrix element as Lellouch-Lüscher-Meyer the (LLM) factor in the following. Equation (3.14) is valid at the center-of-mass energy \( E^*_n \) corresponding to the state in the matrix element on its right-hand side, and the derivative of the pseudophase functions \( \phi \) can be computed numerically. In order to obtain the derivative of the phase shift \( \delta_1 \) however the energy dependence of the scattering amplitude must be parametrized. The first step in the extraction of the pion form factor is hence the determination of the parameters of the \( \rho \) resonance.

\(^5\)The recent determination of the \( \pi\pi \rightarrow \pi\gamma^* \) amplitude [83] uses the same methodology.
4. Numerical Results for Pion-Pion Scattering

4.1. Ensemble Details

In this work we employ two of the $N_f = 2 + 1$ gauge ensembles generated within the CLS effort. A detailed account of the setup and algorithmic parameters can be found in [43]. The scale setting for these ensembles, which proceeds via the Wilson-flow scale $t_0$ [61] as an intermediate scale and subsequent conversion to physical units through a combination of the pion and kaon decay constants, is discussed thoroughly in [84]. We focus here on the aspects relevant to our measurements; some details for the N200 and D200 ensembles of gauge configurations are summarized in table 4.1.

<table>
<thead>
<tr>
<th>$N_s^3 \times N_t$</th>
<th>$m_\pi$ [MeV]</th>
<th>$m_K$ [MeV]</th>
<th>$a$ [fm]</th>
<th>$m_\pi L$</th>
<th>$N_{cfg}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>N200 48$^3 \times 128$</td>
<td>280</td>
<td>460</td>
<td>0.064</td>
<td>4.4</td>
<td>852</td>
</tr>
<tr>
<td>D200 64$^3 \times 128$</td>
<td>200</td>
<td>480</td>
<td>0.064</td>
<td>4.2</td>
<td>559</td>
</tr>
</tbody>
</table>

Table 4.1.: Ensemble details for the gauge configurations used in this work. The quoted pseudoscalar masses and scale are estimates from [43], and $N_{cfg}$ denotes the number of configurations that we have performed measurements on.

The simulations are performed on isotropic lattices of size $N_s^3 \times N_t$ using the Lüscher-Weisz gauge action,

$$S_g[U] = \frac{\beta}{6} \left( c_0 \sum_p \text{tr} \{1 - U(p)\} + c_1 \sum_r \text{tr} \{1 - U(r)\} \right),$$

where the sums run over the oriented plaquettes $p$ and rectangles $r$, $c_0 = 5/3$, $c_1 = -1/12$, and $\beta = 3.55$ for both ensembles. Fermions are simulated using the Wilson-Dirac operator including the Sheikholeslami-Wohlert term [44] needed for...
4. Numerical Results for Pion-Pion Scattering

\( O(a) \) improvement of the bulk action,

\[
D_W(m_0) = \frac{1}{2} \sum_{\mu=0}^{3} \left\{ \gamma_\mu \left( \nabla_\mu^* + \nabla_\mu \right) - a \nabla_\mu^* \nabla_\mu \right\} + ac_{SW} \sum_{\mu,\nu=0}^{3} \frac{1}{4} \sigma_{\mu\nu} F_{\mu\nu} + m_0, \tag{4.2}
\]

with nonperturbatively determined \([46]\) coefficient \( c_{SW} \). All simulations are carried out in the isospin limit, where up and down quark masses are taken to be degenerate, and the bare quark masses \( m_0 \) are tuned such that the trace of the three-flavor mass matrix is constant along the quark mass trajectory,

\[
a \sum_{f=1}^{3} m_{0,f} = \text{const}, \tag{4.3}
\]

so that a heavier-than-physical pion mass implies a lighter kaon mass, a procedure proposed in \([85, 86]\). This scheme facilitates keeping the lattice spacing constant when the sea quark masses are varied, without spoiling the \( O(a) \) improvement \([43]\). In order to keep the lattice spacing constant, the \( O(a) \)-improved coupling \([45]\)

\[
\tilde{g}_0^2 = g_0^2 \left( 1 + \frac{b_g}{N_f} a \text{tr} M \right) \tag{4.4}
\]

related to the bare coupling \( g_0^2 = 6/\beta \), which is controlled in practice, has to be kept constant. While the improvement coefficient \( b_g \) is known to one-loop order in perturbation theory \([87, 88]\), its use can be circumvented altogether by keeping the trace of the bare quark mass matrix constant, which implies a constant trace of the diagonal mass matrix \( M \) with the subtracted quark masses on its diagonal. Then,

\[
\tilde{g}_0 / g_0 = \text{const} \tag{4.5}
\]

along the quark mass trajectory, and hence the lattice spacing is fixed by keeping the bare coupling \( g_0 \) constant.

In order to avoid the freezing of the topological charge as the continuum limit is approached, open boundary conditions are imposed on the gauge field in the temporal direction \([50]\), breaking time translation invariance. Although it has been advocated in \([89]\) to place sources on the boundary in the evaluation of pseudoscalar correlation functions in order to maximize the usable fraction of the lattice, some extra care must be taken when using the stochastic LapH method and extracting not only the ground state but also excited states.

The smearing of quark fields in interpolating operators is based on the three-dim-
4. Numerical Results for Pion-Pion Scattering

Figure 4.1.: Smallest and largest retained eigenvalue of the three-dimensional covariant Laplacian on individual time slices of the lattice normalized by their plateau value. Uncertainties are estimated using 26 evenly-spaced configurations of the N200 ensemble. The normalized smallest eigenvalue is displaced vertically by 0.2 for visibility.

The three-dimensional covariant Laplace operator on each individual time slice of the lattice. The Laplace operator does not alter the transformation properties of the quark fields it acts on and is thus expected to receive contributions from states with vacuum quantum numbers near the boundary. As illustrated in figure 4.1 both the smallest eigenvalue and the largest eigenvalue retained in our smearing scheme deviate significantly from their bulk value near the boundary. Hence in order to keep the smearing of quark fields used in our interpolators constant we employ sources and sinks sufficiently far away from the temporal boundary. Performing measurements only in the central part of the lattice is also advisable in order to not distort the GEVP, because the boundary modifies interpolators in its vicinity into effective interpolators with states with vacuum quantum numbers admixed.

Simulations are performed using the RHMC algorithm to simulate the strange quark, and twisted-mass reweighting [90, 91] is used to stabilize the simulations by avoiding accidental zero-modes of the lattice Dirac operator. On the level of measurements these techniques require a reweighting, and expectation values of primary observables can be computed from expectation values in the theory with the modified action $\langle \ldots \rangle_W$ according to

$$\langle A \rangle = \frac{\langle AW \rangle_W}{\langle W \rangle_W}, \quad (4.6)$$

where the reweighting factor $W = W_{\text{tm}}W_{\text{RHMC}}$ is estimated stochastically during the production of gauge configurations (see [43] for further details).
4. Numerical Results for Pion-Pion Scattering

Even though open temporal boundary conditions were adopted in this simulation effort to ameliorate large autocorrelations in simulation time, observables constructed from fields which have been smoothed using the gradient flow evolve slowly in Monte Carlo time [92]. The largest observed autocorrelation time at this coupling was estimated as $\tau_{\text{int}} = 80(25)$ MDU [43]. In order to mitigate the effects of this residual autocorrelation we perform measurements on configurations separated by 8 molecular dynamics units (MDU) – yielding the numbers of configurations per ensemble quoted in table 4.1 – which are then averaged over four subsequent configurations, so that each bin contains 32 MDU.

<table>
<thead>
<tr>
<th>$n_\rho \cdot \rho$</th>
<th>$N_{\text{ev}}$</th>
<th>line type</th>
<th>scheme</th>
<th>$N_R$</th>
<th>$t_0$</th>
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</thead>
<tbody>
<tr>
<td>N200</td>
<td>$36 \cdot 0.1$</td>
<td>192</td>
<td>fixed (TF, SF, LI8)</td>
<td>5†</td>
<td>32, 52</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>relative (TI8, SF, LI8)</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>D200</td>
<td>$36 \cdot 0.1$</td>
<td>448</td>
<td>fixed (TF, SF, LI8)</td>
<td>5</td>
<td>32, 52</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>relative (TI8, SF, LI8)</td>
<td>2</td>
<td></td>
</tr>
</tbody>
</table>

† The initial inversion runs for $t_0 = 32$ used $N_R = 4$ noise sources, and the fifth noise source was added later. Hence only four noise sources are used for correlators involving the current insertion for $t_0 = 32$.

Table 4.2.: Stout-smearing parameters, number of retained eigenvectors, dilution schemes, number of noise sources, and source times employed in this work.

Quark propagation is estimated using the stochastic LapH method. The stout smearing [60] parameters and the number of retained eigenvectors in the LapH smearing, listed in table 4.2, are chosen such that they result in a similar physical smearing as in previous studies [17]. Eigenvectors are diluted using the interlace-8 scheme for both fixed and relative quark lines as was done in [17]. A finer temporal lattice spacing was used in that reference compared to our lattice spacing, $a/a_t^{\text{ref}} \approx 0.064/(0.12/3.44) \approx 1.8$. Therefore, relative quark lines are diluted in time with only interlace-8 instead of interlace-16 employed in that reference, resulting a similar physical time dilution. The

$$N_{\text{inv}} = 4 \cdot 2 \cdot 8 \cdot 5 + 4 \cdot 8 \cdot 8 \cdot 2 = 832$$

light-quark inversions required per gauge configuration according to (2.58) are performed using the DFL_SAP_GCR solver [59] implemented in openQCD [91], which we have incorporated into the Chroma-based [93] stochastic LapH codebase.\(^1\)

\(^1\)openQCD can be obtained from http://luscher.web.cern.ch/luscher/openQCD/. openQCD-1.4 was used for inversions on the N200 ensemble, and D200 inversions were performed using the
4. Numerical Results for Pion-Pion Scattering

<table>
<thead>
<tr>
<th></th>
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<th>D200</th>
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<tr>
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<td>Inversions</td>
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<td>for fixed lines</td>
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<td>26.9</td>
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<tr>
<td>for relative lines</td>
<td>0.9</td>
<td>10.4</td>
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<td>$O(a)$ counterterm</td>
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<td>2.4</td>
</tr>
<tr>
<td>Meson functions</td>
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<td>Total</td>
<td>3.1</td>
<td>34.7</td>
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</table>

Table 4.3.: Computational cost in 1000 core hours per gauge configuration of the different steps in the stochastic LapH workflow to obtain the correlation functions required in this work. Computations were run on a variety of machines and are only meant to illustrate the orders of magnitude of the cost involved. The cost of stout-smearing the gauge fields is negligible and hence omitted from the table.

In contrast to our stochastic treatment of quark propagation, exact distillation would require 46,080 and 107,520 inversions per gauge configuration of the N200 and D200 ensemble respectively, if correlation functions were to be measured on the central 60 time slices of the lattice as is done here.

4.2. Computational Cost

In table 4.3 we give an overview of the computational cost involved at the different steps of the stochastic LapH workflow. On both ensembles, the computation of eigenvectors of the three-dimensional covariant Laplacian amounts to a fraction at the percent level of the total cost, facilitated by our use of Chebyshev acceleration in the Lanczos method [17]. The eigenvectors are required in both the subsequent inversion run and for the meson function computation, and writing them out to disk accounts for five to ten percent of the total time spent in that task depending on the IO performance of the HPC system.

Solving the Dirac equation for a given right-hand side is the most computationally

---

BlueGene/Q-optimized code (http://hpc.desy.de/simlab/codes/openqcd_bgopt/) built on openQCD-1.2.
expensive individual task at roughly 70% of the resources required per gauge configuration. Inversions on the N200 ensemble were computed using resources on Fionn at the Irish Centre for High-End Computing (ICHEC), and inversions on the D200 ensemble were performed on JUQUEEN at the Jülich Supercomputing Centre (JSC). The corresponding figures in table 4.3 assume the dilution schemes and number of noises indicated in table 4.2. We use one extra noise source in the noise average in addition to the minimum four noise sources required for an unbiased estimate of two-meson–to–two-meson diagrams.

Current functions have to be computed with the unsmear solutions of the Dirac equation in memory and thus necessarily use the same process grid as the inversion runs, rendering their calculation less efficient than the construction of meson functions, which can be performed for each time slice individually in a version of our code with three-dimensional lattice geometry. The estimated cost of the construction of current functions includes all equivalent total momenta in moving frames which we use to increase statistics, and all (nondiagonal) noise combinations are computed.

In the correlator construction on the D200 ensemble we use all available noise combinations for the noise average which do not introduce a bias. On the N200 ensemble, the subset of diagrams in two-pion–to–two-pion correlation functions with quark lines such that the two pions propagate ‘independently’ are estimated using a reduced number of noise combinations, explaining the difference in the correlator construction run times.

The grand total of computer time required to produce the results shown in this work is roughly 2.7 million core hours for the N200 ensemble and 20 million core hours for the D200 ensemble. These figures are smaller than the cost of the generation of these gauge configurations (5.5 and 36 million core hours respectively [43]) by roughly a factor of two.

---

2 The quark propagators can be re-used extensively. For the first steps towards an investigation of string breaking on these ensembles see [94]. There, inversions to treat quark propagation of the strange quark are required as well. The associated cost is not included in the figures in table 4.3.
4. Numerical Results for Pion-Pion Scattering

4.3. Finite-Volume Spectrum

4.3.1. Pion Mass and Dispersion Relation

The pion mass plays an important role in the scattering analysis as is evident from (3.10) – all information on the pion-pion interaction is encoded in the difference between the energies of states with the quantum numbers of two pions and their respective noninteracting energies governed by the pion mass. Additionally, the pion correlation function is our most precise observable and hence provides a stringent check for effects resulting from the open boundary conditions in time which break time translation invariance. We use only the simplest pion interpolating operator of the form

\[ \bar{\chi} \gamma \gamma_5 \psi, \]  

which is the standard interpolator for a pseudoscalar meson.\(^3\) Correlation functions are constructed using the stochastic LapH method as described in chapter 2, and we extract the pion mass from a correlated fit to a single-exponential ansatz. The most pronounced systematic effect in the extraction of the pion mass is the choice of the lower bound of the fit window \(t_{\text{min}}\), signifying a considerable contribution of excited states to the correlation function. Our extraction of the pion mass on the N200 ensemble is illustrated in figure 4.2, and we have checked the stability of these results under variation of \(t_{\text{max}}\), the upper limit of the fit window, which serves as a check of possible temporal boundary effects. In figure 4.3 we show the energies for pions with various momenta on the same ensemble together with the continuum dispersion relation

\[ (aE_\pi)^2 = (am_\pi)^2 + \left( \frac{2\pi a}{L} \right)^2 d^2. \]  

We do not observe discretization effects in the dispersion relation up to momenta with \(d^2 = 6\), while \(d^2 = 4\) is the highest constituent pion momentum in the two-pion interpolating operators employed in our analysis.

On the D200 ensemble, open temporal boundary conditions are expected to have a

\(^3\)In [95] it was advocated to use variationally improved pion interpolators built from spatially extended quark bilinears in the construction of two-pion interpolators, which were shown to have better ground-state overlap at the pion mass \(m_\pi \approx 700\) MeV considered there. Variationally improving the pion interpolator at our pion masses presumably requires including three-pion interpolators which we do not attempt here.
4. Numerical Results for Pion-Pion Scattering

Figure 4.2.: Variation of $t_{\text{min}}$ in the fit to the correlator of a single pion at rest on the N200 ensemble using the time separations $[t_{\text{min}}, t_{\text{max}} = 39a]$. The three panels show fit results for the two source times $t_0/a = 32, 52$ employed in this work individually (center and right), as well as their average (left), whose consistency alludes to negligible boundary effects. The horizontal error band across all three panels shows our pion mass extracted for $t_{\text{min}} = 19$ of the averaged correlator.

Figure 4.3.: Single-pion energies for various momenta $p^2 = \left(\frac{2\pi}{L}\right)^2 d^2$ together with the continuum dispersion relation (4.9) using the mass of a single pion at rest as input. Error bands for the dispersion relation propagating the uncertainty of the pion mass are shown but too small to be visible.

larger effect due to the smaller pion mass, since the lightest contributing boundary state is a two-pion state with vacuum quantum numbers $[84]$. Indeed we observe a sizable $t_{\text{max}}$ dependence of the extracted pion mass when fitting to a single exponential. The pion correlation function in a gauge background with open boundary conditions is expected to have the form $[91, 43]

$$C_{\pi, t_0}(t) \propto \sinh \left[m_\pi (\hat{T} - t - t_0)\right],$$

with the pion source time fixed at $t_0$ and time separation $t$ such that the contribution of excited states with quantum number of the pion is negligible. The functional form derives from the argument that Dirichlet boundary conditions arise naturally in the continuum limit of a scalar lattice theory $[96]$, so that they are the natural
4. Numerical Results for Pion-Pion Scattering

Figure 4.4.: **Left:** Pion mass on the D200 ensemble as $t_{\text{min}}$ is varied in the fit of the source-time-averaged correlator to a single exponential function with $t_{\text{max}} = 30$. **Center and Right:** Pion mass from fits of correlators from both source times individually to (4.10) using $t_{\text{max}} = 40$. The horizontal error band across all three panels shows our pion mass extracted for $t_{\text{min}} = 19$ on the left panel.

Figure 4.5.: Same as figure 4.3 for the D200 ensemble.
boundary conditions for the pion fields in an effective theory [91]. The effective time extent $\hat{T}$ is a parameter in the corresponding theory, and should hence be taken as a free parameter in fits to this form. In principle, using this fit form allows one to fit correlation function data including large time separations, even if the sink gets moderately close to the boundary. For our subsequent analysis however we require the overlap between our single-pion interpolator and the single-pion state, which cannot be readily inferred from fits to (4.10). Instead we use fits to this functional form as a guideline to choose a conservative $t_{\text{max}}$ in the single-exponential fit to the source-time-averaged correlation function, such that the effects of the boundary are smaller than the statistical uncertainty of the pion mass. Varying $t_{\text{max}}$ in the single-exponential fits we observe a plateau at a pion mass consistent with fits to the $\sinh$ fit form of the correlation functions for each source time individually, indicating that for $t_{\text{max}} = 30$ boundary effects are captured by our statistical errors as shown in figure 4.4.

The energies of moving pions on the D200 ensemble are then well described by the continuum dispersion relation up to $d^2 = 6$ with the mass of a pion at rest the only input parameter (see figure 4.5).

<table>
<thead>
<tr>
<th>Ensemble</th>
<th>$m_\pi$</th>
<th>Bruno et al. (2015) [43]</th>
<th>Bruno et al. (2016) [84]</th>
</tr>
</thead>
<tbody>
<tr>
<td>N200</td>
<td>0.09224 (28)</td>
<td>0.09202 (61)</td>
<td>0.09222 (34)</td>
</tr>
<tr>
<td>D200</td>
<td>0.06529 (45)</td>
<td>0.06542 (44)</td>
<td>0.06502 (35)</td>
</tr>
</tbody>
</table>

Table 4.4.: Extracted pion masses on the two ensembles used in this analysis together with their value extracted by other groups.

We give our final values for the pion mass on both ensembles in table 4.4 together with the values extracted during the generation of the ensembles [43] and scale setting [84], and find perfect agreement between the determinations.

4.3.2. Isovector Two-Pion Spectrum

We now discuss the extraction of finite-volume energies from the correlation functions of interpolating operators with the quantum numbers of the $\rho$ meson. Our analysis strategy has previously been described in [97] where results from an anisotropic lattice with Wilson clover fermions were shown. In each irreducible representation we want to utilize not only the ground state but several excited states as well. In order to reliably extract these excited-state energies a generalized eigenvalue problem is solved.
To this end a correlation matrix consisting of a single-site $\rho$ interpolator together with all relevant two-pion operators is constructed in each channel. The two-pion operators are chosen to match the expected noninteracting states and we include one such operator for each state below inelastic threshold.

For each of these correlation matrices $C_{ij}(t)$ we solve the generalized eigenvalue problem (2.13) for a given combination $(t_0, t_d)$. The eigenvectors $\{v_n(t_0, t_d)\}$ are used to define correlation functions $\hat{C}_{ij}(t)$ between ‘optimal’ interpolators according to (2.14). This approach is different from the analyses of [55, 56] which require the solution of the GEVP at different $(t_0, t_d)$, possibly introducing ambiguities between closely spaced levels at different diagonalization times. Due to similar ambiguities in the identification of levels we do not perform the GEVP diagonalization on each bootstrap sample, but use the eigenvectors obtained from the solution of the GEVP on the mean of the data. As a result of our approach off-diagonal elements of the correlation matrix do not vanish exactly at all time separations, possibly introducing deviations from the single-exponential decay beyond the corrections from higher-lying states discussed in [56]. We monitor this effect by varying $(t_0, t_d)$ and requiring consistency between the energy levels extracted for these different pairs. Additionally we demand the results to be stable with respect to including more or less operators as a further check of possible systematic effects in the GEVP.

The finite-volume energies are then accessible through a two-parameter correlated-$\chi^2$ fit to each diagonal element of the rotated correlation matrix with a single-exponential ansatz,

$$\hat{C}_{nn}(t) = Ae^{-E_n t}. \quad (4.11)$$

However for our analysis we employ a different approach which exploits the similarity and correlation between two-pion and single-pion correlation functions. As in [98] but here generalized to arbitrary momenta we define the ratio

$$R_n(t) = \frac{\hat{C}_{nn}(t)}{C_{d_1^2}(t) C_{d_2^2}(t)}, \quad (4.12)$$

for each diagonal element of the rotated correlation matrix $\hat{C}(t)$, with $C_{d_i^2}$ the single-pion correlation function of a pion with momentum-squared $d_i^2$. The ratio is constructed on each bootstrap sample and fit to the functional form

$$R_n(t) = A' e^{-\Delta E_n t}. \quad (4.13)$$
4. Numerical Results for Pion-Pion Scattering

The desired energy is reconstructed from the energy shift $\Delta E_n$ – using the continuum dispersion relation – via

$$aE_n = a\Delta E_n + \sqrt{(am_\pi)^2 + \left(\frac{2\pi a}{L}\right)^2 d_1^2 + \sqrt{(am_\pi)^2 + \left(\frac{2\pi a}{L}\right)^2 d_2^2}}, \quad (4.14)$$

with the pion mass $m_\pi$ determined in the previous section. Similarly the amplitude $A'$ of the rotated correlator is reconstructed from the single-pion overlaps $A_{d_1^2}$ through

$$A = A'A_{d_1^2}A_{d_2^2}. \quad (4.15)$$

This ratio fit strategy is particularly beneficial for weakly-interacting two-pion states, for which the excited state contamination is similar between the numerator and denominator in (4.12) resulting in reduced excited state contamination in the fit for the energy shift. In the isovector channel the two-pion states mix with the $\rho$ meson, but the ratio fits still turn out to be useful. Firstly, at center-of-mass energies sufficiently far away from the resonance region, this mixing is small and the ratio (4.12) still has significantly reduced excited-state contamination. Additionally the excited-state contamination of these ratios has a different form compared to the standard corrections in the single-exponential fits, providing an additional check of the excited-state systematics. In the extraction of Hamiltonian eigenstates with a significant $\rho$-like component there usually appears a bump-like behavior as discussed in [97], which requires some care in the choice of an appropriate fit window.

Figure 4.6 illustrates all these systematic effects for three representative isovector energy levels of the N200 ensemble. The most pronounced effect stems from the choice of the lower limit of the fit window $t_{\text{min}}$ due to excited-state contamination at small time separations, which we address by judiciously choosing the fit range such that this systematic effect is captured by the statistical error shown there. As minimum requirements we demand that the chosen $t_{\text{min}}$ gives a suitable $\chi^2$/d.o.f. < 2 indicating an acceptable quality of the fit, and that

$$|u^2(t_{\text{min}}) - u^2(t_{\text{min}} - \delta t)| < \sigma(t_{\text{min}}), \quad (4.16)$$

where $\sigma(t_{\text{min}})$ is the bootstrap error on $u^2(t_{\text{min}})$ and $\delta t = 3a$.\(^4\)

The ratio fits generally show a very mild dependence on $(t_0, t_d)$, while the num-

\(^4\)This choice of $\delta t$ is similar to the plateau criterion used in [97] given the coarser temporal lattice spacing here.
4. Numerical Results for Pion-Pion Scattering

Figure 4.6.: Variation of $t_{\text{min}}$, GEVP parameters $(t_0, t_d)$ and the number of operators included in the GEVP for three representative energy levels of the N200 ensemble. Each row corresponds to different GEVPs for a single energy level. The dimensionless scattering momentum $u^2$ defined in (3.10) is shown, as it determines the scattering phase shift. The horizontal error band indicates the value extracted from the left panel in each row. In the last row we also show the result of a single-exponential fit to the rotated correlation function, showing its compatibility with the ratio fits used in all other panels. As discussed in subsection 4.3.1, all fits use $t_{\text{max}} = 39$ on this ensemble.
ber of operators included in the GEVP typically has a more pronounced effect at moderately small \( t_{\text{min}} \), as can be seen in the first row of figure 4.6. This situation is commonly reversed for single-exponential fits to the rotated diagonal correlation functions, so that monitoring consistency between the two different fit models provides a further check of the effects of excited states. The last row in that figure shows the mutual consistency between the two fit strategies for an energy level in the resonance region, indicating that ratio fits are valid even for center-of-mass energies where the two pions are not weakly interacting. All other \( t_{\text{min}} \) plots are relegated to appendix A and we simply show the extracted energies in the following.

The low-energy part of the finite-volume spectrum in the isovector irreducible representations relevant to \( \ell = 1 \) pion-pion scattering is summarized in figure 4.7 and figure 4.8 for the N200 and D200 ensemble respectively. Center-of-mass energies are shown in the plots to facilitate comparison between channels with different total momenta. Clearly, excited states can be extracted with good precision, however their interpretation in terms of infinite-volume observables becomes more complicated above the lowest-lying inelastic threshold. The kinematical situation on the N200 is such that the lowest-lying threshold is the two-kaon threshold, which can be treated in the Lüscher framework.\(^5\) Such a coupled-channel analysis would allow us to use the energy levels in the range between \( 2m_K \) and \( 4m_\pi \) in the subsequent phase shift analysis. However, on the N200 ensemble the \( \rho \) resonance occurs well below this energy range, and it is not clear to what extent the more complicated coupled-channel analysis would help constrain its parameters further. Therefore we do not attempt to include multiple scattering channels here.

On the D200 ensemble with its lighter pion mass, the lowest-lying inelastic threshold is the four-pion threshold, above which the interpretation of finite-volume states in the Lüscher framework is currently unknown.\(^6\) The finite-volume spectrum however can still be extracted reliably as we include an interpolating operator for each non-interacting state to be expected in a given irreducible representation. The vector nature of the \( \rho \) resonance requires some of the constituent pions of a four-pion state to carry nonvanishing spatial momentum, pushing the noninteracting energy of the lowest-lying four-pion state in a finite volume to higher energies than \( 4m_\pi \). This consequence of the rotational symmetry does however not extend the energy range in which the Lüscher method may be applied, because the infinite-volume threshold is the relevant quantity there, above which new poles appear in the derivation.

\(^5\) For a recent practical implementation, see [99, 100].

\(^6\) Theoretical progress has been made recently regarding the inclusion of three-particle states in this framework; for a review see [101].
4. Numerical Results for Pion-Pion Scattering

Figure 4.7: **Top:** Finite-volume spectrum on the N200 ensemble in the isovector irreducible representations obtained from ratio fits. The position of each box corresponds to the center-of-mass energy obtained from a Hamiltonian eigenstate in a given irreducible representation, and its width indicates the statistical uncertainty from our extraction. The dashed horizontal line indicates the infinite-volume $K\bar{K}$ threshold. Some states may be missing between the $K\bar{K}$ threshold and the four-pion threshold, as they are not useful to our analysis and we have thus limited the number of interpolators in each irreducible representation. The second excited state in $T_{1u}^+(0)$ is above the energy range shown. **Bottom:** Overlaps of each interpolating operator used in the GEVP with the various eigenstates in each irreducible representation. The fill pattern matches that of the states in the top panel. We use local $\rho$-meson interpolators with matching total momentum as well as two-pion interpolators $\pi(d_1^2)\pi(d_2^2)$, where each pion has definite momentum.
Figure 4.8.: Same as figure 4.7 for the D200 ensemble. States may be missing between the four-pion and infinite-volume $K\bar{K}$ threshold in the irreducible representations except $T_{10}^+(0)$, $A_1^+(1)$ and $B_1^+(2)$. The third excited state in $T_{10}^+(0)$ is above the energy range shown.
in chapter 3 and the diagrammatic series used there is incomplete. Contrary to claims in the literature [102], states above the infinite-volume four-pion threshold are hence not useful for Lüscher-type analyses unless the effect of four-pion states can be quantified, and we do not map out the complete finite-volume spectrum between the four-pion and two-kaon thresholds on the D200 ensemble.

The bottom panels in both figures illustrate the mixing between two-pion interpolators of various constituent pion momenta and the single-site quark bilinear interpolator of a \( \rho \) meson with a given total momentum. We estimate the modulus squared of the overlaps \( Z_i^{(n)} \) of each interpolator used in the GEVP onto the Hamiltonian eigenstates, as defined in (2.4), by forming the ratio

\[
|Z_i^{(n)}(t)|^2 = \left| \frac{\sum_j C_{ij}(t)v_{nj}(t_0, t_d)}{e^{-\frac{E_n}{2}t}\sqrt{C_{nn}(t)}} \right|^2,
\]

using the fitted energies \( E_n \), and taking \( t = 16a \). The overlaps of a given interpolator \( O_i \) onto the various energy eigenstates \( |n\rangle \) which we plot in these figures have an arbitrary overall normalization if no normalization condition is imposed on the interpolators, but their relative contributions to the various states are independent of this normalization.

As expected for the narrow \( \rho \) resonance, local \( \rho \)-meson interpolating operators have significant overlap with energy eigenstates near the resonance mass, which we will determine more precisely in the next section. Sizable mixing with two-pion interpolators is observed if the noninteracting energy of the corresponding two-pion state is near the resonance region. For states which are excited predominantly by a two-pion interpolator, the ratio fits described earlier have very little excited state contamination, so that even highly excited states, for instance in the \( T_{1u}(0) \) and \( A_{1u}(1) \) irreducible representations on the D200 ensemble, can be extracted with good precision.

### 4.4. Pion-Pion Scattering Amplitude

In the case of a single kinematically open scattering channel considered here, and neglecting the effect of higher odd partial waves, each energy level of the finite-volume spectrum corresponds to a value of the \( \ell = 1 \) scattering amplitude at the same center-of-mass energy. The energy-dependent scattering phase shift used to
**4. Numerical Results for Pion-Pion Scattering**

<table>
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<th>irrep</th>
<th>((d_1^2, d_2^2))</th>
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<th>(\chi^2/\text{dof})</th>
<th>(E^*/m_\pi)</th>
<th>((q/m_\pi)^3 \cot \delta_1)</th>
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<td>(A_1^+(4))</td>
<td>(0, 4)</td>
<td>15</td>
<td>0.80</td>
<td>2.629 (84)</td>
<td>1.7 (1.5)</td>
</tr>
<tr>
<td>(E^+(4))</td>
<td>(2, 2)</td>
<td>11</td>
<td>1.90</td>
<td>2.761 (48)</td>
<td>−0.123 (70)</td>
</tr>
</tbody>
</table>

Table 4.5.: Fit parameters and fitted center-of-mass energies for each level of the isovector vector spectrum used in the phase shift analysis on the N200 ensemble. The tuple \((d_1^2, d_2^2)\) denotes the two single-pion correlation functions used in the ratio fits. The minimum time separation included in the fit, the correlated \(\chi^2\) and the corresponding scattering phase shift are also given for each level.

parametrize the scattering amplitude is related to the pseudophase as per (3.12), so that

\[
\delta_1 = -\phi_1 + n\pi, \quad n \in \mathbb{N},
\]

due to the corresponding ambiguity in the inverse cotangent. In table 4.5 and table 4.6 we show all the energy levels from the previous section used in the phase shift analysis together with the phase shift point obtained for each level. The particular quantity shown there is the real part of the inverse scattering amplitude. For the resonant \(\ell = 1\) partial wave, its energy dependence can be described by the Breit-Wigner parametrization

\[
\left(\frac{q}{m_\pi}\right)^3 \cot \delta_1 = \left(\frac{m_\rho^2}{m_\pi^2} - \frac{E^*}{m_\pi^2}\right) \frac{6\pi E^*}{g_{\rho\pi\pi}^2 m_\pi},
\]

66
4. Numerical Results for Pion-Pion Scattering

<table>
<thead>
<tr>
<th>irrep</th>
<th>((d_1^2, d_2^2))</th>
<th>(t_{min}/a)</th>
<th>(\chi^2/\text{dof})</th>
<th>(E^*/m_\pi)</th>
<th>((q/m_\pi)^3\cot\delta_1)</th>
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<td>(T_{1u}^+(0))</td>
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<td>3.436 (23)</td>
<td>5.90 (67)</td>
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<td></td>
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<td>3.986 (76)</td>
<td>-2.5 (1.3)</td>
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<td>(A_1^+(1))</td>
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<td></td>
<td>(1, 2)</td>
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<tr>
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<td>2.5413 (70)</td>
<td>9.5 (1.2)</td>
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<tr>
<td></td>
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<td>0.80 (55)</td>
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<td>3.649 (25)</td>
<td>4.49 (34)</td>
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<td>1.47</td>
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<td>9.5 (1.3)</td>
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<td></td>
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<td>-0.24 (46)</td>
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<tr>
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<td>10.8 (2.4)</td>
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<td></td>
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<td>0.89</td>
<td>3.220 (14)</td>
<td>6.4 (2.5)</td>
</tr>
<tr>
<td></td>
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<td>-0.69 (74)</td>
</tr>
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</tr>
<tr>
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<td>2.841 (17)</td>
<td>14.6 (5.7)</td>
</tr>
<tr>
<td>(E^+(4))</td>
<td>(2, 2)</td>
<td>12</td>
<td>1.38</td>
<td>3.502 (38)</td>
<td>8.4 (3.2)</td>
</tr>
</tbody>
</table>

Table 4.6.: Same as table 4.5 for the D200 ensemble.
4. Numerical Results for Pion-Pion Scattering

<table>
<thead>
<tr>
<th></th>
<th>$\chi^2$/dof</th>
<th>$m_\rho/m_\pi$</th>
<th>$g_{\rho \pi \pi}$</th>
<th>$m_\rho$ [MeV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>N200</td>
<td>0.75</td>
<td>2.741 (16)</td>
<td>5.97 (10)</td>
<td>775 (4)(8)</td>
</tr>
<tr>
<td>D200</td>
<td>1.34</td>
<td>3.901 (41)</td>
<td>6.25 (25)</td>
<td>780 (8)(8)</td>
</tr>
</tbody>
</table>

Table 4.7.: Resonance parameters extracted from the fit of all energy levels below the respective inelastic threshold to a Breit-Wigner parametrization. The uncertainties are estimated from the bootstrap and are thus statistical only. We use the scale determined in [84] for the resonance mass in physical units, where the two quoted uncertainties are the statistical one and the uncertainty of the scale.

due to the narrow width of the $\rho$ resonance. The correlated fit [97] of the energy levels below the inelastic threshold to the Breit-Wigner parametrization yields the resonance parameters given in table 4.7 and is shown in figure 4.9 and figure 4.10 for the two ensembles. The uncertainties quoted there are statistical only; however it is clear from the respective figure that the resonance parameters extracted from the N200 ensemble are stable under reasonable variation of the set of data points included in the fit. With the kinematics of that ensemble we are able to map out the energy dependence of the phase shift up to center-of-mass energies well above the resonance mass before the opening of the $K\bar{K}$ channel invalidates the use of the single-channel Lüscher formalism.

The kinematical situation on the D200 is different to the extent that the resonance mass is just below the four-pion threshold, and the resonance parameters thus have to be determined exclusively from the onset of the rapid phase shift variation. To the best of our knowledge this is the first Wilson-fermion ensemble in the literature featuring a ground state in $T_{1u}^+$ which is predominantly a two-pion state, requiring both a light pion mass and large volume such that the noninteracting two-pion energy is well below the resonance mass,

$$2m_\pi \sqrt{1 + \left( \frac{2\pi}{m_\pi L} \right)^2} < m_\rho. \quad (4.20)$$

Lowering the pion mass further from our current $m_\pi \approx 200$ MeV is hence only useful in the context of Lüscher-type analyses provided the volume is scaled accordingly – because fewer and fewer energy levels are available for the extraction of resonance parameters otherwise – or if four-pion effects can be quantified.\(^7\)

\(^7\)A viable alternative to directly approaching the chiral limit might be to use an effective field theory to extrapolate to physical pion masses. Recently, Unitarized Chiral Perturbation Theory has been used in conjunction with the Lüscher method to demonstrate such an extrapolation [103].
4. Numerical Results for Pion-Pion Scattering

Figure 4.9.: Energy dependence of the real part of the inverse scattering amplitude (top) and corresponding phase shift (bottom) for isovector $\ell = 1$ scattering on the N200 ensemble. The solid line corresponds to a fit of the data to the Breit-Wigner parametrization, and its error band is indicated by the dashed lines. The state above the $K\bar{K}$ threshold is not included in this fit.
Figure 4.10.: Same as figure 4.9 for the D200 ensemble. In the top panel the data point in $A^+_1(4)$ is not shown due to its large error bar (cf. table 4.6), but it yields a precise point in the phase shift plot shown in the bottom panel. The $T^+_{1u}(0)$, $A^+_1(3)$ and $E^+(3)$ data points overlapping with the four-pion threshold are excluded from the fit.
Several competing effects are at work in the low-energy region of pion-pion scattering when increasing the physical spatial extent $L$, as is the case between the two ensembles we consider. The accessible center-of-mass energy range is extended towards the two-pion threshold on purely kinematical grounds. Away from the resonance region and sufficiently close to the threshold, the difference between the noninteracting and interacting energy of a two-pion state is suppressed by a power of the spatial extent $[8]$, requiring an increased accuracy in the energy determination in order to resolve the effect of the interaction. The accurate extraction of the diminishing energy shifts could be impaired by a deteriorating efficiency of the eigenvector dilution in our treatment of quark propagation, since the number of eigenvectors contained in one dilution scales with the physical volume $L^3$ if the dilution scheme is kept fixed. Although at a fixed lattice spacing the only mitigating factor is the increase in statistics due to the use of all-to-all propagators on a lattice with $L/a$ points in each spatial direction, we do not observe a major breakdown of the attainable accuracy in the determination of energies. Due to the large variation in $\cot \phi$ for small pseudophases however, the proximity of the energy of such a low-lying state to its noninteracting value presumably accounts for the somewhat larger error bars of the real part of the inverse scattering amplitude extracted on the D200 ensemble when compared to the N200 data.

Regarding the other end of the accessible energy range, little is known analytically about the transition of the form of finite-volume effects around a threshold; well below the threshold corrections are exponentially suppressed in the spatial extent $L$, and they take the power-law form treated explicitly in the Lüscher method well above the threshold. There should be a smooth transition between the two functional forms around the threshold, and the corrections neglected throughout the derivation of the quantization condition may have a sizable effect already slightly below it. Therefore we do not include the $T_{1s}(0)$, $A_1(3)$ and $E^+(3)$ states overlapping with the threshold in the Breit-Wigner fit on the D200 ensemble.

Finally, in contrast to the resonance mass $m_\rho$, the coupling $g_{\rho\pi\pi}$ is expected to be almost independent of the pion mass [104], and we may hence compare our extracted coupling, which is related to the $\rho$-meson decay width $\Gamma_\rho$ via

$$g^2_{\rho\pi\pi} = 6\pi \frac{m^2_{\rho}\Gamma_{\rho}}{(m^2_{\rho}/4 - m^2_\pi)^{3/2}},$$

with its physical value $g_{\rho\pi\pi}^{\text{phys}} \approx 5.99$ [4], finding reasonable agreement between our determinations at a single lattice spacing and the physical value. Systematic studies
4. Numerical Results for Pion-Pion Scattering

<table>
<thead>
<tr>
<th>$\beta$</th>
<th>$Z_V$ [108]</th>
<th>$\hat{b}_V$ [109, 110]</th>
<th>$am_{PCAC}$ [84]</th>
<th>$c_V$ [109]</th>
</tr>
</thead>
<tbody>
<tr>
<td>N200 3.55</td>
<td>0.7372 (4)</td>
<td>1.0804</td>
<td>0.003150 (11)</td>
<td>-0.02321</td>
</tr>
<tr>
<td>D200 3.55</td>
<td>0.7372 (4)</td>
<td>1.0804</td>
<td>0.001536 (12)</td>
<td>-0.02321</td>
</tr>
</tbody>
</table>

Table 4.8.: Improvement and renormalization constants for the two ensembles used in this work.

of the pion mass dependence of the $\rho$ mass incorporating all available lattice data in an analysis in the framework of Unitarized Chiral Perturbation Theory are currently beginning (see [105] for a recent compilation of $N_f = 2$ results), but require a reliable determination of the lattice spacing. We do not observe a pion mass dependence between the two ensembles considered here, and the Breit-Wigner masses we extract in physical units are consistent with the physical value of $m_{\rho}^{phys} = 775.26(25)$ [4] at our unphysically heavy pion masses.

4.5. Timelike Pion Form Factor

With the Breit-Wigner parametrization of the energy dependence of the scattering amplitude determined in the last section, we now discuss the extraction of the isovector pion form factor in the timelike region. The additional quantities required for a self-contained determination of this resonant form factor are the finite-volume matrix elements of the renormalized vector current between Hamiltonian eigenstates with $\rho$ quantum numbers and the vacuum, which are extracted from correlation functions of the form:

$$D_i(t) = \langle 0|V^{(d,\Lambda)}(t)\mathcal{O}_i^{(d,\Lambda)}(0)|0\rangle,$$  \hspace{1cm} (4.22)

whose construction has been detailed in section 2.4.

The currents $V^{(d,\Lambda)}$ are linear combinations of the renormalized, $O(a)$-improved local vector current $(V_R)$. The renormalization pattern to maintain compatibility with $O(a)$ improvement is complicated by the nondegenerate quark masses in the $N_f = 2 + 1$ setup employed here [106]. The improvement and renormalization of the axial current on these ensembles, which is similar to that of the vector current, is discussed in section 5.1.4 of [107]. The improved bare operator consists of the local

---

8 We set the time where the states of interest are created to zero for notational convenience. In the measurements these source times are determined by the source times of our fixed quark lines.
vector current and the mass-dimension-four operator in the $O(a)$ counterterm,

$$V_{\mu,I} = V_\mu + ac_\mu \partial_\mu T_{\mu\nu},$$  \hspace{1cm} (4.23)$$ which is renormalized according to

$$V_{\mu,R} = Z_V(g_0) \left( 1 + ab_V \text{tr} M + ab_V m_q \right) V_{\mu,I},$$  \hspace{1cm} (4.24)$$ where $m_q$ is the bare subtracted light quark mass and $M$ the diagonal mass matrix of the subtracted light and strange quark masses. In the case of degenerate quark masses the $b_V$ and $b_V$ terms could be combined into a single term, which cannot be done in our setup. In view of $c_V$ and $b_V$ being known only to one loop in perturbation theory, the term proportional to $\tilde{b}_V$ can be readily dropped as it contributes only at order $\tilde{g}_0^2$. Furthermore, while the bare subtracted quark mass is not known on these ensembles, it can be related to the known bare (improved) PCAC mass $m_{PCAC}$,

$$m_q = Z(g_0)m_{PCAC} - (r_m - 1)^{\text{tr} M/N_f} + O(a m^2),$$  \hspace{1cm} (4.25)$$ where $r_m - 1$ vanishes to the order we are working. Consequently, replacing the bare subtracted quark mass by the PCAC mass in (4.24) amounts to

$$m_q \rightarrow m_{PCAC}, \quad b_V \rightarrow \tilde{b}_V = Z b_V,$$  \hspace{1cm} (4.26)$$ with the one-loop results for $Z$ [110] and $b_V$ [109] (see also [107, (5.39)])

$$Z(g_0) = 1 - 0.0703 \tilde{g}_0^2,$$  \hspace{1cm} (4.27)$$

$$b_V(g_0) = 1 + \frac{4}{3} 0.0884 \tilde{g}_0^2.$$  \hspace{1cm} (4.28)$$ Finally, the coupling $\tilde{g}_0^2$ defined in (4.4) and the bare coupling $g_0^2 = 6/\beta \approx 1.69$ for the N200 and D200 ensembles considered here can be used interchangeably in all of the above formulae without spoiling $O(a)$ improvement to one-loop order in perturbation theory. The vector current used in this work,

$$V_{\mu,R} = Z_V \left( 1 + a\tilde{b}_V m_{PCAC} \right) V_{\mu,I},$$  \hspace{1cm} (4.29)$$
4. Numerical Results for Pion-Pion Scattering

with nonperturbative \( Z_V \) [108] and one-loop \( c_V \) [109],

\[
c_V = -\frac{4}{3} 0.0103 g_0^2, \quad (4.30)
\]
is hence formally \( O(a) \) improved to one loop in perturbation theory with numerical values given in table 4.8.

As a first step in our analysis we extract individually the bare matrix elements of the leading-order and mass-dimension-four operator contributing to the current. Since we are interested not only in the matrix element between the ground state and the vacuum, but also want to use the excited states in each irreducible representation, we form the correlation functions between the respective operator and the ‘optimal’ interpolating operators in each symmetry sector,

\[
\hat{D}_n(t) = \sum_i D_i(t) v_{ni}(t_0, t_d), \quad (4.31)
\]
using the eigenvectors obtained from the solution of the GEVP in the determination of the finite-volume spectrum. Up to GEVP corrections and neglecting temporal boundary effects, these optimized correlation functions have the large-time behavior

\[
\hat{D}_n(t) \to \langle 0|V^{(d, \Lambda)}|d\Lambda n \rangle \langle d\Lambda n|\tilde{O}_n^{(d, \Lambda)}|0 \rangle e^{-E_n^{(d, \Lambda)}(t)}, \quad (4.32)
\]
where the overlap between the interpolating operator and the state as well as its energy are the ones extracted from fits to the diagonal elements of the rotated correlation matrix in section 4.3. This suggests three different ratios which tend to the matrix elements of interest,

\[
R_1^{(n)}(t) = \frac{\hat{D}_n(t)}{\hat{C}_{nn}(t) e^{-\frac{1}{2}E_n(t)}},
\]

\[
R_2^{(n)}(t) = \frac{\hat{D}_n(t)}{\langle d\Lambda n|\tilde{O}_n^{(d, \Lambda)}|0 \rangle e^{-E_n(t)}}, \quad (4.33)
\]

\[
R_3^{(n)}(t) = \frac{\hat{D}_n(t) \langle d\Lambda n|\tilde{O}_n^{(d, \Lambda)}|0 \rangle}{\hat{C}_{nn}(t)}.
\]

The three determinations have different excited-state contamination, allowing for a check of this systematic effect in the choice of the range used in the plateau average. Plots of the ratios for three representative energy levels are shown in
4. Numerical Results for Pion-Pion Scattering

Figure 4.11.: Bare finite-volume current matrix element between states with $\rho$ quantum numbers and the vacuum in two irreducible representations on the N200 ensemble. Each figure shows the different ratios of (4.33) for the local vector current (top) and the mass-dimension-four operator required for $O(a)$ improvement (bottom). The solid horizontal line indicates the plateau average obtained from $R_1$, the gray dashed lines its statistical uncertainty, and black dashed lines show the statistical and assigned systematic uncertainty added in quadrature.
4. Numerical Results for Pion-Pion Scattering

Figure 4.12.: Ratio of the bare matrix elements of the $O(a)$-counterterm operator and the leading-order current between states in various irreducible representations at center-of-mass energy $E^*$ and the vacuum on both the N200 ensemble (black error bars) and D200 ensemble (gray error bars) combined. Vertical error bars are statistical only. The energies are plotted in lattice units due to the different pion masses on both ensembles.

Figure 4.11, demonstrating that the ratios which tend to the bare matrix elements show clear plateaux for excited states as well as the ground state in these irreducible representations. However as exemplified in the $E^+(1)$ irrep, the three ratios seem to plateau at slightly different values for a few states. The ratio $R_1$ is expected to be the most reliable given that the overlap of our interpolating operators onto the states of interest, which are required in the other two ratios, have to be reconstructed from single-pion overlaps in the ratio fit strategy used in the extraction of the finite-volume spectrum. We extract the matrix elements from a plateau average of $R_1$ over a suitably chosen range, and assign the smallest of the deviations between the means of the plateau averages of the three ratios as systematic uncertainty. With this procedure the systematic deviations are generally contained within the quoted uncertainty, as is evidenced by the remaining plots detailing the extraction of the bare matrix elements, which we relegate to appendix A. Unlike in the phase shift analysis, systematic uncertainties can be propagated linearly into the final result, since the matrix element enters the timelike pion form factor only linearly.
Some insight regarding the size of cutoff effects can be gained from a comparison of the respective magnitudes of the bare matrix elements of the local current and the $O(a)$-counterterm operator.\textsuperscript{10} For each state, their ratio, shown in figure 4.12, is independent of the current renormalization and allows for an estimate of the native suppression of the counterterm relative to the leading order term. We conclude that cutoff effects could potentially be as large as $O(10\%)$ in the finite-volume matrix elements depending on the value of $c_V$.\textsuperscript{11} With the one-loop value of $c_V$ of the order of two percent however the counterterm is numerically suppressed to the permille level and hence generally beyond the statistical accuracy of our results. On these grounds we also do not propagate the permille-level statistical uncertainties of the renormalization factor and improvement coefficients into our final result, but only use their mean values from table 4.8.

With (3.14) every state below the inelastic threshold together with the corresponding renormalized matrix element is mapped to a form factor data point at the corresponding center-of-mass energy. The data across all irreducible representations is shown in figure 4.13 and figure 4.14 for our two ensembles together with the Gounaris-Sakurai (GS) prediction which is based on the Vector-Meson-Dominance model augmented to incorporate the unstable nature of the $\rho$ meson [112]. Following the notation of [27] the GS parametrization of the pion form factor is given by

$$F_{\pi,GS}(E^*) = \frac{f_0}{q^2 h(E^*) - q^2_\rho h(m_\rho) + b \left(q^2 - q^2_\rho\right) - i\frac{q^3}{E^*}},$$

$$b = -h(m_\rho) - \frac{24\pi}{g^2_{\rho\pi\pi}} \frac{2q^2_\rho}{m_\rho}h'(m_\rho), \quad f_0 = -\frac{m^2_\pi}{\pi} - q^2_\rho h(m_\rho) - b \frac{m^2_\rho}{4}, \quad (4.34)$$

$$h(E^*) = \frac{2}{\pi} \frac{q}{E^*} \ln \left(\frac{E^* + 2q}{2m_\pi}\right),$$

with the scattering momentum at the $\rho$ mass $q_\rho$ defined by

$$m_\rho = 2\sqrt{m^2_\pi + q^2_\rho}. \quad (4.35)$$

The GS parametrization is fully determined by specifying the pion mass and Breit-Wigner parameters of the $\rho$ resonance, which we have extracted in the last section.

\textsuperscript{10}Computing correlation functions using the conserved current in addition to the local vector current employed here would allow for an independent assessment of the size of cutoff effects. We refrained from computing both the local and the point-split current due to limitations on computational resources.

\textsuperscript{11}A recent nonperturbative study with $N_f = 2$ Wilson fermions [111] found $c_V \approx 0.4$, differing substantially from the corresponding one-loop result, which would imply rather large cutoff effects.
4. Numerical Results for Pion-Pion Scattering

| irrep       | renormalized matrix element | LLM factor | $|E_\pi|$ |
|-------------|----------------------------|------------|---------|
| $T^{\pm}_{10}(0)$ | 5.59 (16)(7) | 2.60 (32) | 14.5 (1.5)(0.2) |
| $A^{\pm}_{1}(1)$ | 2.001 (20)(15) | 1.626 (14) | 3.254 (45)(25) |
|             | 6.09 (14)(6)   | 1.52 (13)  | 9.24 (63)(10)  |
| $E^{+}(1)$  | 5.54 (15)(23) | 3.06 (23)  | 17.0 (1.0)(0.7) |
| $A^{+}_{1}(2)$ | 3.28 (4)(12)  | 1.574 (27) | 5.16 (10)(19)  |
|             | 5.75 (18)(24) | 1.139 (77) | 6.54 (39)(27)  |
| $B^{\pm}_{1}(2)$ | 5.39 (10)(2)  | 3.02 (29)  | 16.3 (1.3)(0.1) |
| $B^{\pm}_{2}(2)$ | 3.875 (75)(42)| 2.85 (11)  | 11.05 (48)(12) |
|             | 3.92 (12)(5)  | 1.143 (21) | 4.48 (15)(6)   |
| $A^{+}_{1}(3)$ | 4.61 (12)(2)  | 1.581 (38) | 7.29 (28)(4)   |
|             | 4.44 (15)(2)  | 1.282 (82) | 5.69 (34)(3)   |
|             | 2.56 (5)(11)  | 1.064 (91) | 2.72 (21)(11)  |
| $E^{+}(1)$  | 4.67 (16)(19) | 3.51 (24)  | 16.4 (1.3)(0.7) |
| $A^{+}_{1}(4)$ | 5.67 (28)(50)| 2.09 (33)  | 11.8 (2.4)(1.0) |
| $E^{+}(4)$  | 5.00 (20)(33) | 3.26 (46)  | 16.3 (2.0)(1.1) |

Table 4.9.: Renormalized $O(\alpha)$-improved matrix elements of the isovector part of the electromagnetic current, LLM factor according to (3.14), and final result for the electromagnetic pion form factor in the timelike region for all elastic states on the N200 ensemble. We quote both statistical and systematic uncertainties where appropriate, which are combined in quadrature in subsequent figures.
Figure 4.13.: **Top:** Energy dependence of the electromagnetic pion form factor in the timelike region on the N200 ensemble together with the GS parametrization given by (4.34). The GS parametrization is not a fit to the data, but a prediction based on the resonance mass $m_\rho$ and coupling $g_\rho\pi\pi$ determined in the phase shift analysis. **Bottom:** Deviation of the extracted data points from the GS parametrization. Compared to the top panel, a more pronounced deviation is visible in the resonance region, suggesting a significant correlation.
4. Numerical Results for Pion-Pion Scattering

| irrep       | renormalized matrix element | LLM factor | $|F_\pi|$     |
|-------------|----------------------------|------------|-------------|
| $T_1^+(0)$  | 4.116 (52)(90)              | 1.069 (14) | 4.401 (84)(96) |
|             | 7.25 (24)(11)               | 1.085 (69) | 7.87 (35)(12) |
| $A_1^+(1)$  | 1.221 (9)(21)               | 1.3426 (81)| 1.640 (21)(28) |
|             | 5.70 (6)(10)                | 1.166 (26) | 6.65 (18)(12) |
|             | 7.59 (9)(14)                | 0.993 (37) | 7.54 (24)(14) |
| $E^+(1)$    | 5.43 (8)(13)                | 1.052 (28) | 5.71 (19)(13) |
|             | 8.09 (10)(17)               | 0.816 (14) | 6.60 (11)(14) |
| $A_1^+(2)$  | 1.694 (13)(35)              | 1.1167 (82)| 1.892 (23)(39) |
|             | 7.28 (19)(33)               | 1.062 (38) | 7.73 (42)(35) |
| $B_1^+(2)$  | 6.40 (7)(31)                | 1.081 (36) | 6.92 (24)(34) |
| $B_2^+(2)$  | 1.665 (14)(30)              | 1.368 (12) | 2.277 (29)(41) |
|             | 6.58 (14)(14)               | 1.201 (35) | 7.90 (32)(17) |
| $A_1^+(3)$  | 2.15 (2)(12)                | 1.0016 (84)| 2.15 (3)(12)  |
|             | 1.253 (20)(25)              | 2.71 (22)  | 3.40 (28)(7)  |
|             | 9.35 (36)(16)               | 0.892 (78) | 8.34 (59)(14) |
| $E^+(1)$    | 2.564 (21)(71)              | 1.199 (14) | 3.076 (41)(85) |
|             | 7.77 (46)(16)               | 1.154 (92) | 8.97 (58)(18) |
| $A_1^+(4)$  | 2.463 (29)(14)              | 0.9337 (95)| 2.299 (33)(13) |
| $E^+(4)$    | 3.834 (74)(77)              | 1.312 (28) | 5.03 (17)(10) |

Table 4.10.: Same as table 4.9 but for the D200 ensemble.
4. Numerical Results for Pion-Pion Scattering

Figure 4.14.: Same as figure 4.13 but for the D200 ensemble.
In view of the potentially large systematic effects in this analysis, including the extraction of the bare matrix elements and their cutoff effects, no strong conclusions can be drawn from figure 4.13 and figure 4.14. The GS parametrization describes the enhancement visible in the the data rather well overall, confirming the practical viability of extracting resonant amplitudes from lattice QCD simulations. Taking the data points at face value, the GS parametrization underestimates the peak value of the resonant enhancement in the form factor by roughly 20 percent, in line with the findings of the only other lattice study of the timelike pion form factor [69], which featured one ensemble with a similar pion mass as on the N200 ensemble. Since $\rho - \omega$ mixing is precluded by our isospin-symmetric setup, this result could be indicative of the effects of higher-lying $\rho$ resonances. To turn these measurements into a precision tool however requires a thorough examination of a number of systematic effects. In particular at center-of-mass energies below the resonance region the GS parametrization consistently predicts higher values of the form factor than the extracted data points, possibly indicating an incomplete cancelation of $O(a)$ cutoff effects. Extending the analysis to different lattice spacings will shed light on this issue, and the results shown here using only a single lattice spacing should be interpreted with due care.
5. Concluding Remarks

We have determined the isovector pion-pion scattering amplitude and the isovector part of the electromagnetic pion form factor in the timelike region from $N_f = 2 + 1$ dynamical lattice QCD simulations at a single lattice spacing and two pion masses. The stochastic scheme we employ to treat quark propagation performs efficiently, adding to the evidence suggesting that the stochastic LapH method yields practical all-to-all propagators even in large physical volumes with linear spatial extent exceeding 4 fm.

![Graph showing recent published work for $m_\rho$ and $g_{\rho\pi\pi}$](image)

Figure 5.1.: Summary of recent published work for $m_\rho$ and $g_{\rho\pi\pi}$ with ‘Bulava et al.’ [97], ‘Wilson et al.’ [100], ‘Dudek et al.’ [82], ‘Feng et al.’ [69], ‘Fu and Wang’ [113], ‘ETMC’ [114], ‘GWU’ [115, 116], ‘Lang et al.’ [117], and ‘PACS-CS’ [118].

After extracting the finite-volume spectrum in the elastic region, the Lüscher method is used to calculate phase shifts in a single-channel setup. The isovector $\ell = 1$ partial wave is well described by a Breit-Wigner form and exhibits rapid phase motion indicative of the $\rho$ resonance. As the $\rho$ resonance is the benchmark calculation of Lüscher-type analyses, and in view of the mounting number of lattice studies extracting its Breit-Wigner parameters, clarifying the remaining systematic errors is highly desirable. These include lattice spacing effects and the presence of inelastic thresholds, but also at a more fundamental level, a variety of analysis techniques to
extract the finite-volume spectrum are employed by the different collaborations, such as different fit models and various flavors of the GEVP procedure to extract excited states. Given that resolving small energy differences is the crucial component of Lüscher-type analyses, these subtle differences could potentially have a large impact on the final results. The coupling constant $g_{\rho\pi\pi}$ is particularly sensitive to small shifts of phase shift data points, complicating its extraction to high precision, and a scatter of values extracted for the $\rho$ mass by various collaborations presently exists in the literature, as shown in the summary in figure 5.1. Furthermore, a better understanding of systematic effects in the GEVP becomes even more important when pushing to larger volumes, in view of the denser finite-volume spectrum that entails.

We have also extracted the electromagnetic pion form factor in the timelike region using the framework suggested by Meyer [22], which is conceptionally similar to earlier work by Lellouch-Lüscher [21]. The isotropic regularization employed in the simulations by the CLS consortium allows for a consistent $O(a)$ improvement and renormalization of the vector current required for that calculation, and the corresponding renormalization constant is known nonperturbatively, while $O(a)$ improvement is only implemented perturbatively. The required correlation functions involving the renormalized vector current can be computed in the stochastic LapH framework without spoiling the correct renormalization properties of the operator. Our corresponding analysis is however exploratory in nature, and a careful assessment of associated systematic errors is needed before results with the precision required for phenomenological impact can be quoted. In addition to the systematic effects in the extraction of the Breit-Wigner parameters of the $\rho$ resonance, which are a prerequisite for the Lellouch-Lüscher-Meyer analysis, the matrix elements of the vector current between hadronic states and the vacuum are afflicted with potentially sizable cutoff effects. The contribution of the $O(a)$ counterterm is numerically suppressed mainly by the small (one-loop) value of the improvement coefficient [109]. Therefore a nonperturbative determination of $c_V$ would be highly desirable in conjunction with the recent determination of $b_V$ [119], and extending our analysis to different lattice spacings is a necessary step towards a comprehensive survey of deviations of the pion form factor from the Gounaris-Sakurai model.

From a more exploratory point of view, as the stochastic LapH method provides correlation functions with sufficient accuracy to use in Lüscher-type analyses, more complicated scattering amplitudes are within reach. Due to the favorable scaling of the computational cost of correlator construction in the stochastic LapH approach compared to exact distillation, meson-baryon scattering may be possible with mod-
erate computer resource requirements. Another interesting avenue might be the spectroscopy of three-particle states, although more theoretical work is needed to provide a fully working generalization of the Lüscher method to interpret these states in terms of infinite-volume physics.

In all these endeavors, however, good control over systematic errors at all stages of the analysis is essential, warranting further detailed studies of the benchmark cases. The simulations undertaken by the CLS effort cover a broad range of physical parameters and are therefore ideally suited for a continued investigation of the observables presented in this work.
A. $t_{\text{min}}$-plots for All Energy Levels

In this appendix we show all plots detailing the extraction of the finite-volume isovector two-pion spectrum and the extraction of current matrix elements on the two ensembles used in this work. The extraction of the finite-volume spectrum is the subject of subsection 4.3.2, and the respective plots shown in the following are similar to figure 4.6. The extraction of the current matrix elements is discussed in section 4.5, and the corresponding plots are after the fashion of figure 4.11.

A.1. N200

A.1.1. Extraction of the Finite-Volume Spectrum

\[
\begin{align*}
T_0^+(0), E_0 \\
(t_0, t_d) = (5, 10) \quad N_{\text{op}} = 3
\end{align*}
\]

\[
\begin{align*}
A_1^+(1), E_0 \\
(t_0, t_d) = (5, 10) \quad N_{\text{op}} = 3
\end{align*}
\]

\[
\begin{align*}
(t_0, t_d) = (7, 14) \quad N_{\text{op}} = 3
\end{align*}
\]

\[
\begin{align*}
(t_0, t_d) = (5, 10) \quad N_{\text{op}} = 2
\end{align*}
\]

\[
\begin{align*}
(t_0, t_d) = (7, 14) \quad N_{\text{op}} = 3
\end{align*}
\]

\[
\begin{align*}
(t_0, t_d) = (5, 10) \quad N_{\text{op}} = 2
\end{align*}
\]
A. $t_{\text{min}}$-plots for All Energy Levels

\[ A_1^2(1), E_1 \]
\[ (t_0, t_d) = (5, 10) \; N_{\text{op}} = 3 \]
\[ (t_0, t_d) = (7, 14) \; N_{\text{op}} = 3 \]
\[ (t_0, t_d) = (5, 10) \; N_{\text{op}} = 2 \]

\[ B_1^2(1), E_0 \]
\[ (t_0, t_d) = (5, 10) \; N_{\text{op}} = 2 \]
\[ (t_0, t_d) = (7, 14) \; N_{\text{op}} = 2 \]
\[ (t_0, t_d) = (5, 10) \; N_{\text{op}} = 2 \; \text{single exp.} \]

\[ A_1^2(2), E_0 \]
\[ (t_0, t_d) = (5, 10) \; N_{\text{op}} = 2 \]
\[ (t_0, t_d) = (7, 14) \; N_{\text{op}} = 2 \]
\[ (t_0, t_d) = (5, 10) \; N_{\text{op}} = 3 \]

\[ A_1^2(2), E_1 \]
\[ (t_0, t_d) = (5, 10) \; N_{\text{op}} = 2 \]
\[ (t_0, t_d) = (7, 14) \; N_{\text{op}} = 2 \]
\[ (t_0, t_d) = (5, 10) \; N_{\text{op}} = 3 \]

\[ B_1^2(2), E_0 \]
\[ (t_0, t_d) = (5, 10) \; N_{\text{op}} = 3 \]
\[ (t_0, t_d) = (7, 14) \; N_{\text{op}} = 3 \]
\[ (t_0, t_d) = (5, 10) \; N_{\text{op}} = 2 \]
A. $t_{\text{min}}$-plots for All Energy Levels

For $E_0$, $N_{\text{op}} = 3$ for $(t_0, t_d) = (5, 7, 14)$ and $N_{\text{op}} = 2$ for $(t_0, t_d) = (5, 10)$.

For $E_1$, $N_{\text{op}} = 3$ for $(t_0, t_d) = (5, 7, 14)$ and $N_{\text{op}} = 2$ for $(t_0, t_d) = (5, 10)$.

For $E_2$, $N_{\text{op}} = 3$ for $(t_0, t_d) = (5, 7, 14)$ and $N_{\text{op}} = 2$ for $(t_0, t_d) = (5, 10)$. 

The plots show the dependence of $u^2$ on $t_{\text{min}}/a$ for different energy levels and $N_{\text{op}}$ values.
A. $t_{\text{min}}$-plots for All Energy Levels

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure1}
\caption{Plots showing $E_1^+(3)$, $E_0$ with $(t_0, t_d) = (5, 10)$, $N_{\text{op}} = 2$ alongside $(t_0, t_d) = (7, 14)$, $N_{\text{op}} = 2$ and a single exponential.}
\end{figure}
A. \( t_{\text{min}} \)-plots for All Energy Levels

A.1.2. Extraction of Current Matrix Elements
A. $t_{\text{min}}$-plots for All Energy Levels

\begin{align*}
A_{\text{i}}^{\dagger}(1), E_{\text{i}} & & R_1 \\
R_{\text{CC}}(t) & & R_2 \\
R_{\text{OA}}(t) & & R_3
\end{align*}

\begin{align*}
E_{\text{i}}^{\dagger}(1), E_{\text{0}} & & R_1 \\
R_{\text{CC}}(t) & & R_2 \\
R_{\text{OA}}(t) & & R_3
\end{align*}

\begin{align*}
A_{\text{i}}^{\dagger}(2), E_{\text{0}} & & R_1 \\
R_{\text{CC}}(t) & & R_2 \\
R_{\text{OA}}(t) & & R_3
\end{align*}

\begin{align*}
t/a & & \\
10 & 15 & 20
\end{align*}
A. $t_{\text{min}}$-plots for All Energy Levels
A. $t_{\min}$-plots for All Energy Levels

$R_{CE}(t)$

$R_{OA}(t)$

$t/a$
A. $t_{\text{min}}$-plots for All Energy Levels

\begin{figure}
\centering
\includegraphics[width=\textwidth]{fig1.png}
\end{figure}

\begin{figure}
\centering
\includegraphics[width=\textwidth]{fig2.png}
\end{figure}

\begin{figure}
\centering
\includegraphics[width=\textwidth]{fig3.png}
\end{figure}

95
A. $t_{\text{min}}$-plots for All Energy Levels

![Graph showing $R_{CE}(t)$ and $R_{OA}(t)$ for different energy levels with $t/a$ on the x-axis and $t/a$ on the y-axis.]
A. $t_{\text{min}}$-plots for All Energy Levels

A.2. D200

A.2.1. Extraction of the Finite-Volume Spectrum

![Diagram with $t_{\text{min}}/a$ vs. $u^2$ for different energy levels and time intervals]
A. $t_{\text{min}}$-plots for All Energy Levels

- $A_1^+(1)$, $E_2$
  - $(t_0, t_d) = (5, 10)$ $N_{\text{op}} = 4$
- $E^+(1)$, $E_0$
  - $(t_0, t_d) = (5, 10)$ $N_{\text{op}} = 2$
  - $(t_0, t_d) = (7, 14)$ $N_{\text{op}} = 2$
  - $(t_0, t_d) = (5, 10)$ $N_{\text{op}} = 3$
  - $(t_0, t_d) = (7, 14)$ $N_{\text{op}} = 3$
  - $(t_0, t_d) = (5, 10)$ $N_{\text{op}} = 2$
- $A_1^+(2)$, $E_0$
  - $(t_0, t_d) = (5, 10)$ $N_{\text{op}} = 3$
  - $(t_0, t_d) = (7, 14)$ $N_{\text{op}} = 3$
  - $(t_0, t_d) = (5, 10)$ $N_{\text{op}} = 2$
- $A_1^+(2)$, $E_1$
  - $(t_0, t_d) = (5, 10)$ $N_{\text{op}} = 3$
  - $(t_0, t_d) = (7, 14)$ $N_{\text{op}} = 3$
  - $(t_0, t_d) = (5, 10)$ $N_{\text{op}} = 2$
A. $t_{\text{min}}$-plots for All Energy Levels
A. $t_{\text{min}}$-plots for All Energy Levels

- $A_1^+(3), E_2$ ($t_0, t_d = (5, 10) \ N_{op} = 3$
- $E_1^+(3), E_0$ ($t_0, t_d = (5, 10) \ N_{op} = 2$
- $E_1^+(4), E_0$ ($t_0, t_d = (5, 10) \ N_{op} = 2$
- $E^+(4), E_0$ ($t_0, t_d = (5, 10) \ N_{op} = 2$
A.2.2. Extraction of Current Matrix Elements

\[ R_{\text{CT}}(t) \]

\[ R_{\text{OA}}(t) \]

\[ T_n^1(0), E_0 \]

\[ R_1 \]

\[ R_2 \]

\[ R_3 \]

\[ t/a \]
A. $t_{\text{min}}$-plots for All Energy Levels

\[ R_{\text{OCF}}(t) \]

\[ R_{\text{OA}}(t) \]

\[ t/a \]
A. \( t_{\text{min}} \)-plots for All Energy Levels
A. $t_{\text{min}}$-plots for All Energy Levels

\begin{align*}
R_{\text{CC}}(t) & \quad R_{\text{OA}}(t) \\
R_{\text{CC}}(t) & \quad R_{\text{OA}}(t) \\
R_{\text{CC}}(t) & \quad R_{\text{OA}}(t)
\end{align*}

\begin{align*}
R_{\text{CC}}(t) & \quad R_{\text{OA}}(t) \\
R_{\text{CC}}(t) & \quad R_{\text{OA}}(t) \\
R_{\text{CC}}(t) & \quad R_{\text{OA}}(t)
\end{align*}

\begin{align*}
R_{\text{CC}}(t) & \quad R_{\text{OA}}(t) \\
R_{\text{CC}}(t) & \quad R_{\text{OA}}(t) \\
R_{\text{CC}}(t) & \quad R_{\text{OA}}(t)
\end{align*}
A. $t_{\text{min}}$-plots for All Energy Levels

\[ R_{\text{CU}}(t) \]

\[ R_{\text{OA}}(t) \]

\[ t/a \]
A. $t_{\text{min}}$-plots for All Energy Levels

![Graph showing $t_{\text{min}}$-plots for different energy levels and various labels including $A^+_1(3), E_2$, $E_1'$, $E_{1}\text{'}, E_2'$, and $E_{1}'$.](image-url)
A. $t_{\text{min}}$-plots for All Energy Levels

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1}
\caption{$t_{\text{min}}$-plots for All Energy Levels}
\end{figure}
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