### The Spectrum of Meson States in the Isovector Non-strange $T_{1u}^+$ Channel by the Stochastic LapH Method in Lattice QCD

by

David W. Lenkner

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Advised by Professor Colin Morningstar

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#### Abstract

A new method of estimating quark propagation, known as Stochastic LapH, has provided a way of computing many observables in lattice QCD which have previously been inaccessible due to computational expense. In this work, the first large-scale applications of the Stochastic LapH method to excited meson spectroscopy are presented. We discuss the construction of single-meson and two-meson operators with LapH smearing, and procedures for selecting and correlating large sets of these operators are described. We then present the analysis of a 56 × 56 correlator matrix of operators in the isovector nonstrange  $T_{1u}^+$  channel. We extract the energy of the  $\rho$  meson, and discuss the identification and energy extractions of excited  $\rho$  mesons. Operators are included for all flavor combinations that can result in the I = 1, S = 0total quantum numbers of the desired symmetry channel. The correlation matrix is calculated on 551 configurations of an anisotropic  $24^3 \times 128$  gauge field ensemble with clover-improved Wilson fermions. Good signal quality is obtained even for correlators involving same-time quark lines and isoscalar mesons as part of two-meson operators. Results are compared with experimental values compiled by the Particle Data Group.

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# Contents

1	Intr	roduction	1
<b>2</b>	Lat	tice QCD Overview	9
	2.1	Theoretical Framework	10
	2.2	Discretization of the QCD Action	14
		2.2.1 Wilson Action	14
		2.2.2 Action Improvement	19
	2.3	Numerical Techniques	23
		2.3.1 Monte Carlo Integration	23
		2.3.2 Standard Dirac Matrix Inversion	32
	2.4	Tuning and Setting the Scale	39
	2.5	Extracting Energies from Correlators	41
	2.6	Error Analysis	46
3	Ope	erator Design	48
	3.1	Field Smearing	49
	3.2	Spatially-Extended Operators	53
	3.3	Symmetry Projections	57
		3.3.1 The Need for Definite Momentum for Each Hadron	67
	3.4	Single-Hadron Operator Selection	69
	3.5	A Novel Glueball Operator	72
<b>4</b>	Sto	chastic LapH Method	75
	4.1	Motivation for Stochastic Sub-Sampling	76
	4.2	Stochastic Inversion of a Large Matrix $M$	78
	4.3	The Stochastic LapH Method	82
	4.4	Examples and Implementation Details	89
<b>5</b>	Res	ults	97
	5.1	Multi-Hadron Operator Selection	98
	5.2	$T_{1u}^+$ Correlation Matrix Analysis	101
	5.3	Energy Spectrum for Isovector $T_{1u}^+$ Channel	113

6	Conclusions and Outlook	123
A	Number of Operators and Momenta for Moving Single-Hadrons	125
Bi	ibliography	132

# List of Tables

2.1	Gauge configurations used in this work	41
3.1	Number of LapH Eigenvectors	52
3.2	Meson operator displacement types	54
3.3	Baryon operator displacement types	55
3.4	$O_h$ Irreps and Little Group Subduction	61
3.5	Subduction Onto Continuum Spin	62
3.6	Flavor content of single-hadron operators	65
3.7	Operator Combinations vs. Total Isospin and Strangeness	66
5.1	Single-Hadron $T_1^+$ Operators	101
5.2	Multi-Hadron $T_{1}^{+}$ Operators, I	102
5.3	Multi-Hadron $T_{1_{\mu}}^{i_{\mu}}$ Operators, II	103
5.4	Identification of Single-Hadron Eigenstates	112
A.1	Maximum momentum element by channel, $I = \frac{1}{2}, S = 1$ (K)	126
A.2	Maximum momentum element by channel, $I = 1$ , $S = 0$ $(\pi)$	127
A.3	Maximum momentum element by channel, $I = 0, S = 0$ ( $\eta$ )	128
A.4	Maximum momentum element by channel, $I = \frac{1}{2}$ , $S = 0$ (N)	129
A.5	Maximum momentum element by channel, $I = \frac{3}{2}$ , $S = 0$ ( $\Delta$ )	129
A.6	Maximum momentum element by channel, $I = \vec{0}, S = -1$ (Å)	130
A.7	Maximum momentum element by channel, $I = 1, S = -1$ ( $\Sigma$ )	130
A.8	Maximum momentum element by channel, $I = \frac{1}{2}, S = -2$ ( $\Xi$ )	131
A.9	Maximum momentum element by channel, $I = \vec{0}, S = -3$ ( $\vec{\Omega}$ )	131

# List of Figures

$1.1 \\ 1.2 \\ 1.3 \\ 1.4$	QCD Coupling Constant	$2 \\ 4 \\ 5 \\ 7$
2.1	Single-Meson Wick Contractions	38
3.1 3.2 3.3 3.4 3.5	Quark Smearing ComparisonBaryon Displacement ComparisonTime Reversal Symmetry CheckLocal vs. Definite- $\vec{p} \pi \pi$ ComparisonLapH Glueball Operator	52 56 68 69 73
$\begin{array}{c} 4.1 \\ 4.2 \\ 4.3 \\ 4.4 \\ 4.5 \\ 4.6 \end{array}$	LapH vs. Space-Color Dilution $\dots \dots \dots$	85 86 88 91 93 95
$5.1 \\ 5.2 \\ 5.3 \\ 5.4 \\ 5.5$	Example Effective Masses, Each Two-Meson Flavor Combination 1 Off-diagonal Elements of $\widehat{C}^{(r)}$	104 107 109 110 111
5.6 5.7 5.8 5.9	$ Z_i^{(n)} ^2$ for Multi-Hadron Operators	114 115 116 117
5.10 5.11 5.12 5.13 5.14	$\rho(1450)$ Mass Extraction, Full vs. Single-Hadron-Only Basis 1 $\rho(1570)$ Mass Extraction, Full vs. Single-Hadron-Only Basis 1 $\rho_3(1690)$ Mass Extraction, Full vs. Single-Hadron-Only Basis 1 $\rho(1700)$ Mass Extraction, Full vs. Single-Hadron-Only Basis 1 Additional Excited $\rho$ , Full vs. Single-Hadron-Only Basis 1	117 118 118 119 119

5.15	Additional Excited $\rho$ , Full vs. Single-Hadron-Only Basis	 	120
5.16	$T_{1u}^+$ Spectrum Pattern vs. Experimental States	 	121

### Chapter 1

# Introduction

The existence of quarks was postulated by Gell-Mann [1] and Zweig [2] in 1964 as a way to understand the many hadronic states that were being discovered in accelerators around that time. Just as Mendeleev a century before had organized the elements into a periodic table which made it possible to identify an underlying structure to the atom, Gell-Mann's model made many of these hadronic states understandable in terms of the quarks of which they are comprised. It was not until more than a decade later that Quantum Chromodynamics (QCD) was identified as the dynamical theory governing the interactions of quarks [3], and the gauge bosons that carry their interaction were named gluons.

The bound states of electrons, neutrons, and protons in the chemical elements described by Mendeleev are governed by quantum electrodynamics, which can be studied using perturbation theory in the form of so-called Feynman diagrams. The bound states of QCD are much more difficult to investigate. QCD admits perturbative solutions only for very high energies, much larger than a typical hadron mass scale. At those large energies, the QCD coupling constant  $\alpha_s$  decreases and the behavior of quarks approaches that of freely-moving particles, a phenomenon known as asymptotic freedom [4,5]. At low energies, the coupling becomes stronger and standard perturbative methods fail. The running of the coupling constant  $\alpha_s$  can be seen in Fig. 1.1, along with a comparison of each data point evolved to the Z-boson energy scale using the renormalization group equation, described in Ref. [6]. The agreement of these measurements is a strong confirmation of the validity of perturbative QCD at high energy scales Q.

Given the difficulties of doing QCD calculations, phenomenologists have used Gell-



Figure 1.1: Collection of measurements of the QCD running coupling  $\alpha_s(Q)$ , (left) as a function of energy scale Q. (Right) The RG flow equations have been used [6] to extract predictions of  $\alpha_s(M_Z)$ , the running coupling at the Z-boson mass  $M_Z$ . The yellow band on the right corresponds to the combined world average value of  $\alpha_s(M_Z)$ with error bars, and the line on the left corresponds to that average RG evolved to other scales Q. Data is from Ref. [7].

Mann's quark model to understand mesons as bound states of a quark and an antiquark in a confining potential, and to view baryons as bound states of three constituent quarks in a similarly confining potential. These "quark models" have achieved some success in describing the ground-state hadron spectrum, if various parameters in such models are tuned appropriately. However, higher-lying states and those with so-called "exotic" quantum numbers, are problematic. For example, many quark models, such as that of Ref. [8], predict a large number of excited three-quark states, known as baryons, which are not seen in experiment, and some of the quark-model level orderings do not agree with experiment. Only certain  $J^{PC}$ , where J is spin, P is parity, and C is charge conjugation, are allowed for mesons, which are quarkantiquark states, in the quark model. The forbidden  $J^{PC}$ , such as  $0^{--}, 0^{+-}, 1^{-+}$ , are called exotic, and meson candidates with such exotic quantum numbers have been observed in experiments. Such exotic quantum numbers are possible if the quark and antiquark are bound in an excited gluon field. A good deal of experimental evidence points to a hybrid meson state with I = 1,  $J^{PC} = 1^{-+}$ , known as the  $\pi_1(1600)$  resonance, although further confirmation is needed [9]. Another type of state which is outside the quark model is the glueball, a bound state of massless gluons. Although glueballs have yet to be firmly identified in experiment, the scalar  $0^{++}$  channel contains more mesons than predicted by the quark model [10]. Two possible glueball candidates are the  $f_0(1500)$  and the  $f_0(1710)$  states.

One way of carrying out low-energy calculations in QCD is to formulate the theory on a space-time lattice, and evaluate the path integrals of the theory using Monte Carlo integration. Kenneth Wilson [11] figured out how to formulate QCD on a spacetime lattice in such a way that a key symmetry, known as local gauge invariance, was not destroyed. In quantum field theories, local gauge invariance is intimately connected to renormalizability, which gives predictive power to a quantum field theory. Quark confinement, the complete absence of isolated quarks outside of hadrons<sup>1</sup>, is a key feature of QCD, and Wilson's formulation could explain quark confinement in a certain (non-physical) limit of the theory. Understanding quark confinement remains a key challenge in QCD.

Lattice QCD is an *ab initio* method of investigating the low-energy properties of QCD. Lattice QCD calculations use the relativistic field theory of QCD discretized

<sup>&</sup>lt;sup>1</sup> Experimentally, the relative abundance of fractional-charge particles to baryons has been bounded at  $n_q/n_b \leq 10^{-27}$  [12].



Figure 1.2: A lattice QCD calculation of the heavy-quark potential V(r) as a function of spatial quark separation r (see the blue points labeled  $\Sigma_g^+$ ). The linear rise for large r confirms the phenomenon of quark confinement. The higher line (label  $\Pi_u$ ) represents an excitation of the "flux tube" of gluons between the two heavy quarks. From Ref. [16].

on a space-time grid of finite size and numerically simulate the quark and gluon dynamics via Monte-Carlo algorithms. Through the computation of temporal twopoint correlation functions, one can extract information about the eigenstates of the lattice Hamiltonian and their corresponding energies. In imaginary time, the oscillatory temporal evolution of stationary states maps into exponential decays in time, which provides a means of extracting the finite-volume energies. Under certain conditions [13,14], the infinite-volume spectrum can be deduced from the energies in finite volume.

Lattice QCD has enjoyed a good deal of success in confirming many experimental quantities related to low-energy QCD. For example, calculations of the heavy quark potential V(r), the energy of a pair of heavy quarks fixed at separation r, have provided confirmation of the phenomenon of confinement. One such calculation is shown in Fig. 1.2. The linear rise at larger r is indicative of a string tension resulting from a "flux tube" of gluons connecting the quark-antiquark pair [15].

In addition, the ground state spectrum of hadrons (the energy of the lowest state in each symmetry channel of QCD) has been calculated in lattice QCD with impressive agreement with experiment. One recent lattice spectroscopy calculation is shown in Fig. 1.3, along with experimental results for comparison. Note that these states are



Figure 1.3: A survey of ground state energies in some experimentally well-known symmetry channels, computed with lattice QCD by the BMW collaboration [17].

all ground states in their respective symmetry channels; the states labeled with a "\*" such as the  $K^*$  differ from the un-starred versions by their spin J, and so fall in different symmetry channels. Excited-state energies in a given channel have proven more difficult to extract, as will be discussed presently.

Energies are determined in lattice QCD from the temporal correlations of interpolating operators that create and annihilate the states of interest. These correlations are estimated using the Monte Carlo method. The success of the calculations depends partly on achieving good statistics in the Monte Carlo estimates, but more importantly, on using interpolating operators that are carefully designed. The operators should have definite transformation properties (quantum numbers) under the symmetry group of the lattice, so as to be able to identify the quantum numbers of a given state. They should also create the states of interest, without creating too much contamination from higher-lying states.

An arbitrarily chosen operator could couple to nearly all of the different states within its symmetry channel, but given that we only measure the correlator on a handful of time separations, it is impractical to extract more than the lowest-lying energy from a single correlation function. A more reliable method is to compute a matrix of correlators, the diagonalization of which leads to the eigenstates of the lattice Hamiltonian [13,18]. Unfortunately, the diagonalization process can miss levels that couple weakly to all of the operators used. Thus, it is important to consider large sets of operators that span all states in the energy region of interest. In particular, one should make sure that multi-hadron operators are included as well, since such states may have suppressed couplings to the single-hadron operators. A first calculation of the isovector meson spectrum using only single-hadron operators is shown in Fig. 1.4. The shaded areas indicate energies where bound states might be expected to appear. This plot suggests that the single-hadron operators miss the two-meson energy levels, at least when examining the correlation functions in the range of temporal separations possible in our simulation.

Momenta are quantized in a finite volume and all stationary states are discrete. Techniques have been developed [19–21] to deduce properties of continuum scattering and decay widths from the finite-volume discrete energy levels. The decay of the isovector  $\rho$  meson into two pions is particularly well suited for such a finite-volume analysis. In order to calculate such decay widths and scattering properties on the lattice, it is important to be able to calculate correlators involving two-pion operators.

Multi-hadron operators are difficult to include in lattice QCD calculations. This difficulty stems from the fact that multi-hadron correlators require the calculation of quark propagation between a much larger number of points on the lattice. Propagators are required between all final-time sites and all other final-time sites, not only between the initial and final times in the temporal correlation function. Such quark lines are also necessary in the calculation of isoscalar meson correlators, which have likewise been avoided due to calculational expense.

In this work, a new technique known as the stochastic LapH method [22] is utilized to compute quark propagators in an efficient fashion, which allows multi-hadron correlators to be computable. This method utilizes stochastic estimates of the inverse of the Dirac matrix, which includes variance reduction through noise dilution in a way that works well with Laplacian Heaviside quark field smearing [23]. A description of this method, with preliminary testing, has been carried out in Refs. [22,24,25], showing that it is far more efficient than traditional noise dilution methods. In this work, we review some of these results, but the main focus will be on the first application of this method to meson spectroscopy.

For this first application of the stochastic LapH method which includes both single-meson and two-meson operators, we chose to consider a single symmetry channel. Specifically, we apply the stochastic LapH method to the calculation of the energy spectrum in the bosonic  $(-1)^J = 1$ , isovector I = 1, nonstrange S = 0,  $T_{1u}^+$  sector of QCD, using a large operator basis which includes both single- and two-hadron operators. This channel was chosen for several reasons. First, there are a large number of



Figure 1.4: Our preliminary look at the isovector spectrum using only single-hadron operators. The boxes in this plot indicate the energies, with error bars, of isovector states that we extract using only single-particle operators, on a subset of 170 configurations of a  $24^3 \times 128$  ensemble with  $m_{\pi} \approx 390$  MeV (see later). The letters along the bottom indicate different symmetry sectors (irreducible representations of the lattice symmetry group). The shaded area indicates energies where bound states might be expected, under the approximation that the bound state energies are approximately the sum of the single-hadron energies. The different colors of states simply indicate ground states (black), first excited states (red), second (green), and third (blue) excited states.

excitations of the  $\rho$  meson which are observed in experiment. The "mini-review" in Ref. [26] is devoted to the  $\rho(1450)$  and  $\rho(1700)$  states, which were interpreted originally as a single broad resonance but are now believed to be two distinct states. The four excited states each lie well above multi-hadron thresholds, so our use of multihadron operators may be particularly helpful in delineating these states. Secondly, finite-volume lattice studies of the two lowest states in this channel, the  $\rho(770)$  and a two-pion state in a P-wave, can be used to calculate the  $\rho \to \pi\pi$  decay width in *infinite* volume, and chiral perturbation theory can be used to extrapolate results to the physical pion mass [27]. That particular analysis will not be carried out here, but interest in these calculations has led to a number of studies in this channel, such as Refs. [28,29], with which we can compare certain parts of our results, at least for heavier pion masses and smaller lattice sizes. The lighter pion masses and largest volumes considered in this work are made possible by the stochastic LapH method. Our primary goal is to calculate the spectrum of energy eigenstates below an energy of roughly 2 GeV, with careful attention paid to possible mixing of single-hadron operators with multi-hadron operators. In the process, we will also develop insights that can help streamline future studies, since we plan to apply similar methods to calculate the energy spectrum of QCD in all other symmetry sectors.

This work is organized as follows. In Ch. 2, we briefly review lattice QCD and the computation techniques that we use in conjunction with the Stochastic LapH method. Our operator construction is discussed in Ch. 3, with special attention to the design of good multi-hadron operators with definite symmetry properties. An introduction to the stochastic LapH method is given in Ch. 4, with some demonstrations of its effectiveness. In Ch. 5, we present first calculations of correlator matrices including large sets of such two-hadron operators along with single-hadron operators, and results for the extraction of excited-state energies from these matrices.

### Chapter 2

# Lattice QCD Overview

Putting a field theory onto a finite-extent, discrete space-time lattice offers two advantages. Firstly, the lattice spacing a limits the wavelength of any field fluctuations to 2a, so the momenta relevant to the theory are cut off at a maximum of  $|p| = \pi/a$ . This regulates the divergences that plague analytic calculations in continuum perturbative field theory. Secondly, the number of degrees of freedom in the field is made finite, and so the path integrals of the theory can be estimated via numerical Monte Carlo integration with importance sampling. The first of these two advantages can be utilized independently, as a regularization scheme for perturbative calculations on the lattice [30]. In this work, however, we will focus on the numerical computation of non-perturbative quantities in lattice QCD, especially the computation of the energy spectrum of QCD.

Although a lattice discretization possesses these convenient qualities, there are a number of highly 'inconvenient' aspects to lattice QCD in its actual practice. Large lattices lead to path integrals of very high dimensionality (on the order of 10<sup>8</sup> for the largest lattices in this work), so these integrals can take an enormous amount of CPU-hours to complete. Compounding this issue, certain lattice QCD calculations require the inversion of all-site-to-all-site matrices, so the CPU-time required can scale with numerous powers of the lattice volume.

Yet there is a need for large lattices; on the one hand, the lattice spacing should be small enough that the momentum cutoff  $\pi/a$  does not discard too much of the desired physics, and on the other hand, one wants the total size of the lattice to be sufficiently larger than the Compton wavelength of the lightest particle in the model, the pion. These two properties combine to necessitate large numbers of lattice points, and thus very clever methods for performing the resulting path integrals. Light quark masses (and thus pion masses) carry other hazards as well, in connection with the fermion doubling problem, to be explained below.

This chapter will review some of the methods commonly used to address those challenges, in the course of outlining a typical lattice QCD spectroscopy calculation. In Sec. 2.1, we introduce continuum QCD path integrals in imaginary time, and show how all of the energy eigenstates of QCD are encoded in the results of these integrals. Section 2.2 examines the discretization of the QCD action. Section 2.3 then reviews standard techniques for proceeding from the theoretical grounding of Sec. 2.1 and Sec. 2.2 to arrive numerically at an energy spectrum. These algorithms are well known, and further description can be found in the literature, such as Refs. [31–34]. Also in Sec. 2.3, we briefly preview the new methodological improvement employed in this work, the so-called stochastic LapH method, which will be explained in further detail in Ch. 4. Finally in Secs. 2.4, 2.5 and 2.6, we present standard methodology used to extract excited states from temporal correlation functions (correlators), translate those energies to continuum physical units, and quote statistical errors on those estimates.

#### 2.1 Theoretical Framework

A field theory can be considered solved once all the Green's functions (*n*-point correlation functions) of the theory are known. According to Feynman's path integral formulation of quantum mechanics [35], these *n*-point functions can be calculated via ratios of path integrals involving the action  $S \equiv \int d^4x \mathcal{L}$ , where the Lagrangian density  $\mathcal{L}$  is defined in terms of the fundamental fields of the theory. Thus the Lagrangian serves as the defining feature of a field theory, along with the nature of the fields themselves.

In Euclidean-space QCD, the fundamental fermion fields are Grassmann-valued  $\psi(x)$  and  $\overline{\psi}(x)$ , which are vectors in Dirac spin (four elements), color (3 elements), and flavor ( $N_f$  elements). The fundamental boson field is a gauge field  $A_{\mu}(x)$  which is a complex SU(3) matrix in color and has directional index  $\mu$ . The Euclidean QCD Lagrangian is given by

$$\mathcal{L}_{QCD}(x) = \sum_{f=1}^{N_f} \psi^{(f)}(x) [\gamma_{\mu} D_{\mu} + m^{(f)}] \overline{\psi}^{(f)}(x) + \frac{1}{2} \text{Tr}[F_{\mu\nu}(x) F_{\mu\nu}(x)].$$
(2.1)

The operator  $[\gamma_{\mu}D_{\mu} + m^{(f)}]$  is referred to as the Dirac matrix for flavor f, later denoted by M or  $M^{(f)}$ . Going from lightest to heaviest, the six quark flavors are up, down, strange, charm, bottom, and top. The charm, bottom, and top quark masses are heavy enough that for light hadron physics on the lattice, we can often neglect them. The u and d (up and down) flavors have very similar masses, leading to an approximate symmetry under 'isospin' rotations changing u to d and vice versa. The Euclidean covariant derivative  $D_{\mu}$  in Eq. (2.1) is defined as

$$D_{\mu} = \partial_{\mu} + igA_{\mu}(x), \qquad (2.2)$$

and the field strength tensor  $F_{\mu\nu}$  is defined similarly to that of QED, via

$$F_{\mu\nu}(x) = \frac{-i}{g} [D_{\mu}(x), \ D_{\nu}(x)] = \partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu} + ig[A_{\mu}(x), A_{\nu}(x)].$$
(2.3)

The last term in  $F_{\mu\nu}$  results from the non-Abelian nature of the gauge field, and leads to the self-interactions of gluons, one of the key features that makes QCD richer and more complex than QED. Note that the gauge action  $S_G = \frac{1}{2} \text{Tr}[F_{\mu\nu}F_{\mu\nu}]$  is often written instead as  $\frac{1}{4}F_{\mu\nu}^{(i)}F_{\mu\nu}^{(i)}$ , where  $F_{\mu\nu}^{(i)}$  are scalar coefficients for 8 SU(3) basis matrices, rather than color matrices themselves. These expressions can be shown to be equivalent – see, for example, Ref. [36] – so we use the former notation, which more closely mimics the numerical quantities we will actually compute on the lattice.

We work with the Euclidean field theory, as opposed to the Minkowski-space version. The oscillatory Minkowski path integral weight  $e^{-iS}$  gets Wick-rotated into a Boltzmann-like factor  $e^{-S}$  which can be interpreted as a real probability distribution. The Euclidean theory is obtained from the Minkowski-space one by a change of variables in the time coordinate  $x_4$ ,

$$x_j = x^j = x_j^M = -x_M^j, \quad j = 1...3 \qquad x_4 = x^4 = ix_0^M = ix_M^0, \quad (2.4)$$

with Minkowski-space variables denoted by superscript M. The gamma matrices have also been redefined as compared with the Minkowski-space gamma matrices, such that the Euclidean gamma matrices  $\gamma_{\mu}$ ,  $\mu = 1...4$ , are Hermitian and satisfy

$$\{\gamma_{\mu}, \gamma_{\nu}\} = 2\delta_{\mu\nu}\mathbf{1}.\tag{2.5}$$

This reflects the fact that the Euclidean space metric is  $\delta_{\mu\nu}$  as opposed to  $g_{\mu\nu}$  (thus the name Euclidean), and the distinction between covariant/contravariant indices is lost. As in Minkowski space, a fifth gamma matrix is defined, now  $\gamma_5 \equiv \gamma_1 \gamma_2 \gamma_3 \gamma_4$ . The Euclidean gamma matrices have different commonly-used representations; the representation used in this work is the Dirac-Pauli convention.

As indicated earlier, two-point correlation functions in Euclidean QCD can be expressed as a ratio of path integrals involving the above Lagrangian via  $S_{QCD} = \int d^4x \mathcal{L}_{QCD}$ . For a creation operator  $\overline{O}_i[\psi, \overline{\psi}, A](t_0)$  and an annihilation operator  $O_j[\psi, \overline{\psi}, A](t)$ , the temporal correlation function  $C_{ij}(t - t_0)$  is given by<sup>1</sup>

$$C_{ij}(t-t_0) \equiv \frac{\langle 0|O_i[\psi,\overline{\psi},A](t)\overline{O}_j[\psi,\overline{\psi},A](t_0)|0\rangle}{\langle 0|0\rangle} \\ = \frac{\int \mathcal{D}\psi \mathcal{D}\overline{\psi}\mathcal{D}A O_i[\psi,\overline{\psi},A](t)\overline{O}_j[\psi,\overline{\psi},A](t_0) e^{-S_{QCD}[\psi,\overline{\psi},A]}}{\int \mathcal{D}\psi'\mathcal{D}\overline{\psi}'\mathcal{D}A' e^{-S_{QCD}[\psi',\overline{\psi}',A']}}.$$
 (2.6)

Eq. (2.6) is the main field-theoretical equation upon which lattice QCD spectroscopy is based. Once a suitable set of correlation functions  $C_{ij}$  are numerically evaluated, the stationary state energies of the theory can be extracted from this data, since the expected form of the imaginary-time correlator is<sup>2</sup>

$$C_{ij}(t-t_0) = \sum_{n} \langle 0|O_i|n\rangle \langle n|\overline{O}_j|0\rangle e^{-(t-t_0)E_n}, \qquad (2.7)$$

where  $E_n$  are the energies of each eigenstate  $|n\rangle$  created/destroyed by operators  $O_i$ and  $O_j$ . This spectral representation of the correlation function in imaginary time can be seen by introducing some finite volume limits, and specifying boundary conditions such that the path integral takes the form of a trace

<sup>&</sup>lt;sup>1</sup>For cases where the operators  $O_i$  and  $\overline{O}_j$  have the same quantum numbers as the vacuum, an extra term is included in the correlator subtracting off  $\langle 0|O_i|0\rangle\langle 0|\overline{O}_j|0\rangle/\langle 0|0\rangle$ . This term is treated similarly so will be omitted for the moment.

 $<sup>^{2}</sup>$  Later, we will note a few small modifications to Eq. (2.7) which become necessary when the finite temporal extent of the lattice is comparable to the decay time of these correlators.

$$\int \mathcal{D}\psi \mathcal{D}\overline{\psi} \mathcal{D}Ae^{-S_{QCD}} = \sum_{n} \langle n|e^{-H_{QCD}T}|n\rangle, \qquad (2.8)$$

for finite temporal extent T. It can be shown [37, 38] that the proper boundary conditions to admit this trace interpretation are periodic in space, periodic in time for bosonic fields, and antiperiodic in time for fermionic fields. These boundary conditions also ensure that numerical models of this theory obey time translation invariance, so we can average over  $t_0$  in computing correlation functions.

In order to evaluate the right hand side of Eq. (2.6) on a computer, we first need to deal with the Grassmann-valued quantities, which are naturally not amenable to computers. Fortunately, the fermionic part of the weighting is Gaussian in form, and the integrals over  $\psi$  and  $\overline{\psi}$  can be done analytically. The result involves a product of the determinant of each flavor Dirac operator  $M^{(f)} \equiv \gamma_{\mu} D_{\mu} + m^{(f)}$ , and can be written as

$$C_{ij}(t-t_0) = \frac{\int \mathcal{D}A \ e^{-S_G[A]} \prod_f \det(M^{(f)}[A]) \ \mathcal{F}(M^{-1})}{\int \mathcal{D}A' \ e^{-S_G[A']} \prod_f \det(M^{(f)}[A'])},$$
(2.9)

where  $S_G$  is the gauge action  $\frac{1}{2g^2} \operatorname{Tr}[F_{\mu\nu}F_{\mu\nu}]$ , and the function  $\mathcal{F}$  is some sum of products of  $M^{-1}$ , possibly involving one or more flavors  $M^{(f)}$ . The nature of these combinations of  $M^{-1}$  in  $\mathcal{F}$  is determined by Wick contraction of the quark fields in O and  $\overline{O}$  – each possible way of contracting all  $\overline{\psi}$  and  $\psi$  fields results in a term in the sum, and the products of  $M^{-1}$  within each term are determined by the indices on either side of the  $\psi - \overline{\psi}$  contraction. This rule for  $\mathcal{F}$  is seen most clearly by looking at a few specific examples of its use, as will be done in Sec. 2.3.2 and further in Ch. 4.

Eq. (2.9) is our starting point for numerical computation. In Sec. 2.3, we will look at how to actually calculate the above integral on a computer. The basic elements are a Markov chain of gauge field configurations generated by a Metropolis-Hastings-type algorithm [39, 40], and computation of the needed matrix inverses on each configuration. However before discussing these algorithms, we must demonstrate how the continuum quantities in Eq. (2.9) are introduced on the lattice.

#### 2.2 Discretization of the QCD Action

The discretization of the QCD action is not as simple as replacing derivatives with finite differences. There are some subtleties regarding the important symmetries of the Lagrangian, such as exact local gauge invariance, and chiral symmetry with zero quark masses. The latter symmetry is especially problematic; it is related to the fermion doubling problem [41], which predicts a profusion of unphysical states that emerge for lattice actions which respect chiral symmetry. Nielsen and Ninomiya [42] have shown that it is not possible to reproduce chiral symmetry without either accepting this multiplicity of states, or else violating other important properties of the action such as Hermiticity, locality and translational invariance. In Sec. 2.2.1, we will review our particular choices for dealing with these issues, and give a brief summary of other actions that address the issues in different ways.

While it is advantageous to maintain certain symmetries explicitly for finite spacing, this is not strictly required. Indeed, regardless of how the action is discretized, Lorentz invariance cannot be preserved, due to the restricted rotational symmetry of the lattice itself. The fundamental requirement on lattice discretizations is that they approach the right continuum limit as the spacing shrinks to zero. In that sense, lattice QCD can be thought of as a collection of all discrete theories that reduce to QCD in the continuum limit – that is, whose actions differ by terms that vanish as  $a \rightarrow 0$ .

There is a large class of terms which, being suppressed by powers of the lattice spacing, can be added to the lattice action without affecting the continuum limit. This strategy provides the basis for our solution of the fermion doubling problem, as we employ the so-called Wilson term in our fermion action, which vanishes with the spacing a. Also, we include similarly vanishing "improvement" terms which reduce the discretization errors for finite a, so as to approach the continuum limit faster, as suggested by Symanzik [43]. In Sec. 2.2.2, we discuss such improvement techniques, including the "clover" term [44], and we state the final form for the lattice action used in this work.

#### 2.2.1 Wilson Action

A hypercubic lattice is defined with lattice spacings a,

$$x_{\mu} = n_{\mu}a_{\mu} \quad \text{(no sum over } \mu\text{)},\tag{2.10}$$

with boundary conditions the same as those specified above; periodic in space, periodic in time for bosonic fields, and antiperiodic for fermionic fields. We choose the spatial directions to have a fixed  $a_1 = a_2 = a_3 = a_s$ , and a different spacing for the time direction  $a_4 = a_t$ . Anisotropic lattices offers better temporal resolution in order to extract masses from quickly-decaying temporal correlators [45]. In this work, we choose  $a_s \approx 0.12$  fm, and  $\xi \equiv a_s/a_t \approx 3.5$ . These are targets, rather than exact settings, to be measured after lattices have been generated; during gauge generation, anisotropy is implemented via the bare fermion anisotropy  $\nu$  and the bare gauge anisotropy  $\xi_0$ , parameters in the lattice Lagrangian which we will explain shortly. The tuning of these parameters, as well as more detail on gauge generation for this work, can be found in Ref. [46].

Lattice gauge fields  $U_{\mu}(x)$  are introduced in terms of the continuum gauge fields  $A_{\mu}$  via the gauge transporter G(x, y),

$$U_{\mu}(x) = G(x, x + \hat{\mu}), \qquad G(x, y) = \mathbf{P}e^{ig \int_{\mathcal{C}_{xy}} A_{\nu}(z)dz_{\nu}},$$
 (2.11)

where **P** indicates path-ordering. Any path C from x to y yields a properly-covariant G(x, y), but we choose the straight path linking site x to  $x + \hat{\mu}$ , and U are referred to as "gauge link" variables.

With gauge-covariant  $U_{\nu}(x)$ , one can create gauge-invariant 'plaquettes' as

$$P_{\mu\nu}(x) = \frac{1}{3} \text{ReTr} \big( U_{\mu}(x) U_{\nu}(x+\hat{\mu}) U_{\mu}^{\dagger}(x+\hat{\nu}) U_{\nu}^{\dagger}(x) \big), \qquad (2.12)$$

which in turn can be used to define the unimproved Wilson gauge action,

$$S_{G}^{W} = \frac{5\beta}{3\xi_{0}}\Omega_{s}^{P} + \frac{4\beta\xi_{0}}{3}\Omega_{t}^{P},$$
  
$$\Omega_{s}^{P} = \sum_{x,i(2.13)$$

for bare gauge anisotropy  $\xi_0$  and  $\beta = 2N_c/g = 6/g$  for bare coupling g. This discretized gauge action can be shown to approach the continuum  $S_G$  in the limit of vanishing  $a_{\mu}$ .

For the fermion action, we clearly need some discretization of the covariant derivative  $D_{\mu}$ . This is defined naturally in terms of the gauge link variables U, via

$$[\nabla_{\mu}]_{ax;by} = \frac{1}{2a_{\mu}} \Big[ [U_{\mu}]_{ab}(x)\delta_{x+\hat{\mu},y} - [U_{\mu}^{\dagger}]_{ab}(x-\hat{\mu})\delta_{x-\hat{\mu},y} \Big].$$
(2.14)

We can now formulate a "naïve" discretization of the fermion action  $S_F^{[naive]}$ , so called because it is gauge invariant and seems to mimic the continuum  $S_F$ , but leads to the fermion doubling problem (to be described momentarily). The naïve fermion action is

$$S_F^{[naive]} = \sum_{x,y,f} \overline{\psi}_{a\alpha}^{(f)}(x) \left[ m^{(f)} \delta_{ab} \delta_{\alpha\beta} \delta_{xy} + [\gamma_t]_{\alpha\beta} [\nabla_t]_{ax;by} + \frac{1}{\nu} \sum_{i=1}^3 [\gamma_i]_{\alpha\beta} [\nabla_i]_{ax;by} \right] \psi_{b\beta}^{(f)}(x),$$
(2.15)

where the bare fermion anisotropy  $\nu$  sets the spatial derivatives apart from temporal ones, and is chosen via a procedure to be outlined in Sec. 2.4.

To illustrate the fermion doubling problem, we consider the chiral limit  $m \to 0$ , and for simplicity, set  $\nu = 1$  and  $U_{\mu} = 1$  (inserting zero gauge field  $A_{\mu} = 0$  into Eq. (2.11) gives unit U). In that case, the Dirac matrix in Eq. (2.15) has a simple Fourier transform, and obeys

$$M_{[U,\nu=1]}(p|q) = \delta_{pq} \sum_{\mu} \frac{i}{a_{\mu}} \gamma_{\mu} \sin(p_{\mu}a_{\mu}), \qquad (2.16)$$

$$M_{[U,\nu=1]}^{-1}(p|q) = \delta_{pq} \frac{\sum_{\mu} \frac{i}{a_{\mu}} \gamma_{\mu} \sin(p_{\mu}a_{\mu})}{\sum_{\mu} \frac{1}{a_{\mu}^{2}} \sin(p_{\mu}a_{\mu})^{2}}.$$
(2.17)

This form clearly illustrates that instead of a single pole in the propagator, as expected in the continuum expressions with  $\sin(p) \rightarrow p$ , we now have *sixteen* poles – any of the four elements of  $p_{\mu}$  can be set to  $\pi/a_{\mu}$  while retaining a zero in the denominator of Eq. (2.17). The multiplicity of 16 comes from the possibility of two options (0 or  $\pi/a$ ) for each of four components of  $p_{\mu}$ . These unphysical poles are referred to as the fermion doublers.

Mathematically, these doublers result from the replacement of the derivative (Fourier transform  $\propto p$ ) with the finite difference (Fourier transform  $\propto \sin p$ ). From

a more physical perspective, fermion doubling is related to chiral symmetry. In a continuum theory with fermions, conservation of axial vector current (the Noether current associated with chiral rotation) is violated due to quantum fluctuations, as shown by Adler [47] and Bell and Jackiw [48]. In a lattice regulated theory, however, the existence of a classical symmetry does imply a conserved current [34]. Karsten and Smit [41] demonstrated that the above-mentioned continuum anomaly is canceled on the lattice by the anomaly of unphysical doublers. This deep connection makes it very difficult to address the issue of fermion doubling on the lattice. In fact, it can be shown [42] that no lattice discretization can simultaneously satisfy a) locality, b) chiral symmetry for  $m \to 0$ , c) have the proper continuum limit, and d) lack fermion doubling.

So while there are a variety of ways of dealing with doubling, all of them necessarily sacrifice one of more of the above favorable qualities. A short review of various options is given here, with only a brief discussion of some of the discretization options used in other work, then a more detailed description of the particular action discretization that will be used in this work (the Wilson discretization). The 'Staggered' fermion action [49–51] preserves a remnant of chiral symmetry on the lattice, at the expense of not entirely removing the degeneracy of fermion doublers. This formulation gives rise to four degenerate fermions, referred to as "tastes" as a complement to flavor, and these extra fermions complicate the extraction and identification of excited states. Furthermore, the staggered fermion action is non-local in time, and as a result leads to violations of the positivity of the lattice transfer matrix at small time separations. The lattice transfer matrix is the imaginary time evolution operator in terms of the lattice Hamiltonian,  $e^{-Ht}$ , and should have only positive eigenvalues for any Euclidean time separation  $t = na_t$ . A violation in the positivity of the transfer matrix at small t can cause unphysical aberrations in two-point functions at small time separations, and though these aberrations are presumably small, they can make the extraction of excited states very difficult [52].

The 'Domain-Wall' formulation [53, 54] goes further and preserves *exact* chiral symmetry on the lattice, but does so by introducing a fifth space-time dimension. Violations of chiral symmetry in the zero-quark mass limit are suppressed by a factor of  $\exp(-m_r L)$ , where L is the length of the fifth lattice dimension, and  $m_r$  is some residual mass. However the extra space-time dimension naturally leads to a large increase in computational difficulty, especially since the length of the fifth dimension

should be large enough to make  $\exp(-m_r L)$  small. The Domain-Wall action also leads to a transfer matrix which is not positive-definite.

A third lattice discretization, known as the 'Overlap' fermion action [55, 56], is similar to the Domain-Wall formulation except that the fifth dimension is explicitly integrated in the  $L \to \infty$  limit. The resulting four-dimensional lattice action preserves exact chiral symmetry at finite lattice spacing. However this four-dimensional lattice action still possesses many of the same difficulties as the Domain-Wall action – it is non-local, has a transfer matrix which is not positive-definite, and is computationally expensive.

The approach that we use in this work is one of the earliest, originally proposed by Wilson [44]. In this formulation, a term is introduced into the action which gives a large mass to the doublers, proportional to the inverse lattice spacing, effectively decoupling those spurious modes from the low-energy physics of interest. The additional term explicitly breaks chiral symmetry, and so at first glance might seem less desirable than other actions which preserve at least a remnant of chiral symmetry. However this symmetry breaking can be systematically reduced by the procedure of Symanzik improvement, as well as by the use of stout-smeared gauge link variables, both of which will be discussed shortly. The Wilson action is well-suited to our goal of excited state extraction since the transfer matrix can be shown to be positive definite, for appropriately-chosen smearing and improvement parameters. Also, many numerical tricks have been developed [57] which allow very efficient computations using the Wilson action.

The term that lifts the masses of the doublers is given in terms of a discretization of the covariant second derivative,

$$[\Delta_{\mu}]_{ax;by} = \frac{1}{2a_{\mu}^{2}} \Big[ [U_{\mu}]_{ab}(x)\delta_{x+\hat{\mu},y} + [U_{\mu}^{\dagger}]_{ab}(x-\hat{\mu})\delta_{x-\hat{\mu},y} - 2\delta_{ab}\delta_{xy} \Big],$$
(2.18)

and the (unimproved) anisotropic Wilson fermion action is given as

$$S_F^W = \sum_{x,y,f} \overline{\psi}_{a\alpha}^{(f)}(x) \left[ m^{(f)} \delta_{ab} \delta_{\alpha\beta} \delta_{xy} + [\gamma_t]_{\alpha\beta} [\nabla_t]_{ax;by} - r_t a_t [\Delta_t]_{ax;by} \delta_{\alpha\beta} \right. \\ \left. + \frac{1}{\nu} \sum_{i=1}^3 \left( [\gamma_i]_{\alpha\beta} [\nabla_i]_{ax;by} - r_s a_s [\Delta_i]_{ax;by} \delta_{\alpha\beta} \right) \right] \psi_{b\beta}^{(f)}(x), \qquad (2.19)$$

where the doubler mass terms are weighted by temporal and spatial Wilson parameters  $r_t$  and  $r_s$ .

#### 2.2.2 Action Improvement

The action we have constructed so far consists of the sum of Eqs. (2.13) and (2.19) for the gauge and fermion actions, respectively. This has the proper continuum limit as  $a_{\mu} \rightarrow 0$ , neglecting terms of order  $a_{\mu}^2$ . However, it is possible to improve upon this discretization to achieve a faster approach to continuum behavior, as suggested by Symanzik [58].

The basic program of improvement is easily illustrated in attempting to approximate a derivative by a symmetric finite difference,  $\partial \approx D_2 = [f(x+a) - f(x-a)]/2a$ . In the limit of small a, we can Taylor-expand that expression around x to obtain a series whose leading term is f'(x), as desired. The next term in the expression,  $[a^2/6]f'''(x)$ , vanishes in the continuum limit, but represents an unwanted contribution for finite a. To cancel that, we can consider another finite difference,  $D_4 = [f(x+2a) - f(x-2a)]/4a$ , which expands similarly except with a factor of  $2a^2/3$  in front of the third derivative. In order to achieve cancellation between the  $[a^2/6]f'''(x)$  in  $D_2$  and the  $[2a^2/3]f'''(x)$  in  $D_4$ , we sum those two finite differences with coefficients  $[4/3]D_2 - [1/3]D_4$  to arrive at a new approximation of the derivative whose leading correction is now  $\mathcal{O}(a^4)$ . This prescription for improvement relies on the convergence of the Taylor expansion, that is, that the  $\mathcal{O}(a^4)$  correction is smaller than the  $a^2$  term which was canceled out. Thus in lattice QCD, we expect this improvement program to be beneficial for smaller lattice spacings.

In order to improve the Wilson gauge action in Eq. (2.13), we can consider including  $2 \times 1$  loops  $R_{\mu\nu}(x)$ 

$$R_{\mu\nu}(x) = \frac{1}{3} \operatorname{ReTr} \Big[ U_{\mu}(x) U_{\mu}(x+\hat{\mu}) U_{\nu}(x+2\hat{\mu}) U_{\mu}^{\dagger}(x+\hat{\mu}+\hat{\nu}) U_{\mu}^{\dagger}(x+\hat{\nu}) U_{\nu}^{\dagger}(x) \Big], \quad (2.20)$$

along with the aforementioned  $1 \times 1$  plaquettes  $P_{\mu\nu}$ . The proper coefficients with which to add these loops (corresponding to the 4/3 and 1/3 in the simple example above) were worked out by Lüscher and Weisz [59, 60] as well as by Curci [61]. In general, such coefficients may receive radiative corrections, but in this case, tree-level perturbation theory has been shown [46] to be consistent with non-perturbatively tuned values. We defer a full expression until Eq. (2.27).

A similar improvement strategy can be applied to the Wilson fermion action, as demonstrated by Sheikholeslami and Wohlert [62]. The additional term is expressed in terms of the lattice field strength tensor  $F_{\mu\nu}(x)$  as estimated by an average of the four plaquettes surrounding the lattice point x;

$$[F_{\mu\nu}]_{ab}(x) = \frac{1}{8ia_{\mu}a_{\nu}} \Big[ [L_{\mu\nu}]_{ab}(x) - [L^{\dagger}_{\mu\nu}]_{ab}(x) \Big], \qquad (2.21)$$

$$[L_{\mu\nu}]_{ab}(x) = [U_{\mu}]_{ad}(x)[U_{\nu}]_{de}(x+\hat{\mu})[U_{\mu}^{\dagger}]_{ef}(x+\hat{\mu}-\hat{\nu})[U_{\nu}^{\dagger}]_{fb}(x)$$

$$+ [U_{\nu}]_{ad}(x)[U_{\mu}^{\dagger}]_{de}(x-\hat{\mu}+\hat{\nu})[U_{\nu}^{\dagger}]_{ef}(x-\hat{\mu})[U_{\mu}]_{fb}(x-\hat{\mu})$$

$$+ [U_{\mu}^{\dagger}]_{ad}(x-\hat{\mu})[U_{\nu}^{\dagger}]_{de}(x-\hat{\mu}-\hat{\nu})[U_{\mu}]_{ef}(x-\hat{\mu}-\hat{\nu})[U_{\nu}]_{fb}(x-\hat{\nu})$$

$$+ [U_{\nu}^{\dagger}]_{ad}(x-\hat{\nu})[U_{\mu}]_{de}(x-\hat{\nu})[U_{\nu}]_{ef}(x+\hat{\mu}+\hat{\nu})[U_{\mu}^{\dagger}]_{fb}(x).$$
(2.22)

The addition of this term to the action is referred to as 'clover' improvement, in reference to the arrangement of the four plaquettes in  $L_{\mu\nu}$ .

Another action improvement technique known as "tadpole improvement" was developed by Parisi [63] and Lepage and Mackenzie [64]. It was observed that the definition of the lattice gauge field  $U_{\mu}$  in Eq. (2.11), while setting up a desirable exact gauge invariance on the lattice, introduces extra vertices into the quark action – the leading term proportional to  $\overline{\psi}igA_{\mu}\psi$  is followed by many unwanted terms in the higher-order expansion of the exponential  $e^{ig\int_{C_{xy}}A_{\nu}(z)dz_{\nu}}$ . These are the so-called "tadpole" contributions. They can be reduced in mean field theory by scaling the gauge link variables  $U_{\mu}$  by a factor  $1/u_{\mu}$ , where  $u_{\mu} = \langle \frac{1}{3} \text{ReTr}(U_{\mu}) \rangle$ , since that expectation value deviates from unity only due to tadpole contributions [65]. Since these scaling factors ( $u_s$  and  $u_t$  for our anisotropic lattices) are then both action parameters and also observables, they must be tuned during gauge generation to yield self-consistent values, starting from a perturbative guess (in our case, starting from  $u_s = u_t = 1$  [46]).

The last form of improvement that we use is known as stout-link smearing, developed in Ref. [66]. As the name suggests, it effectively averages the behavior of the gauge fields over a larger area, eliminating ultraviolet fluctuations from the action. The stout-smeared links are then used in place of the usual gauge fields in the fermion action, and also in the observables which will be measured on the resulting ensemble. While other gauge-smearing smearing procedures are available [67], stout-link smearing is prevalent since it has the advantage of being fully analytic, so that it may be used with the HMC algorithm, to be described later.

Stout smearing is defined in terms of 'staples'

$$C_{\mu}[U] = \sum_{\nu \neq \mu} \rho_{\mu\nu} \Big( U_{\nu}(x) U_{\mu}(x+\hat{\nu}) U_{\nu}^{\dagger}(x+\hat{\mu}) + U_{\nu}^{\dagger}(x-\hat{\nu}) U_{\mu}(x-\hat{\nu}) U_{\nu}(x-\hat{\nu}+\hat{\mu}) \Big), \quad (2.23)$$

for real weighting factors  $\rho_{\mu\nu}$ . To preserve the positivity of the transfer matrix, it is necessary to set  $\rho_{\mu4} = \rho_{4\mu} = 0$  (no smearing in the time direction). Also, since the spatial directions of the lattice are assumed to be equivalent, it suffices to set the nonzero values of  $\rho_{ij}$  equal to a single value,  $\rho_{ij} = \rho = 0.14$  [46].

The smearing procedure is defined iteratively, where the original gauge field is  $U^{(0)}_{\mu}(x)$ , and each successive iteration  $U^{(n+1)}_{\mu}$  is given by

$$U_{\mu}^{(n+1)}(x) \equiv e^{iQ_{\mu}^{(n)}(x)}U_{\mu}^{(n)}(x), \qquad (2.24)$$

where

$$Q_{\mu}^{(n)}(x) \equiv \frac{i}{2} \Big( \Lambda_{\mu}^{(n)}(x)^{\dagger} - \Lambda_{\mu}^{(n)}(x) \Big) - \frac{i}{2N} \operatorname{Tr} \Big[ \Lambda_{\mu}^{(n)}(x)^{\dagger} - \Lambda_{\mu}^{(n)}(x) \Big], \qquad (2.25)$$

$$\Lambda_{\mu}^{(n)}(x) \equiv C_{\mu}[U^{(n)}] \ U_{\mu}^{(n)\dagger} \quad (\text{no sum over } \mu),$$
(2.26)

and N is simply that of the gauge group SU(N), so always 3 for this work. The number of smearing iterations  $N_{\rho}$  used in the fermion action is 2, such that our final smeared gauge field is  $\tilde{U}_{\mu} = U_{\mu}^{(2)}$ . The smeared spatial gauge links also necessitate the definition of a new tadpole improvement factor for those links,  $\tilde{u}_s$ . In order to implement a full improvement via gauge field smearing, it is also necessary to use these smeared fields in the interpolating operators, as will be described in Ch 3. The only difference in that case will be our choice of the number of iterations and the smearing constant,  $N_{\rho}$  and  $\rho$ , so we may allow some slight ambiguity in also labeling those smearing gauge fields  $\tilde{U}$ .

To conclude this section, we collect and review the terms in our chosen lattice action, the anisotropic gauge action with tree-level Symanzik improvement,

$$S_G = \frac{5\beta}{3\xi_0 u_s^4} \Omega_s^P + \frac{4\beta\xi_0}{3u_s^2 u_t^2} \Omega_t^P + \frac{\beta}{12\xi_0 u_s^6} \Omega_s^R + \frac{\beta\xi_0}{12u_s^4 u_t^2} \Omega_t^R$$
(2.27)

$$\Omega_s^X = \sum_{x,i < j} 1 - X_{ij}(x), \quad \Omega_t^X = \sum_{x,i} 1 - X_{it}(x)$$
(2.28)

where  $2 \times 1$  loops  $R_{\mu\nu}$  (defined in Eq. 2.20) correct discretization errors in the simpler action built from  $1 \times 1$  plaquettes  $P_{\mu\nu}$  (defined in Eq. 2.12), and a tadpole factor  $u_{\mu}$  divides each gauge link variable. The temporal  $R_{it}$  are arranged such that the length-2 side never extends in the time direction, in order to maintain positivity [46]. The leading discretization effects in this gauge action are  $\mathcal{O}(a_t^2, g^2 a_s^2, a_s^4)$ . For our fermion action, we use the anisotropic clover-improved Wilson action

$$S_{F} = \sum_{x,y,f} \overline{\psi}_{a\alpha}^{(f)}(x) \left[ m^{(f)} \delta_{ab} \delta_{\alpha\beta} \delta_{xy} + [\gamma_{t}]_{\alpha\beta} [\nabla_{t}]_{ax;by} - r_{t} a_{t} [\Delta_{t}]_{ax;by} \delta_{\alpha\beta} \right. \\ \left. + \frac{1}{\nu} \sum_{i=1}^{3} \left( [\gamma_{i}]_{\alpha\beta} [\nabla_{i}]_{ax;by} - r_{s} a_{s} [\Delta_{i}]_{ax;by} \delta_{\alpha\beta} \right)$$

$$\left. + \frac{c_{t} a_{s}}{2 \tilde{u}_{s} u_{t}^{2}} \sum_{i} [\sigma_{ti}]_{\alpha\beta} [F_{ti}]_{ab}(x) \delta_{xy} + \frac{c_{s} a_{s}}{2 \tilde{u}_{s}^{4}} \sum_{i < j} [\sigma_{ij}]_{\alpha\beta} [F_{ij}]_{ab}(x) \delta_{xy} \right] \psi_{b\beta}^{(f)}(x),$$

$$(2.29)$$

where  $\sigma_{\mu\nu} = \frac{1}{2}[\gamma_{\mu}, \gamma_{\nu}]$ , the clover field strength estimate  $F_{ij}$  is given in Eq. (2.21), and the symmetric covariant difference and curvature  $\nabla_{\mu}$  and  $\Delta_{\mu}$  are given in Eqs. (2.14) and (2.18), respectively. For the gauge link variables in F,  $\nabla$ , and  $\Delta$ , we use stoutsmeared variables  $\tilde{U}$  as described in Eq. (2.24). The clover improvement coefficients are determined via tree-level lattice perturbation theory to be  $c_s = 1$ ,  $c_t = \frac{1}{2}(1+\xi^{-1})$ . The Wilson coefficients that scale the doubler mass terms,  $r_s$  and  $r_t$ , are set to unity to one in order to maintain reflection positivity [68]. Lattice artifacts in the fermion action are of order  $\mathcal{O}(g^2a_s, g^2a_t, a_s^2, a_t^2)$ .

The bracketed quantity contracting  $\overline{\psi}$  and  $\psi$  in Eq. (2.29) is our Dirac matrix for a single flavor,  $M^{(f)}[U]$ , the inversion of which is a central challenge in computing hadron correlation functions. The basics of addressing this challenge will be reviewed in Sec. 2.3.2, while our improved inversion method will be introduced in Ch. 4. For the bare quark masses  $m^{(f)}$ , we consider the three lightest flavors  $\{u, d, s\}$ , with exact isospin symmetry  $m^{(u)} = m^{(d)}$  being a good approximation for our purposes. Our tuning of the bare quark masses, and of the bare fermion and gauge anisotropy coefficients  $\nu$  and  $\xi_0$ , will be discussed further in Sec. 2.4.

#### 2.3 Numerical Techniques

Having put together an efficient lattice regularization of QCD, we now delve into the details of how these expressions are actually calculated on a computer. We need to evaluate the integrals in Eq. (2.9), which due to our regularization, are now given in terms of a finite number of real integration variables  $U_{\mu}$  instead of the continuous  $A_{\mu}$ . The evaluation of this integral is difficult, requiring physical insight and innovative algorithms in order to achieve reliable results. Even after the integral is evaluated, the extraction of ground state and excited state energies from the two-point function is a non-trivial procedure, due to the mix of various exponential decays in Eq. (2.7). In the following sections, we review the algorithms that we use to extract actual, numerical energies from the lattice-regularized theory we have developed.

#### 2.3.1 Monte Carlo Integration

In order to efficiently evaluate the ratio of integrals in Eq. (2.9), we can re-interpret the equation as a weighted average of some quantity  $\mathcal{F}(M^{-1}[U])$ , with normalized weighting function w[U] given by

$$w[U] = \frac{e^{-S_G[U]} \prod_f \det(M^{(f)}[U])}{\int \mathcal{D}U' \ e^{-S_G[U']} \prod_f \det(M^{(f)}[U'])},$$
(2.30)

provided that w[U] is real and positive for all U, to admit a probability density interpretation. Under those conditions, we can then estimate Eq. (2.9) by picking some number  $N_{cfg}$  of gauge field configurations  $U^{[n]}$  with probability distribution w[U], and averaging  $\mathcal{F}(M^{-1}[U])$  over those fields,

$$C_{ij}(t-t_0) \approx \frac{1}{N_{cfg}} \sum_{n}^{N_{cfg}} \mathcal{F}(M^{-1}[U^{[n]}]).$$
 (2.31)

This is known as the Theorem of Monte-Carlo Integration. This type of integration proceeds with much greater accuracy than a naïve random sampling, since it preferentially explores the area of integration space that contributes most to the result.

The positivity of the weighting function w[U] is an important requirement, and we take a moment to examine this for our particular definitions of the gauge action  $S_G[U]$ and our Dirac matrix, given in Eqs. (2.27) and (2.29), respectively. The exponentials of the gauge action,  $e^{S_G[U]}$ , are clearly real and positive, so the remaining terms that one might worry about are the determinants of the Dirac matrix. The positivity of the degenerate-mass product det  $M^{(u)}$  det  $M^{(d)}$  can be proven for any Dirac operator that is  $\gamma_5$ -Hermitian, that is, which obeys

$$\gamma_5 M \gamma_5 = M^{\dagger}. \tag{2.32}$$

This property holds for most discretized Dirac operators [33], including the improved Wilson operator used in this work.<sup>3</sup> With this property in mind, we examine the characteristic polynomial of the Dirac matrix,  $P_M(\lambda)$ , the zeroes of which give the eigenvalues of the Dirac operator;

$$P_M(\lambda) = \det[M - \lambda \mathbf{1}] = \det[\gamma_5^2(M - \lambda \mathbf{1})] = \det[\gamma_5(M - \lambda \mathbf{1})\gamma_5]$$
  
= 
$$\det[M^{\dagger} - \lambda \mathbf{1}] = \det[M - \lambda^* \mathbf{1}]^* = P_M(\lambda^*)^*, \qquad (2.33)$$

where we have used  $\gamma_5$  Hermiticity and the fact that  $\gamma_5^2 = 1$  (more detail is in Ref. [33]). Eq. (2.33) shows that if  $\lambda$  is a zero of the characteristic polynomial, then  $\lambda^*$  is also a zero. Therefore, the eigenvalues of M are either real, or come in complex-conjugate pairs, so that any imaginary eigenvalues yield a real and positive contribution when multiplied with their conjugate, and any negative eigenvalues in  $M^{(u)}$  are squared by their corresponding eigenvalue in  $M^{(d)}$  (recall that we operate under the exact isospin approximation,  $m_u = m_d$ ). The positivity of det  $M^{(s)}$  is not

<sup>&</sup>lt;sup>3</sup> The property of  $\gamma_5$ -Hermiticity will also turn out to be convenient later in the calculation of quark propagators  $M^{-1}$ .

guaranteed analytically, but in practice, the strange quark mass is high enough that  $\det M^{(s)}$  is always found to be positive.

The task now turns to that of producing the set of gauge configurations  $U^{[n]}$ whose distribution over the space of all possible U is proportionally to the probability density w[U] in Eq. (2.30). This is done by setting up a Markov chain, each element of which is a gauge field U, and whose stationary-state distribution is w[U]. The transition probability of going from one gauge field U to another field U' at the next configuration in the Markov chain is denoted  $T(U' \leftarrow U)$ , and it must satisfy the following conditions: [31,69]

- 1. The transition probability T is normalized and positive; that is,  $T(U' \leftarrow U) \ge 0$ ,  $\int \mathcal{D}U'T(U' \leftarrow U) = 1$ , for all U, integrating over all possible U'
- 2. w[U] is its fixed-point distribution, that is, w[U] is carried into itself by the transition probability;  $\int \mathcal{D}Uw[U]T(U' \leftarrow U) = w[U']$ , and
- 3. The chain must *get* to this stationary distribution from any starting point, and not get "stuck"; in other words, it must be aperiodic (no closed loops in path space) and irreducible (nonzero probability of getting from any state to any other state, so all are in one communicating class).

A simple statement of such a transition rule, or 'update method', is given by the Metropolis-Hastings algorithm [39, 40]. This algorithm begins with some *proposal* density  $R(U' \leftarrow U)$ , the probability of proposing some field value U' while currently in field state U. It is important that, with repeated applications of R, the probability of arriving at any field U' is nonzero. If the probability of accepting that new field is set at

$$P_{accept}(U' \leftarrow U) = \min\left(1, \frac{R(U' \leftarrow U)w[U]}{R(U \leftarrow U')w[U']}\right),\tag{2.34}$$

then it can be proven [69] that the resulting Markov chain has a fixed-point distribution equal to w[U], and satisfies the three requirements above for the transition probability T. This process has the advantage that the normalization of the distribution function w is irrelevant, since it cancels in the top and bottom of Eq. (2.34). In a pure gauge theory without quarks, or in the so-called 'quenched' approximation<sup>4</sup> where the fermion determinants are set to one, the above Metropolis algorithm stands on its own as a fairly efficient method of exploring U-space. In those cases, the probability distribution can be expressed in terms of the *local* quantity  $S_G(x)$ . Thus, if a change is proposed to a single link variable  $U_{\mu}(x)$ , the update probability  $P_{accept}$  can be calculated quickly based only on a small cluster of sites surrounding x, as illustrated by Creutz [71,72] and others. A variety of local update algorithms are available which improve somewhat on the basic Metropolis scheme; a common choice is the heat bath algorithm [73,74] with overrelaxation steps [75].

When one includes the fermion determinants, however, the situation becomes more difficult. Due to the non-locality of w[U], intensive lattice-wide calculations are necessary in order to get  $P_{accept}$  even for a local change at one  $U_{\mu}(x)$ . Thus a local Metropolis step would take roughly D times as long as in the local case, where Dis the dimensionality of field space. To ameliorate this, one might suggest that the proposal density change a larger number of  $U_{\mu}(x)$  at once – however in that case, one runs into the problem that the acceptance probability drops, and movement in U-space is still slow.

The issue at stake is how to favor various directions of movement in U-space. In Metropolis-style updating, the random proposed steps serve to 'feel out' the gradient of the weight function w, so that downhill moves in w can be made more likely. With no analytic input for the form of the gradient, it must be computed (at least, statistically) by a series of D finite differences, stepping a bit in each direction  $\hat{e}_n$  and recomputing w to get  $\partial w[x_1, x_2, ..., x_D]/\partial x_n$ . For a local action, one can use the fact that

$$\frac{\partial w[x_1, x_2, \dots, x_D]}{\partial x_n} = \frac{\partial w_{loc}[x_n]}{\partial x_n}$$
(2.35)

to reduce the cost of that gradient estimation by a factor of about D. But Eq. (2.35) does not hold (by definition) for global actions, so the 'feeling out' of the gradient is vastly more expensive. Thus we need a more direct computation of  $\vec{\nabla}w$ .

The most prevalent global update method in use in lattice QCD is the Hybrid Monte-Carlo (HMC) algorithm [76]. For an even number of degenerate quarks, such

<sup>&</sup>lt;sup>4</sup> The quenched approximation [70] essentially neglects the effects of 'sea' quarks that are created and annihilated in pairs from the vacuum. This is an uncontrolled omission, accepted in the past simply due to the daunting expense of dynamic gauge generation.
as our  $m^{(u)} = m^{(d)}$ , this algorithm provides an efficient way of generating gauge configurations with full fermion dynamics. The HMC algorithm incorporates the weight function w[U] into a new "Hamiltonian", and allows access to the gradient  $\vec{\nabla}w$  as part of the force that bends classical paths under that Hamiltonian. These classical paths with non-local forces are computed numerically, leading to a process not unlike classical molecular dynamics simulations. The procedure must be modified slightly for the case of a single flavor, yielding the Rational Hybrid Monte-Carlo [77] (RHMC) method, which we use for the strange quark dynamics in this work.

The starting point for HMC is the introduction of a bosonic, complex-valued field  $\Phi_{a\alpha}(x)$  on each color, spin, and space-time. Referred to as the pseudo-fermion field [78], it is used to estimate the fermionic determinants det  $M^{(u)} = \det M^{(d)} = \det M^{(l)}$ , via

$$\det M^{(u)}[U] \det M^{(d)}[U] = (\det M^{(l)}[U])^2 = \int \mathcal{D}\Phi \exp\Big[\Phi^{\dagger} \big(M^{(l)\dagger}[U]M^{(l)}[U]\big)^{-1}\Phi\Big],$$
(2.36)

where we have again used the  $\gamma_5$ -Hermiticity of M, as given in Eq. (2.32). Replacing the determinants on the top and bottom of Eq. (2.9) with this expression, we are able to incorporate  $\Phi$  into an effective action

$$S_e[U,\Phi] = S_G[U] + \Phi^{\dagger} (M^{(l)\dagger}[U]M^{(l)}[U])^{-1}\Phi, \qquad (2.37)$$

with U and  $\Phi$  now comprising the set of fields to be sampled via Monte-Carlo integration. Before integrating though, we introduce one more field variable, a momentum  $\pi$  which is conjugate to U in the fictitious Hamiltonian

$$H[U,\pi] = \frac{1}{2}\pi^{\dagger}\pi + S_e[U,\Phi].$$
 (2.38)

Note that the Hamiltonian depends on  $\Phi$ , but as an external parameter rather than a dynamic variable with a conjugate momentum. The path integral is now cast in terms of  $\Phi$ , U,  $\pi$ ; neglecting the strange quark for the moment,

$$\frac{\int \mathcal{D}\Phi \ \mathcal{D}U \ \mathcal{D}\pi \ O_i(U)\overline{O}_j(U)e^{-H}}{\int \mathcal{D}\Phi \ \mathcal{D}U \ \mathcal{D}\pi \ e^{-H}}.$$
(2.39)

The extra integral over  $\pi$  does not affect the total quantity, merely introducing a factor of  $\int \mathcal{D}\pi e^{-\pi^{\dagger}\pi/2}$  on the top and the bottom. As before, we want to generate an ensemble of  $\Phi, U, \pi$  fields that follow the weight function, only now the effective weight is that of a classical partition function,

$$w[U, \Phi, \pi] = \frac{e^{-H}}{\int \mathcal{D}[\Phi, U, \pi] e^{-H}},$$
(2.40)

with Hamiltonian H as defined in Eq. (2.38).

In order to explore the space of  $[U, \Phi, \pi]$  with a properly-designed transition probability T, the HMC algorithm uses two different mechanisms; one for fixed-energy surfaces (constant H) and another for jumping between those surfaces. Jumps between different H are controlled by changes in  $\pi$  and  $\Phi$ , which happen by fairly straightforward Gaussian generation. Numerous methods exist to sample numbers from a normal distribution, such as the Box-Muller transform [79]. Generation of the  $\Phi$  field is only slightly more complicated since one must apply  $M[U]^{\dagger}$  to the Gaussian distribution of variance  $\frac{1}{2}$ , to pull from the transformed Gaussian distribution  $e^{\Phi^{\dagger}(M^{\dagger}M)^{-1}\Phi}$ . The exploration over fixed-energy surfaces (fixed H) is done via classical evolution with Hamilton's equations,

$$\dot{\pi} = -F = -\frac{\partial S}{\partial U}, \qquad \dot{U} = \pi,$$
(2.41)

where the dot indicates derivatives with fictitious 'time'  $\tau$ .

F is the "force" that allows for Monte Carlo movement in statistically favorable directions without 'testing' movements in other directions first. Clearly, the fermionic force term is not a trivial quantity, being the derivative with respect to U of the second term in Eq. (2.37). These classically-determined steps are preferable to Metropolis-style steps, since each classical trajectory results in significant, global movement of the Markov chain, rather than a random step which may be statistically unfavorable. HMC necessitates an analytic gauge smearing operator, so that the action is smoothly differentiable – thus the use of stout-link smearing. The HMC algorithm exploits the Liouville theorem of statistical mechanics, thereby allowing a global change in the fields with a small change in the action, which ensures a significant probability of acceptance [31, 80].

The integration in  $\tau$  is not done exactly, since it would be wasteful to move smoothly on a scale where the classical path is approximately linear. Instead, the evolution in Eq. (2.41) is approximated via a symplectic integration scheme, such as the second-order Omelyan integrator [81] used in this work. After integrating over some length of fictitious time  $\tau$ , a Metropolis accept/reject step is applied, with  $P_{accept}$ governed by the small incidental change in H. This accept-reject step ensures the condition of detailed balance.

To recap, an HMC update consists of the following major steps;

- 1. Generate a spacetime-color-spin field  $\eta$  filled with Gaussian noise of variance  $\frac{1}{2}$ , and apply  $M^{(l)\dagger}$  to get  $\Phi$ .
- 2. Generate a momentum field  $\pi$  from a Gaussian distribution  $e^{\pi^{\dagger}\pi/2}$ .
- 3. Numerically integrate the canonical equations of motion, Eq. (2.41), for some fixed time  $\tau$  to arrive at a new gauge field U'.
- 4. Accept this movement with a (high) probability given by Eq. (2.34).

The RHMC algorithm follows the same general plan of attack as the HMC, only with some modifications which allow for the treatment of one quark flavor at a time, rather than the two degenerate flavors u and d required by HMC. Another pseudofermion field  $\Phi^{(s)}$  must be introduced, which is used in a similar (but not identical) way as  $\Phi$  in Eq. (2.36); now,

$$|\det M^{(s)}| = \left(\det M^{(s)\dagger} \det M^{(s)}\right)^{\frac{1}{2}} = \int \mathcal{D}\Phi^{(s)}\Phi^{(s)\dagger} \left(M^{(s)\dagger}[U]M^{(s)}\right)^{\frac{1}{2}}\Phi^{(s)}$$
(2.42)

gives us an estimate of the strange quark determinant, so long as det  $M^{(s)} \ge 0$ . As mentioned above, the larger mass of the strange quark in comparison to the light uand d quarks ensures that this determinant is indeed positive, and negative modes are not a problem. The generation of fields  $\Phi^{(s)}$  from a  $\frac{1}{2}$ -variance  $\eta^{(s)}$  is now achieved through  $\Phi^{(s)} = (M^{(s)\dagger}M^{(s)})^{\frac{1}{4}}\eta^{(s)}$ . The necessary fourth root is achieved via a rational approximation, as described in Refs. [82,83]. From this point on the RHMC algorithm proceeds similarly to the HMC, though with an appropriate adjustment to the form of the fermionic force term.

A number of techniques are available that further streamline the HMC and RHMC algorithms. One technique beneficial to this work is multi-scale anisotropic molecular

dynamics [84]. This refinement of the classical-path integration uses a different time step for movement of the temporal gauge links versus those of the spatial gauge links. This is a natural generalization since those links are of physically different sizes, and the classical paths may be expected to have different characteristic scales in those dimensions. Specifically, since the temporal spacing is smaller than the spatial lattice spacing, the corresponding molecular dynamics forces, F, are stronger for  $U_t$ . A smaller step,  $\delta \tau_t < \delta \tau_s$ , facilitates good resolution in those faster-changing contours of the trajectory, without an unnecessarily small step in directions with less classical 'acceleration'.

Another strategy which aims to allow longer integration timescales in some directions is known as Hasenbusch preconditioning [85]. In this technique, the expensive light quark determinant is factored into a form which approximately separates the high and low modes of the Dirac operator,

$$|\det M^{(l)}|^2 = \det \left( M^{(l)\dagger} M^{(l)} + \mu^2 \right) \det \left( \frac{M^{(l)\dagger} M^{(l)}}{M^{(l)\dagger} M^{(l)} + \mu^2} \right).$$
(2.43)

The low modes  $(\lambda \ll \mu)$  show up predominantly in the second term, which becomes roughly  $\prod_{\lambda \ll \mu} \lambda^2 / \mu^2$ , while the first term is then roughly  $\mu^2$ . Then for the high-lying modes  $(\lambda \gg \mu)$ , the first term is roughly  $\prod_{\lambda \gg \mu} \lambda$  while the second term approaches unity. One can now approximate the two determinants by integration over two separate pseudofermion fields; a "heavy" field  $\Phi^{(l)[H]}$  corresponding to the first term in Eq. (2.43), and a new "light" field  $\Phi^{(l)[L]}$  corresponding to the second determinant. It turns out that fermionic forces in this arrangement are usually somewhat smoother, and it has been found [86] that the forces corresponding to  $\Phi^{(l)[L]}$  are considerably smaller than those for  $\Phi^{(l)[H]}$ , so that a larger integration timescale can be used for  $\Phi^{(l)[L]}$ . As in the multiple-timescale integration methods discussed above, this allows for a significant savings in update costs.

Even-odd preconditioning of the clover term [57] is used to further streamline the dynamic gauge generation in this work. Preconditioning is a general method in solving linear systems Mx = y, in which a non-singular R and L are chosen such that the equivalent set of equations

$$LMRx' = Ly, \quad Rx' = x \tag{2.44}$$

is less computationally expensive than the original equation. In our case, a good choice of L and R can be found by noting that the clover Wilson Dirac operator M can be blocked amongst even (e) and odd (o) sites on a 'checkerboard' pattern on the lattice, as

$$M = \begin{pmatrix} M_{ee} & M_{eo} \\ M_{oe} & M_{oo} \end{pmatrix}.$$
 (2.45)

The blocks  $M_{ee}$  and  $M_{oo}$  include the diagonal mass term as well as a Pauli-matrix term for the O(a) improved action, while  $M_{eo}$  includes all terms that hop between even and odd sites. Since  $M_{ee}$  and  $M_{oo}$  do not couple different lattice sites, they are easily invertible. These simple inverses inspire the choice

$$L = \begin{pmatrix} 1 & -M_{eo}M_{oo}^{-1} \\ 0 & 1 \end{pmatrix}, \qquad R = \begin{pmatrix} 1 & 0 \\ -M_{oo}^{-1}M_{oe} & 1 \end{pmatrix},$$
(2.46)

which leads to a diagonal LMRx' = y equation, with

$$LMR = \begin{pmatrix} \hat{M} & 0\\ 0 & M_{oo} \end{pmatrix}, \qquad \hat{M} = M_{ee} - M_{eo} M_{oo}^{-1} M_{oe}.$$
(2.47)

The condition number (the ratio of largest to smallest eigenvalues) of  $\hat{M}$  is typically less than half that of M itself, and the iterative solution of this diagonalized linear system is therefore much faster than the original system. The actual details of iterative inversion, typically based on the conjugate gradient (CG) method, will be discussed in the following section.

One other important technique known as *low-eigenmode deflation* can be used to aid in the HMC and RHMC Dirac matrix inversions. This technique recognizes the physical significance, as well as technical difficulty, of the low-eigenvalue modes of the Dirac operator. The density of these low modes is expected to increase proportionally to the volume as well as to the inverse quark mass [87]. In order to handle these important low modes, a relatively expensive step is taken to project them out, which allows the rest of the orthogonal space (the 'deflated' operator) to be solved much more quickly. Further detail regarding low-mode deflation can be found in Refs. [88, 89].

#### 2.3.2 Standard Dirac Matrix Inversion

We have explained how the path integral in Eq. (2.6) can be discretized, and we have shown how that discretized integral can be written in terms of a Monte-Carlo weighting (Eq. (2.30)) and a function  $\mathcal{F}(M^{-1}[U])$  to be evaluated on gauge configurations drawn from that weighting. This section will focus on the standard techniques for evaluating  $M^{-1}$  itself, and thus  $\mathcal{F}(M^{-1})$ . We have seen that some inversion techniques are already necessary in the gauge generation via HMC and RHMC, and we alluded to the use of the conjugate gradient (CG) iterative solver for this purpose. CG and related algorithms (especially 'biconjugate gradient') are also used in the calculation of  $\mathcal{F}$ , and will be explained briefly here; more detail on these linear solvers can be found in Ref. [90].

The function  $\mathcal{F}$  may involve the Dirac matrix of one or more different flavors, technically  $\mathcal{F}(M^{(u)-1}, M^{(d)-1}, M^{(s)-1})$ , but as the evaluation of each of those flavor contributions to  $\mathcal{F}$  proceeds in the same fashion, we drop the flavor index in this section. In fact, the crux of the problem is largely independent of the form of Mitself, and is basically that of inverting some extremely large, semi-diagonal matrix. The dimension of M is large enough that even storing all of the elements of M or  $M^{-1}$  is impractical. For example, some of the primary lattices used in this work are  $24^3 \times 128$  in space-time, with complex-valued data on three colors and four Dirac spins for each site, which gives  $D_M = 24^3 \times 128 \times 3 \times 4 \approx 2 \times 10^7$ . A vector in this space occupies a tolerable 400 megabytes; a matrix, on the other hand, demands about 100 petabytes.

Fortunately, due to the sparseness of M, we are able to apply M to a vector somewhat efficiently. The conjugate gradient algorithm employs that ability iteratively to solve linear systems  $M\phi = \rho$  for any chosen  $\rho$ . Thus a column of  $M^{-1}$  can be found through solving, for example,

$$M_{a\alpha;b\beta}(x|y)\phi_{b\beta}(y) = \rho_{a\alpha}(x), \quad \rho_{a\alpha}(x) = \delta_{a,2}\delta_{\alpha3}\delta_{x_0,45}\delta_{x_1,4}\delta_{x_2,6}\delta_{x_3,10}$$
(2.48)

to get the column of  $M^{-1}$ 

$$\phi_{b\beta}(y) = M_{b\beta;23}^{-1} \big( y, (45, 4, 6, 10) \big), \tag{2.49}$$

which is the quark propagator going from color 2, spin 3, time 45, and spatial point  $\vec{x} = [4, 6, 10]$  to all other points on the lattice. This basic scenario is known as the 'point-to-all' method, since the propagator is calculated for one source point to all sink points. One solution of an  $M\phi = \rho$  equation is commonly referred to as an 'inversion', though of course it does not lead to a full  $M^{-1}$ , only one column thereof.

The solution of a linear system  $M\phi = \rho$  can be calculated using the conjugate gradient method for some Hermitian and positive-definite M, or using a variant called biconjugate gradient for non-Hermitian M. The conjugate gradient method [90, 91] proceeds by minimizing the quadratic form

$$f(x) = \frac{1}{2}x^{\dagger}Mx - \rho^{\dagger}x,$$
 (2.50)

by taking a finite number of steps  $x^{(n)} \to x^{(n+1)}$ . The step rule has a particularly simple format if one defines a space with the metric  $\langle x|y\rangle_M = x^{\dagger}My$ , with corresponding definitions of M-orthogonality and M-projection. One builds a set of M-orthogonal search directions  $\hat{d}^{(n)}$ , and the step can be expressed as the M-projection of the error vector  $x - x^{(n)}$  onto the search direction  $d^{(n)}$ . The search directions are chosen conveniently via the residual vectors  $Mx^{(n)} - \rho$ , and a solution with any desired residual norm  $|x - x^{(n)}| < \epsilon$  can be efficiently found.

The conjugate gradient method relies on the complete concavity of the quadratic form 2.50, moving downhill somewhat similarly to the 'Steepest Descent' method. This prescription is only guaranteed for Hermitian, positive-definite M; in other cases, f(x) may have saddle points or may be convex in some directions, leading to a diverging iteration for  $\phi$ . The actual Dirac matrix, as we have discussed, is *not* Hermitian, but since  $\gamma_5$ -Hermiticity guarantees that  $M^{\dagger}M$  is Hermitian, we can solve the system  $M^{\dagger}M\phi = M^{\dagger}\rho$ . Alternately, we can try applying a variant of CG known as biconjugate gradient (BiCG), which proceeds via two separate iterators acting in parallel to directly solve the linear system  $M\phi = \rho$  for non-Hermitian M. However BiCG is not guaranteed to converge, and the results must be tested by some measure of the norm of the residual vector  $M\phi - \rho$ , and if that proves higher than some numerical tolerance, the slower CG system must be solved. A significant speedup in the CG and BiCG algorithms can be achieved through the use of Chebyschev acceleration and mixed-precision arithmetic [92].

In general, many linear solutions are necessary in order to calculate  $\mathcal{F}$ , so that in

the point-to-all method, the computation scales with the number of *columns* needed from  $M^{-1}$ . This is an important feature of the iterative matrix inversion methods used in lattice QCD; it is not the number of elements, but the number of columns needed that matters, since one solution of  $M\phi = \rho$  automatically gives you a full column of  $M^{-1}$ . Equivalently there is no way<sup>5</sup> to get a single element of  $M^{-1}$  without also consequently calculating the rest of the elements in that column.

Symmetries of the theory, such as translational invariance, can sometimes greatly reduce the number of such columns needed, but these tricks are not applicable in cases such as multi-hadron and isoscalar meson calculations. These cases are the special target of the new Stochastic LapH inversion method we have developed, a description of which is deferred until Ch. 4. For now, we take a moment to examine the symmetries that allow point-to-all to work for single baryon and isovector mesons, and why those fail for other situations.

In order to understand these difficulties, we introduce a basic form for baryon and meson operators, simpler than the operators we eventually use, but sufficient to illustrate the inversion issues we discuss here. For three quarks, a gauge-invariant, color singlet form is constructed as

$$O_B(\mathbf{p}_0, t_0) = \sum_{\mathbf{x}_0} e^{i\mathbf{p}_0 \cdot \mathbf{x}_0} \varepsilon_{a_0 b_0 c_0} \overline{\psi}_{a_0 \alpha_0}^{(u)}(\mathbf{x}_0, t_0) \overline{\psi}_{b_0 \beta_0}^{(d)}(\mathbf{x}_0, t_0) \overline{\psi}_{c_0 \gamma_0}^{(s)}(\mathbf{x}_0, t_0)$$
$$\overline{O}_B(\mathbf{p}, t) = \sum_{\mathbf{x}} e^{-i\mathbf{p} \cdot \mathbf{x}} \varepsilon_{abc} \psi_{c\gamma}^{(s)}(\mathbf{x}, t) \psi_{b\beta}^{(d)}(\mathbf{x}, t) \psi_{a\alpha}^{(u)}(\mathbf{x}, t), \qquad (2.51)$$

for the source (creation) and sink (annihilation) operators on times t and  $t_0$ . Indices a, b, and c represent color, greek indices represent Dirac spin,  $\psi$  and  $\overline{\psi}$  are the Grassmann fields defined on each lattice site, and  $\varepsilon_{abc}$  is the Levi-Civita tensor. The Fourier sums give each hadron operator a well-defined momentum **p**. In practice, our operators involve a sum over such terms with different coefficients for each spin combination  $\alpha\beta\gamma$ , and involve quark fields at different spatial sites, and different flavors. Furthermore, we eventually will replace simple quark fields with *smeared* quark fields, which couple less to unwanted high-energy modes of the theory – all of

<sup>&</sup>lt;sup>5</sup> Using  $\overline{\gamma_5}$ -Hermiticity, one could also conceivably calculate full rows of  $M^{-1}$  at a time, rather than full columns. There is little reason for this, though, since it would essentially amount to calculating the correlator with a fixed  $t_{final}$  and varying  $t_0$ , which should yield the same results (on average) as the usual two-point function for fixed  $t_0$ .

these complications are deferred until Ch. 3. For now, the operator in Eq. (2.51) will suffice to illustrate a key point about Dirac matrix inversion expense.

If we are interested in a single-baryon correlator, we insert these operators for  $O_B$ and  $\overline{O}_B$  in the path integral Eq. (2.6), which results in the product of Dirac matrix inverses

$$\mathcal{F}(M^{-1}) = \sum_{\mathbf{x}_0, \mathbf{x}} e^{i\mathbf{p}_0 \cdot \mathbf{x}_0} e^{-i\mathbf{p} \cdot \mathbf{x}} \varepsilon_{a_0 b_0 c_0} \varepsilon_{abc} \times M^{(u)-1}_{a\alpha; a_0 \alpha_0}(\mathbf{x}, t | \mathbf{x}_0, t_0) M^{(d)-1}_{b\beta; b_0 \beta_0}(\mathbf{x}, t | \mathbf{x}_0, t_0) M^{(s)-1}_{c\gamma; c_0 \gamma_0}(\mathbf{x}, t | \mathbf{x}_0, t_0)$$
(2.52)

which must be evaluated on each gauge configuration. As discussed earlier, this form for  $\mathcal{F}$  is obtained by contracting each like-flavor  $\psi$  and  $\overline{\psi}$  field to get a factor of  $M^{-1}$ with the same indices, as prescribed by Wick's theorem.

Eq. (2.52) seems to require elements from all columns of  $M^{-1}$ , but in fact the value of either  $\mathbf{x}$  or  $\mathbf{x}_0$  can be fixed; a momentum-fixing sum is not strictly necessary on both times since conservation of momentum will prevent states from mixing for  $\mathbf{p} \neq \mathbf{p}_0$ . The convenient choice is then to leave off the sum over  $\mathbf{x}_0$ , and arbitrarily pick a single value for  $\mathbf{x}_0$  and  $t_0$ . Thus, momentum conservation allows the calculation to proceed using only a few spatial and temporal columns of  $M^{-1}$ ; different columns are still needed for the four source spins and three colors on the chosen  $\mathbf{x}_0$ , for a total of twelve inversions. A few different  $\mathbf{x}_0$  and  $t_0$  can be chosen to increase statistics, if the computation time is available.

Another shortcut is possible for correlators involving only a single isovector or isodoublet meson ( $\pi$  or K), using the conservation of momentum as well as the property of  $\gamma_5$ -Hermiticity. A simple gauge-invariant, color-singlet isovector meson can be created and destroyed, respectively, by

$$\overline{O}_{M}(\mathbf{p}_{0}) = \sum_{\mathbf{x}_{0}} e^{i\mathbf{p}_{0}\cdot\mathbf{x}_{0}} \overline{\psi}_{a_{0}\alpha_{0}}^{(u)}(\mathbf{x}_{0}, t_{0})\psi_{a_{0}\beta_{0}}^{(d)}(\mathbf{x}_{0}, t_{0}),$$
$$O_{M}(\mathbf{p}) = \sum_{\mathbf{x}} e^{-i\mathbf{p}\cdot\mathbf{x}} \overline{\psi}_{a\alpha}^{(d)}(\mathbf{x}, t_{0})\psi_{b\beta}^{(u)}(\mathbf{x}, t_{0}).$$
(2.53)

With these operators in the two-point function, the function  $\mathcal{F}$  after integrating out the fermion fields is

$$\mathcal{F}(M^{-1}) = -\sum_{\mathbf{x}_0, \mathbf{x}} e^{i\mathbf{p}_0 \cdot \mathbf{x}_0} e^{-i\mathbf{p} \cdot \mathbf{x}} M_{b\beta; a_0 \alpha_0}^{(u)-1}(\mathbf{x}, t | \mathbf{x}_0, t_0) M_{b_0 \beta_0; a\alpha}^{(d)-1}(\mathbf{x}_0, t_0 | \mathbf{x}, t), \qquad (2.54)$$

where the negative sign arises from an odd number of Grassmann commutations.

It is not immediately clear why fixing a single  $\mathbf{x}_0$  in Eq. (2.54) would reduce the number of inversions needed, since the second factor of  $M^{(d)-1}$  has sink indices on the right and would still involve all columns of  $M^{-1}$ . Fortunately,  $\gamma_5$ -Hermiticity allows us to rewrite that backwards-propagating quark via

$$M_{b_0\beta_0;a\alpha}^{(d)-1}(\mathbf{x}_0, t_0|\mathbf{x}, t) = [\gamma_5]_{\beta_0\beta_0'} M_{a\alpha';b_0\beta_0'}^{(d)-1*}(\mathbf{x}, t|\mathbf{x}_0, t_0) [\gamma_5]_{\alpha'\alpha}.$$
 (2.55)

Using this identity, we can then calculate the isovector meson correlator with the same ease as the above baryon correlator, restricting the sum to a single  $\mathbf{x}_0$ .

Multi-hadron correlators are much more difficult to calculate in the point-to-all method. This stems from the fact that the different hadrons should each have a fixed momentum in order to generate a well-defined total momentum, such as a zeromomentum two-baryon operator

$$O_{BB} = O_{B,1}(\mathbf{p})O_{B,2}(-\mathbf{p})$$
  
=  $\sum_{\mathbf{x}_1, \mathbf{x}_2} e^{-i\mathbf{p}\cdot\mathbf{x}_1} e^{i\mathbf{p}\cdot\mathbf{x}_2} \varepsilon_{abc} \varepsilon_{def} \psi_{c\gamma}^{(s)}(\mathbf{x}_1, t) \psi_{b\beta}^{(d)}(\mathbf{x}_1, t) \psi_{a\alpha}^{(u)}(\mathbf{x}_1, t)$   
 $\times \psi_{d\gamma'}^{(s)}(\mathbf{x}_2, t) \psi_{e\beta'}^{(d)}(\mathbf{x}_2, t) \psi_{f\alpha'}^{(u)}(\mathbf{x}_2, t).$  (2.56)

With two different positions  $\mathbf{x}_1$  and  $\mathbf{x}_2$ , momentum conservation can serve to fix one, but not the other<sup>6</sup>. Therefore, the multi-hadron correlator requires quark propagators from all points on the source time to all spatial points on the sink time – that is, one needs  $M^{-1}$  elements from all columns with time index  $t_0$ , rather than just columns with a single  $\mathbf{x}_0, t_0$ . This fact is not restricted to two-baryon operators, but also includes two-meson or meson-baryon operators, for example.

Isoscalar meson correlators encounter a similar problem. These flavor-singlet op-

 $<sup>^{6}</sup>$ Alternately, one can place both hadrons at the same point, and not worry about assigning momenta to each hadron separately. This lessens the number of inversions necessary, but leads to other issues – see discussion in Sec. 3.3.1.

erators take a form such as

$$\overline{O}_{M}(\mathbf{p}_{0}) = \sum_{\mathbf{x}_{0}} e^{i\mathbf{p}_{0}\cdot\mathbf{x}_{0}} \overline{\psi}_{a_{0}\alpha_{0}}^{(u)}(\mathbf{x}_{0}, t_{0})\psi_{a_{0}\beta_{0}}^{(u)}(\mathbf{x}_{0}, t_{0}),$$
$$O_{M}(\mathbf{p}) = \sum_{\mathbf{x}} e^{-i\mathbf{p}\cdot\mathbf{x}} \overline{\psi}_{a\alpha}^{(u)}(\mathbf{x}, t_{0})\psi_{b\beta}^{(u)}(\mathbf{x}, t_{0}).$$
(2.57)

The actual isoscalar mesons we use may also include terms with flavors  $\overline{\psi}^{(d)}\psi^{(d)}$  or  $\overline{\psi}^{(s)}\psi^{(s)}$ , to be discussed in the following chapter. But the salient difference between this and the isovector correlator is that the two quarks within the meson can now be Wick-contracted with each other during integration of the fermion fields. The different-time contraction pattern is still possible as well, so that  $\mathcal{F}(M^{-1})$  now has two terms,

$$\mathcal{F}(M^{-1}) = \sum_{\mathbf{x}_{0},\mathbf{x}} e^{i\mathbf{p}_{0}\cdot\mathbf{x}_{0}} e^{-i\mathbf{p}\cdot\mathbf{x}} M_{a\beta;a\alpha}^{(u)-1}(\mathbf{x},t|\mathbf{x},t) M_{a_{0},\beta_{0};a_{0}\alpha_{0}}^{(u)-1}(\mathbf{x}_{0},t_{0}|\mathbf{x}_{0},t_{0}) - \sum_{\mathbf{x}_{0},\mathbf{x}} e^{i\mathbf{p}_{0}\cdot\mathbf{x}_{0}} e^{-i\mathbf{p}\cdot\mathbf{x}} M_{a\beta;a_{0}\alpha_{0}}^{(u)-1}(\mathbf{x},t|\mathbf{x}_{0},t_{0}) M_{a_{0},\beta_{0};a\alpha}^{(u)-1}(\mathbf{x}_{0},t_{0}|\mathbf{x},t).$$
(2.58)

The second term in Eq. (2.58), the 'connected piece', is identical to the isovector meson correlator. The first term, the 'disconnected piece', is what makes isoscalar mesons more difficult; it requires quark lines involving every diagonal element of  $M^{-1}$ on the sink time, each of which demands a new inversion. Since we are interested in a large number of sink times in the correlator, that amounts to a many-fold increase in the amount of inversions needed. The two possible Wick combinations are shown schematically in Fig. (2.1). Later on we will expand on this diagrammatic representation with further labels indicating how the contractions of meson sinks and sources are to be estimated stochastically.

In the past, this disconnected diagram has often been neglected in lattice QCD calculations simply due to difficulty. Yet physical information is contained in this disconnected term, which accounts roughly for the pair production and annihilation of 'sea quarks', an effect accurately modeled by dynamic gauge configurations (those which include the weight of the fermion determinant). In order to access this physics, the *Stochastic LapH* method enables many different quark lines to be estimated with a



Figure 2.1: Shown above are diagrams corresponding to the two Wick contractions of a single-meson to single-meson correlator, as given in Eq. (2.58). The lines represent quark propagators  $M^{-1}$ , whereas the boxes indicate meson operators, including coefficients  $c_{\alpha\beta}$  and momentum sums. The top dot of the meson corresponds to the antiquark, which (before integration of fermion fields) is a  $\psi$  on the source and a  $\chi = \overline{\psi} \gamma_4$  on the sink. In all such diagrams, we hold to the convention that the source time  $t_0$  is on the right, and the sink time t is on the left.

single inversion, without sacrificing accuracy in the final correlator. This new method and some applications thereof will be shown in Chs. 4 and 5.

### 2.4 Tuning and Setting the Scale

There are a number of parameters in our action that must be carefully set. Masses and energies occur only in terms of the lattice spacings  $a_s$  and  $a_t$ . The physical lattice spacings can be inferred after the ensemble of gauge configurations is generated, by looking at some physical observables and choosing a renormalization scheme. We now review how such parameters are determined, and specify their values for the action used in this work; further detail is given in Refs. [46,93].

The basic idea of non-perturbative tuning is to repeat a simulation many times, dialing the different bare parameters to achieve some values for a set of physical observables. This involves repeating the expensive process of gauge generation, so it would seem unrealistic at first glance. However one can make use of the Schrödingerfunction formalism [94] to perform some tuning in an easier regime, then relate those simpler simulation parameters to those on the desired lattices. The 'easier regime' in this work consists of a smaller lattice size  $(12^3 \times 32)$  and a carefully-designed set of boundary conditions in the t and z directions which lift the low modes of the Dirac operator, making inversion much more tractable and reducing autocorrelation time for the molecular dynamics updates [46].

With this technology, each bare parameter can be paired with some physical observable, and the bare parameter can be tuned until the physical observable matches its desired value. For the bare gauge anisotropy  $\xi_0$ , we tune to achieve

$$\frac{R_{ss}(x,y)}{R_{st}(x,\xi y)} = 1,$$
(2.59)

where  $\xi$  is the desired renormalized anisotropy and the Wilson loop ratio R is given by

$$R_{\mu\nu}(x,y) \equiv \frac{\langle 0|\text{Tr } \mathcal{C}(x_{\mu}, x_{\nu})|0\rangle}{\langle 0|\text{Tr } \mathcal{C}(x_{\mu}+1, x_{\nu})|0\rangle},$$
(2.60)

for some gauge field product  $C_{\mu\nu}$  around a rectangle of dimensions  $x_{\mu} \times x_{\nu}$  in the  $\hat{\mu}, \hat{\nu}$ plane. The condition in Eq. (2.59) essentially stipulates that the gauge field strengths in all lattice directions are equal on average. In order to achieve that equality with a renormalized anisotropy  $\xi \approx 3.5$ , we found that a bare value of  $\xi_0 = 4.3$  was needed.

The fermion anisotropy  $\nu$  is tuned using the dispersion relation

$$a_t E(\vec{p}) = \sqrt{a_t^2 m^2 + \xi^{-2} a_s^2 |\vec{p}|^2}$$
(2.61)

for the  $\pi$  and  $\rho$  isovector mesons. This led to a value of  $\nu = 3.4$  for our simulations. These values for the fermion and gauge anisotropies were found to be relatively independent of the bare quark masses.

The quark masses themselves were tuned to reproduce the physical values of

$$s_{\Omega} = \frac{9(m_K^2 - m_{\pi}^2)}{4m_{\Omega}},$$
  
$$l_{\Omega} = \frac{9m_{\pi}^2}{4m_{\Omega}^2},$$
 (2.62)

for the kaon and omega baryon masses  $m_K$  and  $m_{\Omega}$ , and pion mass  $m_{\pi}$ . The main simulations in this work are done on  $24^3 \times 128$  lattices at two different pion masses, tuned for  $m_{\pi} \approx 390$  MeV on one ensemble and  $m_{\pi} \approx 240$  MeV on the other. We later refer to these as simply the  $24^3(390)$  ensemble and  $24^3(240)$  ensembles, respectively. While significantly heavier than the physical pion, these masses represent the lower range of what is feasible with a Wilson action discretization on our lattice sizes. Lighter quark masses lead to a very large condition number on the Dirac matrix, making its inversion extremely costly. The  $m_{\pi} \approx 240$  MeV is at the lower end of what is feasible given computational resource restrictions, and having another ensemble with heavier  $m_{\pi}$  provides some indication of how lattice observables may depend on the pion mass<sup>7</sup>.

For each of our ensembles, the strange quark bare mass is set at  $m_s = -0.0743$ , while the bare light quark masses are set at  $m_l = -0.0840$  for the heavier pion ensemble, and  $m_l = -0.0860$  for the lighter pion ensemble, in units of the inverse temporal lattice spacing. Some preliminary work (such as operator selection tests, to be discussed in the following chapter) has been done on smaller  $16^3 \times 128$  lattices with the heavier  $m_l = -0.0840$  light quark mass. These bare mass parameters can

<sup>&</sup>lt;sup>7</sup>Some predictions of how different observables may vary with the pion mass can be obtained via chiral perturbation theory [95], though simulations at various quark masses must still be performed in order to verify and fix unknown constants in these expected behaviors.

Label	$\operatorname{Size}(L^3 \times T)$	Light Quark $m_l$	$N_{cfgs}$
$16^{3}$	$16^{3} \times 128$	-0.0840	100
$20^{3}$	$20^3 \times 128$	-0.0840	100
$24^3(390)$	$24^3 \times 128$	-0.0840	551
$24^{3}(240)$	$24^3 \times 128$	-0.0860	584
$32^{3}$	$32^3 \times 256$	-0.0860	347

Table 2.1: Gauge configurations used in this work, with  $N_f = 2 + 1$  clover-improved Wilson fermions, a tree-level Lüscher-Weisz gauge action, anisotropy  $\xi \approx 3.5$ . Each ensemble has strange quark mass -0.0743, and a spatial lattice spacing of roughly  $a_s \approx$ 0.12 fm. The labels distinguishing the two 24<sup>3</sup> ensembles, 24<sup>3</sup>(390) and 24<sup>3</sup>(240), are by the approximate pion masses in MeV. The smaller 16<sup>3</sup> and 20<sup>3</sup> ensembles are here used for testing and operator selection purposes only.

be negative due to the Wilson term in the action, since  $m\overline{\psi}\psi$  is not the only nonchiral term in the Lagrangian, and additive mass renormalization is therefore possible. A summary of the gauge configurations used in this work are given in Table 2.1, along with short labels which we use later in referring to those ensembles. Gauge configurations were generated using the CHROMA software suite for lattice QCD [96].

Once the bare parameters are set and a Monte Carlo ensemble is generated, there are a number of ways to obtain an actual value for the lattice spacing. One scheme is to use the physical  $\Omega$  baryon mass to set the scale, directly choosing  $a_t^{-1} \equiv \lambda_{\Omega}/m_{\Omega,phys}$ , where  $\lambda_{\Omega}$  is the measured decay of the  $\Omega$  correlator on the lattice (in the next section, we discus methods to make sure this decay constant is reliably extracted from the data). Another prescription is to extrapolate  $m_{\Omega}$  to the physical value of  $m_{\pi}/m_{\Omega}$ , then set  $a_t$  based on the extrapolated value. These two methods yield similar results for our lattice spacing. Mass ratios also yield smaller statistical errors than individual mass measurements, since different hadron masses often fluctuate together between different gauge configurations. In this work, we will work with ratios with respect to the ground state nucleon mass.

#### 2.5 Extracting Energies from Correlators

Once Monte-Carlo estimates of the temporal correlation functions have been obtained, the task becomes that of extracting the amplitudes and decay constants from these functions. The decay constants are the energies, in units of  $a_t^{-1}$ , of the stationary states in the theory, and the amplitudes contain information about the overlap onto those states of the operators used, as evident from Eq. (2.7). Operators can be constructed using group theoretical projections such that we select states of certain quantum numbers to excite from the vacuum. This has the effect of reducing the number of non-zero overlaps that must be distinguished in a given correlation function, but since many states may have the same quantum numbers, there are still many exponential decays to identify.

For the lowest energy state excited by a given operator, we can rely on the fact that its decay in time is slower than the rest of the contributions. Thus the behavior of any correlation function at large t should be a single exponential decay, and we can fit this region to obtain the ground state energy. Fits should be done by minimizing a *correlated*- $\chi^2$  function, given by [33]

$$\chi^{2}(f) = \sum_{i,j} \left[ f(t_{i}) - \langle C(t_{i}) \rangle \right] \operatorname{Cov}_{ij}^{-1} \left[ f(t_{j}) - \langle C(t_{j}) \rangle \right]$$
$$\operatorname{Cov}_{ij} = \frac{1}{N_{cfg} - 1} \left\langle \left[ C(t_{i}) - \langle C(t_{i}) \rangle \right] \left[ C(t_{j}) - \langle C(t_{j}) \rangle \right] \right\rangle$$
(2.63)

where f represents the fit function with a given set of parameters (amplitude, decay constant, and possibly others), and the averages are over the configurations in the ensemble. The inverse of the covariance matrix accounts for the fact that various points in the correlator are not independent measurements, but are highly correlated since they are measured based on the same gauge configurations and averaged over all of the same initial times. Thus our fit-quality metric applies some lighter weight to fluctuations in data which are not independent, but merely "echoing" other random fluctuations. The actual minimization of the  $\chi^2$  function can be achieved via a simplex or Levenberg-Marquardt algorithm [97, 98].

It is apparent from Eq. (2.63) that a larger number of data points may result in a larger  $\chi^2$ , even if all of the points are equally well-described by the fit form, since these deviations are summed over all points. Thus to obtain a metric for comparing fits with different fit ranges, the  $\chi^2$  is often divided by the number of points, referred to as the  $\chi^2$  per degree of freedom, or  $\chi^2/DOF$ . Ideally this value should be close to one, with  $0.5 < \chi^2/DOF < 1.5$  being acceptable as an approximate rule of thumb. Values much larger than one indicate that the points lie too far away from the best fit curve

(further from the line than expected given their statistical error), suggesting that the fit function cannot accurately describe the data shape. This occurs commonly if one tries to fit a correlator with a single exponential over a range where excited-state contamination may be present, introducing a second exponential into the data. A less common issue is that of  $\chi^2/DOF$  values much less than one, indicating that the fit is "too good," or that the points line up unexpectedly close to the fit curve given their statistical error.

One can also visually inspect the energies present in a correlator based on the "effective mass" function of that correlator,

$$m_{eff}^{(\Delta t)}(t) = \frac{1}{\Delta t} \ln \left[ \frac{C(t)}{C(t + \Delta t)} \right].$$
(2.64)

In the large-t limit, this function levels off to a "plateau" at the ground state energy. A  $\Delta t$  value of 2 or 3 is often a good choice, yielding a measurement with somewhat smaller statistical error than  $\Delta t = 1$ .

The operators we design are likely to excite many different states having the same quantum numbers but different energies, so the large-t limit of these correlators only allows access to the ground state in a given channel. However, by calculating correlation functions between a large number of different operators in the same symmetry channel, one can perform a variational analysis to obtain correlators for a new set of operators which are linear combinations of the original ones, such that the new operators each excite a single energy eigenstate from the vacuum. Ideally, each operator in this new "diagonalized" operator basis will then yield a correlator with a single exponential decay, rather than a sum of exponentials.

The result of this variational analysis is a new set of "rotated" operator basis  $\mathcal{O}_i^{(r)}$ made up of linear combinations of the original operators  $\mathcal{O}_i$ ,

$$\mathcal{O}_a^{(r)\dagger}(t) = v_b^{(a)} \mathcal{O}_b^{\dagger}(t). \tag{2.65}$$

such that these new operators are not correlated with each other, creating a diagonal correlator matrix [13, 18]

$$C_{ab}^{(r)}(t) = \langle 0 | \mathcal{O}_{a}^{(r)}(t_{0}+t) \overline{\mathcal{O}}_{b}^{(r)}(t_{0}) | 0 \rangle = \delta_{ab} \lambda_{a}(t)$$
  
$$= v_{c}^{(a)\dagger} \langle 0 | \mathcal{O}_{c}(t_{0}+t) \overline{\mathcal{O}}_{d}(t_{0}) | 0 \rangle v_{d}^{(b)}$$
  
$$= v_{c}^{(a)\dagger} C_{ab}(t) v_{d}^{(b)}.$$
 (2.66)

If such a rotated basis  $\mathcal{O}^{(r)}$  can be found, the diagonal elements  $\lambda_a(t)$  are equal to the  $N_{op}$  lowest energies in the spectrum excited by the operators involved. The leading corrections to this behavior are exponential decays with  $[E_{N_{op}+1} - E_{N_{op}}]$ , the energy gap between the highest state obtained and next higher state [99].

To find the new operator basis  $v_b^{(a)}$ , we solve the generalized eigenvalue problem

$$C(\tau_D)v^{(a)} = \lambda_a C(\tau_0)v^{(a)} \tag{2.67}$$

for some times  $\tau_D > \tau_0$ , which can be chosen arbitrarily to yield the best diagonalization – that is, a rotated correlator matrix which is diagonal over as wide a *t*-range as possible. In practice, we turn Eq. (2.67) into a standard Hermitian eigensystem

$$\left[C^{-1/2}(\tau_0)C(\tau_D)C^{-1/2}(\tau_0)\right]w^{(a)} = \lambda_a w^{(a)}, \qquad (2.68)$$

and then retrieve the original eigenvectors  $v^{(a)}$  via

$$v^{(a)} = C^{-1/2}(\tau_0) w^{(a)}.$$
(2.69)

Note that  $C(\tau_0)^{1/2}$  is well-defined since we ensure that our correlator matrix is Hermitian and positive definite.

As a measure of how well the rotation succeeded in producing a diagonal  $C^{(r)}(t)$ , we can look at the normalized rotated correlator matrix,

$$\widehat{C}_{ab}^{(r)}(t) = \frac{C_{ab}^{(r)}(t)}{\sqrt{C_{aa}^{(r)}(t)C_{bb}^{(r)}(t)}}.$$
(2.70)

If the new basis  $v^{(a)}$  diagonalizes the correlator matrix for a given *t*-range, then  $\widehat{C}_{ab}^{(r)}(t)$  should be consistent with the identity matrix over that range [24]. This is important since only the diagonal elements of the rotated matrix  $C^{(r)}$  are fit to obtain energy values.

Once the rotated correlator matrix  $C^{(r)}$  has been achieved, its diagonal elements can be analyzed by fitting exponential decays, or by calculating effective masses, to extract energies. One can also perform a simultaneous fit of all elements of the rotated correlator matrix, allowing for any residual off-diagonal signal; however if the rotation is successful, as checked by the normalized rotated correlator matrix, this should be equivalent to simply fitting the diagonal elements.

One more useful metric of the quality of a correlation matrix is the *condition* number, which is defined as the ratio of the largest to smallest eigenvalue of the normalized correlator matrix at a given time separation t:

$$CN(t) \equiv \frac{\max(\lambda[\hat{C}(t)])}{\min(\lambda[\hat{C}(t)])}.$$
(2.71)

As a rule of thumb based on previous experience [24], condition numbers below about 100 indicate operators sufficiently independent<sup>8</sup> for diagonalization, while larger condition numbers indicate that some operators are too dependent on others, and should be dropped, or replaced with other, more independent operators.

The eigenvectors  $v^{(n)}$  contain information about the overlaps of the original operators  $\mathcal{O}_i$  onto the eigenstates  $|n\rangle$ , since the correlator matrix contains those overlaps via

$$C_{ij}(t) = \sum_{n} Z_i^{(n)} Z_j^{(n)*} e^{-E_n t}$$
(2.72)

with

$$Z_i^{(n)} = \langle 0|\mathcal{O}_i|n\rangle.$$
(2.73)

These overlaps  $Z_i^{(n)}$  can be helpful in identifying the nature of a given eigenstate which results from the variational analysis. An estimate of these overlaps can be calculated from the eigenvectors  $v^{(n)}$  via [99]

$$Z_i^{(n)} = C_{ij}(\tau_0) v_j^{(n)} \tilde{Z}_n, \qquad (2.74)$$

where the "rotated" overlaps  $\tilde{Z}n$  are defined as the coefficients of the rotated cor-

<sup>&</sup>lt;sup>8</sup>We have found that larger condition numbers are sometimes tolerable if a large number of configurations are analyzed. This is expected, since a more precise measurement should be able to better distinguish small differences between operators.

relator, in the regime where it only couples to one energy eigenstate,  $C^{(r)}(t)_{nm} = \delta_{nm}\tilde{Z}_n\tilde{Z}_n^*e^{-E_nt}$ . The magnitudes of  $Z_n^{(r)}$  can be obtained from fitting these rotated correlators and taking the square root of the fit amplitude. The phases of  $Z_i^{(n)}$  are irrelevant since they depend on an arbitrary choice of phase of the operators.

### 2.6 Error Analysis

In order to report a statistical error on any quantity estimated in our calculations, we can make use of re-sampling by the jackknife or bootstrap methods. These methods determine the uncertainty in a Monte-Carlo estimate, based on the Monte-Carlo sampling itself. The fact that we can achieve such an estimate is not surprising, since any Monte-Carlo sampling for  $\langle X \rangle$  can also yield an estimate of higher moments  $\langle X^2 \rangle$ , which are the salient quantities in the variance or standard deviation. Calculating these higher moments provides information about the width of the sampling distribution, which, paired with knowledge of how many independent samples one has achieved, should be able to give an estimate of the statistical error in any result.

We consider a quantity F which can be computed on the ensemble  $\mathcal{E}$  composed of N gauge configurations, for which we want to compute a statistical error. The average value of the quantity is of course the average over  $\mathcal{E}$ , denoted by  $\langle F \rangle_{\mathcal{E}}$ . In the jackknife method, we define a "new" ensemble  $\mathcal{J}(i)$  to be the ensemble of all of the original configurations except the  $i^{th}$  one. We then measure the same observable F on each of these jackknife ensembles  $\mathcal{J}(i)$ , to obtain N estimates  $\langle F \rangle_{\mathcal{J}(i)}$ . These new averages  $\langle F \rangle_{\mathcal{J}(i)}$  do not yield independent estimates of F, but their dependence on the original F is well-understood and quantifiable. An estimate of the statistical error on F can then be obtained by [100]

$$\delta F \approx \sqrt{\frac{N-1}{N} \sum_{i=1}^{N} \left( \langle F \rangle_{\mathcal{E}} - \langle F \rangle_{\mathcal{J}(i)} \right)^2}.$$
 (2.75)

Another estimate of the error comes from bootstrap resampling, which can yield asymmetric error bars for data with an asymmetric distribution in  $\mathcal{E}$ . A set of bootstrap ensembles  $\mathcal{B}(j)$  are chosen, with  $j = 1...N_b$  for some suitably large  $N_b$ . We often use  $N_b \approx 2 \times N$ . Each of these bootstrap ensembles is made to consist of Nrandomly-selected configurations from the original ensemble. The bootstrap estimate of the symmetric error is

$$\delta F \approx \sqrt{\frac{1}{N_b} \sum_{i=1}^{N_b} \left( \langle F \rangle_{\mathcal{E}} - \langle F \rangle_{\mathcal{B}(i)} \right)^2}.$$
(2.76)

To obtain an asymmetric bootstrap error estimate, one sorts the bootstrap measurements  $\langle F \rangle_{\mathcal{B}(i)}$  and finds two values  $F_+$  and  $F_-$  which bracket the central 68% (one standard deviation) of the values; these are taken as the high and low ends of the error bar. Both jackknife and bootstrap estimates can be used with *re-binning*, in which the observables are first averaged over fixed-size blocks of consecutive gauge configurations, then that smaller set is subjected to error analysis by resampling. This can give some indication of the amount of autocorrelation between successive configurations pulled from the Markov chain.

# Chapter 3

# **Operator Design**

A crucial step in lattice QCD spectroscopy is the design of appropriate operators with which to build correlation functions. One wants to find operators that possess the following properties:

- 1. They should have minimal coupling to high-energy modes above the energy scale of interest, and have minimal statistical noise,
- 2. They should span all of the lattice states *below* that energy scale that is, for any low-lying state, we can find some operator or operators with a significant overlap onto that state. Finally,
- 3. They should transform irreducibly with a particular representation of the lattice symmetry group. This condition allows us to only compute correlation functions between operators with the same quantum numbers, and also facilitates the identification of lattice eigenstates with continuum ones.

This chapter outlines our method for constructing operators that satisfy these properties. Since these operators have been described in earlier works [101–104], the description here will be somewhat brief, but will suffice to arrive at a final form for the  $M^{-1}$  products and sums that will need to be estimated on each gauge configuration,  $\mathcal{F}$  in Eq. (2.9).

In Sec. 3.1, we present our method for field smearing, which reduces coupling to unwanted high-energy modes (addressing the first objective above). In Sec. 3.2, we demonstrate how quark operators can be combined on different lattice sites to create extended, gauge-invariant meson and baryon operators, which allows for increased coupling with some excited states of interest (see the second point above). A discussion of the symmetry projections that we utilize will be given in Sec. 3.3, addressing the last of our three objectives for operators. In Sec. 3.4, we summarize the final forms for our hadron operators, and present the results of single-hadron operator 'pruning'. Pruning refers to the process of examining effective masses and correlation matrices for all possible operators in a given symmetry channel, using our smaller  $16^3$  gauge configurations, and choosing a subset of operators that satisfies the first two criteria mentioned above. We then run only this subset on the more computationally expensive  $24^3$  and  $32^3$  ensembles. A discussion of recent progress in *multi-hadron* operator pruning, the selection of particular single-hadron operators to combine into multi-hadron operators, will be deferred until Ch. 5. Concluding this chapter, we introduce a novel glueball operator which works at least as well as standard plaquette glueball operators, and can be calculated conveniently from quantities we already need for our LapH quark smearing.

### 3.1 Field Smearing

Field smearing is a way of "smoothing out" the high-frequency fluctuations in the field, or rather, defining operators which do not excite these higher-energy modes very much. Gauge field smearing is applied to the field configurations of the Markov chain, such that the quark action is defined on those smeared gauge links  $\tilde{U}$ , as is the Dirac matrix used in the inversion process,  $M[\tilde{U}]$ . The quark field smearing is defined by an operator S acting on the Grassmann fields  $\psi$  and  $\overline{\psi}$  in mesons and baryons, which then appears in the constructions  $\mathcal{F}(M^{-1})$  mentioned in Eq. (2.6).

Stout-link gauge field smearing was discussed in Sec. 2.2.2 as we presented the discretized fermion action, so we only briefly review it here. As before, only spatial links are smeared so as to preserve positivity of the transfer matrix for all time separations, as explained in Ch. 2. The iteration procedure is defined identically as before, though for our operators we choose  $\rho = 0.1$  and  $N_{\rho} = 10$  smearing iterations, a slightly higher smearing level than used in the action. In choosing smearing levels for operators, one increases the amount of smearing as long as a desired effective mass continues to drop, with its error decreasing or staying relatively constant. At some point, one expects this trend to stop since the physical scales of interest are eventually "smeared out", so that the error bars on observables start to increase

again. Observing this behavior gives a clear indication of what the optimal smearing level is.

The quark field smearing used in this work is known as LapH (Laplacian Heaviside) smearing [23]. As suggested by its name, the LapH smearing operator is defined in terms of the covariant Laplacian (roughly, a measure of curvature on the lattice) and a Heaviside function to cut off modes above a certain curvature. The *covariant* Laplacian is necessary so that smeared fields  $\tilde{\psi}$  and  $\tilde{\overline{\psi}}$  maintain gauge covariance, and hadron operators maintain gauge invariance. Indeed, LapH smearing maintains all of the single-time-slice transformation properties of the original field.

The covariant Laplacian is defined in term of the smeared gauge fields  $\tilde{U}$  via

$$\tilde{\Delta}_{ab}(x,y) = \sum_{k=1}^{3} \left[ \tilde{U}_{k}^{ab}(x)\delta(y,x+\hat{k}) + U_{k}^{\dagger ab}(y)\delta(y,x-\hat{k}) - 2\delta(x,y)\delta^{ab} \right].$$
(3.1)

As a sparse matrix in space and color, one can numerically calculate space-colorvectors  $v_a^{(k)}(x)$  which are eigenvectors of the smeared Laplacian, with corresponding eigenvalues  $\lambda^{(k)}$ . As with the regular Laplacian, the eigenvalues  $\lambda^{(k)}$  will be negative, with higher curvature corresponding to a lower (more negative) eigenvalue. Thus the smearing operator can be defined as

$$\mathcal{S} = \Theta(\sigma_s^2 + \tilde{\Delta}). \tag{3.2}$$

This amounts to projection onto all eigenvectors whose eigenvalues are less than  $\sigma_s^2$ , and amounts to a generalization of a high-frequency cutoff in Fourier space.

In practice, the spacing of the eigenvalues is highly consistent between configurations for a given lattice dimension, and even variations in pion mass have little effect on how many eigenvalues might lie within the cutoff [22]. It follows that Eq. (3.2) can be approximated as a projection onto some fixed number  $N_v$  of the eigenvectors with the lowest curvature (least-negative eigenvalues). Thus, the Hermitian smearing matrix can be written

$$S = \sum_{k=1}^{N_v} v^{(k)} v^{(k)\dagger} = V_s V_s^{\dagger}, \qquad (3.3)$$

where the columns of the matrix  $V_s$  are the eigenvectors of the smeared covariant

Laplacian. The smeared quark fields  $\tilde{\psi}$  are then defined as

$$\tilde{\psi}^{A}_{a\alpha}(x) = \mathcal{S}_{ab}(x, y)\psi^{A}_{b\alpha}(y), \qquad \tilde{\overline{\psi}}^{A}_{a\alpha}(x) = \psi^{A}_{b\alpha}(y)\mathcal{S}_{ba}(y, x).$$
(3.4)

In our calculations, it is more convenient to work with the quantities

$$\chi \equiv \overline{\psi}\gamma_4, \qquad \Omega \equiv \gamma_4 M \tag{3.5}$$

with M being the usual Dirac matrix. The smearing operator is diagonal in spin, and the corresponding smeared field  $\tilde{\chi}$  is simply  $\tilde{\psi}\gamma_4$ .

While the numerical calculation of LapH eigenvectors does represent some overhead cost in CPU usage and disk space, it is relatively inexpensive compared with other parts of lattice QCD calculations, especially Dirac matrix inversion. Importantly, the Laplacian is diagonal in time, making it a much smaller system to solve than Dirac matrix linear systems. The computation of these eigenvectors on each time slice is done via the Krylov-Spectral Restarted Lanczos (KSRL) method, similar to the thick-restarted Lanczos method [105].

The choice of how many eigenvectors to keep, or equivalently what smearing cutoff  $\sigma_s$  to use, is analogous to the choice of  $\rho$  and  $N_{\rho}$  in the gauge-smearing case, in that it is simply a question of tuning to provide the best coupling to low-lying states. Thus, some tests are run at different  $\sigma_s$  values, effective masses are generated for a few example operators, and the smearing level which provides the fast decay to a ground state plateau, with least error, is chosen. An example of this analysis is shown in Fig. 3.1.

As the lattice size increases, the spacing of eigenvalues of the covariant Laplacian becomes more dense in the same way that our discrete momenta values become more dense. Thus, to capture the same physics on a large lattice, we expect to require more eigenvectors roughly in proportion with the volume V. The actual number of eigenvectors determined for each of the gauge configurations used in this work is listed in Table 3.1.



Figure 3.1: An example of how the LapH smearing cutoff  $\sigma_s$  is chosen. The plot shows effective masses for three different nucleon operators, shifted apart by 0.04, for time separation  $t_s = 1$ , plotted against  $\sigma_s^2$ . Results obtained from  $16^3 \times 128$  anisotropic lattices with spacing  $a_s \approx 0.12$  fm, stout-link gauge field smearing,  $N_f = 2 + 1$ . It is observed that choosing  $\sigma_s^2 \approx 0.33$  appears to minimize excited state contamination and statistical noise. From Ref. [22].

Ensemble	$N_v$
$16^{3}$	32
$20^{3}$	64
$24^3(390)$	112
$24^3(240)$	112
$32^{3}$	264

Table 3.1: Number of covariant Laplacian eigenvectors used in quark smearing for the gauge configuration ensembles used in this work. Other gauge configuration parameters are given in Table 2.1.

### **3.2** Spatially-Extended Operators

It is reasonable to imagine that excited states of hadrons may be larger than corresponding ground states because the constituent quarks have greater orbital movement. Therefore, in order to couple to some of these excited states, some hadron operators should be included which have quark fields displaced from each other. This must be done in a way which maintains the gauge-invariance of the operator.

These considerations lead to the covariant displacement operator  $\tilde{D}$  which shifts a quark field in a straight line of length p along  $j^{th}$  direction,

$$\tilde{D}_{j}^{(p)}(x,x') = \tilde{U}_{j}(x)\tilde{U}_{j}(x+\hat{j})...\tilde{U}_{j}(x+(p-1)\hat{j})\delta(x',x+p\hat{j})$$
(3.6)

such that p is referred to as the displacement length and j is one of the spatial directions forward or backward,  $j = \pm 1, \pm 2, \pm 3$ . Note that color indices are implicit on the displacement operators.

To obtain larger, more complicated paths, we can string these operators together, labeling each successive direction  $j_n, n = 1..N$ . Therefore we define smeared, displaced quark fields  $q^A$  and  $\bar{q}^A$  for quark flavor A by

$$\tilde{q}^{A}_{a\alpha[j_1\dots j_N]}(x) = \tilde{D}^{(p)}_{j_1;aa_1}(x, x_1)\tilde{D}^{(p)}_{j_2;a_1a_2}(x_1, x_2)\dots \tilde{D}^{(p)}_{j_N;a_{n-1}a_N}(x_{N-1}, x_N)\tilde{\psi}^{A}_{a_N\alpha}(x_N) \quad (3.7)$$

$$\tilde{\bar{q}}^{A}_{a\alpha[j_1\dots j_N]}(x) = \tilde{\chi}^{A}_{a_1\alpha}(x_1)\tilde{D}^{(p)\dagger}_{j_1;a_1,a_2}(x_1,x_2)\tilde{D}^{(p)\dagger}_{j_2;a_2a_3}(x_2,x_3)\dots\tilde{D}^{(p)\dagger}_{j_N;a_Na}(x_N,x).$$
(3.8)

The notation with smeared, displaced fields gets cumbersome, so we can simplify our notation by defining

$$\tilde{q}^A_{a\alpha[j_1\dots j_N]}(x) \to \ q^A_{a\alpha}(\mathbf{x},t) \qquad \qquad \tilde{\overline{q}}^A_{a\alpha[j_1\dots j_N]}(x) \to \ \overline{q}^A_{a\alpha}(\mathbf{x},t)$$

The displacement path indices  $j_1, j_2...j_N$  are folded into the Dirac spin index  $\alpha$  for each quark, since these two properties are linked for a given operator term. Also the tilde indicating smearing need not be repeated since all of our quark fields are LapH-smeared in the same way. Also, time and spatial components are separated in  $(\mathbf{x}, t)$  since displacement only occurs in spatial directions, and having t explicit will be useful in writing expressions for temporal correlation functions.

The choice of what paths and displacement lengths to employ is determined by smaller-lattice tests, in which we calculate large survey sets of operators and select for

Illustration	Name	Explicit form $( i  \neq  j  \neq  k  \neq 0)$
•	Single-site (SS)	$\delta_{ab} \; \widetilde{\chi}^A_{alpha} \; \widetilde{\psi}^B_{beta}$
0—●	Singly-displaced (SD)	$\delta_{ab} \ \widetilde{\chi}^A_{a\alpha} \ \left( \widetilde{D}^{(p)}_j \widetilde{\psi} \right)^B_{b\beta}$
	Doubly-displaced-L (DDL)	$\delta_{ab} \left( \widetilde{\chi} \ \widetilde{D}_{j}^{(p)\dagger} \right)_{a\alpha}^{A} \left( \widetilde{D}_{k}^{(p)} \widetilde{\psi} \right)_{b\beta}^{B}$
	Triply-displaced-U (TDU)	$\delta_{ab} \left( \widetilde{\chi} \ \widetilde{D}_{j}^{(p)\dagger} \right)_{a\alpha}^{A} \left( \widetilde{D}_{k}^{(p)} \widetilde{D}_{j}^{(p)} \widetilde{\psi} \right)_{b\beta}^{B}$
	Triply-displaced-O (TDO)	$\delta_{ab} \left( \widetilde{\chi} \ \widetilde{D}_i^{(p)\dagger} \right)_{a\alpha}^A \left( \widetilde{D}_j^{(p)} \widetilde{D}_k^{(p)} \widetilde{\psi} \right)_{b\beta}^B$

Table 3.2: The types of displacement path combinations used in meson operators. The lines represent covariant displacements as given in Eq. (3.6), while the filled and hollow circles represent smeared quark and antiquark fields, respectively.

smallest condition number and best coverage of excited states, as discussed in Sec. 2.5. Many of these choices have been discussed in earlier works [25, 106] and paths were chosen with a maximum of three displacements, and with a displacement length p = 3. The path shapes we use for mesons and baryons with three displacements are shown in Figs. 3.2 and 3.3, respectively.

With the development of larger lattices (whose use is made possible by more efficient inversion algorithms), these operator displacements have come to represent a significant amount of computation time, especially for baryon operators. Therefore, some further analysis has been done regarding how many different kinds of paths, and what displacement lengths p, suffice to generate an acceptable operator set. Looking at several representative sets of baryon operators on a small  $16^3$  testing ensemble, we compared dilution lengths of one, two and three lattice units, observing differences in

Illustration	Name	Explicit form $( i  \neq  j  \neq  k )$
٩	Single-site (SS)	$\varepsilon_{abc} \; \tilde{\psi}^A_{a\alpha} \; \tilde{\psi}^B_{b\beta} \; \tilde{\psi}^C_{c\gamma}$
•	Singly-displaced (SD)	$\varepsilon_{abc} \; \tilde{\psi}^A_{a\alpha} \; \tilde{\psi}^B_{b\beta} \; \left( \tilde{D}^{(p)}_j \tilde{\psi} \right)^C_{c\gamma}$
•••	Doubly-displaced-I (DDI)	$\varepsilon_{abc} \; \tilde{\psi}^{A}_{a\alpha} \; \left( \tilde{D}^{(p)}_{-j} \tilde{\psi} \right)^{B}_{b\beta} \; \left( \tilde{D}^{(p)}_{j} \tilde{\psi} \right)^{C}_{c\gamma}$
	Doubly-displaced-L (DDL)	$\varepsilon_{abc} \; \tilde{\psi}^A_{a\alpha} \; \left( \tilde{D}^{(p)}_j \tilde{\psi} \right)^B_{b\beta} \; \left( \tilde{D}^{(p)}_k \tilde{\psi} \right)^C_{c\gamma}$
••	Triply-displaced-T (TDT)	$\varepsilon_{abc} \left( \tilde{D}_{-j}^{(p)} \tilde{\psi} \right)_{a\alpha}^{A} \left( \tilde{D}_{j}^{(p)} \tilde{\psi} \right)_{b\beta}^{B} \left( \tilde{D}_{k}^{(p)} \tilde{\psi} \right)_{c\gamma}^{C}$
	Triply-displaced-O (TDO)	$\varepsilon_{abc} \left( \tilde{D}_{i}^{(p)} \tilde{\psi} \right)_{a\alpha}^{A} \left( \tilde{D}_{j}^{(p)} \tilde{\psi} \right)_{b\beta}^{B} \left( \tilde{D}_{k}^{(p)} \tilde{\psi} \right)_{c\gamma}^{C}$

Table 3.3: The types of displacement path combinations used in baryon operators. The lines represent covariant displacements as given in Eq. (3.6), the filled circles represent smeared quark fields, and the larger open circles represent Levi-Civita color contractions  $\varepsilon_{abc}$ .



Figure 3.2: Effective masses (dt=2) for three nucleon operators, each of which are extended operators which might couple to excited states of the proton. Group theoretically speaking, they are projected onto the lattice irreducible representation  $G_{1g}$ . The labels DDL, DDI, and TDT correspond to displacement paths as outlined in Tables 3.2 and 3.3. In each case, decreasing the displacement length has a relatively small effect on the effective mass observed, leading us towards our choice of reducing the displacement length requirement for baryons. These tests were performed on 22 configurations of a small  $16^3 \times 128$ ,  $m_{\pi} \approx 400 MeV$  ensemble.

the effective mass and condition number of correlator matrices of these operators, as discussed in section 2.5. A typical comparison is shown in Fig. 3.2.

The analysis showed that in each case, the reduction of the displacement length had a relatively small effect on the masses extracted. In the left-most panel of Fig. 3.2, we do see that the smaller operators have slightly less coupling to the baryon excited state; however the amount by which the effective mass drops is not dramatic, and is barely noticeable in the other two operators. Condition number analysis was also performed, as given in Eq. (2.71), and we found that well-conditioned correlator matrices of operators with displacement length three were generally still well-conditioned if the displacement length on all the operators was decreased to two.

Thus a displacement length of two appears to be acceptable, and in some cases even a path length of one seems sufficient. However since we were unable to re-evaluate operator pruning in all baryon symmetry channels, we kept to a displacement length of two to be safe, and still achieve a 2/3 speed-up in the baryon calculation. The displacement length for the computationally less-expensive meson operators was kept at three. As it turned out, another speed-up was utilized for our baryon operator calculations, which came as a consequence of disk space limitations at the stage of LapH baryon operator assembly; however we delay that discussion until Ch. 4 after we have introduced the Stochastic LapH propagator method.

### **3.3 Symmetry Projections**

As mentioned earlier, it is important to choose operators with well-defined lattice transformation properties, so that the correlation matrices we build will be blockdiagonalized among different symmetry sectors. Since our eventual goal is to find stationary states and corresponding energies of the lattice QCD Hamiltonian, this block diagonalization is a major step in the right direction. Also, in constructing operators with known lattice symmetries, one can then subduce these symmetries into different continuum symmetry group representations, thus providing an indication of what physical state corresponds to a particular lattice state (see Table 3.5).

All of the symmetries required of our field-theoretical operators can be approached in a similar way. Given some set of unitary transformations  $U_R$  which transforms lattice operators amongst each other, we first calculate the irreducible matrix representations  $\Gamma_{\lambda\mu}^{(\Lambda)}(R)$  of each transformation R, with  $\lambda$  and  $\mu$  being row and column, respectively. We then design operators that transform with the  $\lambda^{th}$  row of the irreducible representation  $\Lambda$  of that group, meaning that we design operators to satisfy [101]

$$U_R \overline{O}_i^{\Lambda \lambda} U_R^{\dagger} = \sum_{\mu} \overline{O}_i^{\Lambda \mu} \Gamma_{\mu \lambda}^{(\Lambda)}(R), \qquad (3.9)$$

$$U_R O_i^{\Lambda \lambda} U_R^{\dagger} = \sum_{\mu} O_i^{\Lambda \mu} \Gamma_{\mu \lambda}^{(\Lambda)}(R)^*$$
(3.10)

for all group elements R, with index *i* referring to all other possible properties of the operator (for instance, displacement path shapes defined in Tables 3.2 and 3.3). This condition is critical to ensure the orthogonality of operators in different irreducible representations, and to be able to use the results of group subduction to relate lattice irreducible representations to continuum symmetry channels.

The following groups of transformations leave our lattice action unchanged, and so will be addressed in our creation/annihilation operators:

• local SU(3) gauge transformations,

- SU(2) isospin rotations,
- G-parity transformations,
- spatial translations, rotations and reflections possible on a cubic lattice  $(O_h^1)$ .

Gauge symmetry is somewhat different than the others in the list, in that we are only interested in operators transforming with the trivial, one-dimensional representation of SU(3) – that is, we are only interested in color singlet operators. This stipulation leads to the inclusion of the Levi-Civita symbol  $\varepsilon_{abc}$  in baryon operators, and the delta  $\delta_{ab}$  in mesons. For other symmetries in the list, we will be concerned with generating operators transforming with all irreducible representations of the symmetry group.

For isospin symmetry, the requirement of Eq. 3.9 applies with the representation matrices  $\Gamma$  being the Wigner matrices  $D^{(I)}(R_{\tau})$  for any isospin rotation  $R_{\tau}$ , with the rows  $\lambda$  and  $\mu$  being different isospin projections  $I_3$ . These considerations lead to quark-antiquark operators such as  $\overline{u}u + \overline{d}d$ , rather than just  $\overline{u}u$ , reflecting the familiar Clebsch-Gordan coefficients for the tensor product of two two-dimensional irreducible representations of SU(2) into a one- and a three-dimensional irrep.

The strange quark creation/annihilation operators are unaffected by isospin rotations, so that combinations such as  $\overline{ss}$  are isospin singlets, and could mix with an isoscalar  $\overline{u}u + \overline{d}d$  operator. However, there is no issue with keeping these two operators separate in the operator construction phase, since we intend to allow any operators with compatible quantum numbers to mix in a correlator matrix, then diagonalize to find optimized combinations of them.

The G-parity transformation  $\mathcal{G}$  is defined as an application of charge conjugation  $\mathcal{C}$  along with a rotation by  $\pi$  in isospin space,

$$\mathcal{G} = \mathcal{C}e^{-i\pi\tau_2}.\tag{3.11}$$

Like charge conjugation, G-parity eigenstates have eigenvalues of  $\pm 1$ , and the irreducible representation matrices  $\Gamma$  in equation 3.9 are trivially either  $\{1, 1\}$  or  $\{1, -1\}$ . But unlike simple charge conjugation, G-parity is a valid quantum number for some states of nonzero isospin projection  $I_3$ , such as the  $\pi^+$  and  $\pi^-$ . Also, it is worth noting that the combination of a  $\pm 1$  strangeness meson, as in a kaon-antikaon  $KK^c$ , can be projected onto positive or negative G-parity as well.<sup>1</sup> Thus, we need to understand the G-parity transformation behavior not only for our strangeness S = 0 mesons, but also for our kaon and antikaon operators. Specifically, each antikaon operator  $K_A^c$  is constructed from its corresponding kaon operator  $K_A$  such that

$$U_G K_A U_G^{\dagger} = K_A^c, \qquad U_G K_A^c U_G^{\dagger} = -K_A, \qquad (3.12)$$

where the negative sign in the last term comes from the isospin rotation by  $2\pi$  of the light quark fermion field. Thus a kaon-antikaon operator of positive or negative G-parity may be constructed via

$$(K_A K_B^c)^{\pm} = K_A K_B^c \pm U_G K_A K_B^c U_G^{\dagger} = K_A K_B^c \mp K_A^c K_B$$
(3.13)

The last transformation group in our list of symmetries is that of spatial rotations, reflections, and translations. Referring to Eq. (3.9), we require an understanding of how each displaced, smeared building-block operator  $q^A_{a\alpha j}$  transforms under any rotation R, reflection, and translation by **b**;

$$U_{(R,\mathbf{b})}q_{a\alpha j}^{A}(\mathbf{x})U_{(R,\mathbf{b})}^{\dagger} = S(R)_{\alpha\beta}^{-1}q_{a\beta j}^{A}(R\mathbf{x}+\mathbf{b}), \qquad (3.14)$$

$$U_{(R,\mathbf{b})}q^{A}_{a\alpha j}(\mathbf{x})U^{\dagger}_{(R,\mathbf{b})} = \overline{q}^{A}_{a\beta j}(R\mathbf{x} + \mathbf{b})S(R)_{\beta\alpha}$$
(3.15)

where the rotation/reflection matrices S are defined by the three generators  $C_{4y}$ ,  $C_{4z}$ , and parity  $I_s$ ,

$$S(I_s) = \gamma_4, \qquad S(C_{4y}) = \frac{1}{\sqrt{2}}(1 + \gamma_1\gamma_3), \qquad S(C_{4z}) = \frac{1}{\sqrt{2}}(1 + \gamma_2\gamma_1).$$
 (3.16)

These transformation properties govern the left-hand side of equation 3.9. We also need to know the set of representation matrices  $\Gamma^{\Lambda}$  for each irrep  $\Lambda$ . The translation part of the group is implemented via the familiar momentum phases  $e^{-i\mathbf{p}\dot{\mathbf{x}}}$ , so the representation matrices need only be written down for the transformations in the

<sup>&</sup>lt;sup>1</sup>The antikaon is denoted  $K^c$  rather than  $\overline{K}$  to avoid confusion with the designation of source and sink meson operators.

point group  $O_h$  (reflections and rotations). These irreps and our choices<sup>2</sup> for the irreducible representation matrices can be found in Ref. [101]. The fermion irreducible representations are *double-valued*, and these are generated by introducing a new group element corresponding to a rotation by  $2\pi$ , which for fermionic states is a distinct transformation (a rotation by  $4\pi$  is then the identity).

In considering operators with non-zero total momentum, the fixed direction of  $\mathbf{p}$  limits the allowable  $O_h$  transformations. The subset of symmetry operators that leave the momentum invariant is known as the *little group* of  $\mathbf{p}$ . The little group is  $C_{4v}$  for an on-axis momentum such as (1,0,0),  $C_{2v}$  for a planar-diagonal momentum such as (1,1,0), and  $C_{3v}$  for a cubic-diagonal momentum such as (1,1,1). The irreducible representation matrices for the little groups are given in Ref. [101]. Table 3.4 lists the irreducible representations of  $O_h$  and the double-valued representations, and gives the subductions of the point group irreps onto various lattice little groups, indicating which zero-momentum lattice states would be expected to have a moving analogue in which little groups. This information proved useful in the early stages of our operator pruning, choosing the number of operators to consider in each irreducible representation, as discussed in Sec. 3.4.

The group representations denoted in Table 3.4 have subscript g/u to indicate positive/negative eigenvalue, respectively, under spatial parity, for zero-momentum states. The little groups do not include spatial inversion, since parity reverses the momentum. For mesons of strangeness zero, positive or negative G-parity is denoted by a superscript +/-, and G-parity persists as a symmetry of moving hadrons, since it involves only internal quantum numbers. Table 3.5 shows the subduction of various lattice irreducible representations onto continuum spins. The lattice symmetries of parity and G-parity correspond exactly to their continuum counterparts, so the +/superscripts are omitted in Table 3.5.

In constructing the single-hadron operators, we must keep in mind that we intend to build multi-hadron operators from these same data structures. As in the case of

 $<sup>^{2}</sup>$ These representation matrices are a "choice" up to a unitary change of basis.

$\Lambda(O_h)$	$C_{4v}$	$C_{3v}$	$C_{2v}$
$A_{1g}$	$A_1$	$A_1$	$A_1$
$A_{1u}$	$A_2$	$A_2$	$A_2$
$A_{2g}$	$B_1$	$A_2$	$B_2$
$A_{2u}$	$B_2$	$A_1$	$B_1$
$E_g$	$A_1 \oplus B_1$	E	$A_1 \oplus B_2$
$E_u$	$A_2 \oplus B_2$	E	$A_2 \oplus B_1$
$T_{1g}$	$A_2 \oplus E$	$A_2 \oplus E$	$A_2 \oplus B_1 \oplus B_2$
$T_{1u}$	$A_1 \oplus E$	$A_1 \oplus E$	$A_1 \oplus B_1 \oplus B_2$
$T_{2g}$	$B_2 \oplus E$	$A_1 \oplus E$	$A_1 \oplus A_2 \oplus B_1$
$T_{2u}$	$B_1 \oplus E$	$A_2 \oplus E$	$A_1 \oplus A_2 \oplus B_2$
$G_{1g/u}$	$G_1$	G	G
$G_{2g/u}$	$G_2$	G	G
$H_{g/u}$	$G_1\oplus G_2$	$F_1 \oplus F_2 \oplus G$	$G\oplus G$

Table 3.4: Irreducible representations of the lattice point group  $O_h$ , and the subduction of those representations onto the little groups that result from restricting  $O_h$  to only those transformations leaving a given momentum ray unchanged. The last three representations are the double-valued irreps corresponding to fermionic states.

$\Lambda(O_h)$	Continuum Spins $J$ Present
$A_1$	$0, \ 4, \ 6, \ 8, \ 9$
$A_2$	$3,\ 6,\ 7,\ 9$
E	2, 4, 5, 6, 7, 8, 8, 9
$T_1$	$1, \ 3, \ 4, \ 5, \ 5, \ 6, \ 7, \ 7, \ 8, \ 8, \ 9, \ 9, \ 9$
$T_2$	$2, \ 3, \ 4, \ 5, \ 6, \ 6, \ 7, \ 7, \ 8, \ 8, \ 9, \ 9$
$G_1$	1/2, 7/2, 9/2, 11/2, 13/2, 15/2
$G_2$	5/2, 7/2, 11/2, 13/2, 13/2, 15/2
H	3/2, 5/2, 7/2, 9/2, 9/2, 11/2, 11/2, 13/2, 13/2, 15/2, 15/2, 15/2

Table 3.5: Subduction of lattice irreducible representations of  $O_h$  onto onto integer spin J representations of continuum spin SU(2), and below the solid line, subductions of double-valued irreps onto half-integer spin irreps of SU(2). Repeated occurrence of a particular J indicates that after restriction of the continuum irrep to the elements of the lattice subgroup and block diagonalization of these elements, more than one copy of that lattice irrep occur in different blocks. Subduction occurs identically for positive and negative parity and G-parity, so for example the  $A_1$  entry below is equally applicable to  $A_{1g}^+$ ,  $A_{1u}^+$ ,  $A_{1g}^-$ , and  $A_{1u}^-$ , with the same parity and G-parity as the continuum irreps.
$KK^c$  states, we need to know precisely how a single-hadron operator  $O(\mathbf{p})$  transforms not just under its own little group, but also under other elements that would take it to other momenta, for instance to  $O(-\mathbf{p})$ . This requires defining reference rotations  $R_{\text{ref}}^{\mathbf{p}}$  to carry one momentum ray into another. The transformation that appears on the right side of equation 3.9 must be defined for any space group rotation/reflection and translation  $\mathbf{x} \to R\mathbf{x} + \mathbf{b}$ , and the transformation requirement becomes

$$U_{(R,\mathbf{b})}O_{\mathbf{p}\Lambda\lambda i}^{II_{3}}(t)U_{(R,\mathbf{b})}^{\dagger} = O_{\mathbf{p}\Lambda\mu i}^{II_{3}}(t)\Gamma_{\mu\lambda}^{(\Lambda)}(R_{W}^{\mathbf{p}}) \ e^{i\mathbf{b}\cdot R\mathbf{p}},\tag{3.17}$$

with

$$R_W^{\mathbf{p}} = (R_{\text{ref}}^{\mathbf{p}})^{-1} \ R \ R_{\text{ref}}^{\mathbf{p}}.$$
 (3.18)

The actual expressions for these operators are generated automatically via MAPLE procedures which write out coefficients with which to sum the meson and baryon building blocks. The building blocks handled by this routine include proper symmetry under translation and gauge invariance, and are defined as

$$\Phi^{AB}_{\alpha\beta}(\mathbf{p},t) = \sum_{\mathbf{x}} e^{-i\mathbf{p}\cdot(\mathbf{x}+\frac{1}{2}(\mathbf{d}_{\alpha}+\mathbf{d}_{\beta}))} \delta_{ab} \overline{q}^{A}_{a\alpha}(\mathbf{x},t) q^{B}_{b\beta}(\mathbf{x},t)$$
  
$$\overline{\Phi}^{AB}_{\alpha\beta}(\mathbf{p},t) = \sum_{\mathbf{x}} e^{i\mathbf{p}\cdot(\mathbf{x}+\frac{1}{2}(\mathbf{d}_{\alpha}+\mathbf{d}_{\beta}))} \delta_{ab} \overline{q}^{B}_{b\beta}(\mathbf{x},t) q^{A}_{a\alpha}(\mathbf{x},t)$$
(3.19)

for mesons, and

$$\Phi^{ABC}_{\alpha\beta\gamma}(\mathbf{p},t) = \sum_{\mathbf{x}} e^{-i\mathbf{p}\cdot\mathbf{x}} \varepsilon_{abc} q^{A}_{a\alpha}(\mathbf{x},t) q^{B}_{b\beta}(\mathbf{x},t) q^{C}_{c\gamma}(\mathbf{x},t)$$
  
$$\overline{\Phi}^{ABC}_{\alpha\beta\gamma}(\mathbf{p},t) = \sum_{\mathbf{x}} e^{i\mathbf{p}\cdot\mathbf{x}} \varepsilon_{abc} \overline{q}^{C}_{c\gamma}(\mathbf{x},t) \overline{q}^{B}_{b\beta}(\mathbf{x},t) \overline{q}^{A}_{a\alpha}(\mathbf{x},t)$$
(3.20)

for baryons. The smeared, displaced quark fields are written in the simplified notation introduced in Eq. (3.9). In the case of mesons, the momentum phase includes a slight adjustment depending on the displacement vectors  $\mathbf{d}_{\alpha}$ . This phase is necessary in order to preserve fixed G-parity for moving operators, while that symmetry is not relevant for baryons.

The isospin, G-parity and rotation/reflection transformation properties of our final hadrons are then implemented via our MAPLE-generated coefficients, which we here denote as  $c_{\alpha\beta}^{(l)}$  for mesons operators,

$$M_{l}(\mathbf{p}, t) = c_{\alpha\beta}^{(l)} \Phi_{\alpha\beta}^{AB}(\mathbf{p}, t), \qquad (3.21)$$
  
$$\overline{M}_{l}(\mathbf{p}, t) = c_{\alpha\beta}^{(l)*} \overline{\Phi}_{\alpha\beta}^{AB}(\mathbf{p}, t),$$

and  $c_{\alpha\beta\gamma}^{(l)}$  for baryons operators,

$$B_{l}(\mathbf{p},t) = c_{\alpha\beta\gamma}^{(l)} \Phi_{\alpha\beta\gamma}^{ABC}(\mathbf{p},t)$$

$$\overline{B}_{l}(\mathbf{p},t) = c_{\alpha\beta\gamma}^{(l)*} \overline{\Phi}_{\alpha\beta\gamma}^{ABC}(\mathbf{p},t).$$
(3.22)

The superscript (l) represents some particular irreducible representation of  $O_h$  or of one of its little groups if **p** is non-zero, the row  $\lambda$  of that irrep, a particular isospin I, isospin projection  $I_3$ , and strangeness S. The flavor structure of our hadron operators are listed in Table 3.6.

Two-hadron operator construction proceeds in much the same fashion as singlehadron operator construction. In particular, the same Eq. 3.9 is required for irreducible transformation of the multi-hadron operators. The difference is that now our building blocks, instead of being the  $\Phi$  expressions in Eqs. (3.19) and (3.20), are now made up of products of two different complete single-hadron operators,

$$O_{\mathbf{p}\Lambda\lambda i}^{II_3S}(t)O_{\mathbf{p}'\Lambda'\lambda'j}^{I'I_3'S'}(t) \tag{3.23}$$

In this study, we limit ourselves to single-hadron and two-hadron operators since we expect that the coupling between one- and three-particle states should be suppressed. This issue will be addressed in future work. In this work, we focus on obtaining results for the  $I = I_3 = 1, S = 0$  channel, as will be discussed in Ch. 5.

One last symmetry that we consider is time-reversal. For the majority of operators, this symmetry is not important, but for a few of the lowest-energy meson states, it is useful to understand the behavior of backwards-propagating states, since these may be noticeable on a lattice of finite-temporal extent T. If the energies and amplitudes of the backwards-propagating components of our correlators are ensured to be the same as the forward-propagating amplitudes, then correlated- $\chi^2$  fits to these correlation functions can proceed with the two-parameter form  $A(e^{-Et} + e^{-E(T-t)})$ , as opposed

Hadron	$I = I_3$	S	G	Operator Flavor Content
$\Delta^{++}$	$\frac{3}{2}$	0		$\Phi^{uuu}_{lphaeta\gamma}$
$\Sigma^+$	1	-1		$\Phi^{uus}_{lphaeta\gamma}$
$N^+$	$\frac{1}{2}$	0		$\Phi^{uud}_{lphaeta\gamma}-\Phi^{duu}_{lphaeta\gamma}$
$\Xi^0$	$\frac{\overline{1}}{2}$	-2		$\Phi^{ssu}_{lphaeta\gamma}$
$\Lambda^0$	Õ	-1		$\Phi^{uds}_{lphaeta\gamma}-\Phi^{dus}_{lphaeta\gamma}$
$\Omega^{-}$	0	-3		$\Phi^{sss}_{lphaeta\gamma}$
$f,~f',~\eta,~\eta'$	0	0	1	$\Phi^{uu}_{\alpha\beta} + \Phi^{dd}_{\alpha\beta} + U_G (\Phi^{uu}_{\alpha\beta} + \Phi^{dd}_{\alpha\beta}) U_G^{\dagger}$
				$\Phi^{ss}_{\alpha\beta} + U_G \Phi^{ss}_{\alpha\beta} U_G^{\dagger}$
$h,~h',~\omega,~\phi$	0	0	-1	$\Phi^{uu}_{\alpha\beta} + \Phi^{dd}_{\alpha\beta} \ - \ U_G (\Phi^{uu}_{\alpha\beta} + \Phi^{dd}_{\alpha\beta}) U_G^{\dagger}$
				$\Phi^{ss}_{lphaeta} - U_G \Phi^{ss}_{lphaeta} U_G^\dagger$
$b^+, \ \rho^+$	1	0	1	$\Phi^{du}_{lphaeta} + U_G \Phi^{du}_{lphaeta} U_G^{\dagger}$
$a^+, \pi^+$	1	0	-1	$\Phi^{du}_{lphaeta} - U_G \Phi^{du}_{lphaeta} U_G^\dagger$
$K^{+}, K^{*+}$	$\frac{1}{2}$	1		$\Phi^{su}_{lphaeta}$
$\overline{K}^0, \ \overline{K}^{*0}$	$\frac{1}{2}$	-1		$\Phi^{ds}_{lphaeta}$

Table 3.6: Flavor content of single-hadron annihilation operators. The gaugeinvariant, definite-momentum meson and baryon building blocks  $\Phi$  are defined in Eqs. (3.19) and (3.20), respectively. In addition to isospin *I* and strangeness *S*, some light-quark meson operators are characterized by G-parity, as defined in equation 3.11, and effected by unitary transformation  $U_G$ . Note that the isoscalar meson operators for *f*, *h*, etc., can be either both strange or light, which we keep as separate operators but eventually include in the same correlator matrices.

$I = I_z$	$\mathbf{S}$	Single- and Two-Hadron Combinations
0	0	$\eta, \phi, G, \eta\eta, \eta\phi, \eta G, \phi\phi, \phi G, K\overline{K}, \pi\pi$
1	0	$\pi, \pi\pi, \eta\pi, \phi\pi, \pi G, K\overline{K}$
2	0	$\pi\pi$
$\frac{1}{2}$	1	$K, KG, K\pi, K\eta, K\phi$
$\frac{3}{2}$	1	$K\pi$
0	2	KK
1	2	KK
$\frac{1}{2}$	0	$N, N\eta, N\phi, N\pi, NG, \Delta\pi, \Lambda K, \Sigma K$
$\frac{3}{2}$	0	$\Delta, \Delta G, \Delta \eta, \Delta \Phi, \Delta \pi, N\pi, \Sigma K$
$\frac{5}{2}$	0	$\Delta \pi$
0	-1	$\Lambda, \Lambda\eta, \Lambda\phi, \Lambda G, \Sigma\pi, N\overline{K}, \Sigma\pi, \Xi K, \Sigma\pi$
1	-1	$\Sigma, \Sigma\eta, \Sigma\phi, \Sigma G, \Sigma\pi, N\overline{K}, \Delta\overline{K}, \Lambda\pi, \Xi K$
2	-1	$\Delta \overline{K}, \Sigma \pi$
$\frac{1}{2}$	-2	$\Xi,  \Xi\eta,  \Xi\phi,  \Xi G,  \Xi\pi,  \Lambda \overline{K},  \Sigma \overline{K},  \Omega K$
$\frac{3}{2}$	-2	$\Sigma \overline{K},  \Xi \pi$
0	-3	$\Omega,  \Omega\eta,  \Omega\phi,  \Omega G,  \Xi \overline{K}$
1	-3	$\Omega \pi,  \Xi \overline{K}$

Table 3.7: Possible operator combinations for various values of total isospin I, third isospin component  $I_3$ , and strangeness S. The central horizontal line separates bosonic states from fermionic ones. As per the usual convention, the s quark is assigned strangeness -1 such that the kaon  $(\overline{s}u)$  has positive strangeness.

to the three-parameter form  $Ae^{-Et} + Be^{-E(T-t)}$ . The two-parameter form leads to reduced statistical uncertainties in the resulting fit values. The condition C(t) = C(T-t) ensures such a relationship between the forward and backward propagating contributions, and this condition can be satisfied by choosing meson operators which are either even or odd under time reversal. The smeared, covariantly-displaced quark building blocks defined in equation 3.7 transform under time reversal as [101]

$$q^A_{a\alpha j}(\mathbf{x},t) \rightarrow (\gamma_4\gamma_5)_{\alpha\beta}q^A_{a\beta j}(\mathbf{x},T-t),$$
 (3.24)

$$\overline{q}^{A}_{a\alpha j}(\mathbf{x},t) \rightarrow \overline{q}^{A}_{a\beta j}(\mathbf{x},T-t)(\gamma_{4}\gamma_{5})_{\beta\alpha}.$$
 (3.25)

Using these transformation properties, we projected our lowest-energy meson operators onto purely even or purely odd transformation under time reversal. This was applied for the ground state pion  $(I = 1, A_{1u}^-)$ , kaon  $(I = \frac{1}{2}, A_{1u})$  and  $\eta$  isoscalar meson  $(I = 0, A_{1u}^+)$ , expected to be the states of lowest masses in the spectrum. Correlators using the even and odd operators exhibited fairly similar qualities, such as statistical uncertainties and excited-state contamination, with slightly better statistical errors for the odd operators, so those were chosen. Fig. 3.3 shows an example of a numerical test done to verify that our projected meson correlators obeyed the desired time symmetry.

#### 3.3.1 The Need for Definite Momentum for Each Hadron

Building multi-hadron operators as superpositions of products of single-hadron operators of definite momenta is efficient for creating a large number of two-hadron operators. It also produces two-hadron operators whose correlators having dramatically reduced contamination from unwanted higher-lying states, as shown in Fig. 3.4. An alternative method of building a two-pion I = 2 operators is given below:

$$(\pi\pi)^{A_{1g}^+}(t) = \sum_{\mathbf{x}} \pi^+(\mathbf{x}, t) \ \pi^+(\mathbf{x}, t).$$
(3.26)

This operator consists of a product of  $\pi(\mathbf{x}, t)$  fields at a single location, summed over all spatial sites to produce a total zero momentum. We refer to this as a  $\pi\pi$  localfield operator Such a  $\pi\pi$  local-field operator has the advantage that, for the I = 2channel at least, fixing a single  $\mathbf{x}_0$  on the source allows for very efficient computation of correlators using the "point-to-all" method, since it turns out that no same-time



Figure 3.3: Example of time symmetry verification for a particular pion correlator, correlating a single-site (SS)  $A_{1u}^- I = 1$  operator with a singly-displaced operator in that same channel. The black curve shows the correlator with jackknife error bars, and the red curve shows the same correlator flipped in time to show that it matches to within statistical error. Note that the region of single-exponential decay in the correlator appears linear due to the log scale. The correlator is calculated from 25 configurations of our  $16^3 \times 128$ ,  $m_{\pi} \approx 400$  MeV pruning and testing ensemble.



Figure 3.4: Comparison of  $\pi\pi$  local-field operators, such as that expressed in Eq. 3.26, against operators with definite momentum for each meson, as in our own two-hadron operators (building blocks as in equation 3.23). In each case, the  $\pi\pi$  local-field operator shows a dramatic increase in excited state contamination over the definite-momentum operators.

quark lines are necessary for that isospin channel. However, we have found that the lack of definite momentum for each hadron allows the operator to excite much more high-energy state contamination than it would if each hadron had fixed momentum. Figure 3.4 shows a comparison of fixed-momentum  $\pi\pi$  operators against local-field operators, such as that in Eq. (3.26), for two different isospin channels. In each case, the effective masses should eventually plateau at the same value since the lowest state is the same, but the local-field operator shows a much higher value at finite time, such that the actual energy would be nearly impossible to extract.

## **3.4** Single-Hadron Operator Selection

Projecting our smeared, displaced building blocks onto definite symmetry sectors, as outlined above, leads to a very large set of single-hadron operators, and the number of multi-hadron operators possible is also large. Since we expect only a handful of single-hadron states in any channel (based on experimental measurements), it is not necessary to use all of the hundreds of operators that can be designed. To make our spectrum computations practical, it is necessary to narrow down the extensive list to a subset of operators that are effective for extracting the energy levels of interest. We refer to this process as "pruning" the operator sets. We choose operators whose correlators have very small statistical uncertainties and are independent from each other, as determined by the condition number of their renormalized correlation matrices at small time separations. We also take into account their efficacy at producing the states of interest, as determined from small-lattice low-statistics runs. This has been completed for single-hadron operators in all symmetry channels, as discussed in Ref. [25]. We only review and briefly update those results here. New progress on multi-hadron operator pruning will be presented in Ch. 5.

The general procedure for single-hadron operator selection is as follows;

- Calculate the diagonal elements of the correlator matrix (same source/sink operator) for all operators, and discard those that have unacceptably large statistical error.
- Compute the full correlation matrix of the chosen subset of operators, and calculate the condition number  $(CN_{t=1} \text{ in Eq. } (2.71))$  of all possible subsets of those.
- Choose one of those subsets based on the criteria of a maximal set with a low condition number, and verify by variational analysis that these lead to an acceptable preliminary energy spectrum.

These steps were carried out on a small  $16^3$  ensemble, where inversions and operator calculations were inexpensive. More recent work has used our stochastic method (to be described later) on larger  $24^3$  and  $32^3$  ensembles.

For the purposes of computing single-hadron correlation functions, it suffices to compute operators for only one row, since the energies of all rows should be statistically equivalent. However, for those operators which had especially low statistical noise, and thus, were marked for inclusion as part of multi-hadron operators, it was necessary to produce operators for all rows of the irreducible representation, as all of these might appear as terms in multi-hadron operators. Also, for moving mesons and baryons, it is necessary to construct operators in all momentum directions, since these are needed for multi-hadron states with fixed total spin quantum numbers. For instance, an S-wave two-meson operator with zero total momentum might take a form such as

$$O_{MM} = \sum_{\mathbf{p}} M_l(\mathbf{p}, t) M_{l'}(-\mathbf{p}, t)$$
(3.27)

where the sum over  $\mathbf{p}$  ranges over the various directions allowed on the lattice. In an *S*-wave, all of these terms appear with the same coefficient, but in general, they might each have a different coefficient to ensure a given total quantum number of the multi-hadron operator. These coefficient calculations were again automated in MAPLE, with the same goal of obtaining irreducibly-transforming operators, as in Eq. (3.9).

In addition to different momentum directions for single-hadrons, we also need to choose how large in momentum magnitude to explore. Calculating all momenta  $\mathbf{p}$  is unnecessary since we are only interested in a given low-energy region of the spectrum. As a rough guideline for this low-energy region, we focused on energies less than  $E_{\rm cut} \sim 0.5a_t^{-1}$ , corresponding to about two and a half times the mass of our nucleon ground state. This choice was made based on several factors, including computational feasibility, as well as considerations of which energy regions are experimentally well-known, and so would yield useful comparisons.

Based on this cut-off energy  $E_{\text{cut}}$ , we calculated a maximum momentum **p** for each moving single-hadron operator channel as follows:

- 1. For a particular irrep of the little group, use lattice group subduction (see Table 3.4) to infer which stationary  $O_h$  irreps subduce to that little group irrep.
- 2. Based on preliminary spectrum results obtained from small-lattice  $|\mathbf{p}| = 0$  pruning, look up the energies of levels in those  $|\mathbf{p}| = 0$  irreps.
- 3. Estimate the energies of the moving versions of those states by assuming a continuum-like dispersion relation  $E = \sqrt{\mathbf{p}^2 + m_0^2}$ .
- 4. The lightest possible zero-momentum state attainable with any single-hadron operator is obtained by combining it with a pion with opposite momentum; thus, calculate the energies of each of those moving states combined with a pion, assuming no interaction.
- 5. Count how many of those hypothetical [hadron + pion] energy states fall below the cutoff  $E_{\text{cut}}$ , and try to include that many moving hadron operators for the little group.

The results of the process for a few channels in the I = 1, S = 0 sector are shown in Appendix A. Those momenta and all lesser momenta possible were calculated for any operators intended for use in multi-hadron operators, while single-hadron operators (those which were somewhat more noisy but possibly useful for excited-state coupling) were only calculated with  $|\mathbf{p}| = 0$ . Appendix A also shows the number of single-hadron and multi-hadron operators chosen in each channel.

## 3.5 A Novel Glueball Operator

Glueballs are hypothetical bound states of gluons, so it is reasonable to suspect that operators made from gauge links should be important for exciting these states on the lattice. Traditionally, these operators have been made out of loops of gauge links, such as those used in the construction of the lattice gauge action. However, a similarly gauge-invariant quantity can be produced by calculating the eigenvalue of any gauge-covariant lattice operator, such as the gauge-covariant Laplacian. Since some of these eigenvalues are already calculated in the course of LapH smearing, it would be convenient if these could be assembled into a good operator for coupling to glueballs on the lattice.

The simplest such operator is the sum of all eigenvalues of the smeared Laplacian eigenvalues below the cutoff  $\sigma_s$ :

$$G_{\tilde{\Delta}}(t) = -\mathrm{Tr}\Big(\Theta(\sigma_s - \tilde{\Delta}(t)) \ \tilde{\Delta}(t)\Big) = \sum_{\lambda_i < \sigma_s} \lambda_{i,t} \approx \sum_{i=1}^{N_v} \lambda_{i,t}, \qquad (3.28)$$

where  $\hat{\Delta}(t)$  is the covariant Laplacian defined on stout-smeared links on lattice time slice t, and  $\lambda_{i,t}$  denotes the  $i^{th}$  eigenvalue of the negative covariant Laplacian on time t. As discussed earlier, imposing the cutoff  $\sigma_s$  on all configurations is very nearly equivalent to simply keeping a fixed  $N_v$  eigenvectors on every time slice. The glueball operator proposed in Eq. (3.28) should have scalar quantum numbers, since the eigenvalues of the Laplacian are invariant under any spatial rotations and reflections.

We also considered operators in which these eigenvalues were included with various different weightings. Since the lower eigenvalues in the smearing subspace might couple more strongly to the ground state, we tried weighting those lower eigenvalues more heavily by defining

$$G_{\exp(-w\tilde{\Delta})} = -\text{Tr}\Big(\Theta(\sigma_s - \tilde{\Delta}(t)) \ e^{-w\tilde{\Delta}(t)}\Big) \approx \sum_{i=1}^{N_v} e^{-w\lambda_{i,t}}$$
(3.29)

for some positive constant w.



Figure 3.5: A comparison of dt=3 effective masses for scalar glueball operators on 551 configurations of our  $24^3 \times 128$ ,  $m_{\pi} \approx 240 MeV$  ensemble. The plaquette is built from stout-smeared gauge links with  $\rho = 0.1$ ,  $N_{\rho} = 10$ , and is averaged over all spatial directions to obtain a scalar operator  $(J = 0^{++})$ . The other operators are the LapH trace defined in Eq. (3.28) and the LapH trace exponential in Eq. (3.29). The three operators clearly yield very similar signal quality and coupling to ground and excited states.

Tests of  $G_{\tilde{\Delta}}$  and  $G_{\exp(-w\tilde{\Delta})}$  indicated that these LapH-eigenvalue glueball operators are equally as effective as traditional smeared plaquettes in coupling to the ground state in the scalar glueball channel. Figure 3.5 shows that effective masses for these operators have very similar shape and error bars, with possibly a slightly smaller error bar on the LapH eigenvalue-based operators. It is also apparent that there is little difference seen between a simple trace and the weighted sum of eigenvalues in Eq. (3.29). Given that the simple LapH trace is the most straightforward of these (we already have the eigenvalues computed in the course of quark field smearing), we will choose the LapH trace operator for our future calculations involving the scalar sector.

It is interesting to note that the effective masses in Fig. 3.5 appear to decay to a fairly light mass, lower than the energy range traditionally suspected for glueballs based on quenched calculations. Under the quenched approximation (neglecting the fermion determinant in the gauge field integral) the scalar glueball mass has been estimated to be around 1.6 GeV [45]. The glueball effective masses in Fig. 3.5 seem to drop well below 0.2  $a_t^{-1}$ , or below 1 GeV (the exact conversion to GeV depends on what hadron is used to set the scale, but in one scheme [22], the nucleon on sits at roughly 0.21  $a_t^{-1}$ ). This leads us to consider the fact that our scalar glueball operators have the same quantum numbers as a two-pion state in an S-wave, and it is mixing with this lighter state which may result in our glueball effective mass decaying to lower energies at large time. There are also isoscalar meson states possibly mixing, and even kaon-antikaon states may appear. It will be important to take into account any mixing between glueball, single-hadron, and multi-hadron operators in this channel to extract the energies reliably. This will be the subject of future work, and will not be further investigated here.

# Chapter 4

# **Stochastic LapH Method**

The most expensive part of our calculation is the computation of quark propagators, which involves the inversion of the Dirac matrix. Fortunately, the exact inversion of the Dirac matrix is unnecessary, and stochastic estimates of the inverse can improve the efficiency of the calculation without sacrificing accuracy in the hadron masses extracted. In this chapter, we present a new, especially-effective method of estimating quark propagators. This method utilizes the LapH-smeared quark operators discussed in Ch. 3, and enables the calculation of correlator matrices involving both single- and multi-hadron hadron operators.

In Sec. 4.1, we introduce the idea of stochastic subsampling in Monte-Carlo integration, and briefly illustrate how a "noisy" estimate of some configuration-byconfiguration observable can result in little or no additional uncertainty in the ensemble average of that observable. Since the observables of interest to us are built from various products of the inverse of the lattice Dirac matrix, Sec. 4.2 discusses a powerful method of estimating large matrix inverses, involving variance reduction by *noise dilution*.

In Sec. 4.3, we introduce the *stochastic LapH* method, a new propagator calculation method whose merit has been demonstrated recently in Refs. [22,24,25,101,107]. Numerical tests are shown which establish that the stochastic LapH method succeeds especially well at providing low-variance inverse estimates for the LapH-smeared observables that we consider. Not only does the method outperform other noise dilution schemes used in lattice QCD, but its cost also exhibits weak volume dependence which allows it to work well on large lattices. The tests shown in this chapter are primarily on small  $16^3$  lattices, but results in Ch. 5 will be shown on larger  $24^3$  and  $32^3$  lattices. In the last section of this chapter, details of the implementation of stochastic LapH are discussed, especially regarding multi-hadron correlation functions. The large number of Wick contractions involved in these correlators, and the same-time quark lines that are often included, are both conveniently handled in stochastic LapH. In Sec. 4.4, we also discuss the use of noise averaging (permuting various inverse estimates between different quark lines) and explain our choices of when to use it in baryon and meson quark lines. Some practical limitations such as disk space play a role in these choices.

## 4.1 Motivation for Stochastic Sub-Sampling

Imagine that we wish to calculate the ensemble average of some function  $g(\vec{U})$  for some distribution  $p(\vec{U})$  on a very large, many-dimensional space of  $\vec{U}$ . This is clearly analogous to the weighting function on gauge fields and the gauge integral in Eqs. (2.30) and (2.31), but we maintain generality for the moment. The Monte-Carlo method of carrying out such a calculation is to draw some  $N_U$  samples  $\vec{U}_i$  from the distribution  $p(\vec{U})$  using Markov chain updating, then approximate the integral by

$$\langle g(\vec{U}) \rangle_{\vec{U}} = \int \mathcal{D}U \ p(\vec{U}) \ g(\vec{U}) \approx \frac{1}{N_U} \sum_{i=1}^{N_U} g(\vec{U}_i).$$
 (4.1)

For large  $N_U$ , the statistical error on such an estimate can be expressed in terms of the square root of the variance,

$$\sigma_U \approx N_U^{-1/2} \sqrt{\langle g(\vec{U})^2 \rangle_{\vec{U}} - \langle g(\vec{U}) \rangle_{\vec{U}}^2}, \qquad (4.2)$$

where the angle brackets  $\langle ... \rangle_{\vec{U}}$  denote an average over the ensemble  $\vec{U}_i$  generated with distribution  $p(\vec{U})$ . Eq. 4.2 assumes independent sampling from the ensemble, but can be generalized to the case of correlated data [69].

Suppose the function  $g(\vec{U})$  is very expensive to calculate on each  $\vec{U}_i$ , as is the hadronic correlator in lattice QCD which involves products of the inverse of a large matrix. In this case, we can introduce new (unphysical) integration variables  $\vec{\eta}$  such that  $g(\vec{U}, \vec{\eta})$  is much easier to calculate, and such that  $g(\vec{U})$  can be regained by averaging over  $\vec{\eta}$ ,

$$g(\vec{U}) = \int \mathcal{D}\eta \ g(\vec{U}, \vec{\eta}) \approx \frac{1}{N_{\eta}} \sum_{j=1}^{N_{\eta}} g(\vec{U}, \vec{\eta}_j).$$
(4.3)

where  $\vec{\eta}_j$  are sampled with uniform probability density<sup>1</sup>. Using  $N_{\eta}$  subsamples to estimate each  $g(\vec{U}_i)$ , the ensemble average for the observable g can now be written as

$$\langle g(\vec{U}) \rangle_{\vec{U}} = \langle g(\vec{U}) \rangle_{\vec{U},\vec{\eta}} = \int \mathcal{D}U \ \mathcal{D}\eta \ p(\vec{U}) \ g(\vec{U},\vec{\eta}) \approx \frac{1}{N_U N_\eta} \sum_{i=1}^{N_U} \sum_{j=1}^{N_\eta} g(\vec{U}_i,\vec{\eta}_j).$$
 (4.4)

If  $g(\vec{U}, \vec{\eta})$  is much easier to calculate than  $g(\vec{U})$ , and the above estimate is sufficiently accurate, then a significant reduction in computation cost can be achieved. To determine the increase in statistical uncertainty, we can write the observable  $g(\vec{U}, \vec{\eta})$ in terms of its deviation  $\delta$  from the exact  $g(\vec{U})$ , defining  $g(\vec{U}, \vec{\eta}) = g(\vec{U}) + \delta(\vec{U}, \vec{\eta})$ . The Monte-Carlo estimate in Eq. (4.4) can then be written

$$\langle g(\vec{U}) \rangle_{\vec{U},\vec{\eta}} \approx \frac{1}{N_U N_\eta} \sum_{i=1}^{N_U} \sum_{j=1}^{N_\eta} \left[ g(\vec{U}_i) + \delta(\vec{U}_i,\vec{\eta}_j) \right]$$
  
=  $\frac{1}{N_U} \sum_{i=1}^{N_U} g(\vec{U}_i) + \frac{1}{N_U N_\eta} \sum_{i=1}^{N_U} \sum_{j=1}^{N_\eta} \delta(\vec{U}_i,\vec{\eta}_j).$  (4.5)

We can see from Eq. (4.5) that the statistical error on  $\langle g(\vec{U}) \rangle_{\vec{U},\vec{\eta}}$  is due to two sources, corresponding to the first and second terms in the last line in Eq. (4.5). The first term is clearly the same as in Eq. (4.2), the error due to the finite sampling of  $\vec{U}$ . The second term represents the additional variance due to the finite sampling of  $\vec{\eta}$ . In the (somewhat simplified) case that the deviation  $\delta(\vec{U},\vec{\eta})$  is independent of  $\vec{U}$ , the second term is a completely independent sampling from the first term,

$$\langle g(\vec{U}) \rangle_{\vec{U},\vec{\eta}} \approx \frac{1}{N_U} \sum_{i=1}^{N_U} g(\vec{U}_i) + \frac{1}{N_\eta} \sum_{j=1}^{N_\eta} \delta(\vec{\eta}_j)$$
 (4.6)

<sup>&</sup>lt;sup>1</sup> More generally,  $\eta$  can be drawn from some non-uniform distribution, so long as the expectation value of  $g(U, \eta)$  is still g(U), but since the uniform distribution is sufficient for this discussion, it is used here for simplicity.

and the errors would then combine in quadrature,

$$\sigma_{\rm net} = \sqrt{\sigma_U^2 + \sigma_\eta^2} \tag{4.7}$$

$$\sigma_{\eta} = N_{\eta}^{-1/2} \sqrt{\langle \delta(\vec{\eta})^2 \rangle_{\vec{\eta}} - \langle \delta(\vec{\eta}) \rangle_{\vec{\eta}}^2}.$$
(4.8)

The form of Eq. (4.7) conveys the key fact that for some regime where  $\sigma_{\eta} < \sigma_{U}$ , the dependence of  $\sigma_{\text{net}}$  on  $\sigma_{\eta}$  will be very small. In this regime, relaxing  $\sigma_{\eta}$  even by orders of magnitude may have little or no effect on the net statistical error.

In the case that the deviation  $\delta$  is *not* independent of  $\vec{U}$ , equation 4.7 would not strictly apply. However we would still expect a similar phenomenon for small enough  $\delta(\vec{U},\vec{\eta})$ , that the total variance is dominated by that of the first term in Eq. (4.5),  $\sigma_U$ . In that regime, it is greatly advantageous to trade off some accuracy in  $\langle g(\vec{U}_i,\vec{\eta}) \rangle_{\vec{\eta}}$  in favor of computational efficiency, if possible.

#### 4.2 Stochastic Inversion of a Large Matrix M

The relevant observables in lattice QCD are the temporal correlation functions of hadron and multi-hadron operators, which involve the inverse of a very large matrix M. Following the reasoning of Sec. 4.1, we would like to replace the exact  $M^{-1}$ with some less-expensive estimate of that inverse. This estimate will be defined via additional integration variables  $\eta$ , and we only need to sample  $\eta$  enough that uncertainty in our observables approaches the gauge noise.

To exactly invert a very large semi-diagonal matrix M, we iteratively solve for the vector  $X^{(i)}$  in  $MX^{(i)} = \mathbf{e}_i$ , where  $\mathbf{e}_i$  is the  $i^{th}$  basis vector in the space, and repeat for any column i in which  $M^{-1}$  elements are needed. The conjugate gradient and related methods for this task have already been discussed in Ch. 2. In the simplest form of stochastic inversion, we replace the basis vector  $\mathbf{e}$  with a "noise vector"  $\eta$  filled with randomly generated elements. The distribution of random elements must meet the requirements

$$E\left(\eta_{i}\eta_{j}^{*}\right) = \delta_{ij},\tag{4.9}$$

$$\mathbf{E}\left(\eta_{i}\right) = 0,\tag{4.10}$$

where E(A) denotes the expectation value of random variable A over its probability distribution p(A), or  $E(A) \equiv \int A p(A) dA$ . After numerically solving a single linear system  $MX = \eta$ , we then have a consistent and unbiased estimator of the full  $M^{-1}$ through

$$\mathbf{E}\left(X\eta^{\dagger}\right) = \mathbf{E}\left(M^{-1}\eta\eta^{\dagger}\right) = M^{-1}\mathbf{E}\left(\eta\eta^{\dagger}\right) = M^{-1}.$$
(4.11)

Some commonly-used specific forms for the random variable  $\eta$  are:

- Real Gaussian noise, where  $\eta_i$  is selected from a distribution  $p(\eta_i) = \exp(-\eta_i^2)/\sqrt{2\pi}$
- Complex Gaussian noise, where  $\eta$  is selected from the distribution  $p(\eta_i) = \exp(-\eta_i^*\eta_i)/\pi$
- $Z_N$  noise, where  $\eta_i$  takes values  $e^{2\pi n_i/N}$  for random integer  $n_i$  in [0, N-1]
- U(1) noise, where  $\eta_i = \exp(i\theta_i)$  with  $\theta_i$  drawn evenly from the range  $[0, 2\pi)$ .

The particular choice that we use is  $Z_4$  noise<sup>2</sup>, where elements of  $\eta$  are selected at random from [1, i, -1, -i].  $Z_N$  noise was chosen since unlike Gaussian noise, it obeys  $\eta_i \eta_i^* = 1$  (without the need to take an expectation value), which proves useful in inversion with noise dilution. N = 4 was chosen because we found relatively little dependence of correlator variances on N, as long as  $N \ge 4$ . It is easy to see that filling  $\eta$  with  $Z_4$  noise satisfies Eqs. (4.9) and (4.10). The average of any set of evenlyspaced points on the unit circle in the complex plane will be zero, thus Eq. (4.9) holds. Eq. (4.10) can be seen from the fact that the product of two independent  $Z_4$  randoms,  $\eta_i \eta_j$ , is itself another  $Z_4$  random variable.

In a sampling of any complex variables z, a measure of the spread of the distribution is the complex variance

<sup>&</sup>lt;sup>2</sup>The label  $Z_4$  noise refers to the group  $Z_4$  whose representation is exactly the elements [1, i, -1, -i] from which we sample for this type of noise, but the group-theoretical point of view is not important here.

$$\operatorname{Var}(z) = \operatorname{E}(|z - \operatorname{E}(z)|^2) = \operatorname{E}(zz^*) - \operatorname{E}(z)\operatorname{E}(z)^*$$
 (4.12)

Using this definition along with Eqs. (4.9) and (4.10), one can arrive at an expression for the complex variance on some element  $M_{ik}^{-1}$  of the approximate inverse in Eq. (4.11), as

$$\operatorname{Var}([M^{-1}\eta\eta^{\dagger}]_{ik}) = \sum_{j \neq k} M_{ij}^{-1} M_{ij}^{-1*} \qquad \text{(no sum over i,k)}, \tag{4.13}$$

where we have also used the expectation of a product of four  $Z_4$  noises,

$$\mathcal{E}(\eta_i \eta_j^* \eta_k \eta_l^*) = \delta_{ij} \delta_{kl} + \delta_{il} \delta_{jk}^{k \neq l}.$$
(4.14)

The  $k \neq l$  condition on the second term is necessary to avoid double-counting the case where i = j = k = l.

By averaging  $N_{\text{seed}}$  estimates such as in Eq. (4.11) each with different noise vectors  $\eta$ , we can obtain better estimates of  $M^{-1}$ , with the variance decreasing approximately with  $N_{\text{seed}}^{-1}$ . Thus, this basic estimate technically satisfies the goals discussed in the previous section; we have a tunable, unbiased estimate of our observable, and we could (theoretically, at least) adjust the number of noise seeds  $N_{\text{seed}}$  until the statistical error due to stochastic inversion is comparable to the gauge noise. However, it turns out that simple stochastic estimation would require such a large  $N_{\text{seed}}$  as to make the efficiency tradeoff unfavorable.

Fortunately, there is a well-known improvement to this basic stochastic inversion technique. The improvement, known as stochastic inversion with *noise dilution*, involves "projecting out" some of the random noise in  $\eta$  by defining dilution subspaces b and projection operators  $P^{(b)}$  onto these subspaces. If we now numerically solve  $MX^{[b]} = P^{(b)}\eta$  for each subspace b, then we have an estimate of  $M^{-1}$  via

$$E\left(\sum_{b} X^{[b]} \left[P^{(b)}\eta\right]^{\dagger}\right) = E\left(\sum_{b} M^{-1} P^{[b]}\eta\eta^{\dagger} P^{[b]}\right)$$
$$= M^{-1} \sum_{b} P^{(b)} E\left(\eta\eta^{\dagger}\right) P^{[b]} = M^{-1} \sum_{b} P^{[b]} = M^{-1}.$$
(4.15)

The variance on such an estimate should be lower than the basic estimate in

Eq. (4.11), since many of the elements of  $\eta \eta^{\dagger}$  are projected to exactly zero, rather than merely averaging to zero. Another way of seeing this noise reduction is to work out the expression for the variance on some element  $M_{ik}^{-1}$  of the stochastic estimate in Eq. (4.15). That variance comes to

$$\operatorname{Var}\left(\sum_{b} X_{i}^{[b]} \left[P^{[b]} \eta\right]_{k}^{*}\right) = \sum_{j \in b_{k}, j \neq k} M_{ij}^{-1} M_{ij}^{-1*} \qquad \text{(no sum over i,k)}, \tag{4.16}$$

where  $b_k$  is the dilution subspace which contains the element k. This variance should be smaller than the variance in Eq. (4.13), since the terms in Eq. (4.16) are a subset of those in Eq. (4.13), and all of the terms involved are of the form  $zz^*$ , and therefore, real and positive.

The amount of noise reduction depends on the actual matrix itself and the choice of dilution subspaces b. However, we can infer from these expressions that noise reduction through dilution is generally more effective than simply computing more noise seeds. This is clear from the fact that adding more noise seeds diminishes the variance in proportion to  $1/N_{\text{seed}}$ , never actually reaching zero, whereas the variance in Eq. (4.16) drops to exactly zero with a finite amount of effort – namely, when the number of elements in  $b_k$  drops to one, and there are zero terms on the right hand side of Eq. (4.16).

The use of noise dilution does not preclude also averaging over different noise seeds. Just as in simple stochastic estimation, we can append an additional index rto indicate different noise seeds, and sum over those to further reduce variance. Note that the estimation of *products* of inverses requires different noise seeds for each term in the product in order to ensure an unbiased estimate of the product. To see this, consider estimating some product of elements  $M_{ij}^{-1}M_{kl}^{-1}$  using the same noise vector  $\rho$ using stochastic inversion with noise dilution as given in Eq. (4.15). Again employing Eqs. (4.9) and (4.14), we arrive at

where  $b_j$  and  $b_l$  are the subspaces in which elements j and l reside, respectively.

The first term in Eq. (4.17) is the desired product, whereas the second term clearly skews the estimate in the case that j and l are in the same dilution subspace. Since we usually consider matrix products which sum over some common indices between the two  $M^{-1}$  factors, this bias term must be avoided by using a different noise vector  $\rho$  (that is, using different random seeds  $r_1$ ,  $r_2$ , etc, and denoting the vectors  $\eta^{r_1}$ ,  $\eta^{r_2}$ ,...). One needs at least as many noise seeds as there are quark lines in the desired correlator. Some improvement in statistics can be gained by averaging over different permutations of noise seeds in the matrix product estimate, though the gain decreases for further permutations since the different estimates are not necessarily independent. Some discussion of our noise permutation choices follows in Sec. 4.4.

## 4.3 The Stochastic LapH Method

We now focus on the inversion of the lattice Dirac matrix, given in Eq. (2.29). One method of creating subspaces b is to project onto various groups of spins, colors, spatial lattice sites, and time, since those are the original bases in which the Dirac matrix is defined in the action. This approach has been explored in Refs. [108] and [106], among others. However, given the type of quark operators that we intend to use, a more natural option is to define dilution subspaces as *subsets of LapH eigenvectors*, rather than the spatial and and color indices. For all of the quark propagators that we will need in our correlators, the quark on either end is a smeared, displaced object as in Eq. (3.7) and (3.8). Thus the Dirac matrix elements that we need have the form

$$\mathcal{Q}_{a\alpha;b\beta}^{(AB)} = \delta_{AB} \left[ D^{(j_{\alpha})} \mathcal{S} \Omega^{(A)-1} \mathcal{S} D^{(j_{\beta})\dagger} \right]_{a\alpha;b\beta}$$
(4.18)

where the smearing matrix S is defined in Eq. (3.2), and  $\Omega^{(A)}$  is the A-flavor Dirac matrix times  $\gamma_4$ , as noted in Eq. (3.5). The displacement operator D is defined in Eq. (3.6) and its displacement path corresponds to the quark spin indices  $\alpha$  and  $\beta$ . Since the smearing matrix projects onto a subset of low-lying eigenvectors of the covariant Laplacian, we only need elements of  $\Omega$  corresponding to those vectors. Thus, we can define smearing subspaces that span some subset of low-lying eigenvectors, some of the four Dirac spin indices, and time. This is the essence of the stochastic LapH method.

In the stochastic LapH method, noise vectors  $\rho$  are generated as a  $Z_4$  phase for each point in LapH eigenvector/spin/time space, and projectors  $P^{(b)}$  are chosen to project onto certain subspaces in that basis. Sources are created by applying such projectors to  $\rho$ , then using the eigenvector matrix  $V_s$  as in Eq. (3.3) to convert LapH coefficients back to spatial/color coordinates in order to solve

$$\Omega X^{[b]} = V_s P^{(b)} \rho, \tag{4.19}$$

to obtain sinks  $X^{[b]}$ . Next, smeared-displaced source and sink vectors are formed by displacing  $V_s P^{(b)}\rho$ , and by smearing and displacing the  $X^{[b]}$ , to obtain

$$\varrho_{\alpha}^{[b]}(\rho) = D^{(j_{\alpha})} V_s P^{(b)} \rho_{\alpha}, \tag{4.20}$$

$$\varphi_{\alpha}^{[b]}(\rho) = D^{(j_{\alpha})} \mathcal{S} X^{[b]} = D^{(j_{\alpha})} \mathcal{S} \Omega^{-1} V_s P^{(b)} \rho_{\alpha}.$$

$$(4.21)$$

Finally, the contraction of smeared-displaced quarks in Eq. (4.18) can be estimated using

$$\mathcal{Q}_{\alpha\beta}^{(AB)} \approx \delta_{AB} \sum_{b} \varphi_{\alpha}^{[b]}(\rho) \varrho_{\beta}^{[b]}(\rho)^{*}.$$
(4.22)

In some cases, it is useful to estimate this quark propagator in a slightly different way, exploiting the symmetry of  $\gamma_5$ -Hermiticity introduced in Eq. (2.32). This leads to the expression

$$\mathcal{Q}_{\alpha\beta}^{(AB)} \approx \delta_{AB} \sum_{b} \overline{\varrho}_{\alpha}^{[b]}(\rho) \overline{\varphi}_{\beta}^{[b]}(\rho)^{*}$$
(4.23)

with

$$\bar{\varrho}(\rho) = -\gamma_5 \gamma_4 \varrho(\rho), \qquad \bar{\varphi}(\rho) = \gamma_5 \gamma_4 \varphi(\rho).$$
 (4.24)

As before, a better estimate can be achieved in both Eqs. (4.22) and (4.23) by averaging over different noise vectors  $\rho$ , which would then take on another index r for noise seed number.

The separation of the quark line  $\mathcal{Q}$  into two quantities  $\rho$  and  $\varphi$  is very convenient for later stages of the calculation. For example, if one of the quarks in  $\mathcal{Q}$  is part of a meson on the source time and the other is part of a different meson on the sink, one can construct these mesons and store them separately, then contract the dilution index b at the time of constructing correlation matrices. For another example, baryon functions are constructed as [22]

$$\mathcal{B}_{l}^{[b_{1}b_{2}b_{3}]}(\varphi_{1},\varphi_{2},\varphi_{3};t) = c_{\alpha\beta\gamma}^{(l)}\sum_{\mathbf{x}} e^{-i\mathbf{p}\cdot\mathbf{x}}\varepsilon_{abc}\varphi_{a\alpha\mathbf{x}t}^{[b_{1}]}(\rho_{1})\varphi_{b\beta\mathbf{x}t}^{[b_{2}]}(\rho_{2})\varphi_{c\gamma\mathbf{x}t}^{[b_{3}]}(\rho_{3}), \qquad (4.25)$$

for  $\varphi$  as in Eq. 4.21, and similarly for source vector  $\varrho$ . The complex coefficients  $c_{\alpha\beta\gamma}^{(l)}$  are calculated via the group-theoretical considerations discussed in Ch. 3 for each compound set of quantum numbers (*l*). Similarly, a meson function can be defined as

$$\mathcal{M}_{l}^{[b_{1}b_{2}]}(\varrho_{1},\varphi_{2};t) = c_{\alpha\beta}^{(l)} \sum_{\mathbf{x}} e^{-i\mathbf{p}\cdot(\mathbf{x}+\frac{1}{2}(\mathbf{d}_{\alpha}+\mathbf{d}_{\beta}))} \varrho_{a\alpha\mathbf{x}t}^{[b_{1}]}(\rho_{1})^{*} \varphi_{a\beta\mathbf{x}t}^{[b_{2}]}(\rho_{2}).$$
(4.26)

It is important that in the expressions on the right of Eqs. (4.25) and (4.26), the lower indices for color, spin, position and time are all summed over, and the remaining indices are only the dilution subspaces  $[b_1, b_2, ...]$ . This is a key point, since the number of these subspaces b is manageable, and even tensors with three uncontracted dilution indices are still feasible to store on disk.

These baryon and meson functions can be contracted into various hadronic correlators in a convenient fashion, which we will discuss in the following section. They can also be assembled conveniently into multi-hadron operators on a single time slice. The contraction of various dilution indices in these composite single-time-slice operators is then carried out according to the Wick contraction of Grassmann variables, and can be represented concisely by diagrams as in Fig. 2.1 for the case of a single isoscalar meson. In Sec. 4.4 we give examples of such figures for more complicated multi-hadron correlators which will be analyzed in Ch. 5.

While the stochastic LapH method allows these convenient calculational forms, it is not obvious that it should fare any better than color-and-spatial dilution schemes as far as noise reduction is concerned. Thus, we return to the question of numerical tests to verify the efficacy of the method. A large number of dilution schemes were compared on small 16<sup>3</sup> lattices, as shown in Fig. 4.1.  $N_D$  is the number of dilution subspaces per quark line, so that two points appearing at the same  $N_D^{-1/2}$  require the same computational expense, regardless of what the two dilution schemes are.



Figure 4.1: Comparison of statistical error relative to gauge noise for a TDT nucleon correlator at time separation 5, for various dilution schemes on the same set of  $16^3 \times 128$  gauge configurations.  $N_D$  indicates the number of dilution subspaces employed, so dilution schemes at the same  $N_D^{-1/2}$  require the same computational effort. The LapH dilution points in blue clearly decrease to the gauge noise limit significantly faster than the lattice points, approaching  $\sigma_g$  faster by a factor of at least an order of magnitude. From Ref. [22].

Clearly, the LapH noise scheme exhibits far lower statistical errors for similar expense in traditional lattice-color-space dilution. This is a central result of Refs. [22, 24, 25].

While Fig. 4.1 deals with baryonic correlator elements that involve forward-time quark lines, the stochastic LapH method has also been demonstrated to be particularly effective at calculating same-time quark lines. As discussed in Ch. 2, these must be calculated at each sink time and source time desired for a correlation function, and have traditionally been a barrier to the study of multi-hadron and isoscalar correlation functions. Figure 4.2 shows the effective mass of a diagonal correlator of a single-site  $\eta$  isoscalar meson  $(A_{1u}^+)$  in exact inversion versus stochastic LapH inversion. Due to the use of dilution in time as well as LapH eigenvector space, a large reduction in computational expense is achieved, dropping the number of inversions by more than two orders of magnitude. The fact that the additional noise has nearly no effect on the net statistical error is indicative of the regime discussed in Sec. 4.1, where the gauge noise  $\sigma_U$  is the main driver of  $\sigma_{net}$ .

To denote specific LapH dilution schemes, a notation that has been used in previous work [22] writes the number of subspaces spanning each dimension as a triplet, (T,S,L) for time, spin, and LapH eigenvector. Since there are different ways of split-



Figure 4.2: Comparison of  $\Delta t = 2$  effective masses for  $\eta$  isoscalar meson, both connected and disconnected piece included. The stochastic LapH estimate clearly matches the statistical error of the exact calculation, indicating that the noise introduced from stochastic inversion is minimal compared to the gauge noise, while using less than a twentieth the number of Dirac matrix inversions. The errors are calculated via jackknifing, and both effective masses are generated from the same 25 configurations of our 16<sup>3</sup> ensemble, where exact inversion is feasible.

ting up the subspaces – namely, a group of successive indices can go into the same subspace, or every  $n^{th}$  index can go into the same space – these two schemes are referred to as "block" and "interlace," respectively, and an "I" or "B" is inserted into the triplet. For example, if every sixteenth time slice shares a subspace, each spin gets its own subspace, and each group of eight consecutive LapH eigenvectors are allotted to the same subspace, the scheme would be denoted (TI16,S4,LB8). If the subspaces contain only a single index in some dimension, as is true for all indices in exact inversion, we substitute an "F" (full) rather than the number of subspaces, so S4 would be written SF.

In terms of the projection matrices  $P^{(b)}$  introduced in Eq. (4.19), these dilution schemes are defined in the following way. For a particular space (time, spin, or LapH eigenvector), dilution projectors take the form

$$P_{ij}^{(b)} = \delta_{ij} \qquad b = 0 \qquad \text{(none)}$$

$$P_{ij}^{(b)} = \delta_{ij}\delta_{bi} \qquad b = 0, 1, \dots, N-1 \qquad \text{(full)}$$

$$P_{ij}^{(b)} = \delta_{ij}\delta_{b,Ki/N} \qquad b = 0, 1, \dots, K-1 \qquad \text{(interlace-}K)$$

$$P_{ij}^{(b)} = \delta_{ij}\delta_{b,i \mod k} \qquad b = 0, 1, \dots, K-1 \qquad \text{(block-}K)$$

$$(4.27)$$

The dilution projector for the vector space of the quark sources and sinks is the product of three such projectors for time, spin, and LapH eigenvector. The shorthand mentioned above consists of the first letter of a given space (such as S for spin), then B or I for block or interlace, and then the value K for that subspace.

The dilution scheme used in the stochastic LapH curve in Fig. 4.2 is (TI16,SF,LI8) for the same-time quark lines, and (TF,SF,LI8) for the fixed-time quark lines. The number of inversions is then  $8 \times 4$  for each fixed-time quark line. Also, there are two quark lines, and thus, two different noise seeds are required to avoid a bias, so a total of  $8 \times 4 \times 2 = 64$  inversions are needed for the connected diagram. For the disconnected part, we need only one noise seed since the source and sink times reside in different time dilution subspaces<sup>3</sup>, and the bias term in Eq. (4.17) will be zero; thus the number of inversions for the disconnected quark lines is  $16 \times 4 \times 8 = 512$ ,

<sup>&</sup>lt;sup>3</sup>In actuality, there are a few select time separations where the source and sink times may be in the same dilution subspace, names at time separations 16 and 32 since we will use TI16 dilution. In most cases, the effective mass shows the bias to be minimal – a jump in the effective mass at times  $t \pm \Delta t$  would indicate a significant bias, and these are not usually seen. But they are occasionally visible, and since we ended up employing two relative noise vectors in any case, we decided to enforce the use of different noise seeds on the source and sink for time separations 16 and 32.



Figure 4.3: The statistical error relative to the gauge noise of a correlator at time separation 5 of a triply-displaced nucleon operator.  $N_D$  is the number of dilution subspaces per source time and gauge configuration. The LapH dilution scheme at each point is indicated on the graph. For the highest dilution schemes considered, the dependence on volume is seen to be very weak. Figure from Ref. [22].

for a total of 576 inversions. The number of inversions required for the exact method is simply  $N_t \times N_s \times N_v$ , which for  $16^3$  lattices is  $128 \times 4 \times 32 = 16,384$ .

Furthermore, it turns out that the advantage of stochastic LapH increases with volume. The LapH-diluted estimates seem to permit maintaining the same dilution scheme even as the dimension of the Dirac matrix increases in proportion to the lattice volume. Figure 4.3 shows that, for sufficient dilution levels, the dependence of the statistical noise (relative to the gauge noise) is minimal. Thus, even as the number of Laplacian eigenvectors increases with volume (see Table 3.1), it is found that the same dilution scheme choices are sufficient. Each inversion does become more expensive, leading to a scaling approximately with volume V, but this is preferable to scaling with  $V^2$  as in standard Dirac matrix inversion, where the time for each inversion and the number of inversions both scale with volume.

Based on the fact that the ratio of the statistical error over the gauge noise starts to level out at unity around the dilution scheme (TF,SF,LI8), this scheme was chosen for use in source-to-sink quark lines, which are calculated for only a handful of source times widely separated to yield independent measurements. We choose four source times per configuration, spaced roughly evenly over the 128 times, doubling to eight source times for the  $32^3 \times 256$  lattices. For the same-time quark lines, where  $M^{-1}$  is contracted with itself on both the source and sink time of the correlator, quark sources are required on all times, not just the  $t_0$  values chosen. Therefore, a somewhat less intensive dilution scheme (TI16,SF,LI8) is chosen. The dilution subspace choices (TF,SF,LI8) and (TI16,SF,LI8) are referred to as fixed and relative schemes, respectively, and are used in all of the results to follow in Ch. 5.

## 4.4 Examples and Implementation Details

The meson and baryon functions in Eqs. (4.25) and (4.26) are assembled into correlators in the following manner. First, we need to analyze the possible ways that quarks in the source and sink operators can be contracted, so that we know which types of baryon and meson functions need to be computed. That also involves planning out which quark lines should be estimated using the  $\gamma_5$ -Hermiticity trick – that is, exploiting Eq. (4.23) to estimate an antiquark propagator in terms of a forwardspropagating quark line. Secondly, we need to decide on how many noise seeds and how many different noise permutations should be included.

The type of contractions possible depend on the number and flavors of quarks involved. Given that we intend to survey many different isospin sectors, we need to collect all possible contraction diagrams of mesons and baryons in order to determine which noises and quark sources and sinks to insert into meson and baryon functions that we compute. As an example, consider a correlator of a single baryon with some generic flavor content ABC. In terms of the irreducible baryon operators defined in Eq. (3.22) with combined quantum numbers indicated by l, the correlator is given by

$$C_{l\bar{l}}(t_F - t_0) = \frac{1}{N_t} \sum_{t_0} \left\langle B_l(t_F) \overline{B}_{\bar{l}}(t_0) \right\rangle_{U,\psi,\overline{\psi}}$$
$$= c_{\alpha\beta\gamma}^{(l)} c_{\overline{\alpha}\overline{\beta}\overline{\gamma}}^{(\bar{l})*} \left\langle \Phi_{\alpha\beta\gamma}^{ABC}(t_F) \overline{\Phi}_{\overline{\alpha}\overline{\beta}\overline{\gamma}}^{\overline{ABC}}(t_0) \right\rangle_{U,\psi,\overline{\psi}}. \tag{4.28}$$

If we express this in terms of smeared, displaced Grassmann quark fields using equation 3.20, we obtain

$$C_{l\bar{l}}(t_F - t_0) = c^{(l)}_{\alpha\beta\gamma} c^{(\bar{l})*}_{\overline{\alpha}\overline{\beta}\overline{\gamma}} \sum_{\mathbf{x},\overline{\mathbf{x}}} \varepsilon_{abc} \varepsilon_{\overline{a}\overline{b}\overline{c}} e^{-i\mathbf{p}\cdot(\mathbf{x}-\overline{\mathbf{x}})} \\ \times \left\langle q^A_{a\alpha}(\mathbf{x}, t_F) q^B_{b\beta}(\mathbf{x}, t_f) q^C_{c\gamma}(\mathbf{x}, t_F) \ \overline{q}^{\overline{C}}_{\overline{c\gamma}}(\overline{\mathbf{x}}, t_0) \overline{q}^{\overline{A}}_{\overline{c\gamma}}(\overline{\mathbf{x}}, t_0) \overline{q}^{\overline{A}}_{\overline{a\alpha}}(\overline{\mathbf{x}}, t_0) \right\rangle_{U,\psi,\overline{\psi}}, \qquad (4.29)$$

where the brackets indicate averaging over the indicated fields and their corresponding action weighting  $e^{-S}$ . After integration over the fermion fields, we obtain an expression determined by Wick contraction of the quark fields of like flavor, as discussed in Sec. 2.1. The contraction of smeared, displaced quark fields results in quark lines Q defined in Eq. (4.18), and accounting for signs due to Grassmann commutation, Eq. (4.29) becomes

$$C_{l\bar{l}}(t_{F}-t_{0}) = c_{\alpha\beta\gamma}^{(l)}c_{\overline{\alpha}\overline{\beta}\overline{\gamma}}^{(\bar{l})*}\sum_{\mathbf{x},\overline{\mathbf{x}}} \varepsilon_{abc}\varepsilon_{\overline{a}\overline{b}\overline{c}}e^{-i\mathbf{p}\cdot(\mathbf{x}-\overline{\mathbf{x}})} \Big\langle \mathcal{Q}_{a\alpha;\overline{a\alpha}}^{(A\overline{A})}\mathcal{Q}_{b\beta;\overline{b\beta}}^{(B\overline{B})}\mathcal{Q}_{c\gamma;\overline{c\gamma}}^{C\overline{C}} \\ - \mathcal{Q}_{a\alpha;\overline{a\alpha}}^{(A\overline{A})}\mathcal{Q}_{b\beta;\overline{c\gamma}}^{(B\overline{C})}\mathcal{Q}_{c\gamma;\overline{b\beta}}^{C\overline{B}} - \mathcal{Q}_{a\alpha;\overline{b\beta}}^{(A\overline{B})}\mathcal{Q}_{b\beta;\overline{a\alpha}}^{(B\overline{A})}\mathcal{Q}_{c\gamma;\overline{c\gamma}}^{C\overline{C}} - \mathcal{Q}_{a\alpha;\overline{c\gamma}}^{(A\overline{C})}\mathcal{Q}_{b\beta;\overline{b\beta}}^{(B\overline{B})}\mathcal{Q}_{c\gamma;\overline{a\alpha}}^{C\overline{A}} \\ + \mathcal{Q}_{a\alpha;\overline{c\gamma}}^{(A\overline{C})}\mathcal{Q}_{b\beta;\overline{a\alpha}}^{(B\overline{A})}\mathcal{Q}_{c\gamma;\overline{b\beta}}^{C\overline{B}} + \mathcal{Q}_{a\alpha;\overline{b\beta}}^{(A\overline{B})}\mathcal{Q}_{b\beta;\overline{c\gamma}}^{(B\overline{C})}\mathcal{Q}_{c\gamma;\overline{a\alpha}}^{C\overline{A}} \Big\rangle_{U},$$

$$(4.30)$$

where we have written out the color subscripts on  $\mathcal{Q}$  that were implicit earlier.

If we then express each of these quark lines via the stochastic LapH estimate given in Eq. (4.22), we can regroup the factors into products of the baryon function given in Eq. (4.25),

$$C_{l\bar{l}}(t_F - t_0) = \left\langle \mathcal{B}_l^{[b_1 b_2 b_3]}(\varphi_1, \varphi_2, \varphi_3; t_F) \left[ \delta_{A\bar{A}} \delta_{B\bar{B}} \delta_{C\bar{C}} \mathcal{B}_{\bar{l}}^{[b_1 b_2 b_3]}(\varrho_1, \varrho_2, \varrho_3; t_0) - \delta_{A\bar{A}} \delta_{B\bar{C}} \delta_{C\bar{B}} \mathcal{B}_{\bar{l}}^{[b_1 b_3 b_1]}(\varrho_1, \varrho_3, \varrho_2; t_0) - \delta_{A\bar{B}} \delta_{B\bar{A}} \delta_{C\bar{C}} \mathcal{B}_{\bar{l}}^{[b_2 b_1 b_3]}(\varrho_2, \varrho_1, \varrho_3; t_0) - \delta_{A\bar{C}} \delta_{B\bar{B}} \delta_{C\bar{B}} \mathcal{B}_{\bar{l}}^{[b_3 b_2 b_1]}(\varrho_3, \varrho_2, \varrho_1; t_0) + \delta_{A\bar{C}} \delta_{B\bar{A}} \delta_{C\bar{B}} \mathcal{B}_{\bar{l}}^{[b_2 b_3 b_1]}(\varrho_2, \varrho_3, \varrho_1; t_0) + \delta_{A\bar{B}} \delta_{B\bar{C}} \delta_{C\bar{B}} \mathcal{B}_{\bar{l}}^{[b_3 b_1 b_2]}(\varrho_3, \varrho_1, \varrho_2; t_0) \right]^* \right\rangle_{U,\rho}.$$

$$(4.31)$$

The notation  $\rho_1$  and  $\varphi_1$  has been shortened from  $\rho^{[b_1]}(\rho_1)$  and  $\varphi^{[b_1]}(\rho_1)$ , respectively. This contraction of baryon tensors can be conveniently shown diagrammatically, in Fig. 4.4.

As another example, consider the correlation function of two mesons on the source



Figure 4.4: These diagrams represent the terms present in the stochastic LapH expression for a single baryon correlator, resulting from the six ways of Wick-contracting the smeared, displaced quark fields. Each box represents one of the baryon functions as in Eq. (4.31). The fields on the left are the sink times  $t_F$  and the fields on the right are on the source time  $t_0$ , and conjugation of hadron functions on  $t_0$  is implied.

time with a single meson on the sink time. First, the correlator is expressed in terms of meson operators (Eq. (3.21)) and then smeared, displaced quark fields,

$$C_{l\bar{l}''}(t_{F}-t_{0}) = \left\langle M_{l} \; g_{\bar{l}l'}^{(\bar{l}'')} \overline{M}_{\bar{l}} \overline{M}_{\bar{l}'} \right\rangle_{U,\psi,\overline{\psi}}$$

$$= c_{\alpha\beta}^{(l)} g_{\bar{l}l'}^{(\bar{l}'')} c_{\overline{\alpha}\overline{\beta}}^{(\bar{l})*} c_{\overline{\alpha}'\overline{\beta}'}^{(\bar{l})*} \sum_{\mathbf{x},\overline{\mathbf{x}},\overline{\mathbf{x}}'} e^{-i\mathbf{p}\cdot(\mathbf{x}+\frac{1}{2}(\mathbf{d}_{\alpha}+\mathbf{d}_{\beta}))} e^{-i\mathbf{p}\cdot(\overline{\mathbf{x}}+\frac{1}{2}(\mathbf{d}_{\overline{\alpha}}+\mathbf{d}_{\overline{\beta}}))} e^{-i\mathbf{p}'\cdot(\overline{\mathbf{x}}'+\frac{1}{2}(\mathbf{d}_{\overline{\alpha}'}+\mathbf{d}_{\overline{\beta}'}))}$$

$$\times \delta_{ab} \; \delta_{\overline{a}\overline{b}} \delta_{\overline{a}'\overline{b}'} \left\langle \overline{q}_{a\alpha}^{A}(\mathbf{x},t_{F}) q_{b\beta}^{B}(\mathbf{x},t_{F}) \overline{q}_{\overline{b}\beta}^{\overline{B}}(\overline{\mathbf{x}},t_{0}) q_{\overline{a}\alpha}^{\overline{A}}(\overline{\mathbf{x}},t_{0}) \overline{q}_{\overline{b}'\overline{\beta}'}^{\overline{B}'}(\overline{\mathbf{x}}',t_{0}) q_{\overline{a}'\overline{\alpha}'}^{\overline{A}'}(\overline{\mathbf{x}}',t_{0}) \right\rangle_{U,\psi,\overline{\psi}},$$

$$(4.32)$$

where the two-meson combination coefficients  $g_{\bar{l}l'}^{(\bar{l}'')}$  are determined such that the twomeson operator transforms with quantum numbers  $\bar{l}''$ .

The quark fields in Eq. (4.32) are then Wick-contracted in performing the integration over fermion fields, as

$$C_{l\bar{l}''}(t_{F}-t_{0}) = c_{\alpha\beta}^{(l)}g_{\bar{l}l'}^{(\bar{l}')}c_{\alpha\bar{\beta}}^{(\bar{l}')}c_{\alpha'\bar{\beta}'}^{(\bar{l}')*}\sum_{\mathbf{x},\overline{\mathbf{x}},\overline{\mathbf{x}'}}e^{-i\mathbf{p}\cdot(\mathbf{x}+\frac{1}{2}(\mathbf{d}_{\alpha}+\mathbf{d}_{\beta}))}e^{-i\mathbf{p}\cdot(\overline{\mathbf{x}}+\frac{1}{2}(\mathbf{d}_{\overline{\alpha}}+\mathbf{d}_{\overline{\beta}}))}e^{-i\mathbf{p}'\cdot(\overline{\mathbf{x}'}+\frac{1}{2}(\mathbf{d}_{\overline{\alpha}'}+\mathbf{d}_{\overline{\beta}'}))}$$

$$\times \delta_{ab} \,\delta_{\bar{a}\bar{b}}\delta_{\bar{a}'\bar{b}'}\left\langle -\mathcal{Q}_{b\beta;a\alpha}^{(BA)}\mathcal{Q}_{\bar{a}\alpha;\bar{b}\beta}^{(\overline{A}B)}\mathcal{Q}_{\bar{a}'\overline{\alpha}';\bar{b}'\beta'}^{(\overline{A}'B')} - \mathcal{Q}_{\bar{a}\alpha;\bar{b}'\beta'}^{(\overline{A}B')}\mathcal{Q}_{\bar{a}'\overline{\alpha}';a\alpha}^{(\overline{A}B)}\mathcal{Q}_{b\beta;\bar{b}\beta}^{(\overline{B}B)}\right\rangle$$

$$-\mathcal{Q}_{\bar{a}'\overline{\alpha}';\bar{b}\beta}^{(\overline{A}B')}\mathcal{Q}_{b\beta;\bar{b}}^{(BB')}\mathcal{Q}_{\bar{a}\alpha;a\alpha}^{(AA)} + \mathcal{Q}_{\bar{a}'\overline{\alpha}';\bar{b}'\beta'}^{(\overline{A}A)}\mathcal{Q}_{b\beta;\bar{b}\beta}^{(BB')}\mathcal{Q}_{\bar{a}\alpha;a\alpha}^{(\overline{A}A)}$$

$$+\mathcal{Q}_{\bar{a}'\overline{\alpha}';\bar{b}\beta}^{(\overline{A}B')}\mathcal{Q}_{\bar{a}\alpha;\bar{b}'\beta'}^{(BA)}\mathcal{Q}_{b\beta;a\alpha}^{(BA)} + \mathcal{Q}_{\bar{a}'\overline{\alpha}';a\alpha}^{(\overline{A}A)}\mathcal{Q}_{b\beta;\bar{b}\beta'}^{(BB')}\mathcal{Q}_{\bar{a}\alpha;b\beta}^{(\overline{A}B)}\right\rangle_{U}.$$

$$(4.33)$$

Finally those quark lines are expressed in terms of LapH-diluted quark sources and sinks  $\rho$  and  $\varphi$ , and rearranged into products of the meson functions  $\mathcal{M}$ . Unlike the baryonic correlator whose final expression is Eq. (4.31), some of the quark lines are estimated via  $\gamma_5$ -Hermiticity, leading to the inclusion of  $\overline{\rho}$  and  $\overline{\varphi}$  fields in the expression



Figure 4.5: These diagrams represent the six terms in Eq. (4.34) for the stochastic LapH estimation of a two-meson to one-meson correlation function. Each box denotes a meson function  $\mathcal{M}$ , and the lines represent contraction of indices. As in Fig. (4.4), the fields on the left are on the sink time and the fields on the right are on the source time and are to be complex conjugated.

$$\left\langle -\delta_{BA}\delta_{\overline{AB}}\delta_{\overline{A'B'}}\mathcal{M}_{l}^{[b_{0},b_{0}]}(\varrho_{0},\varphi_{0},t_{F})\mathcal{M}_{\overline{l}}^{[b_{1},b_{1}]}(\varphi_{1},\varrho_{1},t_{0})^{*}\mathcal{M}_{\overline{l'}}^{[b_{2},b_{2}]}(\varphi_{2},\varrho_{2},t_{0})^{*} \right. \\ \left. - \delta_{\overline{AB'}}\delta_{\overline{A'A}}\delta_{B\overline{B}}\mathcal{M}_{\overline{l}}^{[b_{0},b_{2}]}(\varphi_{0},\varrho_{2},t_{0})^{*}\mathcal{M}_{\overline{l'}}^{[b_{1},b_{0}]}(\overline{\varrho}_{1},\varrho_{0},t_{0})^{*}\mathcal{M}_{l}^{[b_{1},b_{2}]}(\overline{\varphi}_{1},\varphi_{2},t_{F}) \right. \\ \left. - \delta_{\overline{A'B}}\delta_{B\overline{B'}}\delta_{\overline{A}A}\mathcal{M}_{\overline{l'}}^{[b_{0},b_{1}]}(\varphi_{0},\varrho_{1},t_{0})^{*}\mathcal{M}_{\overline{l}}^{[b_{2},b_{0}]}(\overline{\varrho}_{2},\varrho_{0},t_{0})^{*}\mathcal{M}_{l}^{[b_{2},b_{1}]}(\overline{\varphi}_{2},\varphi_{1},t_{F}) \right. \\ \left. + \delta_{\overline{A'B'}}\delta_{B\overline{B}}\delta_{\overline{A}A}\mathcal{M}_{\overline{l'}}^{[b_{0},b_{0}]}(\varrho_{0},\varphi_{0},t_{0})^{*}\mathcal{M}_{l}^{[b_{2},b_{1}]}(\overline{\varphi}_{2},\varphi_{1},t_{F})\mathcal{M}_{\overline{l}}^{[b_{2},b_{1}]}(\overline{\varphi}_{2},\varrho_{1},t_{0})^{*} \\ \left. + \delta_{\overline{A'B}}\delta_{A\overline{B'}}\delta_{BA}\mathcal{M}_{\overline{l'}}^{[b_{0},b_{1}]}(\varphi_{0},\varrho_{1},t_{0})^{*}\mathcal{M}_{\overline{l}}^{[b_{1},b_{0}]}(\varphi_{1},\varrho_{0},t_{0})^{*}\mathcal{M}_{l}^{[b_{2},b_{2}]}(\varrho_{2},\varphi_{2},t_{F}) \right. \\ \left. + \delta_{\overline{A'A}}\delta_{B\overline{B'}}\delta_{\overline{AB}}\mathcal{M}_{\overline{l'}}^{[b_{0},b_{1}]}(\overline{\varrho}_{0},\varrho_{1},t_{0})^{*}\mathcal{M}_{\overline{l}}^{[b_{0},b_{1}]}(\overline{\varphi}_{0},\varphi_{1},t_{F})\mathcal{M}_{\overline{l}}^{[b_{2},b_{2}]}(\varphi_{2},\varrho_{2},t_{0})^{*} \right\rangle_{U,\rho}.$$
 (4.34)

The profusion of meson tensors in Eq. (4.34) is better represented via the diagrams in Fig. 4.5, following the same diagrammatic conventions as in Fig. 4.4. The usage of  $\gamma_5$ -Hermiticity in calculating certain quark lines is beneficial in that it allows the noise source to always reside on the source time  $t_0$ , and the corresponding quark lines can be estimated via the less noisy (TF,SF,LI8) dilution scheme. In the case of the fully-disconnected diagrams, the internally-contracted quark line on the sink necessitates computing relative-scheme quark lines with noise sources on all times, since the sink time  $t_F$  must be shifted along the lattice time extent to draw out the correlator as a function of time separation.

In each of these expressions, some gain in statistics can be achieved by averaging

over the ordering noise seeds  $\rho_1$ ,  $\rho_2$ ,  $\rho_3$ . This requires no extra Dirac matrix inversion, and so is relatively inexpensive; however the new estimates gained are not independent, so it is not clear how much, if any, ordering over noise seeds is desirable. Indeed, the answer to that question may depend on the exact dilution scheme used, as well as the particular baryon operator in question. In the case of meson correlators, with the dilution schemes we chose originally, (TI16,SF,LI8) and (TF,SF,LI8) for the sametime and fixed-time quark lines, respectively, very little error reduction occurs with the introduction of noise seed permutations.

In the case of baryon operators, we ended up using a form of noise seed permutation and averaging, as a result of a practical issue regarding disk space requirements. For the fixed-scheme dilution setting, there are  $4(t_0) \times 4(\text{spins}) \times 8(\text{LapH subspaces}) =$ 128 dilution subspaces. This makes for baryon functions  $\mathcal{B}$  of a fairly large size, and given that three such indices remain uncontracted, the baryon operators occupy a large amount of disk space. Since we also intend to calculate a large number of baryon operators of various isospin,  $O_h^D$  irreps, and displacement types (the large number of operators can be seen from the tables in Appendix A), it turns out that calculating these baryon operators and storing them would require a prohibitively large amount of data storage space, on the order of one to two petabytes.

In order to reduce storage requirements by a factor of eight, we scaled back the fixed-scheme dilution from (TF,SF,LI8) to (TF,SF,LI4) for baryon operators. In doing so, we sacrificed some accuracy in baryonic correlators, and an investigation was pursued into whether some of this accuracy could be regained via averaging over noise permutations<sup>4</sup> in the baryon-to-baryon correlators. A sample of results are shown in Fig. 4.6.

The use of LI4 dilution and noise averaging is not as effective as LI8 dilution, but for low time separations the error bars do not differ much. This may be acceptable since, in the majority of channels, we hope to achieve a signal early on in time separation via diagonalization of correlator matrices, which typically pulls in the energy plateau to smaller times. Once an optimal set of multi-hadron operators

<sup>&</sup>lt;sup>4</sup>This noise averaging can in fact be implemented by simply enforcing no canonical ordering of the quarks in the baryon function  $\mathcal{B}$ . In the case that noise averaging is not needed, we would establish a canonical ordering of Dirac spins on the three quarks in a baryon, in order to save time in the course of calculating baryon operators. But since the calculation time turns out to be less of an issue than storage space for baryons, we simply relax this canonical ordering to allow any ordering of three Dirac spins, and effectively achieve averaging over noise permutations.



Figure 4.6: Since storage space became a constraining issue in the calculation of baryon operators, we explored the idea of relaxing the LapH-eigenvector dilution level to interlace 4, thereby saving a factor of  $2 \times 2 \times 2 = 8$  in disk space. In order to offset some of the expected loss in accuracy from this, we can average over different noise seed orderings, permuting 1, 2, 3 in Eq. (4.31). The two effective masses shown here indicate that the LI4+noise averaging estimate is significantly more noisy than LI8 estimate, but mainly at larger time separations.

has been chosen, we may eventually rerun some of that final set with LI8 if more precise signals are desired. Since the ground state nucleon is used to set the scale in all channels, that particular baryonic sector was analyzed separately using the more precise LI8 scheme.

## Chapter 5

## Results

The vector isovector (I=1, S=0, P-wave) symmetry sector of QCD offers some unique opportunities for contact between experiment and QCD theory. The lowest state in this sector (for physical pion mass, at least) is a two-pion P-wave resonance, and the parameters of the  $\rho(770)$  decay into two pions have been well-determined experimentally [26]. Lattice studies have recently begun to achieve theoretical predictions [28, 29, 109] of these parameters, using Lüscher's finite-volume method [19]. In those lattice studies, it is found that multi-hadron operators are necessary to precisely extract the first few energy levels in the  $T_{1u}^+$  channel [28].

In this work, our aim is not at the decay parameters of the  $\rho(770)$ , but rather at the full energy spectrum in the  $I=1, S=0, T_{1u}^+$  channel below roughly 2 GeV, using not only two-pion operators but all two-meson operator combinations that can combine with the appropriate total quantum numbers. This larger operator basis should allow us to reliably extract energy levels for the excited states of the  $\rho$  meson as well as the ground state. Experimentally, there are three known excitations of the spin-1  $\rho$  meson, with masses 1450 MeV, 1570 MeV, and 1700 MeV. A fourth state is expected in the lattice  $T_{1u}^+$  channel, namely the  $\rho_3(1690)$ , since spin-3 states also subduce into that irreducible representation. The widths of some of these resonances are very large, such that previous to 1988, the  $\rho(1450)$  and the  $\rho(1700)$  were taken as a single resonance [26]. Four excited  $q\bar{q}$  states are predicted in some relativistic quark models [110], though two of these states lie above 2 GeV. However there are several higher states, in the region of 2 GeV and above, that have been suggested by some experimental analysis but not confirmed [26]. This work will yield comparisons with all of these excited state energies, as well as with other lattice studies in regards to the lowest energy levels in the channel.

This chapter is organized as follows. Section 5.1 discusses the process of selecting multi-hadron operators to employ in the  $T_{1u}^+$  correlation matrix, by examining results on a small number of gauge configurations. We arrive at a general methodology for multi-hadron operator selection that should be useful in future studies. In Sec. 5.2 we present the variational analysis of the correlation matrix of the selected operators on the full ensemble of  $24^3(390)$  gauge configurations, via the procedure outlined in Sec. 2.5 (also sometimes referred to as "correlator matrix diagonalization"). The energy spectrum that emerges from this analysis is summarized in Sec. 5.3 and compared with results from other sources.

In previous chapters we have used the symbols  $\pi$ ,  $\eta$ ,  $\phi$ , K, and  $K^c$  to denote the flavor content of meson operators ( $\overline{u}d$ ,  $\overline{u}u + \overline{d}d$ ,  $\overline{s}s$ ,  $\overline{u}s$ , and  $\overline{s}d$ , respectively, for maximal- $I_3$  creation operators). Thus a  $\pi$  operator may not have the symmetry properties of the commonly-called pion ( $I^G(J^{PC}) = 1^-(0^{-+})$ ,  $m \approx 140$  MeV), but may refer to any isovector quark-antiquark operator. In order to avoid confusion in this chapter, we will always refer to the *physical* mesons with their symbol as well as their mass, in MeV; e.g.,  $\eta(547)$  for the lowest isoscalar pseudoscalar meson, or K(497) for the ground state kaon [26].

### 5.1 Multi-Hadron Operator Selection

Since our lattice QCD action obeys exact isospin symmetry  $(m_u = m_d)$ , we can expect an equivalent mass spectrum for any total isospin projection  $I_3$ , so we choose the maximal value of  $I_3=I=1$  for simplicity, since our single-meson operators then involve a single term  $\overline{u}d$ , for the creation operator  $\overline{O}$ . In order to produce a state of total isospin I=1,  $I_3=1$  as a tensor product of two singe-meson states, we can consider combinations of the form  $\pi\pi$  ( $I=1 \otimes I=1$ ),  $KK^c$  ( $I=\frac{1}{2} \otimes I=\frac{1}{2}$ ), and  $\eta\pi$  and  $\phi\pi$  (I=0 $\otimes I=1$ ). As discussed in Sec. 3.3, the (I=0) operators are divided into those with purely light-quark content  $\overline{u}u + \overline{d}d$  (denoted  $\eta$ ), and those with strange quarks  $\overline{ss}$ (denoted  $\phi$ ).

For each of these two-meson flavor combinations, there are many ways to combine spin, parity and G-parity quantum numbers to achieve a two-meson operator transforming with  $T_{1u}^+$ . Group theoretical coefficients were generated for all of these possibilities, and for all total irreducible representations, via computations in MAPLE.
As a check on these coefficients, operators with different quantum numbers were correlated and checked for consistency with zero.<sup>1</sup> The success of these tests was also a useful check on the validity of our code for combining single-hadron operators into multi-hadron operators, tying them together with the appropriate Wick contraction of indices.

The selection of single-hadron operators has already been discussed in Ch. 3, and also in Refs. [24, 25]. The selection of multi-hadron operators follows the same criteria, but has necessarily proceeded in a somewhat different method. In the singlehadron case, we were able to produce and examine correlation functions of all possible operators of each type, "prune" out the operators with unacceptably large error, then begin to build correlation matrices and examine condition numbers [24]. In the multihadron case, there is a much larger set of operators to start with, due to the different combinations of single-hadron operators in each meson. The criteria of signal quality and condition number is not sufficient to uniquely narrow this large list down to a computationally practical number. Thus, in order to help focus our search for a good operator basis, we undertook a calculation of the two-meson states that might be "expected" based on experimental single-meson masses tabulated by the Particle Data Group [26], imposing the periodic boundary conditions of a cubic box, and assuming no interaction between hadrons. The non-interacting assumption is not generally true (thus the quotations around "expected") but should be acceptable as a rough guide for operator selection purposes.

The resulting "expected" states are translated into lattice irreducible representations for each meson, via group theoretical subductions (see Tables 3.4 and 3.5). For an example, a two-meson combination of an  $\omega(782)$  and a  $\pi(140)$  with momenta (1,1,0) and (-1,-1,0), respectively, could be excited by operators of the form  $[\eta A_1^- \pi A_2^-]$ ,  $[\eta B_1^- \pi A_2^-]$ , or  $[\eta B_2^- \pi A_2^-]$ , in the notation [first meson flavor type, first meson irreducible representation, second meson flavor type, second meson irreducible representation]. This is because the  $\omega(782)$   $(I^G(J^{PC}) = 0^-(1^{--}))$  appears in the  $T_{1u}^-$  stationary irreducible representation, which then subduces onto  $C_{2v}$  little groups  $A_1^-$ ,  $B_1^-$ , and  $B_2^-$ , and the pion  $(I^G(J^{PC}) = 0^-(0^{-+}))$  subduces to  $A_{1u}^-$  on the lattice, which appears in only the  $A_2^-$  representation of  $C_{2v}$ . Once such associations

<sup>&</sup>lt;sup>1</sup>Of note was our test of the definite-G-parity kaon-antikaon operators correlated with singlepions of opposite G-parity. These checks brought to light important features of the kaon-antikaon two-meson combination coefficients, which have been discussed in Sec. 3.3.

were made, our initial approach was to generate correlators and effective mass plots (see Eq. (2.64) for effective mass definition) for all possible displacement type combinations in the these two-meson operators, and examine that set selecting for low statistical error, then subsequently low condition number. This process was carried out for several "expected" levels, and in each case we found that one operator was enough to obtain an acceptable signal for that level. We also found that the multi-hadron operators with the best signal were consistently found to be made up of the least-noisy single-hadron operators, as might be expected. In light of those facts, we verified that the following procedure led to the same operator choices, and proceeded much more efficiently than our original strategy:

- 1. For each hadron combination expected based on experimental single-meson states, use group subduction tables to determine which irreducible representation(s) may contain those states.
- 2. Select the spatial displacement types from those irreducible representations that have the smallest statistical noise, and combine those into a two-meson operator. Such two-meson operators make up the "primary" operator set.
- 3. In a few channels, choose another combination of operators to include as well, selecting from possibly-more-noisy single-hadron operators, to make up a "secondary" set of operators, to ensure saturation of all low-lying states in the Hilbert space.

Our choice of primary and secondary two-meson operators is listed in Tables 5.2 and 5.3, with secondary operators followed by "[2<sup>nd</sup>]." Some combinations of irreducible representations may appear repeated in different "expected" levels, due to subduction of multiple continuum spins into the same lattice symmetry channel, such as for the expected levels  $\pi(140)a_1(1260)$  and  $\pi(140)\pi_1(1400)$  in Table 5.2. In that case we avoid repeating operator choices by choosing the next-best (next-lowest statistical noise) single-hadron operator for one of the mesons, taking care not to duplicate other operators in the primary or secondary set. A list of the single-hadron operators we use is given in Table 5.1, also with qualitative estimates of the "target" experimental state for each single-hadron operator, though these are merely based on the relative energies of the effective masses for each of these operators. It is important to note that these "target" experimental states are not meant as a guarantee that the

Target Exp. State	Operator
$\rho(770)$	$\pi T_{1u}^+$ TDO15
$\rho(770)$	$\pi T_{1u}^+$ SSO
$\rho(770)$	$\pi T_{1u}^+$ TDO3
$\rho(770)$	$\pi T_{1u}^+$ DDL3
$\rho(1450)$	$\pi T_{1u}^+$ DDL4
$ \rho(1450) $	$\pi T_{1u}^+$ DDL8
$ \rho(1570) $	$\pi T_{1u}^+$ SS1
$ \rho(1570) $	$\pi T_{1u}^+$ DDL2
$ \rho_3(1690) $	$\pi T_{1u}^+$ TDO22
$ \rho_3(1690) $	$\pi T_{1u}^+$ DDL12
$\rho(1700)$	$\pi T_{1u}^+$ DDL13
ho(1700)	$\pi T_{1u}^+$ DDL0

Table 5.1: Single-hadron  $T_{1u}^+$  operators of zero momentum used in correlation matrix, along with the "target" experimental state used as a guide in selecting those operators. The acronyms SS, DDL, etc., and following numbers, refer to the displacement types and spatial identification numbers discussed in Ch. 3, and  $\pi$  refers to isovector flavor structure.

given operator will excite that state exclusively – thus the need for correlator matrix diagonalization – but these states are expected to constitute at least part of the linear combination of states produced by the operator. As an example of the signal quality we achieve in correlation functions of multi-hadron operators, effective masses are shown in Fig. 5.1 for each possible two-meson flavor combination in this channel.

#### **5.2** $T_{1u}^+$ Correlation Matrix Analysis

A total of 56 single-meson and two-meson operators were computed, the union of the operators in Tables 5.1, 5.2 and 5.3. These were generated conveniently via the intermediate constructs of meson functions, then two-meson functions, as described in Ch. 4, on all 551 configurations of our  $24^3 \times 128$ ,  $m_{\pi} \approx 390$  MeV ensemble. Correlation

Target Exp. State	Operator
$\pi(140)\pi(140)$	$\pi A_2^-$ SS1 $\pi A_2^-$ SS1 OA
$\pi(140)\pi(140)[2^{nd}]$	$\pi A_2^{-}$ TSD2 $\pi A_2^{-}$ TSD1 OA
$\pi(140)\pi(140)$	$\pi A_2^-$ SS0 $\pi A_2^-$ SS0 PD
$\pi(140)\pi(140)[2^{nd}]$	$\pi A_2^-$ SS1 $\pi A_2^-$ SS0 PD
$h_1(1170)\pi(140)$	$\eta T_{1g}^{-}$ SS0 $\pi A_{1u}^{-}$ SS0
$h_1(1170)\pi(140)[2^{nd}]$	$\eta T_{1g}^{-}$ SD1 $\pi A_{1u}^{-}$ SS0
$K(497)K^{c}(497)$	$KA_2$ ŠS1 $K^cA_2$ SS1 OA
$\omega(782)\pi(140)$	$\eta E^{-}$ SS1 $\pi A_2^{-}$ LSD1 OA
$\pi(140)a_1(1260)$	$\pi A_{1u}^-$ SS0 $\pi T_{1g}^-$ SS0
$\pi(140)a_1(1260)[2^{nd}]$	$\pi A_{1u}^-$ TDO1 $\pi \check{T}_{1q}^-$ SSO
$\pi(140)\pi(140)$	$\pi A_2^-$ SS0 $\pi A_2^-$ SS0 CD
$\phi(1020)\pi(140)$	$\phi E^-$ SS1 $\pi A_2^-$ SS1 OA
$K(497)K^{c}(497)$	$KA_2$ SS0 $K^cA_2$ SS0 PD
$K(497)K^{c}(497)[2^{nd}]$	$KA_2$ SS0 $K^cA_2$ SS1 PD
$\eta(547)\rho(770)$	$\eta A_2^+$ SS1 $\pi E^+$ SS1 OA
$\omega(782)\pi(140)$	$\eta B_1^-$ SS1 $\pi A_2^-$ SS0 PD
$\omega(782)\pi(140)[\text{deg.}]$	$\eta B_2^-$ SS2 $\pi A_2^-$ SS0 PD
$K^*(892)K^c(497)$	$KESS2 \ K^c A_2 SS1 \ OA$
$K^{*}(892)K^{c}(497)[2^{nd}]$	$KESS3 \ K^c A_2 SS0 \ OA$
$h_1(1170)\pi(140)$	$\eta A_2^-$ LSD3 $\pi A_2^-$ SS1 OA
$h_1(1170)\pi(140)[\text{deg.}]$	$\eta E^{-}SS2 \pi A_2^{-}SS1 OA$

Table 5.2: Multi-hadron  $T_{1u}^+$  operators of total zero momentum used in our correlation matrix, along with the "target" experimental state used as a guide in selecting those operators. Notation is similar to that of Table 5.1, with  $\pi$ ,  $\phi$ ,  $\eta$ , K, and  $K^c$  referring to  $q\bar{q}$  operators of different flavor structure. The momentum of each hadron is indicated by the labels OA, PD, and CD, referring to on-axis, planar-diagonal, and cubicdiagonal back-to-back momentum, respectively. The label OA(2) refers to two units of momentum for each direction, (2,0,0). The states followed by "[2<sup>nd</sup>]" indicate operators selected for the "secondary" set as discussed in Sec. 5.1, and those indicated as "[deg.]" are second or third in sets of degenerate states. Continued in Table 5.3.

Target Exp. State	Operator
$\pi(140)\pi(140)$	$\pi A_2^-$ SS1 $\pi A_2^-$ SS1 OA(2)
$\pi(140)\pi(140)[2^{nd}]$	$\pi A_2^-$ SS1 $\pi A_2^-$ TSD0 OA(2)
$\pi(140)a_1(1260)$	$\pi A_2^-$ SS1 $\pi E^-$ SS0 OA
$\pi(140)a_1(1260)[\text{deg.}]$	$\pi A_2^-$ SS1 $\pi A_2^-$ SS0 OA
$\omega(782)a_0(980)$	$\eta T_{1u}^{-} SS0 \ \pi A_{1a}^{-} SS0$
$K_1(1270)K^c(497)$	$KT_{1g}$ SS0 $K^c A_{1u}$ SS0
ho(770) ho(770)	$\pi A_1^+$ SS1 $\pi A_1^+$ SS1 OA
$\rho(770)\rho(770)[\text{deg.}]$	$\pi A_1^+ SS1 \pi E^+ SS1 OA$
$\rho(770)\rho(770)[2^{nd}\text{deg.}]$	$\pi E^+$ SS1 $\pi E^+$ SS1 OA
$\eta(547)b_1(1235)$	$\eta A_{1u}^+$ SS0 $\pi T_{1a}^+$ SS0
$K(497)K^{c}(497)$	$KA_2$ SS0 $K^cA_2$ SS0 CD
$K(497)K^{c}(497)[2^{nd}]$	$KA_2$ SS0 $K^cA_2$ SS1 CD
$\eta(547)\rho(770)$	$\eta A_2^+$ SS0 $\pi B_1^+$ SS1 PD
$\eta(547)\rho(770)[\text{deg.}]$	$\eta A_2^+$ SS0 $\pi B_2^+$ SS2 PD
$\phi(1020)\pi(140)$	$\phi B_1^- SS1 \pi A_2^- SS0 PD$
$\phi(1020)\pi(140)[\text{deg.}]$	$\phi B_2^-$ SS2 $\pi A_2^-$ SS0 PD
$\pi(140)\pi(1300)$	$\pi A_2^-$ SS1 $\pi A_2^-$ TSD0 OA
$a_2(1320)\pi(140)$	$\pi A_2^-$ SS1 $\pi E^-$ TSD1 OA
$\omega(782)\pi(140)$	$\eta E^{-}$ SS1 $\pi A_2^{-}$ SS0 CD
$\omega(782)\pi(140)[2^{nd}]$	$\eta E^{-} SD6 \ \pi A_2^{-} SS0 \ CD$
$K^*(892)K^c(497)$	$KB_1SS1 K^c \overline{A}_2SS0 PD$
$K^*(892)K^c(497)[deg.]$	$KB_2SS3 K^cA_2SS0 PD$
$\pi(140)\pi_1(1400)$	$\pi A_2^-$ SS1 $\pi E^-$ LSD1 OA

Table 5.3: Continued from table 5.2. Multi-hadron  $T_{1u}^+$  operators of total zero momentum used in our correlation matrix (right column), along with the "target" experimental state used as a guide in selecting those operators (left column). Notation is similar to that of Tables 5.1 and 5.2, with  $\pi$ ,  $\phi$ ,  $\eta$ , K, and  $K^c$  referring to  $q\bar{q}$  operators of different flavor structure. The momentum of each hadron is indicated by the labels OA, PD, and CD, referring to on-axis, planar-diagonal, and cubic-diagonal back-toback momentum, respectively. The label OA(2) refers to two units of momentum for each direction, (2, 0, 0). The states followed by "[2<sup>nd</sup>]" indicate operators selected for the "secondary" set as discussed in Sec. 5.1, and those indicated as "[deg.]" are second or third in sets of degenerate states.



Figure 5.1: Effective masses with  $\Delta t = 3$  generated from correlators of a two-meson operator source with the same operator on the sink, for 551 configurations of our  $24^{3}(390)$  ensemble. One operator is shown for each possible flavor combination. The labels indicate the operator, as well as the "target" experimental state, as discussed in Sec. 5.1. Note that each of the correlation functions for these operators contains at least one same-time quark line on the source and sink in one or more of the included Wick contraction diagrams. Statistical errors are computed by the jackknife procedure discussed in Sec. 2.6.

functions were then computed for each pair of operators, enforcing a fixed ordering such that we computed the upper triangle of the matrix, then obtained the other half by Hermiticity  $(C(t) = C(t)^{\dagger})$ . The operators were ordered such that correlators between single- and two-meson operators occurred with the single meson on the sink, allowing the same-time quark line to be estimated by the more accurate fixed scheme (see Sec. 4.3). The analysis of the correlation matrix then follows the procedure outlined in Ch. 2.

The condition number of the full normalized correlator matrix, as described in Eq. (2.71), was found to be unacceptably large, such that diagonalization was impossible. In order to obtain an acceptable condition number, it was necessary to remove some of the very high-energy modes of the correlation matrix by the method of singular value decomposition (SVD) [91]. This method projects the matrix  $C(\tau_0)$  onto a subset of it's eigenvectors whose eigenvalues are greater than some cut-off value  $\lambda_{\rm cut}$ , and  $C(\tau_D)$  onto the same subset<sup>2</sup>. Since C is expected to be positive definite, with lower eigenvalues corresponding to higher energies, the method of SVD amounts to simply leaving out those combinations of operators corresponding to very high-energy modes, which introduce a large amount of statistical noise, and are not needed for the energy spectrum range desired. Of particular importance is the elimination of any negative-eigenvalue modes, which are purely non-physical statistical noise, since the eigenvalues should be positive exponentials of the energies  $e^{-E_n(\tau_D-\tau_0)}$  [99].

The singular-value decomposition is accomplished in several steps; first, we remove the normalization of the diagonal elements of the correlation matrix at  $\tau_0$ ,

$$C_{ij}(t) \rightarrow \frac{C_{ij}(t)}{\sqrt{C_{ii}(\tau_0)C_{jj}(\tau_0)}}.$$
(5.1)

Then, using that correlator matrix normalization, we calculate the eigenvectors u of the normalized correlator matrix on  $\tau_0$ ,

<sup>&</sup>lt;sup>2</sup>To some extent, the SVD analysis of correlator matrices makes it unnecessary to be as stringent as we have been in the operator selection phase of this work, since the subsequent SVD can remove some redundant or extremely high-energy operator combinations from the matrix. However our operator selection process is still important in that we can only feasibly calculate correlator matrices of a certain size due to computational expense and data storage limitations, so keeping all operators and then removing the vast majority of their combinations via SVD is not practical. Still, based on the insights from this calculation, we may keep a larger number of single-hadron operators in future analysis of other channels.

$$C(\tau_0)u = \lambda u. \tag{5.2}$$

Any eigenvectors with eigenvalues  $\lambda > \lambda_{\text{cut}}$  are stored as columns of a matrix U. We then solve a similar generalized eigenvalue problem as in Eq. (2.67), but projecting the correlator matrices onto the eigenvectors u,

(

$$U^{\dagger}C(\tau_0)Uv = \lambda U^{\dagger}C(\tau_D)Uv, \qquad (5.3)$$

in practice using the same trick as in Eq. (2.68) to find the generalized eigenvectors v. We then assemble the generalized eigenvectors v into the columns of a matrix V, and construct the "rotated", SVD-projected correlator matrix as

$$C^{(r)\text{SVD}}(t) = V^{\dagger}U^{\dagger}C(t)UV.$$
(5.4)

It is the diagonal elements of this correlator matrix that are fit in order to determine the energies of the eigenstates corresponding to each v. In this work a cutoff of  $\lambda_{\text{cut}} = 0.05$  is used, which corresponds to a maximum condition number of about 150 for  $\widehat{C}(\tau_0)$ , and causes seven of the lowest eigenvectors u to be disregarded, such that the projected correlator matrix has rank 49 rather than 56. While the calculation of the projection matrix U occurs on  $\tau_0$ , we also verify that the SVD-projected matrix  $U^{\dagger}C(\tau_D)U$  is free of negative eigenvalues.

In Eq. (2.67), we are free to choose  $\tau_0$  and  $\tau_D$  in order to produce a "rotated" correlator matrix  $C^{(r)}$  (or  $C^{(r)SVD}$  with SVD usage) which is as close to diagonal as possible. To that end, we tried several combinations of  $\tau_0$  and  $\tau_D$ , and observed the rotated correlator matrix normalized on *each* time, as in Eq. (2.70), only using the SVD-projected correlator matrix,

$$\widehat{C}_{ij}^{(r)\text{SVD}}(t) = \frac{C_{ij}^{(r)\text{SVD}}(t)}{[C_{ii}^{(r)\text{SVD}}(t)C_{jj}^{(r)\text{SVD}}(t)]^{1/2}}.$$
(5.5)

This gives an indication of how well the new operator basis remains orthogonal at different time separations [24]. Given the large size of the correlator matrix being considered, examining each of the  $N \times (N-1)/2 = 1035$  off-diagonal elements for each diagonalization was not practical. Therefore the off-diagonal elements were sorted according to their statistical significance averaged over time separations,  $\langle \hat{C}^{(r)\text{SVD}}/\text{Err}[\hat{C}^{(r)\text{SVD}}] \rangle_t$ , allowing us to examine any significant off-diagonal elements.



Figure 5.2: In order to verify that the variationally-improved operator basis is orthogonal for all time separations, we examine the rotated normalized correlator matrix  $\hat{C}_{ij}^{(r)\text{SVD}}(t)$  given in Eq. (5.5). The off-diagonal elements of this matrix should be statistically consistent with zero, and small compared to unity [24] to indicate a successful fixed-coefficient diagonalization of the correlator matrix. The curves above represent the five most statistically significant off-diagonal elements, as measured by  $\langle \hat{C}^{(r)\text{SVD}}/\text{Err}[\hat{C}^{(r)\text{SVD}}] \rangle_t$ . The statistical error  $\text{Err}[\hat{C}^{(r)\text{SVD}}]$  is computed via the jackknife procedure discussed in Sec. 2.6. The statistically significant departures from zero at early times (3 and 4) are not a problem since we do not use this time range for energy extraction.

Statistical errors are computed by the jackknife procedure discussed in Sec. 2.6. We found that a choice of  $\tau_0 = 5$  and  $\tau_D = 9$  led to an acceptable diagonalization, as seen from the off-diagonal elements of  $\widehat{C}^{(r)SVD}$  shown in Fig. 5.2.

The diagonal elements of the rotated correlator matrix  $C^{(r)SVD}$  were then fitted to a single exponential form<sup>3</sup>, minimizing the correlated- $\chi^2$  function given in Eq. (2.63). Fit ranges were found for each level that yielded reasonable  $\chi^2/DOF$  values (generally between about 0.5 and 2.0). The fit values and ranges are shown superimposed on the effective masses (Eq. (2.64)) in Figs. 5.3 and 5.4, with best fit values, error, and

<sup>&</sup>lt;sup>3</sup>Fits were also tried using a cosh form, but yielded results indistinguishable from those of the single-exponential fits. This is due to the fact that plateau can be fit at relatively early times for our optimized  $\rho(770)$  operator, rather than attempting to use time separations closer to the middle of the lattice. Fits using a cosh +constant form, to model the next leading contribution of finite size effects, also gave energies matching that from the simple exponential fits.

 $\chi^2/DOF$  listed for each level. Masses are given in units of the inverse temporal lattice spacing  $a_t^{-1}$ . The lattice spacing has been determined in other work [22] as  $a_t^{-1}=5.661(17)$  GeV, though the exact value is not necessarily important here since the observables we report will eventually be expressed as mass ratios against the nucleon mass.

For the higher-energy levels in Fig. 5.4, the signal quality begins to degrade, but a reasonable fit is still found for most levels. In any case, our intent was only to calculate the energy spectrum up to the range of roughly 2 GeV, and these states are at or beyond that energy  $(a_t^{-1} = 5.661(17) \text{ GeV } [22])$ . For higher energies, it is possible that two-nucleon states, or three- and four-hadron states, may become important, though their couplings to single-hadron states are expected to be small. Future studies using the Stochastic LapH method should verify this.

In order to try to identify which of the levels in Figs. 5.3 and 5.4 correspond to the single-hadron states expected in the continuum, we examine the magnitudes of the overlaps  $Z_i^{(n)} = \langle 0 | \mathcal{O}_i | n \rangle$  for each operator  $\mathcal{O}_i$ , as estimated through Eq. (2.74). With the SVD-projected correlator matrix  $U^{\dagger}CU$ , that formula is modified to become

$$Z_{i}^{(n)} = U_{ij} U_{jk}^{\dagger} C_{kl}(\tau_0) U_{lp} v_p^{(n)} \tilde{Z}_n.$$
(5.6)

In general the quark-antiquark operators are expected to excite single-meson states most strongly, so observing  $Z_i^{(n)}$  for a single-hadron operator  $O_i^{[SH]}$  should reveal peaks around the states (n) that correspond most closely to single-meson states in the final optimized set. However, we found that a clearer indicator of these state identifications is the Z value of each optimized single-hadron operator – that is, the Z value of each linear combination  $\mathcal{O}_m^{[SH]'} = \sum_i v_i^{\prime(m)*} \mathcal{O}_i^{[SH]}$  achieved by diagonalizing a correlator matrix of only single-hadron operators  $\mathcal{O}_i^{[SH]}$ . Eq. (2.74) then becomes

$$Z'^{(n)}_{m} \equiv \langle 0 | \mathcal{O}^{[SH]'}_{m} | n \rangle = v'^{(m)*}_{i} C_{ij}(\tau_{0}) v^{(n)}_{j} \tilde{Z}_{n}.$$
(5.7)

It happens that the diagonalization of the single-hadron-only correlator matrix also requires singular value decomposition, resulting in a different set of projection eigenvectors  $u^{[SH]}$  and matrix  $U^{[SH]}$  from Eq. (5.2) for the sub-matrix containing only single-hadron operators. We discovered that the failure to use SVD on a large basis of single-hadron operators can result in an unstable mass extraction for the singlehadron energies. Thus the equivalent of Eq. (5.7) for the case of singular-value de-



Figure 5.3: Effective masses (see Eq. 2.64) with  $\Delta t = 3$  of diagonal correlator elements after variational analysis with the full basis of 56 operators in Tables 5.1, 5.2 and 5.3. Recall that these effective masses tend to the stationary state energies as t becomes large. Correlated- $\chi^2$  fit values are shows as a pair of dotted lines spanning the fit error range, and extending the length of the fit range in t, for a single-exponential fit form. The fit values with error are shown in the legend, where the two digits in parenthesis represent the uncertainty on the last two digits of the reported mean value. Continued in Table 5.4.



Figure 5.4: Effective masses (see Eq. 2.64) with  $\Delta t = 3$  of diagonal correlator elements after variational analysis with the full basis of 56 operators in Tables 5.1, 5.2 and 5.3. Recall that these effective masses tend to the stationary state energies as t becomes large. Correlated- $\chi^2$  fit values are shows as a pair of dotted lines spanning the fit error range, and extending the length of the fit range in t, for a single-exponential fit form. The fit values with error are shown in the legend, where the two digits in parenthesis represent the uncertainty on the last two digits of the reported mean value. Continued from Table 5.3.



Figure 5.5: A plot of  $|Z_m'^{(n)}|^2$  against eigenstate (n) of the full  $56 \times 56$  correlator matrix diagonalization, for each optimized single-hadron operator m, as given in Eq. (5.8). The peaks indicate eigenstates of the full-matrix diagonalization that are strongly excited by a particular optimized single-hadron operator, and allow us to establish which of the full-matrix eigenstates likely correspond to single-hadron states.

composition should contain both the matrix U from the larger diagonalization and the matrix  $U^{[SH]}$  from the single-hadron sub-matrix diagonalization, as

$$Z_m^{\prime(n)} \equiv \langle 0|\mathcal{O}_m^{[\mathrm{SH}]\prime}|n\rangle = v_i^{\prime(m)*} U_{if}^{[\mathrm{SH}]\dagger} U_{fg} U_{gh}^{\dagger} C_{hj}(\tau_0) U_{jk} v_k^{(n)} \tilde{Z}_n.$$
(5.8)

In each graph in Fig. 5.5, the magnitude  $Z'_m^{(n)}Z'_m^{(n)*}$  is plotted against the eigenstate number (n), and the different graphs correspond to different optimized single-hadron operators m. These optimized single-hadron operators were determined using the same  $\tau_0$  and  $\tau_D$ , as well as the same SVD cutoff, as the full-matrix eigenvectors. For most of the optimized single-hadron operators, a clear peak is visible in different places in Fig. 5.5, indicating that these states from the full-matrix variational analysis likely correspond to the single-hadrons in the channel. A list of these correspondences is compiled in Table 5.4, assuming that the states emerging from the single-hadron analysis correspond to the five expected resonances in experiment.

For the multi-hadron operators in the channel, we simply observe the overlaps  $Z_i^{(n)}$  in Eq. (5.6), rather than using optimized operators as in Eq. (5.7). The square of the magnitudes of these Z are plotted in Figs. 5.6, 5.7, and 5.8. In the same way that single-hadron states may be identified in the set of eigenvectors from the diagonalization of the full 56 × 56 matrix, the Z factors in Figs. 5.6, 5.7, and 5.8

Level Number	Continuum Correspondence
0	ho(770)
8	ho(1450)
13	ho(1570)
31	$ ho_3(1690)$
40	ho(1700)
46	?
48	?

Table 5.4: Identification of lattice eigenstates obtained in the  $T_{1u}^+$  channel with continuum single-hadron states. Chosen by observing peaks in the overlaps  $Z_m^{\prime(n)}$  of optimized single-hadron operators onto the levels of the full matrix diagonalization, as shown in Fig. 5.5, and assuming a similar state ordering as in experiment. The identification of the 40<sup>th</sup> level with the  $\rho(1700)$  is somewhat ambiguous, as the 39<sup>th</sup> eigenstate is also strongly excited by the same optimized single-hadron operator, as seen in the fifth plot in Fig. 5.5. However the energy of these two states are very similar, so the choice is not necessarily consequential. The last two excited  $\rho$  states are at the high end of the energy range accessible to this lattice study, so we refrain from identifying them.

allow for tentative identification of which lattice eigenstates correspond to particular continuum two-hadron states. For instance, the second level is mainly a  $\pi\pi$  state with opposite on-axis (OA) momenta, as is clear from the first graph in Fig. 5.6. The first plot on the third row of Fig. 5.6 indicates that the third level is a kaon-antikaon state. From the last graph in the first row of that figure, we see that the fourth level is a  $\pi\pi$  state with opposing planar-diagonal (PD) momenta, e. g. (0,0,1) and (0,0,-1). More of these associations can be inferred, but those will not be discussed in more detail here, since the main states we are concerned with the single-meson states.

While the peaks in Fig. 5.5 confirm that lattice eigenstates do exist which correspond mainly to single-meson content, we still expect that the introduction of multihadron operators into the matrix may affect these energies slightly. This is because these single-hadron states may mix a small amount with nearby two-meson resonances. A comparison of the single-hadron-only mass extraction for the ground state against the full-matrix ground state mass extraction is shown in Fig. 5.9. The ground state energy for the full basis appears slightly lower than that of the single-hadrononly basis, and appears with a somewhat smaller statistical error. This agrees with the effect seen in Ref. [28] in the moving  $p = (1,0,0) T_{1u}^+$  channel, where it was found that neglecting to use both single- and multi-hadron operators can result in an overestimation of the true ground state.

Similar comparisons are shown for the excited  $\rho$  meson levels, between the singlehadron only mass extraction and that from the corresponding level of the full 56 × 56 correlator matrix, are shown in Figs. 5.10, 5.11, 5.12, 5.13, 5.14, and 5.15. It is apparent that the masses are not greatly affected by mixing with nearby two-meson states. However for several single-hadron levels, especially the third level (corresponding to the  $\rho(1570)$  in the continuum), the statistical error is significantly reduced by accurately accounting for coupling in the full single- and two-meson operator basis.

#### 5.3 Energy Spectrum for Isovector $T_{1u}^+$ Channel

In comparisons with experiment, the salient observables on the lattice are not masses but mass ratios of hadrons. Therefore, in compiling the results from the previous section, simultaneous fits were performed of the nucleon ( $G_{1g}$  ground state baryon) energy and the energy of the  $T_{1u}^+$  state of interest. This yields the values in the left column of Fig. 5.16, with experimental values and errors in the right column taken



Figure 5.6: A plot of  $|Z_i^{(n)}|^2$  against eigenstate (n) of the full 56 × 56 correlator matrix diagonalization, for each multi-hadron operator  $\mathcal{O}_i$ , as given in Eq. (2.74). The operators are listed in the top right corner of each plot, and the "target" continuum state for that operator, as derived through symmetry group subductions, is listed below that. The peaks indicate eigenstates that are strongly excited by that operator, and these peaks thus allow us to tentatively associate a particular continuum state with a particular lattice eigenstate of the full-matrix variational analysis. Continued in Figs. 5.7 and 5.8.



Figure 5.7: A plot of  $|Z_i^{(n)}|^2$  against eigenstate (n) of the full 56 × 56 correlator matrix diagonalization, for each multi-hadron operator  $\mathcal{O}_i$ , as given in Eq. (2.74). The operators are listed in the top right corner of each plot, and the "target" continuum state for that operator, as derived through symmetry group subductions, is listed below that. Peaks indicate eigenstates that are strongly excited by that operator, and these peaks thus allow us to tentatively associate a particular continuum state with a particular lattice eigenstate of the full-matrix variational analysis. Continued from Fig. 5.6.



Figure 5.8: A plot of  $|Z_i^{(n)}|^2$  against eigenstate (n) of the full 56 × 56 correlator matrix diagonalization, for each multi-hadron operator  $\mathcal{O}_i$ , as given in Eq. (2.74). The operators are listed in the top right corner of each plot, and the "target" continuum state for that operator, as derived through symmetry group subductions, is listed below that. Peaks indicate an eigenstate that is strongly excited by that operator, and these peaks thus allow us to tentatively associate a particular continuum state with a particular lattice eigenstate of the full-matrix variational analysis. Continued from Fig. 5.7.



Figure 5.9: Comparison of effective masses and fits of ground states from two different correlation matrix analyses. In red, the variational basis included only the single-meson  $T_{1u}^+$  operators in Table 5.1, and in blue, the basis included those same single-hadron operators as well as all of the multi-hadron operators chosen in Tables 5.2 and 5.3. The correspondence of the these two eigenstates from different matrix diagonalization is confirmed by the pattern of Z magnitudes in Fig. 5.5.



Figure 5.10: Comparison of effective masses and fits of the first excited state from the analysis of only single-meson  $T_{1u}^+$  operators in Table 5.1 (red), and the 8<sup>th</sup> level of the larger single- and multi-hadron variational analysis (blue). The 8<sup>th</sup> level is expected to correspond to the first excited  $\rho$  meson, the  $\rho(1450)$ , based on the Z pattern in Fig. 5.5.



Figure 5.11: Comparison of effective masses and fits of the second excited state from the analysis of only the single-meson  $T_{1u}^+$  operators in Table 5.1 (red), and the 13<sup>th</sup> level of the larger single- and multi-hadron variational analysis (blue). The 13<sup>th</sup> level is expected to correspond to the second excited  $\rho$  meson, the  $\rho(1570)$ , based on the Z pattern in Fig. 5.5.



Figure 5.12: Comparison of effective masses and fits of the third excited state from the analysis of only the single-meson  $T_{1u}^+$  operators in Table 5.1 (red), and the 31<sup>st</sup> level of the larger single- and multi-hadron variational analysis (blue). The 31<sup>st</sup> level is expected to correspond to the third excited state in the channel, the  $\rho_3(1690)$ , based on the Z pattern in Fig. 5.5.



Figure 5.13: Comparison of effective masses and fits of the fourth excited state from the analysis of five single-meson  $T_{1u}^+$  operators in Table 5.1 (red), and the 40<sup>th</sup> level of the larger single- and multi-hadron variational analysis (blue). The 40<sup>th</sup> level is expected to correspond to the fourth excited state in the channel, the  $\rho(1700)$ , based on the Z pattern in Fig. 5.5.



Figure 5.14: Comparison of effective masses and fits of the fifth excited state from the analysis of only single-meson  $T_{1u}^+$  operators in Table 5.1 (red), and the 46<sup>th</sup> level of the larger single- and multi-hadron variational analysis (blue). The association of these two levels is made via the pattern of Z magnitudes in Fig. 5.5. This highly excited state may reflect one of the "lower-confidence" proposed states from certain experimental results in Ref. [26], such as the  $\rho(2150)$ , but we also note that it occurs at the upper edge of the energy range accessible to this lattice study, and given the noise at this level, our mass extraction here is less certain than lower states.



Figure 5.15: Comparison of effective masses and fits of the sixth excited state from the analysis of the single-meson  $T_{1u}^+$  operators in Table 5.1 (red), and the 48<sup>th</sup> level of the larger single- and multi-hadron variational analysis (blue). The association of these two levels is made via the pattern of Z magnitudes in Fig. 5.5. This highly excited state may reflect one of the "lower-confidence" proposed states from certain experimental results in Ref. [26], such as the  $\rho(2250)$ , but we also note that it occurs at the upper edge of the energy range accessible to this lattice study, and given the noise at this level, our mass extraction here is less certain than lower states.



Figure 5.16: At left, the energy spectrum in the isovector  $T_{1u}^+$  channel, computed via a large basis of 12 single-hadron and 42 multi-hadron operators, on 551  $24^3 \times$ 128 anisotropic gauge configurations with Wilson clover fermions,  $m_{\pi} = 390$  MeV. The vertical position of each box represents the energy of a state in relation to the nucleon mass, and the vertical thickness of the box indicates the uncertainty on that energy. The right panel shows experimental masses and errors for the five wellconfirmed isovector states that subduce onto the  $T_{1u}^+$  lattice irreducible representation, in comparison to the experimental nucleon mass. The colors indicate first, second, third, and fourth excited states, but are not intended as definite correspondences for each level. The hollow boxes at the top of the left column indicate additional high-energy states that we extract with less certainty.

from Ref. [26].

The first five levels obtained from this ensemble agree fairly well with the pattern seen in experiment. The spacing of the four excited states is slightly larger than that observed in experiment, especially in the the case of the fourth excited state, the  $\rho(1700)$ . However this small aberration is not far outside the statistical error on these higher energies extracted from the lattice calculation. One improvement that might contribute towards a better determination of these states would be to design operators that specifically excite a "spin-3-like" state on the lattice, to achieve a better-understood overlap onto the  $\rho_3(1690)$ . This possibility is being investigated.

The fact that the ratio of the ground state rho meson energy to that of the pion is smaller than the experimental value can be understood via chiral perturbation theory. Both the nucleon and the rho meson mass increase with increasing pion mass as  $m_{\pi}^2$ , but the  $\rho$  mass increase is more mild [111, 112]. The fact that our pion mass is 390 MeV [22] on the ensemble used in this chapter may cause some distortion in the mass spectrum, even in ratios with the nucleon mass. Such speculations should be verified in future studies at lower pion mass, using the same lattice size and methodology. Stochastic LapH quark lines and meson operator functions are already produced and stored for a lighter pion pass of 240 MeV on  $24^3 \times 128$  lattices, as well as on larger  $32^3 \times 256$  lattices.

### Chapter 6

### **Conclusions and Outlook**

In this work we have presented the first full-scale applications of the Stochastic LapH method. Previous work [22, 24, 25] has already demonstrated the efficacy of this method for estimating quark propagation, including from all lattice sites to all other lattice sites, as is required for correlation functions involving multi-hadron or isoscalar meson operators. In Ch. 3, we discussed the construction of LapH-smeared single-hadron and two-hadron operators which transform irreducibly with an irreducible representation of the lattice symmetry group  $O_h^D$  [101]. These can be constructed and stored conveniently as meson, baryon, and multi-hadron functions defined on a single time-slice, facilitating the calculation of large matrices of correlation functions between these operators.

In Ch. 5 a new procedure was developed for the selection of multi-hadron operators that have minimal statistical noise and span the space of states expected to appear in a particular symmetry sector. For the isovector, non-strange  $T_{1u}^+$  sector of lattice QCD, a large matrix of 56 operators was computed on 551 configurations of a  $24^3 \times 128$  anisotropic Wilson clover ensemble with  $m_{\pi} = 390$  MeV. The operator basis included single-meson operators, and two-meson operators with  $\pi\pi$ ,  $\eta\pi$ ,  $\phi\pi$ , and  $KK^c$  flavor combinations. Reliable energy extractions were achieved through the variational method for an unprecedented number of eigenstates. Many of the correlation functions involved in this matrix, especially those involving  $\eta$  mesons, involve a large number of same-time quark lines, for which we still find an acceptable statistical error.

The inclusion of multi-hadron operators appears to lower somewhat the energy extracted for the ground state, agreeing with the findings of Ref. [28]. The larger

operator basis also has the effect in some places of reducing the statistical error of the energy extracted, especially in the case of the second excited state ( $\rho(1570)$ ) energy.

The first five energies extracted agree fairly well with the four well-confirmed  $\rho$  meson masses observed in in the  $I^G(J^{PC}) = 1^+(1^{--})$  and  $I^G(J^{PC}) = 1^+(3^{--})$  channels experimentally [26]. The fifth state appears slightly higher on the lattice than observed in experiment, perhaps due to an effect of the artificially heavy quark mass used in these simulations. Another possible explanation for this discrepancy is the nature of our operator's coupling to spin-3 states that appear in this channel - a better understanding of that coupling is being pursued.

Nonetheless, our analysis has shown that the Stochastic LapH method can be used to generate large correlator matrices of single-hadron and multi-hadron operators, from which a large number of energy eigenstates may be extracted, on lattices with large volume such that the number of Dirac matrix inversions would otherwise make calculations infeasible. Especially given the growing interest in scattering phase shift extractions from lattice studies [29, 109], including multi-hadron operators is recognized as an important capability in lattice QCD. In future work we will apply the Stochastic LapH method towards finite-volume phase shift calculations, and we plan to extract energy spectra in further sectors of the flavor/parity/spin symmetry groups, including fermionic irreducible representations. Future calculations will include larger  $32^3 \times 256$ ,  $m_{\pi} = 240$  MeV gauge configurations, for which quark propagators and meson line ends have already been produced. The insights gained in the current study, such as guidelines for selecting suitable multi-hadron operators for variational analysis, should prove useful in those studies.

# Appendix A Number of Operators/Momenta

As described in Ch. 3, the design of our single-hadron operators is directly related to their intended use in the multi-hadron operators which we construct from them. All direction of momenta are required since these directional sums are integral to creating multi-hadron operators with definite total quantum numbers (for example, summing over all directions with equal phase in order to produce an S-wave). In deciding what *magnitudes* of momentum to consider, we employ the process discussed in Sec. 3.4, which involves utilizing single-hadron spectral estimates to estimate roughly how large a momenta would be required to generate energies beyond our region of interest. Stationary single-hadron energies have been (roughly) estimated in previous work such as [24, 25].

The tables below indicate our estimates as to how large in momenta we should generate moving single-hadron operators. For instance, a  $Max(p_i)$  value of two for a  $C_{4v}$  channel would mean that we build momenta (0, 0, 1), (0, 0, 2), (0, 1, 0), (0, 2, 0), ... for each displacement type chosen. These estimates are approximate in nature – the actual multi-hadron energies will be shifted by interactions – but we recognize this fact in setting a fairly ambitious energy target of 0.5 in lattice units, which we can be comfortable scaling back in certain channels if necessary.

$\Lambda$ (Croup)	$Max(p_i)$ for Ensemble			N
n (Group)	$24^3(390)$	$24^3(240)$	$32^3(240)$	18
$A_1(C_{4v})$	2	2	3	6
$A_2(C_{4v})$	3	3	4	8
$B_1(C_{4v})$	1	2	2	3
$B_2(C_{4v})$	1	1	2	4
$E(C_{4v})$	2	2	3	9
$A_1(C_{2v})$	2	2	2	7
$A_2(C_{2v})$	2	2	2	7
$B_1(C_{2v})$	2	2	2	10
$B_2(C_{2v})$	2	2	2	6
$A_1(C_{3v})$	1	1	2	4
$A_2(C_{3v})$	1	1	2	5
$E(C_{3v})$	1	1	2	9

Table A.1: For each irreducible representation of the little groups for on-axis, planar, and cubic-diagonal momentum, these maximum momentum elements (and all lower momenta magnitudes) were generated for the ensembles shown, in the  $I = \frac{1}{2}$ , S = 1(K) channel. The last column indicates the number of different operators (that is, displacement/spin coefficient combinations) utilized for each of those momenta. Thus the total number of operators produces for a given ensemble is the product  $Max(p_i) \times N_s \times N_{dir}$ , where  $N_{dir}$  is the number of directions that the momentum can be rotated on the lattice – six for on-axis  $C_{4v}$ , twelve for planar-diagonal  $C_{2v}$ , and eight for cubic-diagonal  $C_{3v}$ .

$\Lambda$ (Channe)	$Max(p_i)$ for Ensemble			λτ
A (Group)	$24^3(390)$	$24^3(240)$	$32^3(240)$	118
$A_1^-(C_{4v})$	2	2	3	4
$A_1^+(C_{4v})$	2	2	3	7
$A_2^-(C_{4v})$	3	3	4	7
$A_2^+(C_{4v})$	3	3	4	3
$B_1^-(C_{4v})$	2	2	3	3
$B_1^+(C_{4v})$	0	1	1	1
$B_2^-(C_{4v})$	1	1	2	2
$B_2^+(C_{4v})$	1	1	2	2
$E^{-}(C_{4v})$	2	2	3	5
$E^+(C_{4v})$	2	2	3	6
$A_1^-(C_{2v})$	1	1	2	5
$A_1^+(C_{2v})$	1	2	2	6
$A_2^-(C_{2v})$	2	2	3	6
$A_2^+(C_{2v})$	2	2	2	4
$B_1^-(C_{2v})$	1	1	2	4
$B_1^+(C_{2v})$	1	2	2	6
$B_2^-(C_{2v})$	1	1	2	4
$B_2^+(C_{2v})$	1	2	2	9
$A_1^-(C_{3v})$	1	1	1	2
$A_1^+(C_{3v})$	1	1	2	5
$A_2^-(C_{3v})$	1	1	2	4
$A_2^+(C_{3v})$	1	1	2	2
$E^{-}(C_{3v})$	1	1	1	4
$E^+(C_{3v})$	1	1	2	6

Table A.2: For each irreducible representation of the little groups for on-axis, planar, and cubic-diagonal momentum, these maximum momentum elements (and all lower momenta magnitudes) were generated for the ensembles shown, in the I = 1, S = 0 ( $\pi$ ) channel. The last column indicates the number of different operators (that is, displacement/spin coefficient combinations) utilized for each of those momenta.

$\Lambda$ (Channe)	$Max(p_i)$ for Ensemble			λτ
A (Group)	$24^3(390)$	$24^3(240)$	$32^3(240)$	$N_s$
$A_1^-(C_{4v})$	2	2	3	8
$A_1^+(C_{4v})$	2	2	3	5
$A_2^-(C_{4v})$	3	3	4	5
$A_2^+(C_{4v})$	3	3	4	4
$B_1^-(C_{4v})$	2	2	3	2
$B_1^+(C_{4v})$	0	1	1	3
$B_2^-(C_{4v})$	1	1	2	2
$B_2^+(C_{4v})$	1	1	2	3
$E^{-}(C_{4v})$	2	2	3	8
$E^+(C_{4v})$	2	2	3	6
$A_1^-(C_{2v})$	1	1	2	6
$A_1^+(C_{2v})$	1	2	2	7
$A_2^-(C_{2v})$	2	2	3	7
$A_2^+(C_{2v})$	2	2	2	6
$B_1^-(C_{2v})$	1	1	2	6
$B_1^+(C_{2v})$	1	2	2	4
$B_2^-(C_{2v})$	1	1	2	6
$B_2^+(C_{2v})$	1	2	2	5
$A_1^-(C_{3v})$	1	1	1	6
$A_1^+(C_{3v})$	1	1	2	6
$A_2^-(C_{3v})$	1	1	2	5
$A_2^+(C_{3v})$	1	1	2	4
$E^{-}(C_{3v})$	1	1	1	7
$E^+(C_{3v})$	1	1	2	7

Table A.3: For each irreducible representation of the little groups for on-axis, planar, and cubic-diagonal momentum, these maximum momentum elements (and all lower momenta magnitudes) were generated for the ensembles shown, in the I = 0, S = 0 ( $\eta$ ) channel. The last column indicates the number of different operators (that is, displacement/spin coefficient combinations) utilized for each of those momenta.

	$Max(p_i)$ for Ensemble			M
A (Group)	$24^3(390)$	$24^3(240)$	$32^3(240)$	IVS
$G_1(C_{4v})$	2	2	3	6
$G_2(C_{4v})$	1	2	2	4
$G(C_{2v})$	1	1	2	5
$F_1(C_{3v})$	1	1	1	2
$F_2(C_{3v})$	1	1	1	2
$G(C_{3v})$	1	1	2	4

Table A.4: For each irreducible representation of the little groups for on-axis, planar, and cubic-diagonal momentum, these maximum momentum elements (and all lower momenta magnitudes) were generated for the ensembles shown, in the  $I = \frac{1}{2}$ , S = 0 (N) channel. The last column indicates the number of different operators (that is, displacement/spin coefficient combinations) utilized for each of those momenta.

$\Lambda$ (Croup)	$Max(p_i)$ for Ensemble			M
A (Group)	$24^3(390)$	$24^3(240)$	$32^3(240)$	18
$G_1(C_{4v})$	2	2	3	6
$G_2(C_{4v})$	2	2	3	4
$G(C_{2v})$	1	1	2	5
$F_1(C_{3v})$	1	1	1	3
$F_2(C_{3v})$	1	1	1	3
$G(C_{3v})$	1	1	1	4

Table A.5: For each irreducible representation of the little groups for on-axis, planar, and cubic-diagonal momentum, these maximum momentum elements (and all lower momenta magnitudes) were generated for the ensembles shown, in the  $I = \frac{3}{2}$ , S = 0 ( $\Delta$ ) channel. The last column indicates the number of different operators (that is, displacement/spin coefficient combinations) utilized for each of those momenta.

	$Max(p_i)$ for Ensemble			N
A (Group)	$24^3(390)$	$24^3(240)$	$32^3(240)$	IVS
$G_1(C_{4v})$	2	2	3	8
$G_2(C_{4v})$	1	1	2	5
$G(C_{2v})$	1	1	2	7
$F_1(C_{3v})$	0	1	1	1
$F_2(C_{3v})$	0	1	1	1
$G(C_{3v})$	1	1	1	5

Table A.6: For each irreducible representation of the little groups for on-axis, planar, and cubic-diagonal momentum, these maximum momentum elements (and all lower momenta magnitudes) were generated for the ensembles shown, in the I = 0, S = -1 ( $\Lambda$ ) channel. The last column indicates the number of different operators (that is, displacement/spin coefficient combinations) utilized for each of those momenta.

$\Lambda$ (Croup)	$Max(p_i)$ for Ensemble			$\lambda t$
A (Group)	$24^3(390)$	$24^3(240)$	$32^3(240)$	18
$G_1(C_{4v})$	2	2	3	9
$G_2(C_{4v})$	2	2	2	6
$G(C_{2v})$	1	1	2	8
$F_1(C_{3v})$	1	1	1	6
$F_2(C_{3v})$	1	1	1	6
$G(C_{3v})$	1	1	1	4

Table A.7: For each irreducible representation of the little groups for on-axis, planar, and cubic-diagonal momentum, these maximum momentum elements (and all lower momenta magnitudes) were generated for the ensembles shown, in the I = 1, S = -1 ( $\Sigma$ ) channel. The last column indicates the number of different operators (that is, displacement/spin coefficient combinations) utilized for each of those momenta.

	$Max(p_i)$ for Ensemble			M
n (Group)	$24^3(390)$	$24^3(240)$	$32^3(240)$	IVS
$G_1(C_{4v})$	2	2	2	7
$G_2(C_{4v})$	2	2	2	4
$G(C_{2v})$	1	1	2	4
$F_1(C_{3v})$	1	1	1	1
$F_2(C_{3v})$	1	1	1	1
$G(C_{3v})$	1	1	1	2

Table A.8: For each irreducible representation of the little groups for on-axis, planar, and cubic-diagonal momentum, these maximum momentum elements (and all lower momenta magnitudes) were generated for the ensembles shown, in the  $I = \frac{1}{2}$ , S = -2 ( $\Xi$ ) channel. The last column indicates the number of different operators (that is, displacement/spin coefficient combinations) utilized for each of those momenta.

$\Lambda$ (Group)	$Max(p_i)$ for Ensemble			N
	$24^3(390)$	$24^3(240)$	$32^3(240)$	IVS
$G_1(C_{4v})$	2	2	2	6
$G_2(C_{4v})$	2	2	2	4
$G(C_{2v})$	1	1	2	5
$F_1(C_{3v})$	1	1	1	3
$F_2(C_{3v})$	1	1	1	3
$G(C_{3v})$	1	1	1	4

Table A.9: For each irreducible representation of the little groups for on-axis, planar, and cubic-diagonal momentum, these maximum momentum elements (and all lower momenta magnitudes) were generated for the ensembles shown, in the I = 0, S = -3 ( $\Omega$ ) channel. The last column indicates the number of different operators (that is, displacement/spin coefficient combinations) utilized for each of those momenta.

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