Heavy flavor interactions and spectroscopy from lattice quantum chromodynamics

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Heavy Flavor Interactions and Spectroscopy From Lattice Quantum Chromodynamics

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In the present work, spectroscopy and interactions of hadrons containing heavy quarks is investigated. In particular, a focus is placed on properties of exotic heavy hadronic states, including doubly and triply heavy baryons and doubly heavy tetraquark states. The framework in which these calculations are carried out is provided by lattice quantum chromodynamics, a discrete formulation of the modern theory of the strong interaction. The main body of the thesis had two main project focuses. For the first project, an extensive calculation of the mass spectrum of doubly and triply heavy baryons including both charm and bottom quarks is carried out. The wide range of quark masses in these systems require that the various flavors of quarks be treated with different lattice actions. We use domain wall fermions for 2+1 flavors (up down and strange) of sea and valence quarks, a relativistic heavy quark action for the charm quarks, and non-relativistic QCD for the heavier bottom quarks. The calculation of the ground state spectrum is presented and compared to recent models. For the second project, the interaction potential of two heavy-light mesons in lattice QCD is used to study the existence of tetraquark bound states. The interaction potential of the tetraquark system is calculated on the lattice with 2+1 flavors of dynamical fermions with lattice interpolating fields constructed using colorwave propagators. These propagators provide a method for constructing all-to-all spatially smeared the interpolating fields, a technique which allows for a better overlap with the ground state wavefunction as well as reduced statistical noise. Potentials are extracted for 24 distinct channels, and are fit with a phenomenological non-relativistic quark model potential, from which a determination of the existence of bound states is made via numerical solution of the two body radial Schrödinger equation.
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I would like to dedicate this work to my wife Ekaterina Mastropas and son Luka Mastropas-Brown, who provide the light to my life. Also, to my mother Lisa Lavelle who always encouraged me to reach for the stars. And last but not least, my grandparents Thomas and Joan Lavelle.
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HEAVY FLAVOR INTERACTIONS AND SPECTROSCOPY FROM LATTICE QUANTUM CHROMODYNAMICS
CHAPTER 1

Quantum chromodynamics and heavy hadrons

1.1 Origins of quantum chromodynamics

When beginning a discussion of the theory of quantum chromodynamics, it's worthwhile to reflect on the state of hadronic physics in the early 1960s. During this time experiment was the primary driver of research in particle physics, with almost no theory to speak of save for phenomenological models. Large scale accelerators were running full steam and new experimental results were routinely published at a rate at which theorists could not keep up with developing descriptions of new results.

The study of the strong interaction, both experimentally and theoretically at this time, was a particularly exciting prospect given the fact that the experimental progress was advancing rapidly while there appeared to be no hope of constructing a theoretical picture to explain the landscape of particles that were being produced by accelerator experiments.
Several theories became popular in describing various aspects of the strong interaction, many of them contributing to the eventual development of quantum chromodynamics. Early attempts in studying the strong interaction relied on S-matrix theory (a nice review of which can be found in Ref. [7]). This theory focused on physical observables and avoided a reliance on unphysical constituent fields, something that was attractive to many that had become disillusioned with the apparent need for renormalization in making sense out of field theory calculations. S-Matrix theory relied heavily on fundamental principles such as analyticity and unitarity, and aimed to steer clear of formalisms such as Hamiltonians which were viewed as unnecessary and poorly suited for the description of the strong interaction.

An alternative to S-Matrix theory was found in the theory of current algebra as championed by Gell-Mann [8] (for a historical perspective in line with this discussion, see Ref. [9]). Current algebra calculations began by formulating an underlying field theory, deriving relations from that theory, and keeping those that might be generally true while throwing away those that were of no use. In the end, the underlying field theory was discarded, the general idea being that the underlying field theory was unphysical, but that the relations derived from it could prove to be useful. This methodology has some high profile success, most notably the Adler-Weisberger relation [10], but there didn't exist much in the way of guidelines for determining which field theories relations could be derived. Additionally, it was argued that S-Matrix theory overlooked dynamical issues, something which is crucial in understanding the fundamental behavior of a physical theory.

The description of the spectrum of hadron masses by an underlying flavor symmetry championed by Neeman and Gell-Mann (for a thorough discussion, see Ref. [11]) proved to be very successful in the early 1960's, and consequently SU(3) flavor symmetry was for some time considered fundamental to the understanding of the strong interaction.
The quark model of hadrons extended the symmetry arguments presented by Gell-Mann and postulated that hadrons could be considered as composite objects, composed of quarks (a name that was later famously coined by Gell-Mann from the James Joyce book *Finnegan’s Wake*) with each quark assigned a fractional electrical (and color) charge. Early field theoretical attempts at describing the strong interaction considered the nucleon, pion and electron as elementary particles with the observed hadron spectrum arising from excitations and interactions of these fundamental degrees of freedom. As more and more hadrons were observed experimentally adding to what was later to be deemed the “particle zoo,” it became evident that there was no reason to hold the nucleon and pion as special in the classification of hadrons (save for the lightness of the pion mass which was later explained in the context of chiral symmetry breaking). Thus, the postulate of Gell-Mann that hadrons were composite objects composed of combinations of three flavors of quarks was an attractive one. Although we now know of the existence of three additional quark flavors, the charm, top and bottom, this SU(3) flavor symmetry provided an approximate description of the hadrons containing light quarks and was very successful in its early applications of classifying the hadron spectrum based solely on symmetry arguments.1 In spite of the successes of the quark model, with the discovery of the Δ++ in 1952 (considered to be composed three up quarks), it became clear that the quark model alone was an inadequate description of hadrons. To remedy this apparent violation of Fermi statistics Nambu [12] postulated the existence of a hidden color degree of freedom to the quark model that restored the required antisymmetry of the baryon wavefunctions. The ideas pioneered in the (colored) quark model would eventually play a large role in the development of QCD, but at the time they were not readily accepted by the greater physics community. Part of this

1The reason for this success given the existence of three additional quark flavors is due to the lightness if the up down and strange quark masses in relation to the natural scale of QCD.
was due to dynamical issues with the theory, such as the non-relativistic description of the quarks as hadronic constituents, however the principal obstacle in the acceptance of the quark model as a valid description of hadrons was the complete lack of experimental observation of any free, fractionally charged particles. The quarks themselves were thus considered as a convenient mathematical tool with no physical basis.

The application of quantum field theory to high energy physics had been largely abandoned due to the perceived untrustworthiness of renormalization techniques in dealing with divergences arising in perturbative calculations beyond leading order. Field theory was viewed by many at this time as a fundamentally flawed description of high energy physics, despite the successes of quantum electrodynamics. It was not until the later development and subsequent success of the electroweak theory that interest in field theory once again became popular, albeit with some residual uncertainty remaining as to whether this type of description could be valid in describing the strong interaction.

Indeed, the early ambitions of one of the founding contributors of field theory in its application to the strong interactions, David Gross, was to disprove the validity of quantum field theory in describing Björken Scaling as observed in Deep Inelastic Scattering experiments. This scaling was thought to be attributable to asymptotic freedom, or the idea that the coupling constant must vanish for sufficiently large energy. In order to disprove field theory as a viable contender for describing the strong interaction, one had to prove that a field theory could not be asymptotically free. This seemed to be a straightforward conjecture, as the dominant field theory of the time, quantum electrodynamics, exhibited behavior quite opposite of that of asymptotic freedom, with the effective coupling growing as the energy scale increases. Gross's initial investigation was successful in disproving the possibility of asymptotic freedom for Abelian gauge theories [13]. It was not until working several
years later with his student Frank Wilczek to extend this work to non-Abelian gauge theories [14] that Gross realized that these types of field theories do in fact exhibit asymptotic freedom. This major development in the description of the strong interaction, realized at the same time by Politzer and Sidney [15] acted as the spark that ignited the development of our modern theory of the strong interaction, quantum chromodynamics, as will be described in the following sections.

In light of the importance of the quark model in QCD spectroscopy, we will precede our discussion of QCD with a discussion of the quark model of hadrons.

1.1.1 The quark model of hadrons

The underlying principle of the quark model developed by Gell-Mann and Zweig (see, e.g. [11]) is that hadrons are composed of quarks, which obey an approximate SU(3) flavor symmetry. Below we will outline the main ideas of the quark model and SU(3) flavor symmetry.

We begin by identifying each of the three quark flavors with a vector in flavor space, in the fundamental representation, namely:

\[
\begin{align*}
    u &= \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, &
    d &= \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, &
    s &= \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}
\end{align*}
\] (1.1)

The corresponding anti-quarks are defined in the conjugate representation, providing a \( \mathbf{3} \) and a \( \bar{\mathbf{3}} \) from which to form hadronic states.

With the assumption of an exact SU(3) flavor symmetry, these flavor space
quark fields transform under rotations in flavor space of the form:

\[ q \rightarrow \hat{U}(\theta_i)q, \quad q \in \{u, d, s\} \]

\[ \hat{U}(\theta_i) = e^{-i\theta_i\lambda_i} \]  

where \( \lambda_i \) are the eight generators of SU(3). A useful representation for these generators is provided by the Gell-Mann Matrices, given by:

\[
\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix},
\]

\[
\lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \quad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},
\]

\[
\lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \lambda_8 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix},
\]

These matrices are traceless and Hermitian:

\[ \lambda_i^\dagger = \lambda_i, \quad tr[\lambda_i] = 0, \]  

and satisfy the commutation relations:

\[ [\lambda_i, \lambda_j] = 2i\epsilon_{ijk}\lambda_k \]
which define the SU(3) Lie Algebra. The structure constants $f_{ijk}$ are completely antisymmetric, with the non-zero elements:

$$f_{123} = 1,$$

$$f_{147} = f_{246} = f_{257} = f_{345} = 1/2,$$

$$f_{156} = f_{367} = -1/2,$$

$$f_{458} = f_{678} = \sqrt{3}/2,$$

(1.7)

The expression 1.6 is conventionally written in terms of the hyperspin generators:

$$[F_i, F_j] = i f_{ijk} F_k,$$

(1.8)

with $F_i \equiv 1/2\lambda_i$. As SU(3) is a rank-2 Lie algebra, two of the generators can be simultaneously diagonalized, and these are conventionally chosen to be $F_3$ and $F_8$ (evident in the fact that the corresponding Gell-Mann Matrices are diagonal). From these generators, the operators:

$$T_3 \equiv F_3, \quad Y \equiv 2/\sqrt{3}F_8$$

(1.9)

are defined. The operator $T_3$ is associated with the third component of isospin, while the operator $Y$ is associated with hypercharge.

From the remaining generators, the following ladder operators are formed:

$$T_\pm \equiv F_1 \pm iF_2, \quad U_\pm \equiv F_6 \pm iF_7, \quad V_\pm \equiv F_4 \pm iF_5$$

(1.10)
These ladder operators function to take the quark state from one eigenstate of \( \{T_3, Y\} \) to another. The operators \( T_{\pm} \) act in the SU(2) subspace (isospin) of SU(3) acting as raising and lowering operators for the third component of isospin \( T_3 \). The remaining ladder operators act similarly, stepping discretely through the allowed values in the \( T_3 - Y \) plane. The weight diagrams for the fundamental (3) and adjoint (3) representations of SU(3) in Figure 1.1 provide a clear graphical representation for the effect of these operators in the two dimensional space of the operators \( Y \) and \( T_3 \).

![Weight diagrams for the fundamental and adjoint representations of SU(3).](image)

**FIG. 1.1:** Weight diagrams for the fundamental and adjoint representations of SU(3). The ladder operators take the the eigenstates of hypercharge \( Y \) and third component of isospin \( T_3 \) located at the corners of the triangles along the triangle edges into each other. Diagram from [5].

From the above representation for single quarks, mesons are constructed as combinations of a quark and an anti-quark:

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

(1.11)

Baryons are constructed from three quarks yielding:

\[
3 \otimes 3 \otimes 3 = 10 \oplus 8 \oplus 8 \oplus 1
\]  

(1.12)
From the above decompositions, if SU(3) is a good symmetry, we expect to observe degenerate mesonic octets as well as mesonic singlets, and degenerate baryonic decuplets, octets and singlets. Figure 1.2 shows several experimentally observed octets in both the meson sector and the baryon sector, as well as the $J = 3/2$ baryon decuplet. Although the observed masses of each of the representations are not exactly degenerate due to the explicit breaking of SU(3) symmetry, the SU(3) quark model does indeed provide a good hierarchy by which to classify the light meson and baryon spectra.

![Diagram of SU(3) flavor symmetry](image)

**FIG. 1.2:** Classification of selections of the light meson and baryon spectra by observed hypercharge and isospin. Diagram from [5].

Despite the apparent success of the SU(3) flavor symmetry in describing the structure of the hadron spectrum, with the discovery of the $\Delta^{++}$ came an understanding that the quark model as presented above was inadequate to describe the entirety of the hadronic spectrum. The $\Delta^{++}$ is considered to be a symmetric combination of three up quarks, clearly in violation of the requirement of Fermi statistics that the wavefunction be completely antisymmetric. This fact was remedied with the introduction of an additional internal color degree of freedom, postulated by Nambu [12] in 1965. The idea put forth by Nambu was straightforward: each quark has associated with it an additional internal color degree of freedom, coming in one
of three colors (anti-quarks having an associated anti-color). Hadrons form in one of two colorless combinations: each of three quarks with unique color, or a quark and antiquark with corresponding color/anti-color. The benefit of this in solving the problem introduced with the discovery of the $\Delta^{++}$ is that for a baryon, the color wavefunction can be explicitly anti-symmetrized, yielding an overall anti-symmetric wavefunction for homogeneously flavored baryons. This extension of the vanilla SU(3) flavor quark model allows for a rather complete description of the low-lying, light hadron spectrum, and has proven to be useful beyond the applications of experimental classification in the realm of constructing hadronic operators for lattice QCD as will be subsequently discussed. Before we continue on to a discussion of the modern gauge theory of quantum chromodynamics, we will first comment briefly on several other quark model theories which incorporate symmetries beyond SU(3) flavor.

### Quark models based on other symmetries

Although the original quark model was based on a (colored) SU(3) flavor symmetry, it is possible to attempt to classify the hadronic spectrum by other symmetry groups as well. The isospin symmetry SU(2) (itself a subgroup of the SU(3) flavor symmetry) provides a very accurate description of (a subset of) the low-lying hadron spectrum. Indeed, the degeneracy of the SU(2) representations are broken at the level of only a few percent (the $\pi^\pm, \pi^0$ splitting is roughly 3.5%) indicating that masses of the up and down quarks are very nearly degenerate. The SU(3) flavor symmetry discussed above and used as the basis of the original quark model is broken at the level of 20%, as can be seen by the mass differences for baryon octet and decuplet members (the $\Omega$ mass only differs by the average mass of the $\Delta$ decuplet by $\sim 15\%$). This level of symmetry breaking is not surprising, as the mass of the strange quark is roughly 20 times heavier than that of the up and down
quarks. Flavor symmetry breaking is not the only mechanism contributing to the non-degeneracy of the observed hadron spectrum, however.

Other contributing factors beyond the quark mass differences include Coulomb energy difference between pairs of quarks as well as hyperfine effects. The Coulombic contribution is expected to be of $\mathcal{O}(\alpha^2/R_0)$, and for typical intra-hadronic distances ($R_0 \sim 0.8 \text{ fm}$) these effects contribute at the order of several MeV. Electromagnetic hyperfine splittings are expected to contribute corrections proportional to $\frac{2\alpha}{3}$, also expected to contribute at the level of several MeV.

Beyond SU(3) symmetry, one could consider including the next lightest quark in the flavor symmetry and using SU(4) flavor to classify states. The heaviness of the charm quark (at roughly 250 times larger than the up and down quark masses) badly breaks SU(4) flavor symmetry. An interesting alternative to extensions of the flavor symmetry is to include the observed SU(2) spin symmetry alongside the SU(3) flavor symmetry and classifying states by a combined SU(6) spin-flavor symmetry. For baryons, the three quark combinations would decompose into the following subgroups:

$$6 \otimes 6 \otimes 6 = 56 \oplus 70 \oplus 70 \oplus 20$$

If we consider the the baryon $J = 1/2$ octet and $J = 3/2$ decuplet to be described by an SU(6) symmetry (which now includes the spin degrees of freedom), we would require a representation that includes $8 \times (2S + 1) = 16$ members for the octet and $10 \times (2S + 1) = 40$ members for the decuplet. Thus, the octet and decuplet can be described as the 56 dimensional representation of the SU(6) symmetry group.

Similarly, the mesonic $q\bar{q}$ states decompose as:

$$6 \otimes \bar{6} = 35 \oplus 1$$
To describe the pseudoscalar meson octet requires $8 \times (2S + 1) = 8$ members and for the vector meson nonet (a combination of the octet and singlet $8 \oplus 1$), we require $9 \times (2S + 1) = 27$ members, which is described by the 35 dimensional representation of SU(6) shown above.

It is clear that the SU(6) symmetry is able to provide a relevant hierarchical framework by which to classify the low lying hadron spectrum by both spin and flavor, but it fails to provide a proper relativistic treatment of the fermions as spinors through the artificial separation of the intrinsic and orbital angular momentum of the fermions.

Additionally, the approximate flavor symmetries utilized by all flavors (pun intended) of the quark model are not a fundamental aspect of the strong interaction, but rather an accidental symmetry due to the lightness of several of the quark masses with respect to the characteristic scale of the strong interaction. In the following section, we will present the modern framework for the strong interaction, a relativistic gauge theory that extends the basic idea of colored quarks to be a fundamental symmetry from which the dynamics of the theory are derived.

### 1.2 Quantum Chromodynamics

Quantum chromodynamics (QCD) is considered today to be the best candidate for a complete description of the strong interaction. Not only does it provide a mechanism by which to explain the origins of the hadron spectrum as it is observed experimentally, it also exhibits features unique to the strong interaction such as asymptotic freedom (and conversely infrared slavery). This latter feature provides an explanation for the experimental non-observation of free quarks, a problem that hindered the development of a constituent theory of hadrons and the strong interaction for some time. The fundamental degrees of freedom in quantum chromo-
dynamics, are spin-1/2 fermionic quarks and spin-1 bosonic gluons which interact via a hidden color charge, based on an underlying SU(3) color gauge symmetry. The basic properties of the six known quarks are presented in Table 1.2, with the quantum number assignments for the quarks motivated by the successes of the quark model.

The assignment of quark as spin-1/2 fermions draws from several veins of supporting evidence the first of which is the consistency of the hadron spectrum with the angular momentum states based on spin-1/2 constituents and labeled by $J^{PC}$. Experimentally, electron nucleon deep inelastic scattering (DIS) as well as high energy electron-positron collider experiments both provide evidence that suggest the half integer nature of the hadronic constituent spin. In DIS, an electron interacts with the nucleon constituents via a transversely polarized photon which will only be absorbed if the hadronic constituents have half integer spin. The similarities between angular momentum distributions of hadronic and muonic jet structures support the spin-1/2 nature of the quarks. In high energy electron positron collisions, the (angular momentum distribution of the) two-jet structure of the outgoing hadrons is similar to that of outgoing $\mu^+\mu^-$ pairs. The underlying mechanism that governs this behavior is thought to stem from the hadronization of the quarks that are produced shortly after the $e^-e^+$ collision, with the hadrons produced retaining the angular distribution of the initial quark anti-quark pairs.

Experimental study of both vector meson decay widths as well as Drell-Yan processes support the idea that the quarks have fractional charges of $1/3, 2/3$ as required by the quark model assignments. Additionally DIS experiments, which effectively count the number of quarks with a given flavor weighted by the quark charge, are consistent with the notion of fractionally charged quarks.

Although it isn’t observed directly due to color confinement, the idea that QCD relies on an internal SU(3) color symmetry is supported by by several experimental
indications as well, the first of which being the very existence of triply flavor
degenerate baryons such as the $\Delta^{++}$ (as described in our discussion of the need for
a colored quark model). Although it was not understood at the time, this simple
postulation to remedy an existing theory with experimental evidence would live on
to become the foundation for the modern theory of the strong interaction. Other
experimental evidence for a three color theory can be drawn from experimental ob-
servables which have an expected relation to the number colors in the theory. An
example of this is the cross section of the process $\pi^0 \rightarrow \gamma \gamma$ whose width is expected
to be proportional to the square of the number of colors $N_c^2$. Such experimental
probes of the internal color symmetry of QCD support the idea of three colors of
quarks.

Below we will outline basic principles of QCD followed by a discussion of some of
the key features that result from the non-abelian nature of the theory. We will then
discuss several key points associated with the symmetries of the QCD Lagrangian,
including chiral symmetry and the chiral anomaly.

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<tr>
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<td>-1/2</td>
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<td>0</td>
</tr>
<tr>
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<td>2/3</td>
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<td>0</td>
</tr>
<tr>
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<td>b</td>
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<td>-1/3</td>
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<td>1/2</td>
<td>2/3</td>
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<td>0</td>
</tr>
</tbody>
</table>

TABLE 1.1: Quantum numbers associated with the six known quarks. In addition to
these values the strange/bottom are are assigned -1 unit of strangeness/bottomness,
while the charm/top are assigned +1 unit of charm/topness.
1.2.1 QCD from Yang-Mills fields

As motivated above, QCD is believed to be a theory of fermion fields carrying color charge. By imposing the requirement of local (non-Abelian) SU(3) gauge invariance, bosonic gauge fields (gluons) arise naturally as the force carriers of the theory. Below we will outline the basic ideas of such non-Abelian gauge theories, as pioneered by the work of Yang and Mills [16].

We begin with the free Lagrange density for a single flavor of fermion (the generalization to multiple flavors is straightforward):

\[ \mathcal{L} = \bar{\psi}(x) (i\gamma \mathcal{D} - m) \psi(x). \]  \hspace{1cm} (1.15)

where \( \gamma \mathcal{D} \equiv \gamma_\mu \partial^\mu \) and \( m \) is the mass of the single fermion field under consideration.

The fermion fields are assumed to be 4-component Dirac spinors, and three component vectors in color space

\[ \psi(x) \equiv \psi(x)^\alpha_a, \]  \hspace{1cm} (1.16)

where greek indices indicate spinor labels and roman indices denote color labels. For the following discussion, these indices will be suppressed unless necessary for the sake of clarity. The requirement is then imposed that the Lagrange density Eqn. 1.15 is invariant under local SU(3) rotations in color space, with the fermion fields \( \bar{\psi}, \psi \) transforming as:

\[ \psi(x) \to e^{-i\omega(x)\lambda_\mu/2} \psi(x) \equiv U(\omega) \psi(x) \]  \hspace{1cm} (1.17)

\[ \bar{\psi}(x) \to \bar{\psi}(x) e^{i\omega(x)\lambda_\mu/2} \equiv \bar{\psi}(x) U^\dagger(\omega) \]  \hspace{1cm} (1.18)
Here, the parameters \( \omega_i(x), i = 1 \ldots 8 \), are real, and the \( \lambda_i \) are the familiar Gell-Mann matrix representation of the generators of SU(3) (given by Eqn. 1.4). Naively performing this transformation of the Lagrangian density 1.15 finds the appearance of an additional term, stemming from the invariance of the derivative term in the Lagrangian. This stems from the requirement of a \textit{local} invariance \( (\omega = \omega(x)) \). The dependence on \( \omega \) will be suppressed in the following unless necessary for clarity.

\[
\mathcal{L} \rightarrow \mathcal{L}' = \bar{\psi}(x) U^\dagger (i\mathcal{D} - m) U \psi(x) \\
= \bar{\psi}(x) (i\mathcal{D} - m) \psi(x) + i\gamma^\mu \bar{\psi}(x) U^\dagger (\partial_\mu U) \psi(x) \\
= \mathcal{L} + \mathcal{L}_{\text{int}} \tag{1.19}
\]

The appearance of this interaction term signifies that the imposition of a local SU(3) gauge invariance requires an interacting theory. To retain the gauge invariance of the theory the derivative is redefined as:

\[
\mathcal{D}_\mu \equiv \partial_\mu + igA_\mu, \tag{1.20}
\]

and the Lagrange density becomes:

\[
\mathcal{L} = \bar{\psi}(x) (i\mathcal{D} - m) \psi(x). \tag{1.21}
\]

Once again applying the gauge transformation, it is found that the following expression must be must hold to retain gauge invariance:

\[
-gU^\dagger A'_\mu U + iU^\dagger (\partial_\mu U) = -gA_\mu. \tag{1.22}
\]
This expression implies that the field $A_\mu$ has a component corresponding to each of the eight generators of SU(3), and can be written as:

$$A_\mu = \frac{\lambda_i}{2} A^i_\mu.$$  \hspace{1cm} (1.23)

The relation Eqn. 1.22 also implies the following transformation property for the vector potential field:

$$A_\mu \rightarrow A'_\mu = U \left( A_\mu - \frac{i}{g} \partial_\mu \right) U^\dagger.$$  \hspace{1cm} (1.24)

The remaining ingredient missing form the Lagrange density thus far are mass and kinetic energy terms for the gauge fields. A mass term for the gauge fields is incompatible with a gauge invariant theory, as it would be proportional to $A^j_\mu A^i_\mu$, which is not a gauge invariant quantity. The kinetic energy term is obtained by constructing a field strength tensor (analogous to that for non-Abelian theories) for the non-Abelian fields:

$$F^{ij}_{\mu\nu} = \frac{\lambda^j_i}{2} = \partial_\mu A^j_\nu - \partial_\nu A^j_\mu + ig \left[ A_\mu A_\nu \right]$$  \hspace{1cm} (1.25)

with:

$$F^{ij}_{\mu\nu} = \partial_\mu A^j_\nu - \partial_\nu A^j_\mu - ig f_{jkl} A^k_\mu A^l_\nu,$$  \hspace{1cm} (1.26)

where the $f_{jkl}$ are the structure constants of SU(3) given by Eqn. 1.1.1.

It is important to note that the commutator in Eqn. 1.25 is exactly zero in the case of an Abelian theory, such as QED. The appearance of this non-zero commutator gives rise to one of the most interesting aspects of QCD, confinement, as will be discussed below.

With this field strength tensor, a gauge invariant kinetic energy term for the Yang-Mills fields can be included in the Lagrange density:
\[ \mathcal{L} = \bar{\psi}(x)(i\mathcal{D} - m)\psi(x) - \frac{1}{4} F^j_{\mu\nu} F^{j\mu\nu}, \]

with the factor of $1/4$ being the conventional normalization. From the requirement of an internal SU(3) color gauge symmetry, the QCD Lagrangian is constructed.

### 1.3 Features of the QCD Lagrangian

The QCD Lagrangian Eqn. 1.27 exhibits several unique features that will be briefly discussed in this section. These features arise from several sources: the non-Abelian nature of the Yang-Mills theory as discussed above, the accidental approximate symmetry of the up and down quarks and their relatively light mass in comparison with the natural scale of QCD, and anomalously broken symmetries. Several of these features such are not unique to the theory of quantum chromodynamics and are common to both the electroweak theory as well as quantum electrodynamics (QED). The most striking difference between QED and QCD is the nature of the running of the coupling in QCD, as will be discussed presently.

#### 1.3.1 Running of the coupling and asymptotic freedom

In quantum electrodynamics, upon renormalization of the theory it is found that the bare coupling appearing in the QED Lagrangian is not the same coupling measured in experiments, but rather what is accessible experimentally is a dressed coupling. When implementing the renormalization procedure, non-analytic terms are absorbed into a redefinition of the bare coupling. This phenomenon is interpreted as a screening of the bare coupling by polarization of the QED vacuum arising from the existence of virtual fermion anti-fermion pairs. These contributions arise from diagrams like that shown in the left side of Fig. 1.3.
If a probe of $Q^2$ (defined as $-(p)^2$, where $p^\mu$ is the four-momentum) is used to test the effective QED coupling, it is found that this screening becomes smaller and the effective coupling increases as $Q^2$ increases. Because of this, the coupling constant in QED is energy dependent:

$$\alpha (Q^2) = \frac{\alpha (m^2)}{1 - \frac{\alpha(m^2)}{3\pi} \log \left( \frac{Q^2}{m^2} \right)}, \quad (1.28)$$

where $Q^2$ is taken to be much greater than the mass of the particles in question ($Q^2 \equiv -(p^2) \gg m^2$).

In quantum chromodynamics, the theory contains the same screening of the effective coupling by the fermion loops as shown in the left hand side of Fig. 1.3. Due to the non-Abelian nature of the theory however, the gauge fields carry charge themselves, and the theory contains self-interactions between gauge fields. This fact was apparent from the appearance of the non-vanishing commutator in Eqn. 1.25, which gives rise to cubic and quartic gauge field interactions as illustrated in Fig. 1.4. This inherent non-linearity in the gluonic interactions gives rise to additional contributions to the QCD coupling, arising from diagrams illustrated in the bottom right of Fig. 1.3. As the gluons themselves are charged, the effect of such loops is to produce an *antiscreening* of the QCD coupling. The (spin-1) charged gluons behave...
as permanent magnetic color dipoles, aligning themselves parallel to any external chromomagnetic field and increasing the strength of the field. The result of this is that the QCD vacuum is effectively a paramagnetic medium, with the fermionic screening of the effective coupling competing with the gluonic antiscreening. The level of fermionic screening is dependent on the number of fermion flavors, and the level of antiscreening is dependent on the underlying gauge group of the Yang-Mills theory. For an SU(3) gauge symmetric theory such as QCD, the effective coupling of the theory is given by

$$\alpha_s(Q^2) = \frac{12\pi}{(33 - 2N_f) \log \left( \frac{Q^2}{\Lambda_{QCD}^2} \right)}$$  \hspace{1cm} (1.29)

where $N_f$ is the number of fermion flavors, and $\Lambda_{QCD}$ is the characteristic scale of the strong interaction.

Several determinations of the QCD coupling, both experimental and theoretical, are presented in Fig. 1.5
1.3.2 Symmetries of the QCD Lagrangian

The QCD Lagrangian satisfies the symmetries of the Poincaré group, including the discrete symmetries C, P, and T, leading to a natural classification of the QCD fields as eigenstates of these operators.

The classical QCD Lagrangian possesses an additional approximate $U(N_f) \otimes U(N_f)$ chiral symmetry (for $N_f$ fermion flavors), under independent rotations of the left and right handed fermion fields:

\begin{align}
\psi(x)_L & \rightarrow U_L \psi(x)_L & \bar{\psi}(x)_L & \rightarrow \bar{\psi}(x)_L U_L^\dagger \\
\psi(x)_R & \rightarrow U_R \psi(x)_R & \bar{\psi}(x)_R & \rightarrow \bar{\psi}(x)_R U_R^\dagger 
\end{align}

where $\psi(x)_{L,R} = \frac{1}{2} (1 \mp \gamma_5) \psi(x) = P_{L,R} \psi(x)$, and $U_{L,R}$ are elements of the group
U (N_f). This symmetry becomes exact in the limit of massless fermions, as can be seen explicitly upon examination of the free QCD Lagrangian with the left and right handed states projected:

\[ \mathcal{L} = \bar{\psi}(x) (i \slashed{D} - m) \psi(x) \]  
\[ = \bar{\psi}(x)_L i \slashed{D} \psi(x)_L + \bar{\psi}(x)_R i \slashed{D} \psi(x)_R - m \bar{\psi}(x)_L \psi(x)_R - m \bar{\psi}(x)_R \psi(x)_L \quad (1.34) \]

where we have used the relations:

\[ P_L P_R = P_R P_L = 0 \quad (P_L)^2 = (P_L)^2 = 1 \quad (1.35) \]
\[ (P_L + P_R) = 1 \quad P_{L,R} \gamma_\mu = \gamma_\mu P_{R,L} \quad (1.36) \]

This symmetry decomposes as:

\[ U(N_f)_L \otimes U(N_f)_R = SU(N_f)_L \otimes SU(N_f)_R \otimes U(1)_L \otimes U(1)_R \]
\[ = SU(N_f)_V \otimes SU(N_f)_A \otimes U(1)_V \otimes U(1)_A \quad (1.37) \]

For the moment, we shall restrict our focus to \( N_f = 2 \) for simplicity, however extending the following discussion to three flavors of light quarks is straightforward. The symmetries in Eqn. 1.37 correspond to the following transformations for SU(2) flavors:

\[ U(1)_V : \psi(x) \rightarrow e^{-i\theta \gamma_5} \psi(x) \quad (1.39) \]
\[ SU(2)_V : \psi(x) \rightarrow e^{-i\frac{\theta}{2} \gamma_5} \psi(x) \quad (1.40) \]
\[ U(1)_A : \psi(x) \rightarrow e^{-i\gamma_5 \theta} \psi(x) \quad (1.41) \]
\[ SU(2)_A : \psi(x) \rightarrow e^{-i\gamma_5 \frac{\theta}{2}} \psi(x) \quad (1.42) \]
Here, the parameters $\theta_0, \theta_i (i = 1 \ldots 3)$ are a real valued continuous variables, the $\tau_i (i = 1 \ldots 3)$ are the generators of $SU(2)$, and $\gamma_5 \equiv \gamma_0 \gamma_1 \gamma_2 \gamma_3$ is the anti commuting product of the Dirac gamma matrices.

From Noether’s theorem, invariance of the theory under these transformations implies conservation of the currents:

$$j^\mu \equiv \bar{\psi} (x) \gamma^\mu \psi (x) \quad j^{\mu a} \equiv \bar{\psi} (x) \gamma^\mu \frac{T}{2} \psi (x) \tag{1.43}$$

$$j^{\mu 5} \equiv \bar{\psi} (x) \gamma^\mu \gamma_5 \psi (x) \quad j^{\mu 5a} \equiv \bar{\psi} (x) \gamma^\mu \gamma_5 \frac{T}{2} \psi (x) \tag{1.44}$$

The vector currents $j^\mu$ and $j^{\mu a}$ are associated with the conservation of baryon number and isospin, respectively, the experimental observation of which has been historically well verified in high energy physics.

The axial currents $j^{\mu 5}$ and $j^{\mu 5a}$ on the other hand, have no obvious physical manifestation. The explicit conservation of both the vector and axial vector symmetries above would presume the existence of iso-vector parity partners, an example being positive parity states around roughly the same mass as the pion iso-triplet. As these are not observed experimentally, it is assumed that the $SU(2)_A$ symmetry is spontaneously broken, giving rise to a triplet of nearly-degenerate pseudo-goldstone bosons. If the chiral symmetry were exact, these bosons would be massless, but the explicit chiral symmetry breaking by the masses of the up and down quarks leads to the pions being relatively light with respect to other states composed of two light quarks, such as the rho meson. The $U(1)_A$ symmetry on the other hand is explicitly broken by another, less obvious source: the axial anomaly. A detailed discussion of axial anomalies in quantum field theories is beyond the intended scope of the current work, however the source of the axial anomaly can be understood as arising from the lack of invariance of the integration measure upon quantization of the classical field theory. The effect of this symmetry breaking is evident upon calculation of the
divergence of the iso-singlet axial vector current, given by:

\[
\partial_\mu j^\mu_S = \frac{g^2 N_c}{23 \pi^2} \epsilon^{\alpha \beta \mu \nu} F_{\alpha \beta}^c F_{\mu \nu}^c
\]  

(1.45)

It is worth noting here that this type of anomalous symmetry breaking is a result of the quantization of the theory and therefore is a feature of many quantum field theories, including QED.

This concludes our discussion of the key features of QCD. We will not shift focus to several effective theories that are useful in the study of QCD and hadronic physics.

1.4 Effective theories for heavy quarks

Similar to those symmetries that manifest themselves in QCD for due to the separation of scales between the lightness of the light quark masses and \( \Lambda_{QCD} \), symmetries also arise in the QCD Lagrangian as the mass of the quarks becomes very large (for the following discussion, we will refer to the mass of the heavy quark as \( m_Q \)). Indeed, in the limit \( m_Q \rightarrow \infty \), the part of the QCD Lagrangian containing the heavy flavors attains an exact \( SU(2N_{f}^{\text{heavy}}) \) spin-flavor symmetry. The consequence of the flavor symmetry is that properties of heavy quark states that remain finite in the limit \( m_Q \rightarrow \infty \) should be independent of the heavy quark flavor. The additional spin symmetry (which is the source of the factor of two above) arises from the fact that when expanding the QCD Lagrangian in powers of \( \frac{1}{m_Q} \), the magnetic moment dependence \( \Sigma \cdot B \) enters at \( \mathcal{O} \left( \frac{1}{m_Q} \right) \).

For \( \Lambda_{QCD} \ll m_Q \) heavy quarks contained in QCD bound states contribute little to the dynamics and as such a natural treatment is to integrate out the energy scale introduced by the heavy quark mass. There are two effective theories commonly
used which approach the treatment of heavy quarks from different perspectives. Heavy quark effective theory (HQET) (see Ref. [17] and references therein for a good overview) treats the heavy quark from an almost classical point of view, and is derived in the explicit $m_Q \to \infty$ limit. At leading order, the heavy quarks in this theory exhibit exact $SU(2N_f^{heavy})$ spin-flavor symmetry, with corrections entering at $\mathcal{O}\left(\frac{1}{m_Q}\right)$. The drawback to this approach is that it cannot be used for hadrons containing more than a single heavy quark, the reasons for which will become apparent below. In contrast to HQET, non-relativistic QCD (NRQCD) [18] aims to treat the heavy quarks non-relativistically by decoupling the upper and lower components of the Dirac spinor and systematically removing terms in the Lagrangian that couple the two (independent) two-component spinors through a given order in $\frac{\not{p}}{m_Q}$ (the NRQCD expansion parameter, where $\not{p}$ is the momentum of the heavy quark). Below we will outline the frameworks for each of these effective theories, as both will be used for different purposes in the present work.

1.4.1 Heavy quark effective theory

Heavy quark effective theory builds from the assumption that the heavy quark mass is much greater than the characteristic scale of QCD interactions: $\Lambda_{QCD} \ll m_Q$. In this limit, the heavy quark acquires an additional spin-flavor symmetry as discussed above. The goal of HQET is to make this symmetry more apparent by writing the heavy quark Lagrangian as an expansion in powers of the inverse heavy quark mass:

$$\mathcal{L} = \mathcal{L}_0 + \frac{1}{m_Q} \mathcal{L}_1 + \frac{1}{m_Q^2} \mathcal{L}_2 + \ldots$$ (1.46)

The usual treatment of this expansion is to retain the leading order term as the Lagrangian of HQET, while treating terms higher order in $\frac{1}{m_Q}$ as perturbations whose effects could be included order by order if desired.
Typical momentum exchanges arising from interactions of the heavy quark with the light degrees of the theory will be of $\mathcal{O}(\Lambda_{QCD})$. Because of this, a heavy quark interacting within a QCD bound state will experience only negligible changes to its momentum when interacting with the light degrees of freedom (ldof). Consider a heavy quark with initial momentum $p^\mu_i = m_Q v^\mu$, and final momentum $p^\mu_f = m_Q v^\mu + k^\mu$ after interaction with the ldof as pictured in Figure 1.6. Here, $k^\mu$ is a small residual momentum of the interaction and is of the order $\Lambda_{QCD}$. The velocity of the heavy quark $v^\mu = \frac{k^\mu}{m_Q}$ does not change in the limit $\Lambda_{QCD} \ll m_Q$:

\[
\delta v^\mu = \frac{\delta p^\mu}{m_Q} \sim \frac{\Lambda_{QCD}}{m_Q} \to 0.
\]

Furthermore, the large mass limit allows for simultaneous specification of the heavy quark position and velocity:

\[
[v, x] = \frac{1}{m_Q} [p, x] = \frac{i\hbar}{m_Q} \to 0.
\]

Because of this, the heavy quarks in HQET are defined to be eigenstates of both position and velocity. In its rest frame, the heavy quark has four velocity $v^\mu = (1, \mathbf{0})$, and it acts simply as a static color source. It should be noted that the theory contains no restriction on the spatial components of the velocity requiring them to be non-relativistic, as is the desired treatment for this effective theory. This
is easily remedied however, as it's always possible to boost to a frame of reference in which a single heavy quark is at rest. When dealing with two heavy quarks with different velocities however, this argument does not hold, therefore HQET is not a theory that can handle multiple heavy quarks within the same hadron.

To derive the explicit form of the HQET Lagrangian, we begin with the section of the QCD Lagrangian that describes the heavy quark field, which we shall refer to as $Q$:

$$\mathcal{L} = \bar{Q} \left( i \slashed{D} - m_Q \right) Q.$$  \hspace{1cm} (1.49)

In this form, the limit $m_Q \to \infty$ is not easily taken and the symmetries associated with this limit are opaque. To make the symmetries more explicit, the upper and lower components of the heavy quark fields are projected out with the use of the idempotent operators (here $\not\!v \equiv v_\mu \gamma^\mu$):

$$P_\pm = \frac{(1 \pm \not\!v)}{2} \hspace{1cm} (1.50)$$

which satisfy the properties:

$$P_\pm^2 = P_\pm, \hspace{1cm} P_+ + P_- = 1, \hspace{1cm} P_+ P_- = P_- P_+ = 0. \hspace{1cm} (1.51)$$

The projected components of the heavy quark field are then given by:

$$h_v = e^{imQv \cdot x} P_+ Q, \hspace{1cm} \xi_v = e^{imQv \cdot x} P_- Q, \hspace{1cm} (1.52)$$

where an explicit dependence on the heavy velocity has been included as we are now working in the heavy quark limit. The heavy quark field is now rewritten as:
\[ Q = P_+ Q + P_\cdot Q = e^{-i m Q\nu \cdot x} (h_v + \xi_v), \]  

(1.53)

with the constraints that \(\not\! h_v = h_v\) and \(\not\! \xi_v = -\xi_v\). Plugging this back into the Lagrangian Eqn. 1.49, we find:

\[
\mathcal{L} = e^{i m Q\nu \cdot x} (\bar{h}_v + \bar{\xi}_v) (i \not\! \partial - m_Q) e^{-i m Q\nu \cdot x} (h_v + \xi_v) \\
= (\bar{h}_v + \bar{\xi}_v) (i \not\! \partial - m_Q (\not\! \gamma - 1)) (h_v + \xi_v) \\
= \bar{h}_v i \not\! \partial h_v + \bar{\xi}_v (i \not\! \partial - 2m_Q) \xi_v \\
+ \bar{\xi}_v (i \not\! \partial - m_Q (\not\! \gamma - 1)) h_v + \bar{h}_v (i \not\! \partial - m_Q (\not\! \gamma - 1)) \xi_v 
\]  

(1.54)

where we have used the aforementioned constraints: \(\not\! h_v = h_v\) and \(\not\! \xi_v = -\xi_v\). As the production of heavy quark-antiquark pairs is a highly energetic process, the last two terms in the Lagrangian above can be neglected as they will only impact processes which lie well above the energy threshold that has been established as an upper limit for the effective theory; namely \(m_Q\). The second term describes a heavy quark excitation with a mass of \(2m_Q\). Because of this, the propagation of this state will be suppressed by a power of \(\frac{1}{m_Q}\) in relation to the leading order term in the Lagrangian and can be neglected as well. We are then left with the following HQET Lagrangian:

\[
\mathcal{L}_{HQET} = \bar{h}_v i \not\! \partial h_v \\
= \bar{h}_v P_+ i \not\! \partial P_+ h_v \\
= \bar{h}_v P_+ i (\gamma^\mu P_\mu - D_\mu P_+ h_v \\
= \bar{h}_v i v \cdot D h_v 
\]  

(1.55)
where we have used the identity \( P_+ \gamma^\mu = (\gamma^\mu + \gamma^\mu P_-). \) This Lagrangian will provide the foundation for implementing heavy quarks in the static limit on the lattice for the present work. We now turn our attention to an alternative effective theory for heavy quarks, NRQCD.

### 1.4.2 Non-relativistic QCD

Just as HQET relies on the fact that the heavy quark momentum is much less than the characteristic scale of QCD, so does the effective theory NRQCD [18]. The two theories differ in their treatment of the expansion which leads to the Lagrangian for the heavy quark flavors. While HQET keeps only the leading order term and treats all terms higher order in \( \frac{1}{m_Q} \) as perturbations, NRQCD seeks to build a non-relativistic theory by decoupling the upper and lower components of the heavy quark field to any required order in \( \frac{1}{m_Q} \). This treatment of the expansion has the benefit that it allows for the inclusion of multiple NRQCD quarks within a single hadron (in contrast to HQET). The drawback of including terms beyond leading order in the expansion in powers of \( \frac{1}{m_Q} \) is that these terms are necessarily of mass dimension \( d > 4 \) making continuum NRQCD an explicitly non-renormalizable theory. This undesirable trait is remedied by tuning the expansion parameters in the NRQCD Lagrangian to produce the results of the full theory which effectively shifts the bare mass and coupling to account for the inclusion of these higher order effects which are explicitly neglected (due to the truncated expansion).

Below we will briefly outline the key ideas in the derivation of the NRQCD Lagrangian. This derivation relies on the use of a Foldy-Wouthuysen-Tani (FWT) transformation [19] to systematically decouple the upper and lower components of the heavy quark field by placing the non-commuting terms in the phase of iterative field redefinitions. This transformation has the added benefit in that it provides a
natural route for the expansion of the heavy quark Lagrangian in inverse powers of the heavy quark mass as will be seen below. We begin with the heavy quark part of the QCD Lagrangian:

\[ \mathcal{L} = \bar{Q} \left( i \slashed{D} - m_Q \right) Q. \] (1.56)

We wish to use the projectors \( P_\pm = \frac{1}{2} \left( 1 \pm \gamma_0 \right) \) to decouple the upper and lower components of the heavy quark spinor in the Dirac basis. The difficulty in applying this procedure stems from the fact that the projectors \( P_\pm \) do not commute with the spatial components of the gamma matrices: \( [P_\pm, \gamma_i] \neq 0 \) necessitating the removal of the explicit \( \gamma_i \) dependence from the Lagrangian. As mentioned above, this is accomplished with the use of Foldy-Wouthuysen-Tani transformations on the heavy quark field, the first of which is defined as:

\[ Q = Q^{(1)} e^{i \gamma^j D_j / 2 m_Q}. \] (1.57)

Inserting this into Eqn. 1.56 and expanding the exponentials, we find:

\[ \mathcal{L} = \bar{Q}^{(1)} \left( \gamma^0 D_0 - m_Q \right) Q^{(1)} \]

\[ + \frac{1}{m_Q} \bar{Q}^{(1)} \left[ -\frac{1}{2} D^i D_i - \frac{ig}{8} [\gamma^i, \gamma^j] F^{ij} - \frac{ig}{2} \gamma^i \gamma^0 F^{ij} \right] Q^{(1)} + \mathcal{O} \left( \frac{1}{m_Q^2} \right) \] (1.58)

The non-commutativity of the Lagrangian with the term \( \gamma^j D_j \) has now been shifted to an \( \mathcal{O} \left( \frac{1}{m_Q} \right) \) term, and the Lagrangian is decoupled to leading order. All terms of \( \mathcal{O} \left( \frac{1}{m_Q} \right) \) commute with the \( \gamma_i \) save for the last term above, which has an odd number of spatial gamma matrices. The FWT transformation can be applied iteratively to decouple the heavy quark field components through any order in \( \frac{1}{m_Q} \) by inserting the non-commuting operator into the phase of the
redefinition as illustrated above. To remove all non-commuting operators through and including order \( \frac{1}{m_Q} \) requires three such FWT transformations. Following these transformations, it is customary (although not necessary as it only introduces an overall energy shift to quantities calculated within the theory) to perform one last rescaling of the quark field in order to remove the mass term from the Lagrangian. This final field redefinition is given by:

\[
Q = e^{-im_Q \gamma^0 x^9} \tilde{Q}^{(3)}
\]

where the superscripted field \( \tilde{Q}^{(3)} \) is the result of three iterations of FWT transformations.

After this, the NRQCD Lagrangian, decoupled through \( \mathcal{O} \left( \frac{1}{m_Q^3} \right) \), is given by:

\[
\mathcal{L} = \bar{Q} \left[ i \gamma^0 D^0 - \frac{1}{2m_Q} D^i D_i - \frac{ig}{8m_Q} \left[ \gamma^i, \gamma^j \right] F^{ij} \right. \\
\left. - \frac{g^2}{8m_Q^2} \gamma^0 \left( D_i^j F_j, - \frac{1}{2} \left[ \gamma^i, \gamma^j \right] \{ D_i, F_j, 0 \} \right) \right] \tilde{Q} + \mathcal{O} \left( \frac{1}{m_Q^3} \right)
\]

(1.60)

Using the identity \( P_+ + P_- = 1 \), this Lagrangian can now easily be separated into the upper and lower components \( P_+ Q = h \), and \( P_- Q = \xi \). where \( h \) acts to create a heavy quark, while \( \xi \) creates a heavy anti-quark. The Lagrangian presented in Eqn. 1.60 is used as the basis for the lattice NRQCD action that will be discussed in Chapter 2.

This concludes the discussion of continuum effective theories for heavy quarks.
1.5 Chiral perturbation theory

As was mentioned in 1.3.2, QCD acquires additional vector and axial vector symmetries in the limit of vanishing quark mass. Because of this, one would expect to observe experimentally a doubling of the hadron spectrum, with degenerate parity partners for every observed hadron. As this is not observed experimentally, it is postulated that the axial vector symmetry is spontaneously broken, leading to the formation of a non-zero chiral condensate given by $\langle \bar{q}q \rangle$. For each spontaneously broken degree of freedom, we expect to observe a massless Nambu-Goldstone boson. For an SU(N) chiral symmetry, we therefore expect $N^2 - 1$ massless Goldstone bosons, one for each generator of the symmetry group. The low-lying mesonic spectrum of QCD contains a nearly degenerate triplet of light pseudoscalar mesons $(\pi^\pm, \pi^0)$ contained within an octet of light pseudoscalar mesons with very similar masses. The finite mass of the pion triplet is interpreted to be caused by the explicit chiral symmetry breaking of the QCD Lagrangian by the fermion mass. From this perspective, it seems natural that the low energy dynamics of QCD can be described by an effective theory which possesses exact chiral symmetry with the masses of the light degrees of freedom entering as small perturbations. Chiral Perturbation Theory (ChiPT) seeks to provide a description of the dynamics of the asymptotically free states of QCD (hadrons) composed of light quarks, while providing insight into how the physical observables of QCD scale with the masses of the light quarks. In the following section, we will sketch the fundamentals of ChiPT for the light mesons, and then detail the primary modifications necessary when moving to a description of light baryons as well as baryons containing heavy quarks, as well as the use of partial quenching in ChiPT.
1.5.1 ChiPT for mesons

In choosing a field representation for the effective theory, we need a representation of the coset space $SU(N)_L \times SU(N)_R / SU(N)_V$, that is the space of transformations that do not leave the vacuum invariant. The number of elements in this coset space is equal to the number of Goldstone bosons generated by the spontaneously broken symmetry (8 for $SU(3)$, 3 for $SU(2)$). A useful unitary representation for elements of $SU(N)$ that represent the mesonic fields is the exponential representation, given by:

$$U = e^{i/2 \lambda^a \phi}, \quad (1.61)$$

For $SU(2)$, the explicit form of the matrix valued field $U \equiv U^a \lambda^a$ is given by:

$$U = \begin{pmatrix} \pi_0 & \pi^+ \\ \pi^- & -\pi_0 \end{pmatrix}, \quad (1.62)$$

and for $SU(3)$:

$$U = \sqrt{2} \begin{pmatrix} \frac{1}{\sqrt{2}} \pi^0 + \frac{1}{\sqrt{6}} \eta & \pi^+ & K^+ \\ \pi^- & -\frac{1}{\sqrt{2}} \pi^0 + \frac{1}{\sqrt{6}} \eta & K^0 \\ K^- & \bar{K}^0 & -\frac{2}{\sqrt{6}} \eta \end{pmatrix} \quad (1.63)$$

These fields transform as:

$$U \to U_L U \bar{U}_R \quad (1.64)$$

under chiral rotations, with $U_{L/R}$ as in Eqn. 1.30.

It can be shown that at vanishing momenta, the Goldstone bosons of massless QCD do not interact, thus providing motivation for the low energy expansion of the effective Lagrangian in powers of the momentum:
\[ \mathcal{L}_{\text{eff}} = \mathcal{L}^{(0)} + \mathcal{L}^{(2)} + \mathcal{L}^{(4)} + \ldots \]  

(1.65)

Within the Lagrangian this translates to ordering terms by the number of derivatives which, upon acting on a quark field, produces a single power of the quark momentum. In terms of the matrix valued fields of Eqns. 1.62 and 1.63, the effective Lagrangian will be a function of the field itself and powers of derivatives acting on the matrix valued field:

\[ \mathcal{L} = \mathcal{L} (U, \partial U, \partial^2 U, \ldots) \]  

(1.66)

The astute reader will have noticed that only even powers appear in the expansion above, and this is due to the requirement that the Lagrangian be a Lorentz scalar, which constrains the derivative operators to appear in pairs in terms within the Lagrangian. The zeroth order term in the Lagrangian contains zero derivatives and zero powers of the quark fields, making at a trivial additive constant which can be neglected. Because of this, the leading order term in the effective chiral Lagrangian will be \( \mathcal{L}^{(2)} \) which contains only one unique term:

\[ \mathcal{L}^{(2)} = c_1 \text{tr} \left( \partial_\mu U^\dagger \partial^\mu U \right) . \]  

(1.67)

The low energy constant (LEC) \( c_1 \) is determined to be \( f^2/4 \) by expanding the fields \( U \) in Eqn. 1.67 and requiring the standard form of the kinetic term for the individual Goldstone fields:

\[ \mathcal{L}^{(2)} = \frac{1}{2} \partial_\mu \phi^a \partial^\mu \phi^a + \mathcal{O}(\phi^4) . \]  

(1.68)

The above Lagrangian describes massless fields that are invariant under chiral transformations by construction. As has been discussed, the mass term in the QCD
Lagrangian explicitly breaks the chiral symmetry. To include the quark masses in the effective Lagrangian while still retaining invariance under chiral transformations, one introduces a mass matrix $M$ for the effective theory and require that it transforms as:

$$M \rightarrow U_R M U_L^\dagger.$$

(1.69)

With the above transformation property, we can include a mass term in the effective Lagrangian that is explicitly invariant under chiral transformations. The lowest order term in $M$ that can be included is given by:

$$\mathcal{L}_M = \frac{f^2 B_0}{2} tr \left( M U^\dagger + U M^\dagger \right),$$

(1.70)

where the parameter $B_0$ is (at lowest order in the chiral expansion) related to the value of the chiral condensate as: $3f^2 B_0 = -\langle \bar{q}q \rangle$ (this can be seen by taking the derivative of the energy density of the effective Lagrangian with respect to the quark mass and comparing to the same quantity in QCD). Including this term in the effective Lagrangian, and expanding the fields $U$ to order $\phi^2$ we find (for SU(3), where $M = \text{diag}(m_u, m_d, m_s)$):

$$\mathcal{L}^{(2)} = \partial_\mu \pi^+ \partial^\mu \pi^- + \frac{1}{2} \left( \partial_\mu \pi^0 \right)^2 + \partial_\mu K^+ \partial^\mu K^- + \frac{1}{2} \left( \partial_\mu K^0 \right)^2 + \frac{1}{2} \left( \partial_\mu \eta \right)^2$$

$$- B_0 (m_u + m_d) \pi^+ \pi^- - \frac{B_0}{2} (m_u + m_d) \pi^0 \pi^0 - B_0 (m_u + m_s) K^+ K^-$$

$$- B_0 (m_d + m_s) K^0 \bar{K}^0 - \frac{B_0}{6} (m_u + m_d + 4m_s) \eta \eta$$

$$- \frac{B_0}{\sqrt{3}} (m_u - m_d) \pi^0 \eta.$$

(1.71)

From this expression, we are able to read off the masses of the Goldstone bosons
in terms of the quark masses as (in the isospin symmetric limit with $m_u = m_d = m_l$):

\begin{align}
M^2_f &= 2B_0 m_l, \\
M^2_K &= B_0 (m_l + m_s), \\
M^2_n &= \frac{2B_0}{3} (m_l + 2m_s). 
\end{align}  
(1.72)

From these expressions and the relativistic dispersion relationship, it is clear that for the purposes of power counting a single power of the mass matrix $M$ in the effective Lagrangian will contribute at $\mathcal{O}(p^2)$ in the low energy expansion. The expression Eqn. 1.72 (and similar equations derived at higher orders in the chiral expansion) are extremely useful in guiding extrapolations of results from lattice QCD calculations which are often carried out at unphysical quark masses to the physical quark mass. Similar expressions will be used in guiding extrapolations for spectroscopy calculations carried out in the present work, however explicit derivation of the formulae used will not be presented as it is beyond the intended scope of this work. For this reason, the following sections will focus on the modifications necessary to the basic framework of ChiPT in its application to (heavy) baryons, as well as the incorporation of partial quenching.

This concludes our discussion of ChiPT for the mesonic sector. In the next section we will shift our focus to ChiPT for heavy baryons.

1.5.2 ChiPT for (heavy) baryons and partial quenching

As the framework for deriving the effective Lagrangian for baryons in chiral perturbation theory is very similar to the methods presented above, we will focus on the primary differences in deriving ChiPT for baryons as opposed to mesons,
and present new definitions and redefinitions (e.g. for field variables) as needed. Furthermore, in consideration of the main focus of this dissertation, we will restrict our focus to the application of baryonic chiral perturbation to the heavy baryon sector.

The main conceptual difference between ChiPT for light mesons and for baryons is that we no longer expect the baryonic masses to be small in relation to $\Lambda_{QCD}$, and that the masses of the baryons are not expected to vanish in the limit of vanishing quark masses. In building an effective theory for heavy baryons, it is useful to follow the heavy quark methods presented in section 1.4.1. It should be noted that when applying these methods to baryons, only the scale of the average mass of the baryon multiplet can be removed, as the SU(3) mass splittings transform non-trivially under chiral transformations. As such, the mass splittings are treated as perturbations (a valid treatment as the splittings are small in comparison with the average mass).

Below we will present an overview of the construction of the leading order chiral effective Lagrangian for heavy baryons which will provide context that can help to frame the discussions of chiral extrapolations that will be presented in later chapters of this dissertation.

ChiPT for baryons

The matrix valued Goldstone boson field is given by Eqn. 1.63, with the additional field definitions:

$$\xi \equiv e^{iU/f}, \quad U = \xi^2 \equiv e^{2iU/f},$$

which transform as:

$$\xi \rightarrow U_R \xi K^{-1}(U_R, U_L, U),$$

(1.73)
where the non-linear function \( K \) is defined (implicitly through Eqn. 1.74) as:

\[
K(U_L, U_R, U) \equiv \sqrt{U_R U_L^* U_R^* U_L}
\]  

(1.75)

The field \( \xi \) is introduced as a convenience in constructing the axial and vector currents that couple the mesons to the baryons:

\[
V^\mu \equiv \frac{1}{2} (\xi \partial^\mu \xi^\dagger + \xi^\dagger \partial^\mu \xi)
\]  

(1.76)

\[
A^\mu \equiv \frac{1}{2} (\xi \partial^\mu \xi^\dagger - \xi^\dagger \partial^\mu \xi)
\]  

(1.77)

Just as with the HQET we wish to treat the baryonic fields as heavy, and write the baryon momentum as:

\[
p^\mu = m_B v^\mu + k^\mu
\]  

(1.78)

which explicitly separates out the residual momentum \( k^\mu \ll m_B \) (here \( m_B \) is the baryon mass). The baryon fields are then projected rewritten as eigenstates of velocity:

\[
B_v^\pm(x) = e^{im_B v x} P_{\pm} B
\]  

(1.79)

For SU(3) (on which our attention will be focused for the remainder of this section) the fields \( B_v \) are collected in a complex traceless non-Hermitian matrix for SU(3):

\[
B_v = \sqrt{2}
\begin{pmatrix}
\frac{1}{\sqrt{2}} \pi^0 + \frac{1}{\sqrt{6}} \eta & \pi^+ & K^+
\frac{1}{\sqrt{2}} \pi^0 - \frac{1}{\sqrt{6}} \eta & K^0
\end{pmatrix}
\]  

(1.80)
For the following discussion, we will restrict our attention to SU(3). The baryonic Dirac spinor at rest is not a chiral eigenstate, and therefore we seek that the left and right handed components transform in the same way under chiral rotations to facilitate the removal of the mass term. As a matter of convenience, the transformation is written in terms of the transformation matrix $K(L, R, U)$ (with $L = U_L$ and $R = U_R$) as in Eqn. 1.75 and is given by\(^2\):

$$B \rightarrow K(L, R, U) B K(L, R, U)^{-1}$$  \(1.81\)

Following from Eqn. 1.79, we find spin operators $S_\nu^\mu$ which satisfy:

\begin{align*}
v \cdot S_\nu &= 0, \quad (1.82) \\
S_\nu^2 B_\nu &= -\frac{3}{4} B_\nu \quad (1.83) \\
\{S_\nu^\mu, S_\nu^\nu\} &= \frac{1}{2} (v_\mu v_\nu - g_\mu^\nu), \quad (1.84) \\
[S_\nu^\mu, S_\nu^\nu] &= i\epsilon^{\mu\nu\alpha\beta} v_\alpha S_{\nu,\beta} \quad (1.85)
\end{align*}

From these relations, bilinears in the baryon fields can be rewritten entirely in

\(^2\)It should be noted here that this is not the only choice of the representation for the $SU(3)_L \times SU(3)_R \times U(1)_Y$ transformations, however it proves to be the most useful for connecting the transformation properties of the baryon and mesonic fields via field redefinition. Another possible representation of the baryon fields is given by: e.g. $(B_L, B_R) \rightarrow (L B_L L^\dagger, R B_R R^\dagger)$.
allowing the leading order effective Lagrangian to be written down independent of the gamma matrices. The explicit form of this LO Lagrangian is given by:

$$\mathcal{L}^0_v = i\bar{B}_v (v \cdot \mathcal{D}) B_v + 2D\bar{B}_v S^\mu_v \{ A_\mu, B_v \}
+ 2F\bar{B}_v S^\mu_v [A_\mu, B_v] + \frac{1}{4} f^2 \overline{\partial_\mu U} \partial_\mu U^\dagger + aM (U + U^\dagger)$$

with the covariant derivative that acts on the baryon field given by:

$$\mathcal{D}^\mu B_v \equiv \partial^\mu B_v + [V^\mu, B_v]$$

The Lagrangian Eqn. 1.91 describes general heavy baryon fields $B_v$. These baryon fields will generally contain one two or three heavy quarks. In the simplest case of a triply heavy baryon, chiral effects will only enter at one loop order, and the chiral dependence of the mass of a triply heavy baryon can generally be neglected to leading order. Doubly heavy baryons will behave much in the same way as a singly heavy meson, as the two heavy quarks can be treated as a single heavy di-quark in the large mass limit. An effective Lagrangian using as fundamental degrees of freedom quarks and heavy di-quarks (utilizing NRQCD to describe the heavy quark
fields) was constructed in Ref. [20]. Building on this, an exhaustive analysis of the (partially quenched) chiral mass dependence of doubly heavy baryon masses has been carried out in Ref. [21]. Formulae from the latter are used as the basis for chiral extrapolations performed in the present work. Similar expressions for the (partially quenched) chiral mass dependence of singly heavy baryons were derived in Ref. [22], in which the heavy quarks were treated using HQET. For the present work, the expressions for baryon masses presented in [22] have been extended (many thanks to William Detmold and Stefan Meinel) to include the leading order $1/M_Q$ corrections, allowing for an explicit distinction between $S = 1/2$ and $S = 3/2$ baryon states.

**Partial Quenching**

Partial quenching refers to incorporation of differing masses for the sea and valence quark (those bound in the asymptotically observable states of QCD, such as baryons/mesons). The behavior of such a theory (particularly the behavior of observables as a function of the sea and valence quark masses) is of great interest in lattice QCD where computational limitations have traditionally constrained the feasibility of carrying out calculations at very light quark masses. This constraint is much less pronounced for the valence quark sector and thus studying the expected quark mass dependence of observables in a partially quenched theory is highly desirable.

Partially quenched QCD includes six extra quarks into the theory: three bosonic *ghost* quarks, and three fermionic *sea* quarks. The interpretation of these fields is that the valence quarks form asymptotic QCD bound states, while the sea quarks contribute only in virtual quark anti-quark pairs. The ghost quarks are added to facilitate this differentiation. The quark field for the partially quenched theory is given by:
\[ q = \left( u, d, s, j, l, r, \bar{u}, \bar{d}, \bar{s} \right)^T \]  \hspace{1cm} (1.93)

with masses given by (here the \( M \) are 3 \( \times \) 3 diagonal matrices):

\[
m = \left( M_v, M_s, \tilde{M} \right) = \text{diag} (m_u, m_d, m_s, m_j, m_l, m_r, m_u, m_d, m_s), \hspace{1cm} (1.94)
\]

where, as is evident by the second line, \( \tilde{M} = M_v \). The motivation for the addition of six extra quarks is evident upon considering the mass matrix for the quark fields above and its effect in evaluating the fermionic part of the QCD path integral.

Consider the QCD partition function, given by:

\[
Z_F[U] = \int D[\psi, \bar{\psi}, U] e^{-S_F[\psi, \bar{\psi}, U]} \hspace{1cm} (1.96)
\]

\[
= \int D[\psi, \bar{\psi}, U] e^{\bar{\psi}D[U,m]\psi} \hspace{1cm} (1.97)
\]

where \( D \) is the Dirac operator, with its dependence on the fermion mass matrix explicitly shown. The integral in Eqn. 1.96 is bilinear in the quark fields, and is easily evaluated. For fermion fields, it is equal to the determinant of the Dirac operator \( \det (D[U, M]) \), while for boson fields it is equivalent to the inverse of the determinant of the Dirac operator \( \det (D[U, M])^{-1} \). For the partially quenched theory we find that only the determinant of the sea quark fields remains:
The effect of the additional bosonic degrees of freedom is to exactly cancel the contribution of the valence quarks to the fermion determinant. As will be discussed in the next chapter, the fermion determinant is representative of all closed quark loops on the lattice, so the ultimate result of the partially quenched theory is to allow for the separate prescription of sea and valence quark masses.
CHAPTER 2

Lattice quantum chromodynamics

The development of quantum chromodynamics as a description of the mechanisms governing the strong interaction was a great triumph of modern particle physics. The non-abelian gauge theory used to describe the strong interaction leads to some rather remarkable features, such as linear confinement and asymptotic freedom. The description of the strong force by a non-Abelian theory has serious implications for carrying out theoretical calculations in QCD, as the usual perturbative expressions that had proven so incredibly successful for QED are applicable to only the high energy region of the theory where the coupling constant is small. In order to perform calculations in the low energy regime (i.e. hadronic physics) where the QCD coupling is large, a new computational methodology was developed to circumvent reliance on the traditional perturbative techniques. In this chapter, the theory and methodology of lattice quantum chromodynamics is introduced, as well as its application in the calculation of selected hadronic properties that will be the main focus of this thesis.
2.1 Introduction of the discrete Euclidean path integral

The seminal work of Kenneth Wilson in 1974 [23] provided the first formulation of QCD in the context of a discretized space-time lattice. To introduce this methodology, we begin with a discussion of the Feynman integral in Euclidean space. Consider the QCD path integral in Minkowski space:

\[ Z = \int \mathcal{D} [\psi, \bar{\psi}, A_\mu] e^{iS_{QCD}^M [\psi, \bar{\psi}, A_\mu]}, \]  

(2.1)

where \( S_{QCD}^M [\psi, \bar{\psi}, A_\mu] \) is the continuum Minkowski space QCD action and \( \mathcal{D} [\psi, \bar{\psi}, A_\mu] \) is the integration measure. It is clear that the evaluation of this expression will be extremely difficult due to fluctuations for particular values of \( S_{QCD}^M [\psi, \bar{\psi}, A_\mu] \). The usual prescription for avoiding these violent fluctuations is to carry out a Wick rotation rotating to Euclidean space (imaginary time), letting:

\begin{align*}
x_4 &= ix_0^M, \quad x_i = -x_i^M \quad (2.2) \\
\partial_4 &= -i\partial_0^M, \quad \partial_i = \partial_i^M \quad (2.3)
\end{align*}

Here and below we differentiate between the Euclidean quantities from their Minkowski space counterparts by denoting the latter with a superscript \( M \). With these redefinitions, the gamma matrices and space-time metric in Euclidean space are given by:
\[ \gamma_4 = \gamma_0^M, \quad \gamma_i = -i \gamma_i^M \]  
(2.4)

\[ \{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu} \]  
(2.5)

with \(\delta_{\mu\nu}\) (the 4-dimensional kronecker delta) representing the Euclidean space metric.

After rotating to Euclidean time, the path integral is given by:

\[ Z = \int \mathcal{D}[\psi, \bar{\psi}, A_\mu] e^{-S_{QCD}[\psi, \bar{\psi}, A_\mu]} \]  
(2.6)

where:

\[ S_{QCD}[\psi, \bar{\psi}, A_\mu] = S_F[\psi, \bar{\psi}, A_\mu] + S_g[\psi, \bar{\psi}, A_\mu], \]  
(2.7)

\[ S_F[\psi, \bar{\psi}, A_\mu] = \int d^4x \: \bar{\psi}(x) \left( i \partial_\mu \bar{\psi} + m \right) \psi(x), \]  
(2.8)

\[ S_g[A_\mu] = \frac{1}{4g^2} \sum_{i=1}^{8} \int d^4x \: F^{(i)\mu}_\mu F_{(i)\mu} \]  
(2.9)

As illustrated above, the exponent is now transformed into a positive definite quantity that can be interpreted as a partition function of a statistical mechanical system. The potentially violent fluctuations in the path integral due to the phase are now absent, and the above expression lends itself to numerical evaluation much more readily than its Minkowski space counterpart. This partition function can be used to evaluate Euclidean correlation functions, such as:
\[ \langle \mathcal{O}_N (t_N) \ldots \mathcal{O}_2 (t_2) \mathcal{O}_1 (t_1) \rangle \]
\[ \equiv \frac{1}{Z} \int \mathcal{D} [\psi, \bar{\psi}, A_\mu] \mathcal{O}_N (t_N) \ldots \mathcal{O}_2 (t_2) \mathcal{O}_1 (t_1) e^{-S_{QCD} [\psi, \bar{\psi}, A_\mu]} \]

where the operators on the left side of the equation are understood to be quantum mechanical Hilbert space operators, and those on the right are functionals of the QCD fields. By considering the partition function and correlation function in Hilbert space, a relationship between the path integral and the spectrum of the theory may be derived. The asymptotic time (taking \( t \to T \), for \( T \) large) partition function for a quantum mechanical system with Hamiltonian \( H \) is given by:

\[ Z_T = \text{tr} [e^{TH}] = \sum_n < n | e^{TH} | n > = \sum_n e^{E_n T} \]
\[ = e^{E_0 T} \left( 1 + e^{-\Delta_1 T} + e^{-\Delta_1 T} + \ldots \right) \]

(2.11)

where the time \( T \) is understood to eventually be taken to \( \infty \), and \( |n > \) are energy eigenstates of the Hamiltonian with energies \( E_n \). In the last step we have simply pulled out the leading order behavior for the partition function for large \( T \) and defined \( \Delta_i \equiv E_i - E_0 \). The correlation function for a set of operators \( \mathcal{O}_N (t_N) \ldots \mathcal{O}_2 (t_2) \mathcal{O}_1 (t_1) \) is given by:

\[ \langle \mathcal{O}_N (t_N) \ldots \mathcal{O}_2 (t_2) \mathcal{O}_1 (t_1) \rangle \]
\[ = \frac{1}{Z_T} \text{tr} [e^{-t_N H} \mathcal{O}_N \ldots e^{-t_2 H} \mathcal{O}_2 e^{-t_1 H} \mathcal{O}_1] \]

(2.12)
Utilizing the completeness relation:

\[ 1 = \sum_n |n><n| \]  

(2.14)

Eqn. 2.12 can be rewritten as:

\[
\langle \mathcal{O}_N (t_N) \ldots \mathcal{O}_2 (t_2) \mathcal{O}_1 (t_1) \rangle = \\
\frac{1}{Z_T} \sum_{n_1, n_2 \ldots n_N} < n_N | e^{-(T-t_N)H} \mathcal{O}_N | n_{N-1} > \ldots \\
< n_2 | e^{-t_2 H} \mathcal{O}_2 | n_1 > < n_1 | e^{-t_1 H} \mathcal{O}_1 | n_N > \\
= \frac{1}{Z_T} \sum_{n_1, n_2 \ldots n_N} e^{-(T-t_N)E_N} < n_N | \mathcal{O}_N | n_{N-1} > \ldots \\
\quad \quad \quad e^{-t_2 E_{n_2}} < n_2 | \mathcal{O}_2 | n_1 > e^{-t_1 E_{n_1}} < n_1 | \mathcal{O}_1 | n_N >
\]  

(2.15)

For large times only terms with \( E_N = 0 \) survive and Eqn. 2.15 becomes:

\[
\langle \mathcal{O}_N (t_N) \ldots \mathcal{O}_2 (t_2) \mathcal{O}_1 (t_1) \rangle = \\
\sum_{n_1, n_2 \ldots n_{N-1}} < 0 | \mathcal{O}_N | n_{N-1} > \ldots < n_2 | \mathcal{O}_2 | n_1 > < n_1 | \mathcal{O}_1 | 0 > \\
\quad \quad \quad e^{-t_{N-1} E_{n_{N-1}}} \ldots e^{-t_2 E_{n_2}} e^{-t_1 E_{n_1}}
\]  

(2.16)

The above expression allows the path integral representation of correlation functions of Hilbert space operators to be related to a sum of amplitudes multiplied by exponential decay factors which are related to the energy spectrum of the theory.

For the particularly simple case for a correlation function of the operator \( \mathcal{O} (t) \)
and its adjoint $\bar{O}(t_0)$ the above expression becomes:

$$\langle O(t) \bar{O}(t_0) \rangle = \sum_n |\langle n|O|0 \rangle|^2 e^{-E_n t}$$  \hspace{1cm} (2.17)

### 2.1.1 Discretization prescription

In order to evaluate expressions of the form Eqn. 2.10, an ultraviolet regulator is introduced in the form of a lattice spacing $a_{s,t}$, which is used to define the Euclidean QCD action on a discrete space-time lattice with total volume $V = (a_t N_t) (a_s N_s)^3$ resulting in an expression of finite dimension. Here, the lattice spacing in the temporal direction $a_t$ in this definition has been isolated from the spatial lattice spacing $a_s$, which allows for the possibility to choose $a_t \neq a_s$ which can be useful in extracting information from lattice correlation functions at small time separations. The finite extent of the space-time volume is implemented with (anti-)periodic boundary conditions, and provides an infrared regulator in addition to the ultraviolet cutoff given by $a_t^{-1}$.

This discretization of the action must be chosen such that:

$$\lim_{a_{s,t} \to 0} S_{\text{Latt}} (a_{s,t}, \psi, \bar{\psi}, A_\mu) = S_{\text{QCD}} (\psi, \bar{\psi}, A_\mu).$$  \hspace{1cm} (2.18)

The lattice action is also constrained such that it obeys the symmetries of the continuum action as closely as possible. The introduction of a lattice spacing allows a great deal of freedom in choosing various discretization schemes that may be advantageous for particular calculations. When doing so however, great care must be taken in insuring that no undesired lattice artifacts are introduced (as will be illustrated below in the description of Wilson's fermion action). In practice, the fermion and gauge actions are treated separately as will be outlined below.
\[ \langle \mathcal{O}_N(t_N) \ldots \mathcal{O}_2(t_2) \mathcal{O}_1(t_1) \rangle \]
\[ = \frac{1}{Z_{\text{latt}}} \int_V \mathcal{D}[\psi, \bar{\psi}, A_\mu] \mathcal{O}_N(t_N) \ldots \mathcal{O}_2(t_2) \mathcal{O}_1(t_1) e^{-S_{\text{latt}}[a_{s,t}, \psi, \bar{\psi}, A_\mu]} \]

(2.19)

with the lattice partition function given by:

\[ Z_{\text{latt}} = \int_V \mathcal{D}[\psi, \bar{\psi}, A_\mu] e^{-S_{\text{latt}}[a_{s,t}, \psi, \bar{\psi}, A_\mu]}. \]

(2.20)

Although this expression has been transformed into a well defined, finite-sized problem, the magnitude of the required calculation is intractable for all practical purposes. In Section 2.3, we discuss how to confront this problem and numerically evaluate the discretized path integral. For the moment, let us turn our attention to a discussion of various discretization methods for the gauge and fermion sectors, followed by a presentation of those used in the present work.

### 2.2 Discretization of gauge and fermion actions

We begin by introducing the naive discretization of the free fermion action, which highlights the role of the gauge fields as link variables in the lattice formulation. Once the formalism has been introduced in the naive case, several alternative formulations of the lattice fermion action are briefly reviewed that address specific issues in the fermion action, such as fermion doubling, discretization errors and chiral symmetry. We conclude this section by presenting the naive discretization of the lattice action for the gauge field sector.
2.2.1 Fermion actions for light quarks

Consider the continuum Euclidean fermion action for free quarks:

\[ S_F[\psi, \bar{\psi}] = \int dx^4 \bar{\psi}(x) (\not{\partial} + m) \psi(x) \quad (2.21) \]

where we have omitted flavor and color indices for brevity, and we restrict our discussion to one quark flavor as the extension to multiple flavors for our purposes is trivial. We seek to find a discretized form by introducing a minimum space time discretization parameter \( a \). For the following discussion, we will assume that \( a_s = a_t = a \), i.e. isotropic lattice spacing. A naive prescription for the discretization of this action is carried out by replacing the derivative with a symmetric first order approximation from a Taylor series expansion, and the four dimensional integral by a sum over all sites on the lattice:

\[ x \rightarrow na \]

\[ \partial_\mu \psi(x) \rightarrow \frac{\psi(n+\mu) - \psi(n-\mu)}{2a} \quad (2.22) \]

\[ \int dx^4 \rightarrow a^4 \sum_{n \in V} \]

With these replacements, our discretized fermion action reads:

\[ S_F[\psi, \bar{\psi}] = a^4 \sum_{n \in V} \sum_{\mu=1}^{4} \bar{\psi}(n) \gamma_\mu \left( \frac{\psi(n+\mu) - \psi(n-\mu)}{2a} \right) + m\bar{\psi}(n)\psi(n) \quad (2.23) \]

As in continuum QCD, our gauge fields enter by requiring the theory to be
invariant under local SU(3) rotations in color space, given by the following set of transformations:

\[
\psi(n) \rightarrow \Omega(n) \psi(n), \quad \bar{\psi}(n) \rightarrow \bar{\psi}(n) \Omega^\dagger(n)
\] (2.24)

Here the \( \Omega(n) \) are SU(3) matrices in color space acting at the lattice point \( n \). Upon applying these transformations, the lattice action Eqn. 2.23 is found to acquire terms of the form \( \bar{\psi}(n) \Omega^\dagger(n) \Omega(n \pm \hat{\mu}) \psi(n) \) (where \( \hat{\mu} \) is the unit vector in the \( \mu \) direction) which violate gauge invariance. To remedy this, new directional fields \( U_\mu(n) \) are introduced into the theory in order to restore gauge invariance. These gauge fields obey the following transformation properties:

\[
U_\mu(n) \rightarrow \Omega(n) U_\mu(n) \Omega^\dagger(n + \hat{\mu}),
\] (2.25)

where the gauge fields \( U_\mu(n) \) are SU(3) valued and are interpreted as links between adjacent lattice sites. With the introduction of these gauge link variables, the gauge invariant lattice action for fermions in the naive discretization prescription is given by:

\[
S_F[\psi, \bar{\psi}] = a^4 \sum_{n \in V} \sum_{\mu=1}^{4} \bar{\psi}(n) \gamma_\mu \left( \frac{U_\mu(n) \psi(n + \mu) - U_{-\mu}(n) \psi(n - \mu)}{2a} \right) + m\bar{\psi}(n) \psi(n)
\] (2.26)

where the definition \( U_{-\mu}(n) \equiv U_\mu^\dagger(n - \hat{\mu}) \) has been introduced for notational convenience. The relationship of these SU(3) valued gauge links to the continuum gauge
fields $A_\mu(x)$ in the limit $a \to 0$ will be discussed in Section 2.2.3. For now we turn our attention to a discussion of various prescriptions for the discretization of the fermion action that address specific issues that present themselves in lattice calculations.

**Doubling and Wilson fermions**

The naive discretization of the fermion action suffers from a lattice artifact commonly referred to as the fermion doubling problem. To illustrate this problem, consider the Dirac operator in the free ($U_\mu(n) = 1$) naive fermion action:

$$S_F[\psi, \bar{\psi}] = a^4 \sum_{n,m \in V} \bar{\psi}(n) D(n|m) \psi(n) \quad (2.27)$$

where:

$$D(n|m) = \sum_{\mu=1}^{4} \gamma_\mu \left( \frac{\delta_{n+\mu,m} - \delta_{n-\mu,m}}{2a} \right) + m \delta_{n,m} \quad (2.28)$$

In momentum space, the free Dirac operator becomes:

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

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

$$= \frac{1}{|A|} \sum_{n,m \in \Lambda} e^{-i(p-q) \cdot n} a \tilde{D}(p) \quad (2.29)$$
with:

\[ \hat{D}(p) = m + ia^{-1} \sum_{\mu} \gamma_\mu \sin(p_\mu a) \]  

(2.30)

where we have utilized the Fourier transform identity:

\[ \delta_{n-n'} = \delta_{n_1,n'_1}\delta_{n_2,n'_2}\delta_{n_3,n'_3}\delta_{n_4,n'_4} = \frac{1}{|A|} \sum_{n \in A} e^{ip(n-n')a} \]  

(2.31)

Taking the inverse of the Dirac operator, the naive free Dirac propagator is given by:

\[ \hat{D}^{-1}(p) = \frac{m - ia^{-1} \sum_{\mu} \gamma_\mu \sin(p_\mu a)}{m^2 + a^{-2} \sum_{\mu} \sin(p_\mu a)^2} \]  

(2.32)

Due to the periodicity of the lattice formulation, the lattice momentum values are restricted to lie in the range \(-\pi/a < p_\mu \leq \pi/a\). It is clear from the expression above that although the continuum Dirac propagator has a single pole at \(p_\mu = (0, 0, 0, 0)\), the lattice Dirac propagator has additional poles whenever the momentum components are \(\{0, \pm\pi/a\}\). These 16 poles \(\vec{p}_k, k = 1 \ldots 16\) are interpreted as distinct fermion states and are related by the 16 symmetry transformations:

\[ T_k \equiv S_k e^{-i\vec{p}_k \cdot x} \]  

(2.33)

where \(S_k\) is the Dirac space structure of the transformation which has been isolated from the spatial transformation.

For momentum near a given pole \(p = \vec{p}_k + k\) with \(k\) small, the naive fermion propagator Eqn. 2.32 can be expanded about the pole yielding:
\[
D(p)^{-1} = \frac{m - i a^{-1} \sum_\mu \gamma_\mu \sin(p_\mu a)}{m^2 + a^{-2} \sum_\mu \sin(p_\mu a)^2} \\
= \frac{m - i \sum_\mu \gamma_\mu k_\mu \cos(\bar{p}_\mu a)}{m^2 + k^2} + \mathcal{O}(a) \\
= S_k \frac{m - i \sum_\mu \gamma_\mu k_\mu}{m^2 + k^2} S_k^{-1} + \mathcal{O}(a)
\]  

(2.34) 

(2.35) 

(2.36)

where we have used \( \gamma_\mu^k \equiv S_k^{-1} \gamma_\mu S_k = \gamma_\mu \cos(\bar{p}_\mu a) \). From the above expressions, it is clear that the continuum limit of the naive fermion action has sixteen distinct fermions:

\[
\psi(x)_k = T_k \psi(x), \quad \bar{\psi}(x)_k = \bar{\psi}(x) T_k^\dagger.
\]  

(2.37)

all of which can be pair produced to contribute at tree level to all processes. One might expect that a restriction on calculations such that \( p \sim 0 \) for all calculated observables might suffice in solving this problem, however the effects of the doublers would contribute at the one loop order in that scenario. In order to deal with this fermion doubling problem it is necessary to modify the naive fermion action with the introduction of additional terms that will remove the unwanted doublers while preserving a single species of fermion. One approach for doing this is to modify the dispersion relation such that, at low energies, the unwanted doublers are removed. This is achieved by making the energies of the unwanted poles \( \sim 1/a \) such that as the lattice spacing is increased, the energies of the doublers becomes so large as to not contribute to the low energy physics of interest. One method, developed by Ken Wilson requires adding to the naive fermion action a discretization of the second derivative \( D^2 \):
The coefficient \( r \) is traditionally set to \( r = 1 \), a convention that is used presently. Calculating the momentum space Dirac operator once again for the Wilson action, we find:

\[
D(p) = D_{\text{naive}}(p) + D_W(p) = m + ia^{-1} \sum_\mu \gamma_\mu \sin(p_\mu a) + a^{-1} \sum_\mu (1 - \cos(p_\mu a)) \tag{2.40}
\]

From this expression it is clear that the Wilson term vanishes for the zero momentum pole only, while remaining finite for the remaining values of \( p \) in the Brillouin zone. To better see that the additional poles do not propagate, it is useful to look at the momentum space propagator:

\[
D^{-1} = \frac{m - ia^{-1} \sum_\mu \gamma_\mu \sin(p_\mu a) + a^{-1} \sum_\mu (1 - \cos(p_\mu a))}{\left(m + a^{-1} \sum_\mu (1 - \cos(p_\mu a))\right)^2 + a^{-2} \sum_\mu \sin^2(p_\mu a)}
\]

\[
= \frac{m - i \sum_\mu \gamma_\mu p_\mu}{m^2 + 2ma^{-1} \sum_\mu (1 - \cos(p_\mu a)) + 2a^{-2} \sum_\mu (1 - \cos(p_\mu a))} + \mathcal{O}(a^2)
\]

\[
= \frac{-i\gamma_\mu p_\mu + m}{p^2 + m^2} \tag{2.42}
\]

where in the last line we have taken the limit as \( a \to 0 \). From Eqn. 2.42 it is obvious that the continuum limit of the Wilson action permits only one propagating fermion.
Clover fermion action

As stated above, the Wilson action has been derived from a discretized version of the operator $\bar{\psi}(x) D^2 \psi(x)$. The process of adding discretized operators to a lattice action to achieve a particular result is a common procedure, and a systematic framework for improving actions through a given order in the lattice spacing $a$ is provided by Symanzik improvement. For systematic improvement through a given order in the lattice spacing, the improvement program begins by considering an effective theory that describes the lattice action at finite (but very small) $a$ (which lies near the continuum). All operators are identified up to a given order in $a$, and are then discretized. Appropriate linear combinations of the discretized operators are then taken in order to provide cancellation at a given order in the lattice spacing.

When applying this procedure to the naive fermion action, it is found that there are two dimension 5 operators of interest:

$$\bar{\psi}(x) \slashed{D} \psi(x) \quad \bar{\psi}(x) \sigma_{\mu\nu} F_{\mu\nu} \psi(x)$$

(2.43)

Rewriting the first of these operators as:

$$\slashed{D} \slashed{D} = D^2 + \frac{1}{2} \sigma_{\mu\nu} F_{\mu\nu} \psi(x)$$

(2.44)

the Wilson term can be obtained through an appropriate linear combination of the operators (which works to remove the fermion doublers). To remove discretization errors through $\mathcal{O}(a^2)$, one can discretize the second operator above, commonly called the Sheikholeslami - Wohlert or clover term, after the group who wrote down this improved action for the first time. Here we should note that the Wilson and Clover terms typically come with the coefficients $r$ and $c_{sw}$ respectively, which are typically
set to unity. Below we will present the explicit form for the clover action.

\[ S_{SW} = S_W + c_{sw} a^5 \sum_n \sum_{\mu<\nu} \bar{\psi}(x) \frac{1}{2} \sigma_{\mu\nu} F_{\mu\nu}^{\text{Latt}} \psi(x) \] (2.45)

The clover action adds a discretization of the operator \( \sigma_{\mu\nu} F_{\mu\nu} \) to the Wilson action. A particular choice for discretization of the field strength tensor is given by:

\[ F_{\mu\nu}^{\text{Latt}} = -\frac{i}{8a^2} \left( Q_{\mu\nu}(n) - Q_{\nu\mu}(n) \right) \] (2.46)

with:

\[ Q_{\mu\nu}(n) \equiv U_{\mu,\nu}(n) + U_{\nu,-\mu}(n) + U_{-\mu,-\nu}(n) + U_{-\nu,\mu}(n) \] (2.47)

where \( U_{\mu,\nu} \) is a simple \( 1 \times 1 \) loop of gauge links in the \( \mu, \nu \) plane given by:

\[ U_{\mu,\nu} = U_\mu(n) U_\nu(n + \mu) U_{-\mu}(n + \mu + \nu) U_{-\nu}(n + \nu) \] (2.48)

This simple lattice object is called the plaquette, and is commonly used in the construction of the gauge action as will be discussed below.

### 2.2.2 Heavy quark actions

As discussed in Section 1.4.1, there are several effective theories common for dealing with heavy quarks in the continuum. Here, we present the propagator in the static limit of HQET as well as the Lattice NRQCD action used in the current work. After this, we briefly present the relativistic treatment of heavy quarks where lattice improvement is used as a tool to systematically remove discretization errors that become large for heavy quark masses.
Lattice static quarks

In HQET, the two component positive energy Dirac spinor can be represented by a Wilson line that propagates only in the temporal direction. The usual lattice discretization of the lattice propagator for a static heavy quark is given by:

\[
S(\vec{x}, t, t_0) = \frac{(1 + \gamma_4)}{2} \prod_{t' = t_0}^{t} U_4^\dagger(\vec{x}, t')
\]  

Non-relativistic heavy quark action

For the present work, a non-relativistic heavy quark action is used for the bottom quarks. This is a discretization of NRQCD as presented in Section 1.4.2. The bottom quark is represented on the lattice by a two component spinor field and the Lattice NRQCD action is given by:

\[
S_\psi = a^3 \sum_{\vec{x}, t} \psi^\dagger(x, t) [\psi(x, t) - K(t) \psi(x, t - a)].
\]  

Here:

\[
K(t) = \left(1 - \frac{a \delta H|_t}{2}\right) \left(1 - \frac{a H_0|_t}{2n}\right)^n U_0^\dagger(t - a)
\]

\[
\times \left(1 - \frac{a H_0|_{t-a}}{2n}\right)^n \left(1 - \frac{a \delta H|_{t-a}}{2}\right).
\]  

with:

\[
H_0 = -\frac{\Delta^{(2)}}{2m_b}, \tag{2.52}
\]

\[
\delta H = -c_1 \frac{(\Delta^{(2)})^2}{8m_b^3} + c_2 \frac{ig}{8m_b^2} \left( \nabla \cdot \vec{E} - \vec{E} \cdot \nabla \right) - c_3 \frac{g}{8m_b^2} \sigma \cdot \left( \vec{\nabla} \times \vec{E} - \vec{E} \times \vec{\nabla} \right) - c_4 \frac{g}{2m_b} \sigma \cdot \vec{B} + c_5 \frac{a^2 \Delta^{(4)}}{24m_b} - c_0 \frac{a (\Delta^{(2)})^2}{16n m_b^2}. \tag{2.53}
\]

Here \( U_0(t-a) \) represent temporal gauge links. For doubly bottom hadrons, the naturally small expansion parameter is the velocity \( v^2 \). The leading order term \( H_0 \) is of \( \mathcal{O}(v^2) \), while the first four terms in \( \delta H \) are of \( \mathcal{O}(v^4) \). The remaining terms in \( \delta H \) are included to correct discretization errors in \( H_0 \) and temporal derivatives. For singly bottom hadrons, the expansion parameter is \( \frac{\Lambda_{QCD}}{m_b} \) and the operator containing \( c_4 \) is of the same order in \( \frac{\Lambda_{QCD}}{m_b} \) as the leading order \( H_0 \). All other operators enter at higher order.

More details of this particular discretization of the continuum NRQCD action can be found in Ref. [24] and the references therein.

**Relativistic heavy quark action**

As the mass of the charm quark is below the threshold of applicability for a non-relativistic treatment on the current lattices, we use instead a relativistic heavy quark action in the Fermilab interpretation [25]. Beginning with a clover fermion action, a distinction is made between the spatial and temporal directions and Symanzik improvement is carried out to remove discretization errors in the action of \( \mathcal{O}((am_c)^n) \), resulting in four bare parameters in the improved action that must be determined in order to ensure cancellation of these errors. The relativistic
heavy quark action is then given by: $S = S_0 + S_B + S_E$, where:

\[ S_0 = \sum_x \bar{Q}(x) \left[ m_0 + \gamma_0 D_0 - \frac{a}{2} D_0^2 + \nu \left( \gamma_i D_i - \frac{a}{2} D_i^2 \right) \right] Q(x), \quad (2.54) \]

\[ S_B = \sum_x \bar{Q}(x) \left( -\frac{a}{4} c_B \sigma_{i,j} F_{i,j} \right) Q(x), \]

\[ S_E = \sum_x \bar{Q}(x) \left( -\frac{a}{2} c_E \sigma_{0,j} F_{0,j} \right) Q(x), \]

where $F_{i,j}$ is the QCD field strength tensor. The anisotropy parameter $\nu$, bare mass $m_0$, and the chromomagnetic and chromoelectric coefficients $c_B, c_E$ remain to be determined. Perturbative lattice QCD relates $c_B, c_E$ to the anisotropy $\nu$ (see eg. [26]) by:

\[ c_B = \frac{\nu}{u_0^3}, \quad c_E = \frac{(1 + \nu)}{2u_0^3}, \quad (2.55) \]

with the average lattice plaquette given by:

\[ u_0 = \left( \frac{1}{3} \sum_p Tr(U_p) \right)^{1/4}, \quad (2.56) \]

leaving only the bare mass $m_0$ and anisotropy $\nu$ to be determined non-perturbatively.

### 2.2.3 Gauge actions

The discretization of the gauge action $S(U_p)$ can be performed in a variety of ways, although it must obey the symmetries of the QCD gauge action and converge to the continuum QCD gauge action upon taking the continuum limit. Before we present the Wilson gauge action (the most straightforward prescription), we will first take a look at what types of gauge invariant objects can be constructed on the lattice. We have seen before that the requirement of gauge invariance for a lattice
action suggests that the gauge links transform as:

\[ U_{\mu}(x) \rightarrow \Omega(x) U_{\mu}(x) \Omega^{\dagger}(x + \mu) \quad (2.57) \]

We can then consider a chain of gauge links, representing a specific path from one space time point to another. The Euclidean space gauge transporter given is by:

\[
P [U] = U_{\mu_0}(x_0) U_{\mu_1}(x_0 + \mu_0) \ldots U_{\mu_{k-1}}(x_1 - \mu_{k-1}) \quad (2.58)
\]

\[
\equiv \prod_{x_i, \mu_i \in P} U_{\mu}(x_i) \quad (2.59)
\]

The gauge transporter is a product of the enforcement of space-time translational symmetry. The effect of the gauge transporter is to translate a fermion field from one point in space time to another.

\[
\bar{\psi}(x_1) P [U] \psi(x_2) \rightarrow \bar{\psi}(x_1)' P [U'] \psi(x_2)'
\]

\[
= \bar{\psi}(x_1) \Omega^{\dagger}(x_1) \Omega(x_1) P [U'] \Omega^{\dagger}(x_2) \Omega(x_2) \psi(x_2) \quad (2.60)
\]

\[
= \bar{\psi}(x_1) P [U] \psi(x_2) \quad (2.61)
\]

From the transformation properties of a single gauge link it is clear that, upon performing a gauge transformation on the gauge transporter, all of the internal gauge rotation matrices cancel among themselves and only those at the endpoints of the path remain. By attaching a fermion field to either end of the transporter as in Eqn. 2.60, we form a gauge invariant object (recalling the gauge transformation properties of the lattice fermion fields). An alternative method for constructing
gauge invariant objects from the gauge transporter would be to take the trace of a *closed loop* of gauge links.

\[ tr [P[U]] \rightarrow tr [P[U']] \]

\[ = tr [\Omega(x_0) P[U] \Omega^\dagger(x_0)] = tr [P[U]] \]

A straightforward gauge invariant action for the gauge fields can be constructed by considering simple closed loops of gauge links. The simplest such closed loop is given by the plaquette presented in Eqn. 2.48. The simplest gauge invariant gauge action is constructed by taking combinations of only single plaquettes, and is realized in the Wilson gauge action, given below:

\[ S_G[U] = \frac{2}{g^2} \sum_{n \in \Lambda} \sum_{\mu < \nu} \text{Re}\{tr [1 - U_{\mu\nu}(n)]\}. \]  

To see that the Wilson gauge action is indeed equivalent to the QCD gauge action, we note that the lattice gauge links transform just as a continuum transporter. Therefore we may relate the lattice gauge link, a single link gauge transporter, to the lattice gauge fields:

\[ U_\mu(n) = e^{iaA_\mu(n)}. \]

Using this relation, we may Taylor expand the gauge links as:

\[ U_\mu = 1 + iaA_\mu(n) + O(a^2) \]

\[ U_\mu = 1 - iaA_\mu(n - \mu) + O(a^2) \]

With these relations, we may expand the lattice plaquette making use of the
well known Baker-Campbell-Hausdorff formula (given by by Eqn. 2.31), and then expanding the fields about $n$

$$A_\mu (n + \nu) = A_\mu (n) + a \partial_\nu A_\mu (n)$$ \hspace{1cm} (2.69)

it is straightforward to show that the plaquette is:

$$U_{\mu\nu} (n) = \exp \left[ it a^2 \partial_\mu A_\nu (n) - \partial_\nu A_\mu (n) + i [A_\mu (n), A_\nu (n)] \right] + \mathcal{O} (a^3)$$

$$= \exp \left[ it a^2 F_{\mu\nu} + \mathcal{O} (a^3) \right]$$ \hspace{1cm} (2.70)

Inserting this into the expression for the Wilson action, we find that upon taking the real part of the trace of the plaquette, the $\mathcal{O} (a^2, a^3, a^5)$ terms cancel and we are left with leading order contributions at $\mathcal{O} (a^4)$ with $\mathcal{O} (a^6)$ corrections. To obtain the correct dimensionality for associating the sum over lattice sites with a continuum integral, we require that the four dimensional sum be accompanied by a factor of $a^4$, therefore we see that the leading order discretization effects of the Wilson gauge action are $\mathcal{O} (a^2)$:

$$S_G [U] = \frac{2a^4}{g^2} \sum_{n \in \Lambda} \sum_{\mu,\nu} \frac{1}{4} \text{tr} \left[ F_{\mu\nu} (n)^2 + \mathcal{O} (a^2) \right]$$ \hspace{1cm} (2.71)

### 2.3 Evaluation of the Euclidean path integral

#### 2.3.1 Fermions in the path integral

In order to evaluate expressions of the form 2.19, we must rely on a Monte Carlo evaluation of the integral over the gauge fields, as a brute force calculation would be prohibitively expensive. Before beginning the discussion of how this process is
carried out however, we will first discuss how the Grassman valued fermion fields are treated in the evaluation of the path integral. First, consider the lattice partition function:

\[ Z = \int D[\psi, \bar{\psi}, U] e^{-S_{\text{Last}}[\psi, \bar{\psi}, U]}. \]  

(2.72)

\[ = \int D[U] e^{-S_G[U]} \int D[\psi, \bar{\psi}] e^{-S_F[\psi, \bar{\psi}, U]} \]  

(2.73)

\[ = \int D[U] e^{-S_G[U]} Z_F[U] \]  

(2.74)

\[ = \int D[U] e^{-S_G[U]} \]  

(2.75)

Written in this form, it’s clear that the integration over the fermion fields can be carried out prior to the integration over the gauge fields. Furthermore, provided that the lattice fermion action is bilinear in the fermion fields (or can be rewritten in this form with an appropriate field redefinition) the integration over the fermion fields can be carried out analytically. With the aid of the Matthews-Salam formula for integration over bilinears of fermion fields, the fermionic integral is rewritten as:

\[ Z_F[U] = \int D[\psi, \bar{\psi}] e^{-S_F[a_{t,t}, \psi, \bar{\psi}, U]} \]  

(2.76)

\[ = \int D[\psi, \bar{\psi}] e^{\bar{\psi} D[U] \psi} \]  

\[ = \det [D[U]] \]  

This fermion determinant is computationally very expensive, as the full Dirac operators has \( O(V^2) \) entries. In early lattice calculations where computational resources were much more limited than presently, this fermion determinant was often set to unity. This unphysical act, called the quenched approximation, corresponds
to neglecting all closed fermion loops on the lattice as will be discussed below. The quenched approximation introduces a systematic uncertainty into the calculation whose effects are extremely difficult to properly estimate. Additionally, the quenched approximation does not correspond to continuum QCD in the chiral limit, although partially quenched theories do, making quenched calculations a less apt probe of quantities in continuum QCD.

We now turn to the evaluation of the numerator in the fermionic part of the path integral. In general lattice calculations could involve correlation functions between $N$ operators, all of which can be arbitrary functions of the fermion and gauge fields $\bar{\psi}, \psi, U$:

\[
\langle \mathcal{O}_1 (\bar{\psi}, \psi, U), \mathcal{O}_2 (\bar{\psi}, \psi, U) \ldots \mathcal{O}_N (\bar{\psi}, \psi, U) \rangle_F = \int \mathcal{D} [\psi, \bar{\psi}, U] \mathcal{O}_1 (\bar{\psi}, \psi, U), \mathcal{O}_2 (\bar{\psi}, \psi, U) \ldots \mathcal{O}_N (\bar{\psi}, \psi, U) e^{-S_{\text{Latt}}[\psi, \bar{\psi}, U]}.
\]

Here the subscript $F$ denotes the integration over fermion fields only. In order to evaluate expressions of this form, we construct the generating functional by adding to the fermion action quark and antiquark sources $\bar{\theta}, \theta$:

\[
W [\theta, \bar{\theta}] = \int \left( \prod_{k=1}^{N} d\psi_k d\bar{\psi}_k \right) \exp \left( \bar{\psi} D \psi + \bar{\theta} \psi + \psi \bar{\theta} \right)
\]

\[
= \det[D] \exp (-\bar{\theta} D^{-1} \theta).
\]

By taking derivatives with respect to the sources, one is able to iteratively construct the expectation value of any number of fermion fields (here we restrict our
attention to pairwise combinations of quark creation and annihilation operators):

\[
\langle \psi_{i_1} \bar{\psi}_{j_1} \ldots \psi_{i_n} \bar{\psi}_{j_n} \rangle_F = \frac{1}{Z_F} \frac{\partial}{\partial \theta_{j_1}} \frac{\partial}{\partial \theta_{i_1}} \ldots \frac{\partial}{\partial \theta_{j_n}} \frac{\partial}{\partial \theta_{i_n}} Z_F
\]  

(2.80)

Applying this method with a single fermion creation and annihilation operator, the full quark propagator matrix is defined as:

\[
\langle \psi \bar{\psi} \rangle_F = D^{-1}
\]  

(2.81)

Generalizing the process of taking functional derivatives of the generating functional to an arbitrary number of fields, one arrives at the result:

\[
\langle \psi_{i_1} \bar{\psi}_{j_1} \ldots \psi_{i_n} \bar{\psi}_{j_n} \rangle_F
\]

\[
= \frac{1}{Z_F} \int \left( \prod_{k=1}^{N} d\psi_k d\bar{\psi}_k \right) \psi_{i_1} \bar{\psi}_{j_1} \ldots \psi_{i_n} \bar{\psi}_{j_n} e^{\bar{\psi} D[U] \psi}
\]

\[
= (-1)^n \sum_{P(1,2,...,n)} \text{sign} (P) D^{-1}_{i_1,j_{P_1}} D^{-1}_{i_2,j_{P_2}} \ldots D^{-1}_{i_n,j_{P_n}}
\]  

(2.82)

known as Wick’s Theorem (here \( P(1,2,\ldots,n) \) represents all permutations of the \( n \) fermions). It should be noted that the fermionic expectation value for an odd number of fermions fields vanishes, due to the nature of the Grassman algebra describing fermions.

### 2.3.2 The fermion propagator and fermion determinant

We now return to our discussion of the fermion determinant, and its relation to closed loops of fermion propagators. We begin by looking at a particularly insightful
representation of the fermion propagator Eqn. 2.81 in the limit of a large quark mass. We first rewrite the Dirac operator as (here we use the Wilson action for illustrative purposes):

\[
D = C (1 + \kappa H) , \quad \kappa = \frac{1}{2 (am + 4)} , \quad C = m + \frac{4}{a} \quad (2.83)
\]

\[
H (n|m) = \sum_{\mu = \pm 1}^{\pm 4} (1 - \gamma_{\mu}) U_{\mu} (n) \delta_{n + \mu, m} \quad (2.84)
\]

The Dirac operator in this form is commonly referred to as the hopping expansion, and is convenient for expansion in large fermion mass, as \( \kappa \to \infty \) as \( m \to 0 \). The constant \( C \) is commonly reabsorbed into a redefinition of the fields, and will be neglected here. With the Dirac operator in the form 2.83, the fermion propagator can then be expanded in powers of the hopping parameter \( \kappa \) in a geometric series:

\[
D^{-1} (n|m) = (1 - \kappa H)^{-1} = \sum_{j=0}^{\infty} \kappa^{j} H^{j} . \quad (2.85)
\]

In general, the \( j \)th power of \( H \) is given by:

\[
H^{j} (n|m) = \sum_{\mu = \pm 1}^{\pm 4} \left( \prod_{i=1}^{j} (1 - \gamma_{\mu_{i}}) \right) P_{\mu_{1} \ldots \mu_{j}} (n) \delta_{n + \mu_{1} + \ldots + \mu_{j}, m} \quad (2.86)
\]

with \( \mu_{1} \ldots \mu_{j} \) representing a path of link variables and the delta function enforcing that the path end at the lattice points \( n \) and \( m \). From this expression, it is clear that the lattice fermion propagator can be viewed as a sum over all paths of links connecting the two points \( n \) and \( m \).

Returning to the fermion determinant, with the hopping expansion we may
rewrite $\text{det} \ [D]$ as:

$$
\text{det} \ [D] = \text{det} \ [1 - \kappa H] = \exp \left( \text{tr} \ \ln \ (1 - \kappa H) \right) 
= \exp \left( - \sum_{j=1}^{\infty} \frac{1}{j} \kappa^j \text{tr} \ [H^j] \right)
$$

(2.87)

(2.88)

The trace over the powers of the hopping matrix $H$ enforces that all paths of gauge links begin and end at the same spatial point. Because of this, the contribution of the fermion determinant to the path integral is to include all closed loops of fermions, or vacuum polarization loops into the path integral.

### 2.3.3 Evaluation of the gauge field path integral

As previously mentioned, the evaluation of the path integral over all gauge fields is an insurmountable task for any modern computational technology, so one must instead rely on a Monte Carlo evaluation of the path integral over the gauge degrees of freedom. This approach gives a reliable estimator of the actual value of observables while still maintaining a reasonable computational cost.

After treating the fermion fields analytically as described above, what remains is:

$$
\langle \mathcal{O} (\tilde{\psi}, \psi, U) \rangle = \frac{1}{Z} \int \mathcal{D} [U] \mathcal{O}' (U, D_{f_1}^{-1} (U) \ldots D_{f_n}^{-1} (U)) 
\times (\text{det} \ [D_{f_1}] \ldots \text{det} \ [D_{f_n}]) \ e^{-S_G [U]}
$$

(2.89)

where we have assumed $n$ flavors of quarks, and the function $\mathcal{O}' (U, D_{f_1}^{-1} (U) \ldots D_{f_n}^{-1} (U))$ represents the functional dependence of the operator
\( \mathcal{O} (\bar{\psi}, \psi, U) \) on the gauge fields and fermion propagators after integration over the fermionic degrees of freedom. The goal of the Monte Carlo approach is to approximate this integral by the discrete sum:

\[
\langle \mathcal{O} (\bar{\psi}, \psi, U) \rangle = \lim_{N \to \infty} \frac{1}{N} \sum_{U'} \mathcal{O}' (U, D_{f_1}^{-1} (U') \ldots D_{f_n}^{-1} (U'))
\]

with the gauge field configurations \( U' \) drawn from the distribution:

\[
dP[U] = \frac{\mathcal{D}[U] (\det [D_{f_1}] \ldots \det [D_{f_n}]) e^{-S_G[U]}}{\int \mathcal{D}[U] e^{-S_G[U]}}
\]

Below we will detail the process by which the gauge fields are generated according to the distribution Eqn. 2.91.

**Markov chain process**

In order to generate gauge field configurations \( U' \) according to the distribution 2.91, an iterative process is used generating a Markov chain of gauge field configurations from an initial configuration that eventually converges to the required distribution. Beginning from an arbitrary initial gauge field configuration \( U_0 \), successive configurations are generated iteratively:

\[
U_0 \rightarrow U_1 \rightarrow U_2 \ldots \rightarrow U_N
\]

and each iteration of the Markov process is referred to as a single step in simulation time. Configurations spaced closely in simulation time are strongly correlated, a feature called autocorrelation, and great care must be taken in both sampling configurations at intervals that reduce autocorrelation as well as accounting for the
effects of the autocorrelation when computing values of observables measured on the configurations.

The Markov process is characterized by the transition probability:

\[ P(U_n = U' | U_{n-1} = U) = T(U' | U) \]  

(2.93)

which is the probability for transitioning to the final configuration \( U' \) from the initial configuration \( U \). It should be noted here that the transition probability is dependent on the initial and final gauge field configurations, but not on the Markov chain time step \( n \). Transition probabilities obey the following relations:

\[ 0 < T(U' | U) \leq 1, \quad \sum_{U'} T(U' | U) = 1. \]  

(2.94)

The first of these relations is just a normalization condition for the probability, while the second is a statement that the probability to jump from a configuration to \textit{any} other configuration (including itself) is equal to unity. For a given transition probability, it is required that once the configurations have reached equilibrium (i.e. once we have reached the desired distribution) the system will remain in equilibrium. This is achieved by the following condition, known as the \textit{balance condition}:

\[ \sum_{U} T(U' | U) P(U) = \sum_{U} T(U | U') P(U') \]  

(2.95)

Applying the normalization condition 2.94 to the balance equation 2.95, it is clear that once equilibrium is reached, successive applications of \( T \) will lead the system to remain in the equilibrium state. One caveat that must be mentioned at this point is that all points in configuration space must be accessible with a
finite number of applications of the operator $T$. If one imposes the restriction that $T$ be strictly positive for all $U'$, $U$ then the Markov process is aperiodic in $U$ and all configurations can be reached. In practice, some algorithms may have trouble accessing all sectors of configuration space, and special care must be taken in ensuring that the configuration space is correctly sampled. Having presented the general background for Markov processes, we now proceed to the outline the most basic framework for constructing a Markov chain.

The Metropolis algorithm

One of the most straightforward approaches to generating a Markov chain iteratively is called the Metropolis algorithm. Given a configuration $U_{n-1}$, the function of the Metropolis algorithm is advance the Markov process one step in simulation time producing a new configuration $U_n$. As the algorithm has at its core an accept/reject step, the newly chosen $U_n$ may or may not be unique from $U_{n-1}$. Before going on to outline the basic form of the Metropolis algorithm, we need to briefly comment on a modification to the balance condition 2.95 often used for the sake of calculational ease. It is clear from Eqn. 2.95 that if the equality were to hold term by term, then the balance equation would be satisfied. The resulting equation:

$$T (U'|U) P (U) = T (U|U') P (U')$$  \hspace{1cm} (2.96)

is called the detailed balance equation. It should be noted that this is not a necessary condition, but it is a sufficient requirement to meet the condition of the balance equation. This rather stringent requirement however is often used in the practice as lends itself rather nicely to implementing a clean, easy-to-determine accept/reject step.

We now outline the steps required to advance from a configuration $U_{n-1}$ to a
configuration $U_n$ using the Metropolis algorithm. For the following it is assumed that we are working with the probability density $P(U) = e^{-S(U)}$. The first step is to choose some selection probability $T_0(U'|U_{n-1})$ that will produce a configuration $U'$ that will be a candidate for the next step in the Markov chain. The choice of $T_0(U'|U_{n-1})$ is arbitrary provided that it will reach (or can be made to reach) all areas of the configuration space. This selection probability is often chosen to be symmetric, satisfying:

$$T_0(U'|U) = T_0(U|U')$$

(2.97)

for reasons that will become clear below.

Once a candidate configuration has been selected, the new configuration is chosen with an acceptance probability given by:

$$T_A = \min\left(1, \frac{T_0(U|U') e^{-S(U')}}{T_0(U'|U) e^{-S(U)}}\right)$$

(2.98)

If the candidate configuration is accepted, the next configuration in the Markov chain is set equal to the candidate configuration $U_n = U'$. If the candidate configuration $U'$ is not accepted, the new configuration $U_n$ is set equal to the previous configuration $U_{n-1}$ and a new candidate is again generated.

With the choice Eqn. 2.98 for the acceptance probability, the total transition probability $T \equiv T_0 T_A$ satisfies the detailed balance condition:
As stated above, using a symmetric selection probability is advantageous as it reduces Eqn. 2.98 to:

\[
T(U'|U) e^{-S[U']} = T_0(U'|U) \min \left( 1, \frac{T_0(U|U') e^{-S[U']}}{T_0(U'|U) e^{-S[U]}} \right) e^{-S[U]}
\]

\[
= \min \left( T_0(U'|U) e^{-S[U']}, T_0(U|U') e^{-S[U]} \right)
\]

\[
= T_0(U|U') \min \left( 1, \frac{T_0(U'|U) e^{-S[U]}}{T_0(U|U') e^{-S[U']}} \right) e^{-S[U']}
\]

\[
= T(U|U') e^{-S[U']}
\]  \hspace{1cm} (2.99)

As stated above, using a symmetric selection probability is advantageous as it reduces Eqn. 2.98 to:

\[
T_A = \min \left( 1, \frac{T_0(U|U') e^{-S[U']}}{T_0(U'|U) e^{-S[U]}} \right)
\]

\[
= \min \left( 1, \frac{e^{-S[U']}}{e^{-S[U]}} \right)
\]

\[
= \min \left( 1, e^{-\Delta S[U', U]} \right)
\]  \hspace{1cm} (2.100)

with \( \Delta S[U', U] \equiv S[U'] - S[U] \). Therefore when making only local updates to the configurations, only those nearby links that are affected by the changed link need to be calculated to calculate the change in the action. As it stands, this transition probability will minimize the action \( S \), as any increase in \( S \) will cause the candidate configuration to be rejected while any decrease will be accepted. In practice, to increase the acceptance rate (and therefore the stability of the algorithm), the left hand side of the min (. . . . . .) function is usually chosen to be a number \( r \), randomly chosen from \( r \in [0, 1) \). This modification to the acceptance can be regarded in as a way to account for quantum fluctuations that would allow one configuration to fluctuate into another configuration although the probability barrier is too high for this to occur "classically".
As a concrete example, consider the one link update to the Wilson gauge action. Recall that the Wilson gauge action was built as a sum over all distinct plaquettes on the lattice. Because of this, updating a single link will affect the six plaquettes (in four dimensions) that share that particular link (see Fig. 2.1).

![Diagram of plaquettes](image)

**FIG. 2.1:** Three dimensional representation of plaquettes affected by a single link update to the Wilson gauge action.

The effect of this local change to the action $S$ may be written as:

$$
\Delta S = S[U'(n)]_{loc} - S[U''(n)]_{loc}
$$

$$
= -\frac{\beta}{N} \text{Re}\{ \text{tr} [(U'(n) - U(n)) A] \} 
$$

(2.101)

where the invariant (under the single link update) quantity $A$, given by:
\[ A = \sum_{i=1}^{6} P_i = \sum_{\mu \neq \nu} (U_{\nu} (n + \mu) U_{-\mu} (n + \mu + \nu) U_{-\nu} (n + \nu) \]
\[ + U_{-\nu} (n + \mu) U_{-\mu} (n + \mu - \nu) U_{\nu} (n - \nu) \]  
(2.102)

represents the sum of the "staples" that constitute the remainders of the plaquettes that contain the updated link \( U'(n) \).

From Eqns. 2.101, 2.102 it's clear that a selection probability that updates the configurations only locally is advantageous in the minimal computational cost required to calculate the change in the action. In order to further take advantage of this, once the staples are calculated for a particular link variable and the object \( A \) constructed, the single link of interest is often updated several times before proceeding. This can provide several steps in the Markov chain for a single computation of the "staples" \( A \), increasing the computation efficiency.

As stated above, although the selection probability \( T_0 \) is chosen at the discretion of a practitioner of lattice QCD, it is advantageous to choose updates that do not too radically change the action. Because of this, for single link updates, the update is usually chosen such that \( U'(n) = X U(n) \) with \( X \in SU(3), X \sim 1 \). For the single link updating Metropolis algorithm, a common choice for updating the sites is to systematically work through a grid of lattice sites, updating one at a time.

There now exist a wide array of algorithms for generating gauge field configurations. These will not be discussed in detail in this work.

### 2.4 Lattice spectroscopy

One type of calculation that lattice QCD lends itself to particularly well is the determination of ground and excited state spectra of hadrons. While typical
hadronic energies are too low for perturbative treatments to be of much use, most lie well within the realm of applicability for non-perturbative treatment will lattice calculations. Additionally, we have already shown that the correlation function of an operator and its adjoint has a particularly simple relationship to the spectrum of lattice states that overlap with the operator. To extract hadronic masses from a lattice QCD calculation, one must compute the correlation function:

$$ C^\Phi(t - t_0) = \sum_{\vec{x}} e^{-i\Phi \vec{x}} \langle \mathcal{O}(\vec{x}, t) \tilde{\mathcal{O}}(\vec{x}_0, t_0) \rangle $$  \hspace{1cm} (2.103) $$

where the operator $\mathcal{O}_B(\vec{x}_0)$ creates a hadron at $t_0$ and the sum over $\vec{x}$ is used to project the final state to a definite momentum $\vec{p}$. The correlation function expected to behave as a sum of exponentials as in Eqn. 2.17:

$$ \langle \mathcal{O}(t) \tilde{\mathcal{O}}(t_0) \rangle = \sum_n |<n|\mathcal{O}|0>|^2 e^{-E_n t} = \sum_n |A_n|^2 e^{-E_n t} $$
$$ \sim |A_0|^2 e^{-E_0 t} \left( 1 + \mathcal{O}(e^{-\Delta E_1 t}) \right). \hspace{1cm} (2.104) $$

where $\Delta E_1$ is the energy splitting between the lowest lying state that couples to the operator and the next excited state.

If we consider a basis of operators $\mathcal{O}_i$ that all couple to a desired state, we can construct a matrix of correlation functions, given by:

$$ C^\Phi_{ij}(t - t_0) = \sum_{\vec{x}} e^{-i\Phi \vec{x}} \langle \mathcal{O}_i(\vec{x}, t) \tilde{\mathcal{O}}_j(\vec{x}_0, t_0) \rangle. \hspace{1cm} (2.105) $$

The individual components of this correlator matrix will each have different couplings to the desired state, and will obey the relation:
\[ \langle \mathcal{O}_i (\vec{x}, t) \mathcal{O}_j (\vec{x}_0, t_0) \rangle \sim A_0^i \left(A_0^jight)^* e^{-E_0 t} \left(1 + \mathcal{O} \left(e^{-\Delta E_{1t}}\right)\right). \]  

(2.106)

Using the above relation increases the effectiveness of extracting a given mass, as fitting a matrix of correlation functions requires at most \(N_{\text{ops}} + N_{\text{masses}}\) fitting parameters (where \(N_{\text{ops}}\) is the number of interpolating operators and \(N_{\text{masses}}\) is the number of masses to be extracted from the calculation). This scales linearly with the number of operators used, while the number of data points to be fit scales as \(N_{\text{ops}} \times N_t\) if the correlation function is calculated for all lattice time slices. For now we will turn our attention to the form of the interpolating operators \(\mathcal{O}_i\).

### 2.4.1 Operator construction for spectroscopy calculations

**Covariant Operators**

One method for constructing interpolating operators for hadrons uses a covariant formulation in which a quark and antiquark (or three quarks) are combined with a product of Dirac gamma matrices in order to achieve the desired transformation properties of the state in question:

\[ \mathcal{O}_M (x) = \bar{q}_{f_1} (x) \Gamma q_{f_2} (x), \]  

(2.107)

\[ \mathcal{O}_B (x) = \epsilon_{a,b,c} \bar{q}_{f_1}^a (x) \left( (q_{f_2}^b (x))^T \Gamma q_{f_3}^c (x) \right) \]  

(2.108)

In Table 2.4.1, the gamma matrices for several covariant mesonic operators are presented, along with the states with which overlap is expected. The only disadvantage to this method is that it has does not lend itself readily to the construction of a large basis of interpolating operators for a particular hadronic state. Because of
this, smearing techniques must be used. Operator smearing is a method by which the point like interpolating operators are multiplied by products of gauge links to provide a more realistic spatial distribution, and in practice this produces a better overlap of the correlation function with the low lying states in the spectrum. We will return to the topic of smearing when discussing interpolating operators used in the present work for charmed bottom baryon spectroscopy. For now, we turn our attention to the construction of interpolating operators motivated by the quark model.

**TABLE 2.1: Gamma matrices for selected covariant mesonic interpolating operators**

<table>
<thead>
<tr>
<th>State</th>
<th>$J^{PC}$</th>
<th>$\Gamma$</th>
<th>Particles</th>
</tr>
</thead>
<tbody>
<tr>
<td>Scalar</td>
<td>$0^{++}$</td>
<td>$1, \gamma_4$</td>
<td>$f_0, a_0, K_0^*$, ...</td>
</tr>
<tr>
<td>Pseudoscalar</td>
<td>$0^{-+}$</td>
<td>$\gamma_5, \gamma_4 \gamma_5$</td>
<td>$\pi^+, \pi^0, \eta, K^\pm, K^0$, ...</td>
</tr>
<tr>
<td>Vector</td>
<td>$1^{--}$</td>
<td>$\gamma_i, \gamma_4 \gamma_i$</td>
<td>$\rho^\pm, \rho^0, \omega, K^*, \phi$, ...</td>
</tr>
<tr>
<td>Axial Vector</td>
<td>$1^{++}$</td>
<td>$\gamma_5$</td>
<td>$a_1, f_1$, ...</td>
</tr>
<tr>
<td>Tensor</td>
<td>$1^{+-}$</td>
<td>$\gamma_i \gamma_j$</td>
<td>$h_1, b_1$, ...</td>
</tr>
</tbody>
</table>

**Quark model operators**

Using the quark model as a guide, it is straightforward to construct local hadronic operators to be used in spectroscopy calculations. For the present discussion, we assume an $SU(2)$ chiral symmetry, and include the strange, charm, and bottom quarks as well. We wish to construct eigenstates of isospin $I, I_z$, angular momentum $J, J_z$, and parity $P$, along with the flavor quantum numbers of the heavy quarks. For a single quark, we can therefore specify $(I, I_z) = (1/2, \pm 1/2)$, $(J, J_z) = (1/2, \pm 1/2)$, $P = \pm$ and $(S, C, B) = 0, 1$. We write the single quark field located at the point $x$ as: $f_{I_s, J_s, P}^I (x) = f_{J_s, P}^I (x)$. For now, we will suppress the color indices until they are relevant for the discussion. The construction of quark model operators to be used in lattice calculations is straightforward using a Clebsch-
Gordan approach [27], where the spin and isospin indices of the single quark field are summed over with the appropriate Clebsch-Gordan weights to project to the desired three quark angular momentum and isospin eigenstate. For two (mesonic) and three quark (baryonic) operators, this can be represented as:

\[ \mathcal{O}^{I_1 I_2}_{J_1 J_2} (x) = \sum_{I_1, J_1} \sum_{J_2} W^{I_1 I_2}_{I_1 J_1} W^{J_1 J_2}_{J_1 J_2} W^{P}_{P_1 P_2} f^{I_1}_{J_1, P_1} (x) f^{I_2}_{J_2, P_2} (x) \]  

(2.109)

\[ \mathcal{O}^{I_1 I_2}_{J_1 J_2, P} (x) = \sum_{I_1, J_1} \sum_{J_2, J_3} \sum_{J_1, J_2, J_3} W^{I_1 I_2}_{I_1 J_1} W^{J_1 J_2}_{J_1 J_2} W^{J_2 J_3}_{J_2 J_3} W^{P}_{P_1, P_2, P_3} \times f^{I_1}_{J_1, P_1} (x) f^{I_2}_{J_2, P_2} (x) f^{I_2}_{J_3, P_3} (x) \]  

(2.110)

where the Clebsch-Gordan coefficients \( W \) are well known and easily determined. In the above expressions, we have chosen to separate the spin and parity of the quark wavefunctions, writing them as \( f^{I_2}_{J_2, P_2} (x) \) as opposed to using a single spinor index for both spin and parity: \( f^{I_2}_{J_2} (x) \). This distinction is useful in the construction of the quark model wavefunctions as it allows for easy (anti)symmetrization of the full (baryon) meson wavefunction based on the symmetry of both the spin, flavor and parity wavefunctions. This process of constructing wavefunctions lends itself well to automation, allowing for the construction of a basis of operators with which to construct a matrix of correlation functions from which to extract hadronic masses.

The above operators can be written succinctly as a sum over individual terms, as:

\[ \mathcal{O}^{I_1 I_2}_{J_1 J_2} (x) = \sum_{\tilde{I}} W^{I_1 I_2 \tilde{J}_1 \tilde{J}_2 P}_{\tilde{I}} \mathcal{O}^{\tilde{I}} (x) \]  

(2.111)
where the super-index \( \tilde{t} \), given by:

\[
\tilde{t} = \{ I_1^1, I_2^2, J_z^1, J_z^2, P_1, P_2 \} \quad (\text{mesons},) \tag{2.113}
\]

\[
\tilde{t} = \{ I_1^1, I_2^2, J_z^3, J_z^2, P_1, P_2, P_3 \} \quad (\text{baryons}) \tag{2.114}
\]

contains all of the spin and isospin components of the quark operators and the super-weights are given by:

\[
W_{\tilde{t}}^{I_1, I_2, J_z, J_z, P} \equiv W_{I_1}^{I_1} W_{I_2}^{I_2} W_{J_z}^{J_z} W_{P_1}^{P_1} W_{P_2}^{P_2} \quad (\text{mesons}), \tag{2.115}
\]

\[
W_{\tilde{t}}^{I_1, I_2, J_z, J_z, P} \equiv W_{I_1}^{I_1} W_{I_2}^{I_2} W_{J_z}^{J_z} W_{J_z}^{J_z} W_{P_1}^{P_1} W_{P_2}^{P_2} W_{P_3}^{P_3} \quad (\text{baryons}). \tag{2.116}
\]

For the present discussion, we will focus on the construction of baryonic operators. The above construction methods are sufficient to construct an operator basis for baryons with \( J \leq \frac{3}{2} \). If we wish to construct baryonic interpolating operators that will couple to angular momentum eigenstates with \( J > \frac{3}{2} \), we must turn to non-local operators, as a combination of three spin-1/2 objects can at most yield a spin-3/2 object. In the continuum, the spatial components of the derivative operator can be written in a spherical harmonic basis, the components of which transform as spin-1 objects. For convenience, we will make the definitions:

\[
D_0 \equiv 1, \quad D_1 \equiv \partial_z, \quad D_2 \equiv \frac{\partial_x - i\partial_y}{\sqrt{2}}, \quad D_3 \equiv \frac{\partial_x + i\partial_y}{\sqrt{2}}. \tag{2.117}
\]

Combining spin-1 derivative operators with the spin-1/2 quark fields therefore allows for the construction of objects with arbitrarily high angular momentum, provided one is willing to keep adding derivatives to the quark field operators. For
our purposes we fill focus on at most a single derivative operator acting on each quark field, which can produce a three quark baryonic state with maximum angular momentum of $J = \frac{9}{2}$. The interpolating operators for threes states are given by:

$$
O_{J_1,J_2,J_3}^{I_1,I_2} (x) = \sum_{I_1',I_2',J_z,J_z} \sum_{P_1,P_2} \sum_{d_1,d_2,d_3} \sum_{d_1',d_2',d_3'} W_{I_1',I_2',J_z}^{J_1,J_2,J_3} W_{P_1',d_1}^{J_z,d_2} W_{P_2',d_2}^{J_z,d_3} W_{J_3'}^{P_3,d_3'} \\
\times D_{d_1} f_{J_z}^{I_1} (x) D_{d_2} f_{J_z}^{I_2} (x) D_{d_3} f_{J_z}^{I_3} (x) \quad (2.118)
$$

where here the indices $d_i$ can take on the values 0, 1, 2, 3 and the $D_{d_i}$ are given by Eqns. 2.4.1. The weights $W_{J_1,J_2,J_3}^{I_1,I_2,J_z}$ are now products of weights that first project the single quark with derivative operators to a given angular momentum, then project to the three quark state angular momentum. When the derivative operator is discretized the operators 2.118 will be composed of terms that look like:

$$
\mathcal{O} (\vec{x}) \equiv U (\vec{x}, t) f_{J_z}^{I_1} (\vec{x} \pm \hat{i}_1, t) U (\vec{x}, t) f_{J_z}^{I_2} (\vec{x} \pm \hat{i}_2, t) U (\vec{x}, t) f_{J_z}^{I_3} (\vec{x} \pm \hat{i}_3, t) \\
\quad (2.119)
$$

with:

$$
\vec{t} \equiv \{ I_1^1, I_1^2, J_1^1, J_1^2, P_1, P_2, \pm i_1, \pm i_2 \} \quad (\text{mesons}), \quad (2.120)
$$

$$
\vec{t} \equiv \{ I_2^1, I_2^2, J_2^1, J_2^2, J_3^1, J_3^2, J_3^3, P_1, P_2, P_3, \pm i_1, \pm i_2, \pm i_3 \} \quad (\text{baryons}) \quad (2.121)
$$

We can then write the above operators as a sum over terms similar to Eqn. 2.111 as:
\[ O_{J,J_z,P}^{I,I_z}(x) = \sum_{\tilde{r}} W_{\tilde{r}}^{I,I_z,J,J_z,P} O^{\tilde{r}} \]  

(2.122)

\[ (2.123) \]

where the vector index \( \tilde{r} \) now contains all of the spin and isospin components of the quark operators and the super-weights are given by:

\[ W^{I,I_z,J,J_z,P}_{I_1,I_2,J_1,J_2,\pm i_1,\pm i_2} W^P_{P_1,P_2} \]  

(2.124)  

\[ W^{I,I_z,J,J_z,P}_{I_1,I_2,J_1,J_2,\pm i_1,\pm i_2,\pm i_3} W^P_{P_1,P_2,P_3} \]  

(2.125)  

In considering states with such large angular momenta, one must take into consideration how the explicit breaking of spatial rotational invariance by the lattice discretization will effect the spectrum of angular momentum eigenstates. When the full rotational symmetry of the continuum is reduced to the rotational subgroup \( O(4) \), the continuum irreducible representations (irreps) of the full rotational group are mapped onto a group of lattice irreps associated with the \( O(4) \) group. The mapping of the continuum states onto the lattice irreps is given in Table 2.2. The \( J = \frac{1}{2} \) and \( J = \frac{3}{2} \) angular momentum states are unambiguously mapped to the lattice irreps \( G_1 \) and \( H \) respectively, allowing for a straightforward identification of the states that couple to the local baryonic operators from Eqns. 2.109 with their continuum angular momentum states. For states with \( J > 3/2 \), this is not necessarily the case, as the continuum irreducible representations are mapped into multiple lattice irreps. Because of this, the operators constructed according to Eqn. 2.118 will fall into different lattice irreps. Each of these operators will overlap with the desired continuum state as the lattice spacing is taken to zero, however
operators from different lattice irreps will have very small overlap with each other at finite lattice spacing. From a group theoretical perspective, one can determine linear combinations of the naive lattice operators given by Eqn. 2.118 from each lattice irrep with appropriate weights such that they will have maximum overlap with the desired continuum state. For details of this approach, see e.g. Ref. [27].

This concludes our discussion of the construction of non-local baryonic operators for use in spectroscopy calculations. In section 2.6.1, this methodology will be revisited in the context of colorwave propagators.

2.5 Interactions and exotic states from lattice calculations

When considering interactions in lattice calculations, it has long been known that Euclidean space calculations cannot provide information on the real time dynamics of hadronic systems. To circumvent this difficulty, several lattice methodologies have been developed to determine information of hadronic interactions without explicitly considering the real time dynamics of the system. One method, developed by Lüscher [28] leverages the fact that lattice calculations are necessarily performed in finite volume to our advantage. By studying the finite volume scattering problem in the continuum, one can derive relations between the elastic scattering phase shift of a two particle system in a finite periodic box with the energy levels of the

<table>
<thead>
<tr>
<th>$J$</th>
<th>$\Lambda$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/2</td>
<td>$G_1$</td>
</tr>
<tr>
<td>3/2</td>
<td>$H$</td>
</tr>
<tr>
<td>5/2</td>
<td>$H \oplus G_2$</td>
</tr>
<tr>
<td>7/2</td>
<td>$G_1 \oplus H \oplus G_2$</td>
</tr>
</tbody>
</table>

TABLE 2.2: Lattice irreducible representations in which the continuum angular momentum eigenstates are mapped to.
system. We will not discuss this methodology here, but instead turn our attention to an alternate approach for the determination of interaction properties from lattice calculations that relies on the inclusion of two heavy quarks to the system under study.

As discussed in Section 1.4.1, in the static limit of HQET, a heavy flavor quark in its rest frame acts as a color source, propagating only in the temporal direction. If two hadrons are put on the lattice, each containing a heavy static quark, then one is immediately provided with a well defined separation for the two hadrons as the spatial separation of the two heavy quarks with the hadrons. Utilizing this, the energy of the multi-hadron system $E(r)$ can be calculated as a function of spatial separation. If one subtracts from this multi-hadron energy the rest energy of the two particles (determined from the lattice) for the limit $r \rightarrow \infty$, then one is left with a well defined two-hadron potential as determined from the lattice:

$$V(r) \equiv E_{H_1,H_2}(r) - M_{H_1} - M_{H_2}. \quad (2.126)$$

This formalism is used in the present work to probe the properties of two meson systems when each meson contains a single heavy quark, the model being two $B$ mesons.

### 2.6 Colorwave Formalism

Consider a general operator for a two quark mesonic state:

$$\mathcal{O} (\vec{x}) = \bar{q}_1(x) \Gamma q_2(x) \quad (2.127)$$

where we assume for simplicity that the two quarks have different flavors. We seek to calculate the correlation function with localized interpolating fields: (averaged
over spatial source and sink locations to increase statistics)

\[
C(t, t_0) = \sum_{x,y} \langle \mathcal{O}(y) \mathcal{O}^\dagger(x) \rangle \\
= \sum_{x} \sum_{y} \text{tr} \left( S_1(x, t_0|y, t) \Gamma S_2(y, t|x, t_0) \Gamma \right)
\] (2.128)

Following the methodology presented in [29], we now consider any complete set of orthonormal states \( \{ \phi_i(x) \} \) which satisfy:

\[
\sum_i \phi_i^*(x) \phi_i(y) = \delta(x - y), \quad \sum_x \phi_i^*(x) \phi_j(x) = \delta_{ij}.
\] (2.129)

By inserting the completeness relation of Eqn. 2.129 twice into the two point function of Eqn. 2.128:

\[
C(t, t_0) = \sum_{x,x'} \sum_{y,y'} \langle S_1(x, t_0|y', t) \delta(y - y') \Gamma S_2(y, t|x', t_0) \delta(x - x') \Gamma \rangle \\
= \sum_{x,x'} \sum_{y,y'} \left( \sum_i \phi_i^*(y) \phi_i(y') \Gamma S_2(y, t|x', t_0) \sum_j \phi_j^*(x) \phi_j(x') \Gamma \right) \\
= \sum_{i,j} S_1^{ij}(t_0, t) \Gamma S_2^{ij}(t, t_0) \Gamma
\] (2.130)

where we have defined:

\[
S^{ij}(t_0, t) \equiv \sum_{x,y} \phi_i^*(y) S(y, t; x, t_0) \phi_j(x)
\] (2.131)

A convenient choice for the \( \{ \phi_i(x) \} \) is a plane wave basis: \( \phi_i(x) \equiv \phi_p(x) = e^{-ipx} \delta_{s,s'} \delta_{c,c'} \). The delta functions here operate on color and spin. This choice of basis greatly reduces the computational cost of contractions because a substantial part of the work can be done analytically. With this choice of basis, we define \( S^{ij}(t, t_0) \equiv S^{p,p'}(t, t_0) \) to be colorwave propogators. It is also evident that the
colorwave propagators can be also viewed as a generalization of gauge fixed wall source propagators. The use of these propagators allows us to implement spatial smearing at the source and sink of our correlation functions. In the limit where all momenta are summed over in equation 2.131, all to all point-point propagators are recovered. However, introducing a maximum momentum cut off $p_{cut}^2$ we are able to introduce and control the effective amount of spatial smearing\(^1\).

### 2.6.1 Colorwave propagators with non-local operators

In the previous section, we presented the colorwave formalism and its application to the construction of hadronic correlation functions. Here, we wish to describe the non-local baryonic operators as described in Section 2.4.1 in the language of the colorwave formalism. To begin, we will look at a single term from a baryonic operator as described by Eqn. 2.119.

We now replace the quark operators with their Fourier transform and we find that a single term becomes:

\(^1\)It should be noted that smearing is achieved only in fixed gauge. In our case we use the Coulomb gauge, which is a smooth gauge allowing to project out high energy modes if the cut off $p_{cut}^2$ is kept small. However, no gauge dependence is introduced to our correlation functions as they are gauge invariant by construction.
\[ \mathcal{O}(\vec{x}, t)_{\pm i_1, \pm i_2, \pm i_3} = \sum_{\vec{p}_1, \vec{p}_2, \vec{p}_3} U(\vec{x}, t)_{\pm i_1} f_1(\vec{p}_1, t) e^{-i\vec{p}_1 \cdot \vec{x} \pm i_1} \]
\[ \times U(\vec{x}, t)_{\pm i_2} f_2(\vec{p}_2, t) e^{-i\vec{p}_2 \cdot \vec{x} \pm i_2} \]
\[ \times U(\vec{x}, t)_{\pm i_3} f_3(\vec{p}_3, t) e^{-i\vec{p}_3 \cdot \vec{x} \pm i_3} \]
\[ = \sum_{\vec{p}_1, \vec{p}_2, \vec{p}_3} f_1(\vec{p}_1, t) f_2(\vec{p}_2, t) f_3(\vec{p}_3, t) \]
\[ \times U(\vec{x}, t)_{\pm i_1} U(\vec{x}, t)_{\pm i_2} U(\vec{x}, t)_{\pm i_3} \]
\[ \times e^{-i(\vec{p}_1 \cdot \vec{i}_1 + \vec{p}_2 \cdot \vec{i}_2 + \vec{p}_3 \cdot \vec{i}_3)} e^{-i\vec{P} \cdot \vec{x}} \]
\[ = \sum_{\vec{p}_1, \vec{p}_2, \vec{p}_3} f_1(\vec{p}_1, t) f_2(\vec{p}_2, t) f_3(\vec{p}_3, t) L(\vec{x}, t)_{\vec{P}_1, \vec{P}_2, \vec{P}_3} \pm i_1, \pm i_2, \pm i_3 \quad (2.132) \]

where \( \vec{P} \equiv \vec{p}_1 + \vec{p}_2 + \vec{p}_3 \), and we have defined:

\[ L(\vec{x}, t)_{\vec{P}_1, \vec{P}_2, \vec{P}_3} \equiv U(\vec{x}, t)_{\pm i_1} U(\vec{x}, t)_{\pm i_2} U(\vec{x}, t)_{\pm i_3} e^{-i(\vec{P}_1 \cdot \vec{i}_1 + \vec{P}_2 \cdot \vec{i}_2 + \vec{P}_3 \cdot \vec{i}_3)} e^{-i\vec{P} \cdot \vec{x}} \quad (2.133) \]

Using this for our operators, we may construct baryonic correlation functions as follows:

\[ C(t - t_0) = \sum_{\vec{x}_1, \vec{x}_2} \langle \mathcal{O}(\vec{x}_1, t) \mathcal{O}(\vec{x}_2, t_0) \rangle \]
\[ C(t - t_0) = \sum_{\vec{x}_1, \vec{x}_2} \sum_{\vec{t}_1, \vec{t}_2} W_{\vec{t}_1} W_{\vec{t}_2}^* \left\langle \mathcal{O}(\vec{x}_1, \vec{t}_1) \mathcal{O}(\vec{x}_2, t_0) \right\rangle \quad (2.134) \]
\[ C(t - t_0) = \sum_{\vec{x}, \vec{x}', i, j} (W_{\vec{i}, \vec{j}}) \left< \mathcal{O}(\vec{x}', t)_{\pm i_1, \pm i_2, \pm i_3} \bar{\mathcal{O}}(\vec{x}, t_0)_{\pm i_1, \pm i_2, \pm i_3} \right> \]

\[ = \sum_{\vec{x}, \vec{x}', i, j} \sum_{\vec{p}_1, \vec{p}_2, \vec{p}_3} \sum_{\vec{p}'_1, \vec{p}'_2, \vec{p}'_3} \langle f_3(\vec{p}'_1, t) f_2(\vec{p}'_2, t) f_3(\vec{p}'_3, t) \bar{f}_3(\vec{p}_3, t_0) \bar{f}_2(\vec{p}_2, t_0) \bar{f}_1(\vec{p}_1, t_0) \rangle \]

\[ \times W_{\vec{i}, \vec{j}} \left< L(\vec{x}', t)_{\pm i'_1, \pm i'_2, \pm i'_3} L^\dagger(\vec{x}, t)_{\pm i_1, \pm i_2, \pm i_3} \right> \]

(2.135)

\[ C(t - t_0) = \sum_{\vec{x}, \vec{x}', i, j} (W_{\vec{i}, \vec{j}}) \sum_{\vec{p}_1, \vec{p}_2, \vec{p}_3} S_{\vec{p}_1, \vec{p}_2, \vec{p}_3}^{\vec{i}, \vec{j}}(t, t_0) S_{\vec{p}_3}^{\vec{i}, \vec{j}}(t, t_0) \]

\[ \times \left< L(\vec{x}', t)_{\pm i'_1, \pm i'_2, \pm i'_3} L^\dagger(\vec{x}, t)_{\pm i_1, \pm i_2, \pm i_3} \right> \]

\[ = \sum_{i, j} (W_{\vec{i}, \vec{j}}) \sum_{\vec{p}_1, \vec{p}_2, \vec{p}_3} S_{\vec{p}_1, \vec{p}_2, \vec{p}_3}^{\vec{i}, \vec{j}}(t, t_0) S_{\vec{p}_3}^{\vec{i}, \vec{j}}(t, t_0) \]

\[ \times \sum_{\vec{x}'} \left< L(\vec{x}', t)_{\pm i'_1, \pm i'_2, \pm i'_3} \sum_{\vec{x}} \left< L^\dagger(\vec{x}, t)_{\pm i_1, \pm i_2, \pm i_3} \right> \right> \]

(2.136)

This concludes our discussion of the colorwave formalism as applied to non-local baryonic operators.
CHAPTER 3

Charmed bottom baryon spectroscopy

Experimental observations of charmed and bottom baryons date back to the mid 1970s with the discovery of the $\Lambda_c^+$, and to the early 1990s with the discovery of the $\Lambda_b$. Since that time, the experimental spectrum has filled out with many very precise measurements of the ground state energies of singly charmed and bottom baryons. In the past 10 years, results from BaBar and Belle, as well as the D0 and CDF experiments at Fermilab have provided more precise measurements of heavy flavor ground and excited states as well as a first glimpse of several new states, most notably the controversial $\Omega_b$ at CDF [30] and D0 [31] and the $\Xi_{cc}$ at SELEX [32, 33]. Although the former controversy has been resolved by a more recent measurement at the LHCb [34], the latter observation has still received no experimental verification to date, and is generally in disagreement with most current theoretical results by $\sim 200$ MeV. It is controversies like these, as well as the prospect of observations of new states that make this an exciting time for lattice QCD. The opportunities for heavy flavor spectroscopy from the lattice are threefold: 1) Lattice
results can help to resolve controversies like the ones presented above (providing a model-independent point of comparison for current experimental measurements). 2) Lattice results can help to provide predictions for as yet unobserved states and 3) Spectroscopy calculations can help to pin down values for the low energy constants (LECs) of chiral perturbation theory (a job that lattice calculations are uniquely suited for), helping to aid in the understanding of hadronic physics at low energies.

The predictive power of lattice QCD is especially exciting in the context of the upcoming increase in operating energy at the LHC scheduled for 2014.

The renewed interest in heavy baryon spectroscopy within the lattice community is reflected by the array of recent calculations of the spectra of singly, doubly, and triply heavy baryons [35, 36, 37, 38, 39, 40, 41, 42, 43]. Early calculations performed in the quenched approximation explored the charmed [35] as well as the charmed and bottom [42] baryon spectra, however quenching introduces a systematic uncertainty into the calculation which is extremely difficult to quantify. Moreover, from the perspective of chiral perturbation theory, the quenched version of QCD does not contain full QCD and therefore the low energy constants extracted from chiral extrapolations of values obtained in quenched calculations are not the same as those that are found in the chiral expansions for full QCD. Thus these extracted coefficients cannot be used in studying the low energy dynamics of hadronic physics.

A dynamical (2+1 flavor) calculation presented in Ref. [40] provided an extensive exploratory study of both singly and doubly charmed and bottom baryon masses, using an improved clover action to treat the charm and bottom quarks relativistically. Extensive details of this work (including tables of all the calculated baryon masses) were not published however, the available results being restricted to several figures containing values for singly and doubly charmed and bottom mass splittings.

In Ref. [39], singly bottom hadron mass splittings were calculated using domain
wall valence quarks (with a lightest pion mass around 290 MeV) on dynamical configurations with 2+1 flavors of Kogut-Susskind sea quarks with a lattice spacing of $\sim 0.124$ fm. The static quark action was used for the bottom sector, and several predictions were made for the masses of bottom baryons, including the mass of the $\Xi_b^*$ which has yet to be observed experimentally. The mass of the $\Omega_b$ was also calculated, and found to be in agreement with the observation of the CDF collaboration, providing early evidence to help quell the controversy surrounding this state.

Building on the singly bottom results presented in [39], Ref. [38] calculated the masses of bottom baryons including up to three bottom quarks. This calculation utilized domain wall fermions for both the sea and valence sectors on configurations generated by the RBC UKQCD collaboration [44]. The NRQCD action [45] was used for the bottom quark, allowing the splittings between various spin states to be calculated. Additionally, the first determination of the $\Omega_{bb\bar{b}}$ mass was presented. The spectrum of excited states of this triply bottom state was then examined in detail in [37], with the same computational details as in [38], providing the extensive study of the excited state spectrum of multiply heavy states on the lattice.

Recent calculations of the charmed baryon spectrum were carried out in Refs. [41], [43] and [46] each utilizing an improved clover action [47] for a relativistic treatment of the charm quarks. For the light quark sector, Liu et al. utilized domain wall fermions in the valence sector and Kogut-Suskind sea quarks with the lightest pion mass around 290 MeV. As this calculation was limited to states with $J = 1/2$ chiral extrapolations had to be treated very carefully, as chiral expansion formulae for baryon masses relate the $J = 1/2$ and $J = 3/2$ spin partners. Briceno and Lin used a mixed action approach for the light sector as well, with clover improved valence quarks on configurations with HISQ sea quarks. For their calculation, the $J = 1/2$ and $J = 3/2$ spin partners were calculated, allowing the chiral extrapolations to be
guided by heavy hadron chiral perturbation theory. The mixed action approach to
the light quark sector in these calculations can present some difficulties, once such
being the necessity of mixed action ChiPT in performing chiral extrapolations once
the lattice calculation has been carried out. The more recent work presented in [46]
was performed at the physical point using reweighting techniques to tune the up
down and strange quarks to their physical masses.

The interest in heavy hadron spectroscopy has not been limited to the lattice
community, and there has been significant recent progress in theoretical calculations
of the charmed and bottom baryon spectra as well using various theoretical mod­
ells [48] [49] [50] [51]. Included among these calculations several determinations of the
doubly heavy baryons which contain charm and bottom quarks. With the exception
of the early quenched heavy hadron study [35], this sector of doubly heavy states
remains largely unexplored in lattice calculations, and there is no existing experi­
mental data on charmed bottom baryons. This is a void that the present work will
seek to fill, while at the same time reinforcing the existing lattice calculations of the
charmed and bottom baryon spectra with a calculation using a single action for the
light quark sector.

3.1 Details of the lattice calculation

The gauge field ensembles for this spectroscopy calculation were generated by
the RBC/UKQCD collaboration [1] utilize the Iwasaki gauge action [52, 53]. These
gauge configurations include 2 + 1 (up down and strange) flavors of light quarks. The
fermion action utilized for these light quarks is the domain wall action [54, 55, 56],
where an additional fifth dimension is introduced as a means of preserving chiral
symmetry at finite lattice spacing. In this formalism, the four dimensional light
fermions exist on the boundaries of the fifth dimension. In the limit that this
additional dimension becomes infinite, one obtains an exact chiral symmetry for these fermion light nodes. In practice, this additional dimension must have finite extent, and in the current work the length $L_5/a = 16$. Additionally, the Domain wall height is set to be $aM_5 = 1.8$. Details about this particular action are beyond the scope of this work, but can be found in [57].

Two ensembles with the above parameters were utilized with different lattice spacings: a coarse lattice spacing with $a \sim 0.11$ fm and a fine lattice spacing with $a \sim 0.08$ fm. Additionally these ensembles were computed using various sea quark masses, and we utilize four different sea quark masses (two for the coarse and two for the fine ensembles).

Valence quark propagators were generated with these configurations, with the valence quark masses not restricted to equal that of the sea quark mass (partial quenching). This partial quenching was carried out in the interest of achieving a wide range of quark masses on which to perform chiral extrapolations. Table 3.1 provides details of all of the ensembles used in the spectroscopy calculation.

<table>
<thead>
<tr>
<th>Ensem.</th>
<th>$N_f^3$</th>
<th>$am_{ud}^{(sea)}$</th>
<th>$am_{s}^{(sea)}$</th>
<th>$a$ (fm)</th>
<th>$am_{ud}^{(val)}$</th>
<th>$am_{s}^{(val)}$</th>
<th>$m^{(vv)}_{\pi}$ (MeV)</th>
<th>$m^{(vv)}_{\eta_s}$ (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>24$^3$</td>
<td>0.01</td>
<td>0.04</td>
<td>0.1139(18)</td>
<td>0.01</td>
<td>0.04</td>
<td>419(7)</td>
<td>752(12)</td>
</tr>
<tr>
<td>B</td>
<td>24$^3$</td>
<td>0.005</td>
<td>0.04</td>
<td>0.1119(17)</td>
<td>0.001</td>
<td>0.04</td>
<td>245(4)</td>
<td>761(12)</td>
</tr>
<tr>
<td>C</td>
<td>24$^3$</td>
<td>0.005</td>
<td>0.04</td>
<td>0.1119(17)</td>
<td>0.002</td>
<td>0.04</td>
<td>270(4)</td>
<td>761(12)</td>
</tr>
<tr>
<td>D</td>
<td>24$^3$</td>
<td>0.005</td>
<td>0.04</td>
<td>0.1119(17)</td>
<td>0.005</td>
<td>0.04</td>
<td>336(5)</td>
<td>761(12)</td>
</tr>
<tr>
<td>E</td>
<td>24$^3$</td>
<td>0.005</td>
<td>0.04</td>
<td>0.1119(17)</td>
<td>0.005</td>
<td>0.03</td>
<td>336(5)</td>
<td>665(10)</td>
</tr>
<tr>
<td>F</td>
<td>32$^3$</td>
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<td>0.03</td>
<td>0.0849(12)</td>
<td>0.002</td>
<td>0.03</td>
<td>227(3)</td>
<td>747(10)</td>
</tr>
<tr>
<td>G</td>
<td>32$^3$</td>
<td>0.004</td>
<td>0.03</td>
<td>0.0849(12)</td>
<td>0.004</td>
<td>0.03</td>
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</tr>
<tr>
<td>H</td>
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<td>0.0848(17)</td>
<td>0.006</td>
<td>0.03</td>
<td>352(7)</td>
<td>749(14)</td>
</tr>
</tbody>
</table>

TABLE 3.1: Properties of the gauge field ensembles [1] and the light/strange propagators computed on them. $am_f^{(sea)}$ sea quark masses for flavor $f$, and $a$ is the lattice spacing (determined in Ref. [2]). The valence quark masses used for the calculation of the light and strange quark propagators are denoted by $am_f^{(val)}$. Lastly, the corresponding pion and kaon masses are presented.

For the bottom quarks, the NRQCD action presented in section 2.2.2 is used. For the charmed sector, the relativistic heavy quark action is used (see section 2.2.2).
The parameters $\nu$ and $m_0$ for this action were tuned non-perturbatively, as we will now discuss.

### 3.2 Tuning the relativistic heavy quark action

In order to tune the parameters $\nu$ and $m_0$ for the charmed sector, we calculate the dispersion relation of $J/\Psi$ as well as the spin averaged charmonium mass using the Chroma software package for Lattice QCD [58] for calculating correlation functions:

$$c^2 = \frac{\tilde{M}_{|p^2|=1}^2 - \tilde{M}_{|p^2|=0}^2}{(2\pi/L)^2}, \quad \tilde{M} = \frac{1}{4}M_{\eta_c} + \frac{3}{4}M_{J/\psi} \quad (3.1)$$

Here, we use only the single momentum value to tune the dispersion relation as it provides a clean estimate of the true dispersion relation in the region of parameter space near the physical point of $c^2 = 1$. In practice, the tuning procedure began by calculating the correlation functions:

$$C_{\eta_c, J/\psi}^p(t) = \sum_x e^{-p \cdot x} \langle \mathcal{O}_{\eta_c, J/\psi}(x, t_{\text{src}} + t) \mathcal{O}_{\eta_c, J/\psi}(x_{\text{src}}, t_{\text{src}}) \rangle \quad (3.2)$$

(with $\mathcal{O}_{\eta_c} = \bar{c}\gamma_5 c$, $\mathcal{O}_{J/\psi} = \bar{c}\gamma_i c$) with a two randomly placed sources on each configuration (an average was later taken over the source locations). The masses $M_{\eta_c}, M_{J/\psi}$ were then extracted using single exponential fits. From these masses, $c^2$ and $\tilde{M}$ were determined from the above relations, using the mass of the $\eta_c$ in the determination of $c^2$. Next, a linear dependence of both quantities on both $\nu$ and $m_0$
was assumed of the form:

\[
f_M(\nu, m_0) = \delta^M + C^M_\nu \nu + C^M_{m_0} m_0 \\
f_c(\nu, m_0) = \delta^c + C^c_\nu \nu + C^c_{m_0} m_0.
\]

The optimal values of \(\nu\) and \(m_0\) were then determined iteratively by minimizing the function:

\[
\chi^2 \equiv \left[ \bar{Y} - \bar{F}(\nu, m_0) \right]' C^{-1} \left[ \bar{Y} - \bar{F}(\nu, m_0) \right]
\]

where:

\[
\bar{Y} \equiv \begin{bmatrix}
M(\nu, m_0) - M_{\text{phys}} \\
\bar{c}(\nu, m_0) - 1
\end{bmatrix},
\bar{F}(\nu, m_0) \equiv \begin{bmatrix}
f_M(\nu, m_0) \\
f_c(\nu, m_0)
\end{bmatrix}
\]

and \(C\) is the jackknife estimate of the covariance matrix of \(\bar{Y}\). The results of this minimization are presented in Table 3.2.

### 3.3 Covariant baryon interpolating operators

For the present calculation, covariant interpolating operators were constructed for the baryon and mesonic sectors. We begin with operators of the form:
\[ O_5[q,q',q'']_\alpha = \epsilon_{abc} (C\gamma_5)_{\beta\gamma} q_\beta^a q_\gamma^b (P_+ q'')^c_\alpha, \] (3.7)

\[ O'_5[q,q',q'']_\alpha = \epsilon_{abc} (C\gamma_5)_{\beta\gamma} \left[ q_\beta^a q_\gamma^b (P_+ q')^c_\alpha + q_\beta^a q_\gamma^b (P_+ q)^c_\alpha \right], \] (3.8)

\[ O_j[q,q',q'']_\alpha = \epsilon_{abc} (C\gamma_j)_{\beta\gamma} q_\beta^a q_\gamma^b (P_+ q'')^c_\alpha. \] (3.9)

where \( a, b, c \) are color indices, \( \alpha, \beta, \gamma \) are spinor indices, \( C \) is the charge conjugation matrix, and \( P_+ \) is the positive-parity projector

\[ P_+ = \frac{1}{2}(1 + \gamma_0). \] (3.10)

The operators \( O_5 \) and \( O'_5 \) have positive parity and spin 1/2. The operator \( O_j \) (where \( j = 1, 2, 3 \)) has positive parity but couples to both spin 1/2 and spin 3/2 in general. Using the projectors

\[ P^{(1/2)}_{jk} = \frac{1}{3} \gamma_j \gamma_k, \] (3.11)

\[ P^{(3/2)}_{jk} = \delta_{jk} - \frac{1}{3} \gamma_j \gamma_k, \] (3.12)

we are able to project to definite spin, creating the operators \( O^{(1/2)}_j \) and \( O^{(3/2)}_j \) given by:

\[ O^{(1/2)}_j[q,q',q'']_\alpha = \left( P^{(1/2)}_{jk} O_k[q,q',q''] \right)_\alpha, \] (3.13)

\[ O^{(3/2)}_j[q,q',q'']_\alpha = \left( P^{(3/2)}_{jk} O_k[q,q',q''] \right)_\alpha. \] (3.14)

In Table 3.3, we tabulate these operators alongside all of the baryonic states considered in this work.
<table>
<thead>
<tr>
<th>Hadron</th>
<th>$J^P$</th>
<th>Operator(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Lambda_c$</td>
<td>$\frac{1}{2}^+$</td>
<td>$O_5[u, d, c]$</td>
</tr>
<tr>
<td>$\Sigma_c$</td>
<td>$\frac{1}{2}^+$</td>
<td>$O_j^{(1/2)}[u, u, c]$</td>
</tr>
<tr>
<td>$\Sigma_c^*$</td>
<td>$\frac{3}{2}^+$</td>
<td>$O_j^{(3/2)}[u, u, c]$</td>
</tr>
<tr>
<td>$\Xi_c$</td>
<td>$\frac{1}{2}^+$</td>
<td>$O_5[u, s, c]$</td>
</tr>
<tr>
<td>$\Xi_c^*$</td>
<td>$\frac{1}{2}^+$</td>
<td>$O_j^{(1/2)}[u, s, c], \quad O_5[u, s, c]$</td>
</tr>
<tr>
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<td>$O_j^{(3/2)}[u, s, c]$</td>
</tr>
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<td>$O_j^{(1/2)}[s, s, c]$</td>
</tr>
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<td>$O_j^{(3/2)}[s, s, c]$</td>
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</tr>
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<td>$O_j^{(3/2)}[c, c, u]$</td>
</tr>
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<td>$\Omega_{cc}$</td>
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<td>$O_j^{(1/2)}[c, c, s]$</td>
</tr>
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</tr>
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<td>$O_5[u, d, b]$</td>
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<td>$\frac{1}{2}^+$</td>
<td>$O_j^{(1/2)}[u, u, b]$</td>
</tr>
<tr>
<td>$\Sigma_b^*$</td>
<td>$\frac{3}{2}^+$</td>
<td>$O_j^{(3/2)}[u, u, b]$</td>
</tr>
<tr>
<td>$\Xi_b$</td>
<td>$\frac{1}{2}^+$</td>
<td>$O_5[u, s, b]$</td>
</tr>
<tr>
<td>$\Xi_b'$</td>
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<td>$O_j^{(1/2)}[u, s, b], \quad O_5[u, s, b]$</td>
</tr>
<tr>
<td>$\Xi_b^*$</td>
<td>$\frac{3}{2}^+$</td>
<td>$O_j^{(3/2)}[u, s, b]$</td>
</tr>
<tr>
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<td>$O_j^{(1/2)}[s, s, b]$</td>
</tr>
<tr>
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<td>$O_j^{(3/2)}[s, s, b]$</td>
</tr>
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<td>$O_j^{(1/2)}[b, b, u]$</td>
</tr>
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<td>$O_j^{(3/2)}[b, b, u]$</td>
</tr>
<tr>
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<td>$O_j^{(1/2)}[b, b, s]$</td>
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</table>

TABLE 3.3 – Continued on next page
TABLE 3.3 - continued from previous page

<table>
<thead>
<tr>
<th>Hadron</th>
<th>$J^P$</th>
<th>Operator(s)</th>
</tr>
</thead>
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</tr>
<tr>
<td>$\Omega_{bbb}^*$</td>
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<td>$O_j^{(3/2)}[b, b, b]$</td>
</tr>
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<td>$\frac{1}{2}$</td>
<td>$O_5[u, c, b]$</td>
</tr>
<tr>
<td>$\Xi'_{cb}$</td>
<td>$\frac{1}{2}$</td>
<td>$O_j^{(1/2)}[u, c, b], \quad O_5'[u, c, b]$</td>
</tr>
<tr>
<td>$\Xi_{cb}^*$</td>
<td>$\frac{3}{2}^+$</td>
<td>$O_j^{(3/2)}[u, c, b]$</td>
</tr>
<tr>
<td>$\Omega_{cb}$</td>
<td>$\frac{1}{2}$</td>
<td>$O_5[s, c, b]$</td>
</tr>
<tr>
<td>$\Omega'_{cb}$</td>
<td>$\frac{1}{2}$</td>
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</tr>
<tr>
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<td>$\frac{3}{2}^+$</td>
<td>$O_j^{(3/2)}[s, c, b]$</td>
</tr>
<tr>
<td>$\Omega_{cbb}$</td>
<td>$\frac{1}{2}$</td>
<td>$O_j^{(1/2)}[c, c, b]$</td>
</tr>
<tr>
<td>$\Omega'_{cbb}$</td>
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<td>$O_j^{(3/2)}[c, c, b]$</td>
</tr>
<tr>
<td>$\Omega_{cbb}$</td>
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<td>$O_j^{(1/2)}[b, b, c]$</td>
</tr>
<tr>
<td>$\Omega_{cbb}^*$</td>
<td>$\frac{3}{2}^+$</td>
<td>$O_j^{(3/2)}[b, b, c]$</td>
</tr>
</tbody>
</table>

| TABLE 3.3: Heavy-baryon operators. |

For the mesonic sector, we use operators of the form:

\[ O^{(M)}_5[\bar{q}, q'] = \bar{q}\gamma_5 q', \]  
\( (3.15) \)

\[ O^{(M)}_j[\bar{q}, q'] = \bar{q}\gamma_j q'. \]  
\( (3.16) \)

To construct a basis of operators constructed with this methodology, Gaussian smearing was applied to the operators as given by:

\[ \tilde{q} = \left(1 + \frac{r_s^2}{2n_s} \Delta^{(2)}\right)^{n_s} q, \]  
\( (3.17) \)
where the gauge-covariant three-dimensional lattice Laplace operator, $\Delta^{(2)}$, is defined as

$$\Delta^{(2)} q(x, t) = -\frac{1}{a^2} \sum_{j=1}^{3} \left( U_j(x, t) q(x + a\hat{j}, t) - 2q(x, t) + U_{-j}(x, t) q(x - a\hat{j}, t) \right).$$

(3.18)

Different levels of smearing were used for the the various flavors of quark, as presented in Table 3.4. For the present analysis, the smearings were applied to either all of the heavy quarks, or none of the heavy quarks with the light quarks always being smeared at the source and sink. This provides a basis of two interpolating operators for each state in question.

<table>
<thead>
<tr>
<th>Data set</th>
<th>$a r_S, n_S$ (light/strange)</th>
<th>$a r_S, n_S$ (charm)</th>
<th>$a r_S, n_S$ (bottom)</th>
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</thead>
<tbody>
<tr>
<td>$24^3 C53$</td>
<td>3.08, 30</td>
<td>2.12, 70</td>
<td>1.41, 10</td>
</tr>
<tr>
<td>$32^3$</td>
<td>3.08, 30</td>
<td>2.83, 70</td>
<td>1.89, 10</td>
</tr>
</tbody>
</table>

TABLE 3.4: Parameters used for the smearing of the quark fields in the baryon and meson interpolating operators.

Once the operators have been constructed, zero-momentum projected two point functions were calculated as:

$$C(t) = \sum_{\vec{x}} \langle O(\vec{x}, t + t_0) \bar{O}(\vec{x}_0, t + t_0) \rangle,$$

(3.19)

where the operator at the source and sink can either be smeared or unsmeared.
3.4 Mass extraction procedure

With a basis of two operators for each state in question, a matrix of correlation functions can be constructed as:

\[ C_{i,j}(t) \sim A_0^i (A_0^j)^* e^{-E_0 t} (1 + \mathcal{O}(e^{-\Delta E_1 t})) . \tag{3.20} \]

In order to reduce contamination from excited states and allow for fitting at earlier time ranges, we performed two exponential fits of the form:

\[ f_{i,j} \left( A_i, E_0, \tilde{E}, t \right) = \left( t \right) A_0^i (A_0^j)^* \left( e^{-E_0 t} + e^{-\tilde{E} t} \right) . \tag{3.21} \]

where the extracted energy \( \tilde{E} \) is understood to act as a bucket for excited state contamination and not to provide an accurate measure of the energy of the first excited state. The fits were performed by minimizing the function:

\[ F \left( A_i, E_0, \tilde{E} \right) = \left[ C_{i,j}(t) - f_{i,j} \left( A_i, E_0, \tilde{E}, t \right) \right] \times C_{i,j,k,l}^{-1}(t,t') \left[ C_{k,l}(t') - f_{k,l} \left( A_i, E_0, \tilde{E}, t' \right) \right] \tag{3.22} \]

with the observed covariance matrix calculated as:

\[ C_{i,j,k,l} (t,t') = \frac{1}{N-1} \left\langle C_{i,j} (t) - \langle C_{i,j} (t) \rangle_N \right\rangle_N \left\langle C_{k,l} (t') - \langle C_{k,l} (t') \rangle_N \right\rangle_N , \tag{3.23} \]

where \( N \) is the number of configurations and \( \langle \ldots \rangle_N \) represents the average over gauge field configurations of the enclosed quantity.
To facilitate the above process, first, single exponential fits were carried out, yielding an energy $E'_0$. This energy was then used as the initial guess for the ground state of the two exponential fit, helping to stabilize the fitting procedure. The fitting ranges were chosen such that $\chi^2/d.o.f. \leq 1$ with the minimum possible statistical uncertainty as estimated by the inverse of the covariance matrix. Furthermore, in anticipation of the eventual chiral extrapolation that would be performed, the fitting ranges for chiral partner states (e.g. $\Lambda, \Sigma, \Sigma^*$) were chosen to be as similar as possible. To aid in the choice of fitting range, effective mass plots were considered. The effective mass for a correlation function is given by:

$$m_{eff} \left( t + \frac{1}{2} \right) = \ln \frac{C(t)}{C(t + \frac{1}{2})}.$$  \hspace{1cm} \text{(3.24)}$$

The effective mass is a useful tool for determining when a correlation function has little ground state contamination as it will exhibit a plateau region when the correlation function is dominated by a single exponential. In Fig. 3.4 several example effective mass plots are shown for the $32^3, m_{sea} = m_{val} = 0.006$ ensemble.

The results of the fitting described above are presented in Tables 3.5 and 3.6.

The statistical uncertainty (arising from the fact that these quantities were calculated in a Monte Carlo simulation) was determined using a jackknife resampling procedure, where the correlation function for a each individual configuration is systematically removed and the fit redone on each reduced configuration population. The statistical uncertainty is then given by $\sqrt{N} \times \sigma$, where $\sigma$ is the variance of the energies obtained from the resampled population and $N$ is the number of configurations. To obtain an estimate of the systematic uncertainty associated with the choice of fitting window, the fitting window was shifted by one time slice and the fit performed again. The difference between this newly extracted mass and that of the original fit was taken to be the systematic uncertainty associated with the choice of
FIG. 3.1: Example effective mass plots for the $32^3$, $m_{sea} = m_{vol} = 0.006$ ensemble.
<table>
<thead>
<tr>
<th>State</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>A</th>
<th>F</th>
<th>G</th>
<th>H</th>
</tr>
</thead>
<tbody>
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<td>...</td>
<td>...</td>
<td>...</td>
<td>1.69142(59)(3)</td>
<td>1.69289(38)(36)</td>
<td>...</td>
<td>1.28212(44)(3)</td>
<td>1.28340(31)(23)</td>
</tr>
<tr>
<td>( J/\psi )</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>1.75306(56)(31)</td>
<td>1.75566(55)(29)</td>
<td>...</td>
<td>1.32889(70)(68)</td>
<td>1.32917(50)(22)</td>
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<td>...</td>
<td>...</td>
<td>...</td>
<td>0.24817(89)(11)</td>
<td>0.24873(35)(17)</td>
<td>...</td>
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<td>( \Upsilon )</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>0.28431(49)(38)</td>
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<td>...</td>
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<td>...</td>
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<td>1.4029(29)(30)</td>
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<td>1.463(20)</td>
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<td>0.8736(61)(31)</td>
<td>0.630(24)(25)</td>
<td>0.642(10)(1)</td>
<td>0.6661(64)(36)</td>
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<td>1.4550(28)(30)</td>
<td>1.4694(26)(11)</td>
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<td>1.0895(37)(32)</td>
<td>1.1021(21)(13)</td>
</tr>
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<td>1.5158(30)(46)</td>
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<td>1.5190(34)(48)</td>
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<td>1.1372(47)(15)</td>
<td>1.1405(43)(15)</td>
<td>1.1537(22)(17)</td>
</tr>
<tr>
<td>( \Xi_c^* )</td>
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<td>1.553(11)(5)</td>
<td>1.536(8)(20)</td>
<td>1.5608(43)(94)</td>
<td>1.5796(43)(19)</td>
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<td>0.873(34)(3)</td>
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<td>1.572(10)(6)</td>
<td>...</td>
<td>1.1859(31)(1)</td>
<td>1.1814(26)(48)</td>
</tr>
<tr>
<td>( \Omega_c^* )</td>
<td>...</td>
<td>...</td>
<td>1.578(6)(16)</td>
<td>1.6145(42)(11)</td>
<td>1.6233(42)(35)</td>
<td>...</td>
<td>1.2126(43)(36)</td>
<td>1.2108(44)(71)</td>
</tr>
</tbody>
</table>

Table 3.5: Extracted masses for each configuration presented in Table 3.1 for mesons and singly heavy baryons. Singly/doubly heavy states were fitted with two exponential functions. Here the first number in parenthesis is the statistical uncertainty, while the second is the systematic uncertainty determined by adjusting the choice of fitting window.
<table>
<thead>
<tr>
<th>State</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>F</th>
<th>G</th>
<th>H</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ξ_{cc}</td>
<td>2.0804(29)(10)</td>
<td>2.0804(39)(33)</td>
<td>...</td>
<td>2.084(3)(27)</td>
<td>2.0931(28)(16)</td>
<td>1.562(4)(12)</td>
<td>1.565(3)(12)</td>
</tr>
<tr>
<td>Ξ_{cc}'</td>
<td>2.131(38)(29)</td>
<td>2.1315(53)(4)</td>
<td>...</td>
<td>2.135(4)(41)</td>
<td>2.1465(29)(2)</td>
<td>1.5951(60)(68)</td>
<td>1.5999(53)(59)</td>
</tr>
<tr>
<td>Ξ_{cb}</td>
<td>1.4068(44)(22)</td>
<td>1.419(12)(1)</td>
<td>...</td>
<td>1.4125(72)(44)</td>
<td>1.412(13)(8)</td>
<td>1.0772(82)(39)</td>
<td>1.0768(74)(2)</td>
</tr>
<tr>
<td>Ξ_{cb}'</td>
<td>1.37(16)(7)</td>
<td>1.44(41)(1)</td>
<td>...</td>
<td>1.439(32)(1)</td>
<td>1.4386(99)(37)</td>
<td>1.088(10)(7)</td>
<td>1.0900(87)(60)</td>
</tr>
<tr>
<td>Ξ_{bb}</td>
<td>1.4482(77)(63)</td>
<td>1.450(5)(59)</td>
<td>...</td>
<td>1.452(5)(88)</td>
<td>1.4545(56)(45)</td>
<td>1.104(14)(2)</td>
<td>1.102(8)(11)</td>
</tr>
<tr>
<td>Ξ_{bb}'</td>
<td>0.7150(54)(22)</td>
<td>0.711(6)(70)</td>
<td>...</td>
<td>0.712(5)(85)</td>
<td>0.715(5)(11)</td>
<td>0.5739(80)(26)</td>
<td>0.5866(37)(56)</td>
</tr>
<tr>
<td>Ξ_{bb}</td>
<td>0.735(6)(55)</td>
<td>0.730(54)(57)</td>
<td>...</td>
<td>0.730(5)(88)</td>
<td>0.764(11)(1)</td>
<td>0.5851(94)(40)</td>
<td>0.6011(37)(72)</td>
</tr>
<tr>
<td>Ω_{cc}</td>
<td>...</td>
<td>2.1215(61)(27)</td>
<td>2.139(2)(18)</td>
<td>2.1391(18)(8)</td>
<td>...</td>
<td>1.6085(23)(11)</td>
<td>1.6133(56)(10)</td>
</tr>
<tr>
<td>Ω_{cc}'</td>
<td>...</td>
<td>2.1683(89)(20)</td>
<td>2.1854(25)(4)</td>
<td>2.1884(19)(2)</td>
<td>...</td>
<td>1.641(3)(18)</td>
<td>1.647(2)(17)</td>
</tr>
<tr>
<td>Ω_{cb}</td>
<td>...</td>
<td>1.4482(71)(47)</td>
<td>1.4639(30)(10)</td>
<td>1.4570(42)(71)</td>
<td>...</td>
<td>1.116(4)(24)</td>
<td>1.1265(28)(95)</td>
</tr>
<tr>
<td>Ω_{cb}'</td>
<td>...</td>
<td>1.4754(64)(75)</td>
<td>1.4836(30)(14)</td>
<td>1.479(3)(30)</td>
<td>...</td>
<td>1.133(32)(23)</td>
<td>1.144(2)(65)</td>
</tr>
<tr>
<td>Ω_{bb}</td>
<td>...</td>
<td>1.4932(75)(86)</td>
<td>1.500(62)(1)</td>
<td>1.495(79)(1)</td>
<td>...</td>
<td>1.145(73)(21)</td>
<td>1.1577(23)(69)</td>
</tr>
<tr>
<td>Ω_{bb}'</td>
<td>...</td>
<td>0.738(5)(15)</td>
<td>0.756(31)(1)</td>
<td>0.753(3)(18)</td>
<td>...</td>
<td>0.610(4)(14)</td>
<td>0.6121(34)(47)</td>
</tr>
<tr>
<td>Ω_{bb}</td>
<td>...</td>
<td>0.755(6)(21)</td>
<td>0.776(3)(24)</td>
<td>0.774(3)(24)</td>
<td>...</td>
<td>0.6263(45)(45)</td>
<td>0.6313(21)(34)</td>
</tr>
</tbody>
</table>

### Table 3.6: Extracted masses for each configuration presented in Table 3.1 for doubly and triply heavy baryons. Doubly heavy states were fitted with two exponential functions while triply heavy states were fitted with single exponential functions. Here the first number in parenthesis is the statistical uncertainty, while the second is the systematic uncertainty determined by adjusting the choice of fitting window.
3.5 Chiral and continuum extrapolations

As this spectroscopy calculation has been performed using several unphysical pion masses, in order to obtain a final result that is comparable to experimental results (as well as provide useful predictions for baryons that have yet to be observed) we must perform an extrapolation of our results to the physical pion mass. One complicating factor stems from the fact that the calculation was performed using partial quenching in the light quark sector in order to extend the range of pion masses beyond those offered by the set of gauge field configurations used. Because of this, the baryon masses in the current calculation (containing light valence quarks) are expected have a dependence on both the sea and valence quark masses. Although partial quenching is an unphysical tool utilized in lattice calculations to combat the computational expense of lowering the pion mass, theoretical tools are available to assist in performing extrapolations of partially quenched calculations in both the valence and sea sectors to the physical point. Partially quenched chiral perturbation theory (PQ\(\chi\)PT) [59] is an effective field theory in which the sea and valence quark masses are not constrained to have the same value. This is achieved by the introduction of (unphysical) bosonic ghost quark fields that contribute negatively to the mass of the sea quarks (see Section 1.5). An expansion in powers of the sea and valence quark masses is then performed for quantities of interest, allowing the sea and valence quark mass dependence can to be studied to a given order. Early applications [59] of partially quenched chiral perturbation theory in the analysis of lattice calculation results aimed at studying the effects of fully quenching one flavor of quarks while leaving others unquenched, a situation encountered in calculations where it was prohibitively expensive to include a second dynamical fermion mass in the generation of the gauge field ensembles. Successful applications of PQ\(\chi\)PT expressions in lattice calculations include the study of the dependence
on variations in the sea and valence quark masses of a variety of hadronic properties, such as electromagnetic properties [60] [61] [62], decay constants [63] [64] [65], and even generalized parton distributions [66] in addition to hadron masses [67] [68] [69] [70] [71] [72] As with $\chi$PT, PQ$\chi$PT has been extended to include symmetries associated with heavy quarks. Partially quenched heavy hadron chiral perturbation theory (PQ HH$\chi$PT) constructs the chiral Lagrangian to include heavy quark symmetries in both the infinite mass limit as well as the NRQCD framework which includes $O(1/m_Q)$ corrections. Expressions have been derived for the sea and valence mass dependence of singly [22] and doubly heavy [69] baryon masses, the latter relying on quark-diquark symmetry to relate the properties of singly heavy mesons to doubly heavy baryons. As the chiral expansion for SU(3) is thought to have poor convergence properties, we will allow our extrapolations to be guided by SU(2) HH PQ$\chi$PT. For singly heavy baryons, we extend existing expressions [22] for the baryon masses to include $O(1/m_Q)$ corrections, while for the doubly heavy sector, we use the expressions presented in Ref. [69]. To include finite volume effects that appear from performing the calculation in a finite sized box, we include corrections to the chiral functions taken from Ref. [73]

In addition to the light quark mass dependence, the dependence on the finite lattice spacing must be accounted for. In order to accomplish this, we parameterize the lattice spacing dependence with a coefficient $c_a$ for each of the chiral extrapolations, then set this parameter to zero in quoting our final results. Below we present the formulae used for our extrapolations, ordered by the heavy quark content of the states.
3.5.1 Singly heavy extrapolation formulae

For the singly heavy sector, we have baryons containing either a single bottom or single charm quark. As partially quenched expressions for the masses of these singly heavy baryons have previously only appeared in the literature in the $m_Q \to \infty$ limit (see Ref. [22]), the expressions used in the present work have been extended to include the effects of $\mathcal{O}(1/m_Q)$ corrections to the chiral Lagrangian. For the purposes of chiral extrapolations, we have three multiplets of states based on the strangeness content that will have different expressions for the light quark mass dependence. For the strangeness $S = 0$ sector, we have the $\{\Lambda_Q, \Sigma_Q, \Sigma_Q^*\}$ multiplet which is expected to exhibit the strongest leading order light quark mass dependence due to the existence of two light valence quarks in the interpolating operators.

The light pseudoscalar mass dependence for this multiplet is given by:

$$
\begin{bmatrix}
M_{\Lambda} \\
M_{\Sigma} \\
M_{\Sigma^*}
\end{bmatrix}
= M_0 + \begin{bmatrix}
0 \\
\Delta_{\Sigma,\Lambda} \\
\Delta_{\Sigma^*,\Lambda}
\end{bmatrix} + \frac{f^2}{8} \begin{bmatrix}
\hat{\lambda}_{\Lambda} \\
\hat{\lambda}_1 \\
\hat{\lambda}_1
\end{bmatrix} m_{\pi}^2 + \frac{f^2}{4} \begin{bmatrix}
\hat{\lambda}_4 \\
\hat{\lambda}_3 \\
\hat{\lambda}_2
\end{bmatrix} m_{\pi,\pi}^2 + \begin{bmatrix}
\bar{M}_{g_3,\Lambda}^{(3/2)} \\
\bar{M}_{g_3,\Sigma}^{(3/2)} \\
\bar{M}_{g_3,\Sigma^*}^{(3/2)}
\end{bmatrix} g_3^2 + \begin{bmatrix}
\tilde{M}_{g_2,\Sigma}^{(3/2)} \\
\tilde{M}_{g_2,\Sigma^*}^{(3/2)}
\end{bmatrix} g_2^2
$$

(3.25)

where the $\hat{\lambda}_i$ are the low energy constants (LECs) of the theory (normalized by the bare parameter $\lambda$ from the chiral Lagrangian) and the $\tilde{M}_{B,gi}$ are the parts of the loop contribution for baryon $B$ proportional to the coupling $g_i^2$ (with this coupling divided out). These terms along with the finite corrections are given in Appendices A.1 and A.3, respectively.

For the strangeness $S = 1$ sector, we expect the multiplet $\{\Xi_Q, \Xi_Q', \Xi_Q^*\}$ to have an additional leading order dependence on the valence sea quark mass, unconstrained.
between $S$ and $T$ baryons leading to two additional fit parameters. The light and strange pseudoscalar mass dependence is then given by:

$$
\begin{bmatrix}
M_\Xi \\
M_\Xi' \\
M_\Xi^{*}
\end{bmatrix}
= M_0 + \begin{bmatrix}
0 \\
\Delta_{\Xi';\Xi} \\
\Delta_{\Xi^{*};\Xi}
\end{bmatrix} + \frac{f^2}{8} \begin{bmatrix}
\frac{\bar{\lambda}_1}{2} \\
\bar{\lambda}_1
\end{bmatrix} m_{\pi,vv}^2 + \frac{f^2}{4} \begin{bmatrix}
\frac{\bar{\lambda}_2}{2} \\
\bar{\lambda}_2
\end{bmatrix} m_{\pi,ss}^2 + \frac{f^2}{4} \begin{bmatrix}
\frac{\bar{\lambda}_4}{2} \\
\bar{\lambda}_4
\end{bmatrix} m_{\pi,ss}^2
$$

$$(3.26)$$

As the values of $g_1$, $g_2$, $g_3$ have been previously determined in Ref. [74], it is useful to constrain their values while performing the chiral extrapolations in the interest of stabilizing the fits. This is accomplished by adding two additional constraint terms to the above formulae of the form: $(g - g_0)^2 / \sigma_g^2$. Here $g$ is the value of either $g_1$ or $g_2$ as determined in the aforementioned reference, and $\sigma_g$ is the width, determined by adding in quadrature to the statistical uncertainty of the $g_0$s a 10-30% width to account for $\mathcal{O}(1/m_Q)$ corrections\textsuperscript{1}. For the singly bottom states the width was chosen to be 10% while for the charm states the width was chosen to be 30%, as the infinite mass limit is a much better approximation for the bottom sector than the charmed. The constraining parameters and their associated widths are given in Table 3.8.

For singly heavy states containing two strange quarks, the leading order dependence is expected to come from the mass of the valence $\eta_s$. Additional higher order effects could enter at one loop order introducing a dependence on the sea pion mass as well. We therefore make the following ansatz in fitting the singly heavy states

\textsuperscript{1}It should be noted here that this reduces the effective number of degrees of freedom by 2
<table>
<thead>
<tr>
<th></th>
<th>$g_0$</th>
<th>$\sigma_g(Q = b)$</th>
<th>$\sigma_g(Q = c)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$g_2$</td>
<td>0.84</td>
<td>0.22</td>
<td>0.32</td>
</tr>
<tr>
<td>$g_3$</td>
<td>0.71</td>
<td>0.15</td>
<td>0.25</td>
</tr>
</tbody>
</table>

TABLE 3.7: Constraining parameters for singly heavy chiral extrapolations

<table>
<thead>
<tr>
<th></th>
<th>$g_0$</th>
<th>$\sigma_g(QQ = bb)$</th>
<th>$\sigma_g(QQ = cb)$</th>
<th>$\sigma_g(QQ = cc)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$g_1$</td>
<td>0.449</td>
<td>0.10</td>
<td>0.18</td>
<td>0.27</td>
</tr>
</tbody>
</table>

TABLE 3.8: Constraining parameters for doubly heavy chiral extrapolations

containing two strange quarks:

$$
\begin{bmatrix}
M_{\Omega} \\
M_{\Omega^2}
\end{bmatrix} = M_0 + \begin{bmatrix} 0 \\ \Delta^* \end{bmatrix} + C_n m_{\pi vv} + C_\pi m_{\pi ss}^2
$$

(3.27)

3.5.2 Doubly heavy extrapolation formulae

To guide our extrapolations for doubly heavy baryons with strangeness $S = 0$, we rely on SU(2) versions of the relations presented in Ref. [69]:

$$
\begin{bmatrix}
M_{\Xi} \\
M_{\Xi^*}
\end{bmatrix} = M_0 + \begin{bmatrix} -(1/2) \\ (1/4) \end{bmatrix} \Delta_H + \frac{f^2 \tilde{\sigma}}{2} m_{\pi vv}^2 - f^2 \tilde{\sigma}' m_{\pi ss}^2 + g_1 \begin{bmatrix} \tilde{M}^{(3/2)}_{\Xi QQ} \\
\tilde{M}^{(3/2)}_{\Xi^* QQ}
\end{bmatrix}
$$

(3.28)

Here $M_0$ is the chiral limit mass, $\Delta_H$ the chiral limit mass splitting, and $\tilde{\sigma}^{(r)}$ the LEC of the chiral theory (again normalized by the bare parameter $\lambda$ in the Lagrangian).

The chiral loop corrections $\tilde{M}^{(3/2)}_{\Xi QQ}$, $\tilde{M}^{(3/2)}_{\Xi^* QQ}$ are presented in Appendix A.2, with the finite volume corrections to these terms presented in Appendix A.3. Once again, we constrain the parameter $g_1$ with the value from Ref. [74] by adding a term of the form $(g - g_0)^2 / \sigma_g^2$. Again, the width is chosen to be dependent on the heavy quark content of the state, with slightly larger widths (from 20% - 60%) chosen than for the singly heavy states to account for quark diquark symmetry breaking effects.
These constraining parameters and their associated widths are presented in Table 3.8.

For doubly heavy states containing one strange quark, we assume the same dependence as in Eqn. 3.27.

3.5.3 Triply heavy extrapolation formulae

Triply heavy baryons contain no valence light or strange quarks, we obtain no additional information by varying the valence light and strange quark masses. Additionally, there is no reason to expect that any sea quark dependence from one loop contributions should enter in the same way to the various triply heavy states. This significantly reduces the number of data points available as input to the chiral extrapolations, as we perform individual fits for each of the triply heavy states. In light of this limitation, we make the ansatz that the triply heavy states will have only a lattice spacing dependence of the form:

\[ M_{\Omega^{(*)}_{qqq}} = M_0 + c_a a^2 \]  

(3.29)

3.5.4 Fitting procedure and results

In order to perform the chiral extrapolations, we make use of the formulae presented in the previous section. To each extrapolation formula we add a lattice spacing dependence of the form: \( c_a a^2 \), giving us a fit function \( f(\nu) \) dependent on a set of fit parameters here denoted by \( \nu \).
For the states of interest we construct the vector:

\[ \bar{\mathbf{y}} = \left[ \begin{array}{c} \bar{M}_1 \\ \bar{M}_2 \\ \vdots \end{array} \right] - N_c \bar{M}_c - N_b \bar{M}_b, \]  

(3.30)

where the bar denotes the average over jackknife ensembles, and the values \( \bar{M}_{c,b} \) are the spin averaged masses of the doubly heavy meson states, and \( N_{c,b} \) are the number of charmed and bottom quarks in the state in question. This subtraction is carried out in order to reduce any residual \( \mathcal{O} ((amg)^n) \) error from the tuning of the charmed quark mass, as well as to remove the energy shift introduced by the use of NRQCD for the bottom sector. It should be noted here that the masses in \( \bar{\mathbf{y}} \) have been converted to physical units by multiplying by the inverse lattice spacing. The covariance matrix \( \tilde{\mathcal{C}} \) is then calculated, with the covariances between different gauge field ensembles set identically to zero. In order to include the statistical uncertainty associated with the determination of the lattice spacing, we augment the covariance matrix by adding the lattice spacing uncertainty in quadrature with the covariance:

\[ \tilde{\mathcal{C}} (M_1, M_2) = \mathcal{C} (M_1, M_2) + \bar{M}_1 \bar{M}_2 \frac{(e_{a-1})^2}{(a^{-1})^2} \]  

(3.31)

We then numerically determine the values of the fit parameters \( \{\mathbf{\nu}^0\} \) that minimize the function:

\[ \chi^2 \equiv [\bar{\mathbf{y}} - f(\mathbf{\nu})]' \tilde{\mathcal{C}}^{-1} [\bar{\mathbf{y}} - f(\mathbf{\nu})] \]  

(3.32)

The uncertainty on the fit parameters are determined from the inverse of the covariance matrix (over jackknife ensembles), as are the uncertainties for the extrapolated masses themselves. An estimate of the systematic uncertainty associated with the
choice of fitting window was obtained by moving the fitting window by one time slice for all states and then performing the extrapolation again for this new fitting range. In order to facilitate this process, covariant fits were not used in these additional extrapolations. The difference in these new results with the original extrapolation was then taken to be the systematic uncertainty. In evaluating the goodness of the fit, we use both \( \chi^2/d.o.f. \) as well as the quality of fit \( Q(\chi^2, d.o.f.) \), which provides a measure of the probability of obtaining a given \( \chi^2 \) from a fit with a fixed number of degrees of freedom.

The fitted parameters for these extrapolations are presented in Tables 3.9, 3.10, 3.11, 3.12, and the extrapolated masses presented in Tables 3.13, 3.14. An example of the chiral extrapolation for the singly charmed sector is presented in Fig. 3.5.4.

TABLE 3.9: Fit parameters for singly heavy extrapolations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>{\Lambda_c, \Sigma_c, \Sigma_c^*}</th>
<th>{\Xi_c, \Xi_c', \Xi_c^*}</th>
<th>{\Lambda_b, \Sigma_b, \Sigma_b^*}</th>
<th>{\Xi_b, \Xi_b', \Xi_b^*}</th>
</tr>
</thead>
<tbody>
<tr>
<td>( M_0 ) (MeV)</td>
<td>664(73)</td>
<td>753(45)</td>
<td>286(63)</td>
<td>1089(82)</td>
</tr>
<tr>
<td>( \Delta_{\Sigma,\Lambda} ) (MeV)</td>
<td>288(59)</td>
<td>157(44)</td>
<td>256(47)</td>
<td>265(74)</td>
</tr>
<tr>
<td>( \Delta_{\Sigma^*,\Lambda} ) (MeV)</td>
<td>368(56)</td>
<td>231(44)</td>
<td>265(74)</td>
<td>296(75)</td>
</tr>
<tr>
<td>( (\tilde{\lambda}_3 f^2) ) (MeV)(^{-2} \times 10^{-3} )</td>
<td>1.87(76)</td>
<td>0.45(13)</td>
<td>1.94(55)</td>
<td>0.21(19)</td>
</tr>
<tr>
<td>( (\tilde{\lambda}_1 f^2) ) (MeV)(^{-2} \times 10^{-4} )</td>
<td>-0.9(2.1)</td>
<td>1.6(7)</td>
<td>3.3(1.8)</td>
<td>-7.0(2.9)</td>
</tr>
<tr>
<td>( (\tilde{\lambda}_4 f^2) ) (MeV)(^{-2} \times 10^{-4} )</td>
<td>4.6(3.0)</td>
<td>2.1(2.0)</td>
<td>4.2(2.7)</td>
<td>2.0(3.4)</td>
</tr>
<tr>
<td>( (\tilde{\lambda}_2 f^2) ) (MeV)(^{-2} \times 10^{-4} )</td>
<td>1.6(2.1)</td>
<td>0.2(1.8)</td>
<td>1.2(2.2)</td>
<td>6.1(3.3)</td>
</tr>
<tr>
<td>( C_s^S ) (MeV)(^{-1} \times 10^{-4} )</td>
<td>N/A</td>
<td>3.3(5)</td>
<td>N/A</td>
<td>0.78(86)</td>
</tr>
<tr>
<td>( C_{\eta_s}^T ) (MeV)(^{-1} \times 10^{-4} )</td>
<td>N/A</td>
<td>3.0(7)</td>
<td>N/A</td>
<td>-2.3(1.2)</td>
</tr>
<tr>
<td>( g_3 )</td>
<td>0.72(0.22)</td>
<td>0.75(0.24)</td>
<td>0.70(0.15)</td>
<td>0.71(0.15)</td>
</tr>
<tr>
<td>( g_2 )</td>
<td>0.72(0.31)</td>
<td>0.80(0.32)</td>
<td>0.83(0.22)</td>
<td>0.84(0.22)</td>
</tr>
<tr>
<td>( c_a ) (MeV)(^3 \times 10^3 )</td>
<td>3.5(3.7)</td>
<td>2.8(3.9)</td>
<td>2.6(4.8)</td>
<td>-1.0(4.9)</td>
</tr>
<tr>
<td>( \chi^2/d.o.f. )</td>
<td>1.2</td>
<td>0.45</td>
<td>1.0</td>
<td>0.81</td>
</tr>
<tr>
<td>( Q )</td>
<td>0.31</td>
<td>0.91</td>
<td>0.41</td>
<td>0.62</td>
</tr>
</tbody>
</table>
TABLE 3.10: Fit parameters for doubly heavy extrapolations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$\Omega_{cc}^{(*)}$</th>
<th>$\Omega_{cb}^{(*)}$</th>
<th>$\Omega_{bb}^{(*)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$M_0$ (MeV)</td>
<td>675(42)</td>
<td>739(33)</td>
<td>583(25)</td>
</tr>
<tr>
<td>$\Delta_H$ (MeV)</td>
<td>39(7)</td>
<td>41(4)</td>
<td>117(4)</td>
</tr>
<tr>
<td>$(\sigma f^2)$ (MeV)$^{-2} \times 10^{-4}$</td>
<td>-1.1(1.2)</td>
<td>-1.4(1.1)</td>
<td>-1.3(7)</td>
</tr>
<tr>
<td>$(\sigma' f^2)$ (MeV)$^{-2} \times 10^{-4}$</td>
<td>-1.8(1.7)</td>
<td>-1.4(1.5)</td>
<td>-1.4(1.2)</td>
</tr>
<tr>
<td>$g_1$</td>
<td>0.36(0.13)</td>
<td>0.47(9)</td>
<td>0.24(9)</td>
</tr>
<tr>
<td>$c_a$ (MeV)$^3 \times 10^3$</td>
<td>4.4(3.8)</td>
<td>8.9(3.8)</td>
<td>3.6(2.4)</td>
</tr>
<tr>
<td>$\chi^2/d.o.f.$</td>
<td>0.61</td>
<td>1.39</td>
<td>0.75</td>
</tr>
<tr>
<td>$Q$</td>
<td>0.83</td>
<td>0.20</td>
<td></td>
</tr>
</tbody>
</table>

TABLE 3.11: Fit parameters for doubly heavy extrapolations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$\Omega_{ccc}$</th>
<th>$\Omega_{ccb}$</th>
<th>$\Omega_{cc}^{*}$</th>
<th>$\Omega_{cb}$</th>
<th>$\Omega_{bb}$</th>
<th>$\Omega_{bb}^{*}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$M_0$ (MeV)</td>
<td>200(10)</td>
<td>222(12)</td>
<td>200(9)</td>
<td>228(11)</td>
<td>206(10)</td>
<td></td>
</tr>
<tr>
<td>$c_a$ (MeV)$^3 \times 10^3$</td>
<td>2.8(1.1)</td>
<td>3.4(1.2)</td>
<td>1.5(1.0)</td>
<td>2.0(1.1)</td>
<td>-0.2(1.1)</td>
<td></td>
</tr>
<tr>
<td>$\chi^2/d.o.f.$</td>
<td>0.3</td>
<td>0.01</td>
<td>0.3</td>
<td>0.05</td>
<td>0.43</td>
<td>0.03</td>
</tr>
<tr>
<td>$Q$</td>
<td>0.90</td>
<td>0.62</td>
<td>0.83</td>
<td>0.51</td>
<td>0.85</td>
<td></td>
</tr>
</tbody>
</table>

TABLE 3.12: Fit parameters for triply heavy extrapolations.

<table>
<thead>
<tr>
<th>Baryon</th>
<th>Lattice (GeV)</th>
<th>Expt. (GeV)</th>
<th>Baryon</th>
<th>Lattice (GeV)</th>
<th>Expt. (GeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Lambda_c$</td>
<td>2.269(44)(24)</td>
<td>2.286</td>
<td>$\Lambda_b$</td>
<td>5.607(51)(29)</td>
<td>5.619</td>
</tr>
<tr>
<td>$\Sigma_c$</td>
<td>2.494(36)(14)</td>
<td>2.454</td>
<td>$\Sigma_b$</td>
<td>5.818(48)(32)</td>
<td>5.811</td>
</tr>
<tr>
<td>$\Sigma^*$</td>
<td>2.569(40)(20)</td>
<td>2.518</td>
<td>$\Sigma_b^*$</td>
<td>5.826(49)(39)</td>
<td>5.832</td>
</tr>
<tr>
<td>$\Xi_c$</td>
<td>2.462(34)(13)</td>
<td>2.467</td>
<td>$\Xi_b$</td>
<td>5.860(61)(11)</td>
<td>5.791</td>
</tr>
<tr>
<td>$\Xi_c^*$</td>
<td>2.595(37)(96)</td>
<td>2.575</td>
<td>$\Xi_b^*$</td>
<td>5.978(53)(10)</td>
<td>-</td>
</tr>
<tr>
<td>$\Omega_c$</td>
<td>2.667(38)(24)</td>
<td>2.645</td>
<td>$\Omega_b$</td>
<td>6.008(53)(19)</td>
<td>-</td>
</tr>
<tr>
<td>$\Omega_c^*$</td>
<td>2.690(41)(16)</td>
<td>2.685</td>
<td>$\Omega_b^*$</td>
<td>6.066(50)(4)</td>
<td>6.071</td>
</tr>
</tbody>
</table>

TABLE 3.13: Extrapolated masses for singly heavy states. The first number in parenthesis is the estimated statistical uncertainty, and the second is the estimated systematic uncertainty due to the choice of fitting window.
<table>
<thead>
<tr>
<th>Baryon</th>
<th>Lattice (GeV)</th>
<th>Baryon</th>
<th>Lattice (GeV)</th>
<th>Baryon</th>
<th>Lattice (GeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Xi_{cc}$</td>
<td>3.600(22)(27)</td>
<td>$\Xi_{cb}$</td>
<td>6.919(38)(23)</td>
<td>$\Xi_{bb}$</td>
<td>10.167(31)(80)</td>
</tr>
<tr>
<td>$\Xi^*_{cc}$</td>
<td>3.688(23)(27)</td>
<td>$\Xi^*_{cb}$</td>
<td>6.949(39)(4)</td>
<td>$\Xi^*_{bb}$</td>
<td>10.199(31)(65)</td>
</tr>
<tr>
<td>$\Omega_{cc}$</td>
<td>3.703(24)(21)</td>
<td>$\Omega_{cb}$</td>
<td>7.082(45)(78)</td>
<td>$\Omega_{bb}$</td>
<td>10.230(30)(23)</td>
</tr>
<tr>
<td>$\Omega^*_{cc}$</td>
<td>3.787(23)(27)</td>
<td>$\Omega^*_{cb}$</td>
<td>7.113(46)(46)</td>
<td>$\Omega^*_{bb}$</td>
<td>10.268(30)(20)</td>
</tr>
<tr>
<td>$\Omega_{ccc}$</td>
<td>4.794(9)</td>
<td>$\Omega_{ccb}$</td>
<td>7.989(11)</td>
<td>$\Omega^*_{ccb}$</td>
<td>8.012(12)</td>
</tr>
<tr>
<td>$\Omega_{cbb}$</td>
<td>11.177(9)</td>
<td>$\Omega^*_{cbb}$</td>
<td>11.206(11)</td>
<td>$\Omega^*_{cbb}$</td>
<td>14.370(10)</td>
</tr>
</tbody>
</table>

TABLE 3.14: Extrapolated masses for doubly and triply heavy states. The first number in parenthesis is the estimated statistical uncertainty, and the second is the estimated systematic uncertainty due to the choice of fitting window.

FIG. 3.2: Example of chiral/continuum extrapolations for singly charmed states. The different line types represent the extrapolation evaluated at coarse and fine lattice spacings and the continuum limit represented by dashed, dotted and solid lines respectively (with green, blue and orange error bands respectively). Circles and squares represent fine and coarse lattice results respectively.
CHAPTER 4

Heavy Flavor Interactions and
Four Quark States from the Lattice

The calculation of hadronic forces from first principles allows insight into how interactions of the fundamental quark and gluonic degrees of freedom manifest themselves at the hadronic level. Lattice QCD is an excellent tool for calculating hadronic observables in the low energy regime. Although lattice calculations in Euclidean space are not well suited for the study of real-time scattering processes, two methods can be used to extract interaction information from the lattice. Lüscher’s method [75], which was briefly discussed in Section 2.5, relates the elastic scattering phase shift of a two particle system in a finite periodic box with the energy levels of the system. An alternate method, used in the present work, extracts the interaction energy as a function of hadron separation. This method is only applicable for systems of hadrons containing more than one heavy quarks which can be treated in the static approximation providing a definite spatial position for the hadrons.
Phenomenologically, two heavy-light meson systems (which we will denote as HLHL) have become interesting in the study of tetraquark bound states \cite{76} \cite{77} \cite{78}. It has long been known that the binding of a $Q\bar{Q}qq$ (with $q = u, d$) system increases with the mass ratio of the heavy to light quark flavours \cite{79}, thus $c\bar{c}qq$ and $b\bar{b}qq$ systems are excellent candidates in the search for exotic four quark bound states. In Ref. \cite{78} a distinction was made between two types of tetraquark bound states: molecular, in which the four quarks exhibit a single physical two-meson (singlet-singlet) component, and the more exotic compact bound states. The latter would involve a complicated color space structure in which quark pairs form color vectors which then combine to form a colorless four quark state \cite{78}. In spite of this complicated color structure, compact bound states can be interpreted as a mixture of various two meson (color singlet) components \cite{80}. The expected features that would characterize a molecular bound state would be a small binding energy and a bound state RMS radius greater than that of the sum of the two particle sizes, i.e.:

$$\Delta R \equiv \frac{RMS_{4q}}{RMS_{M_1} + RMS_{M_2}} > 1$$

A compact state, on the other hand, would be more tightly bound and have a smaller RMS radius than the molecular state. In Ref. \cite{81} doubly heavy four quark states were modeled as hadronic molecules interacting via a meson exchange potential. Several of the doubly bottom bound states were found to be deeply bound and spatially compact, making them excellent candidates for tetraquark bound states. It is with these ideas in mind that we may begin to search for the signature of compact bound states on the lattice.

Lattice calculations of the interaction potential of the heavy-light heavy-light system were first performed over 20 years ago (see eg. Ref. \cite{82}), however only recently have these simulations included fully dynamical fermions for the light up and
down quarks [83, 84, 85, 86]. The study of tetraquark states from lattice calculations had remained unexplored until only recently with Ref [85] hinting at the possibility of a bound tetraquark state in one heavy-light heavy-light channel that exhibits a particularly wide and deep potential well when compared with other channels. In Ref. [86] this particular channel was investigated further by fitting lattice potentials with a simple potential model and numerically solving the two body Schrödinger equation to extract a binding energy\(^1\). In the present work we perform a calculation similar to ([85], [86]) using the anisotropic clover Wilson action for the light quarks. Using a highly constrained phenomenological potential model, we then present a quantitative determination of a bound state energy in the HLHL system.

An inherent difficulty in making comparisons between theoretical models and lattice calculations performed in the static limit stems from the omission of the heavy quark spin in the static limit. As \(m_H \to \infty\), the integer valued \((J = 0, 1)\) angular momentum eigenstates of a single heavy light meson map onto a single static limit eigenstate with \(J = 1/2\). The energies of the non-static angular momentum eigenstates also converge to a single energy corresponding to the \(J = 1/2\) eigenstate. Although the two spaces map onto each other, there is not a simple one to one correspondence between static limit eigenstates and their non-static counterparts, and care must be taken in making identifications between the two spaces. Previous lattice studies of HLHL interaction energy ([82], [87] for example) performed in the quenched approximation and included uncontrolled systematic errors because of this. Recently dynamical quarks have been used to calculate the HLHL interaction energy using a complete set of quantum numbers which exploits the full set of symmetries of the HLHL system [88].

\(^1\)The recent work of Ref. [86] appeared as a preprint while this manuscript was at its final stages of preparation.
4.1 Background

4.1.1 Heavy-Light states

The quark model view of a heavy-light meson is of a heavy anti-quark $\bar{Q}$ coupled to a light quark $q$. The relevant quantum numbers to describe such a state are total angular momentum $J$ and its projection along some axis (here arbitrarily chosen to be $\hat{z}$) $J_z$, and the parity $P_i$ as well as the relevant flavor quantum numbers. For our interests, we choose $\bar{Q} = \bar{b}$ and $q = \{u, d\}$. Therefore all states then have bottomness $b = +1$, and are otherwise classified by total isospin and the third component of isospin $(I, I_z) = (1/2, \pm 1/2)$. Throughout this work, we make the assumption that we fit our correlation functions with a sufficiently large $t_{\text{min}}$ such that contributions from excited states have died out and we extract only the ground state energy. Furthermore, we assume that states with non-zero orbital angular momentum $L$ are at sufficiently high energies as to have a negligible contribution to the ground state energies which we extract. We are then free to speak of the spin and total angular momentum interchangeably.

In heavy quark effective theory, spin dependent contributions enter into the heavy quark action at order $1/m_H$, and in the static limit ($m_H \to \infty$) the heavy quark acts as a static color source. This means that the spin of the HL meson comes only from the light degrees of freedom. Because of this, the physical HL meson states with $J = (0, 1)$ become degenerate in the static limit, with both represented by a single $J = 1/2$ state. The relevant angular momentum classification is then $(J, J_z) = (1/2, \pm 1/2)$. With the above flavor assignments, the lowest energy excitations of the B spectrum with $J^P = \{0, 1\}^-$ (coupling to the static $J^P = 1/2^-$ B) are $B_{0,\pm}$ and $B^*$, and for $J^P = \{0, 1\}^+$ (coupling to the static $J^P = 1/2^+ B_1$), the ground state $B_1(5721)^0$ (neglecting excited states).
4.1.2 Heavy-Light Heavy-Light states

When constructing states with a pair of HL mesons, care must be taken in determining a relevant set of quantum numbers that fully exploit the symmetries of the problem. The flavor quantum numbers for a Heavy-Light Heavy-Light (HLHL) system are straightforward, and for a $\bar{Q}q\bar{Q}q$ (with $q = \{u, d\}$) there are two isospin combinations, an isospin triplet with $I = 1$ and an $I = 0$ singlet. For a HLHL pair separated by a vector $\vec{r}$ the rotational symmetry is broken to rotations around the separation axis. Total angular momentum $J$ is therefore no longer a conserved quantity, though its projection along the axis of separation (arbitrarily taken to be $z$) is still conserved. The system will also be symmetric or antisymmetric under parity as well as reflections through a plane containing the separation axis, which we shall call $P_\perp$. This last transformation can be accomplished by a parity transformation followed by a rotation of $\pi$ about an axis perpendicular to the reflection plane. States with $J_z = \pm 1$ are not invariant under this transformation (being mapped onto each other), but their average is an eigenstate of $P_\perp$. Lastly we choose to classify HLHL states by intrinsic parity $P_i$, defined to be the product of the intrinsic parities of the two light quarks, and (full) parity $P$, defined as the product of the intrinsic parity transformation and coordinate inversion of the two particle spatial wavefunction. We will use both parity quantum numbers in our classification of states.

4.2 Methodology

4.2.1 HL and HLHL interpolating fields

A general interpolating operator coupling to a single heavy-light state is given by:

$$\mathcal{O}_{HL}(\vec{x}) = \bar{\Phi}(\vec{x}) \Gamma q(\vec{x})$$

(4.1)
with $\Gamma$ chosen to achieve the desired angular momentum and parity quantum numbers. For pseudoscalar HL states, $\Gamma = \gamma_5, \gamma_i$ (with $i = 1, 2, 3$), corresponding to a particle in the static limit with $J^P = 1/2^-$, which we will refer to simply as $B$. $J = 1$ meson states with $\Gamma = 1, \gamma_i\gamma_5$ correspond to a state with $J^P = 1/2^+$, which we shall refer to as $B_1$. We make the choice $\Gamma = \gamma_5$ for $O_B$ and $\Gamma = 1$ for $O_{B_1}$. As it will be useful in the analysis of HLHL states, it should be noted that for these choices of $\Gamma$, correlation functions constructed from $O_B$ interpolating fields will consist of only upper (positive parity) components in the Dirac basis of the light quarks while those constructed from $O_{B_1}$ will consist of only lower (negative parity) components. This is explicitly shown in Appendix A.4. The states are classified by the additional flavor quantum numbers $(I, I_z) = (1, \pm 1)$ for $q = \{u, d\}$.

For HLHL states, we want to create states with definite $(I, I_z, |J_z|, P, P_i)$ and displacement $\vec{r}$ at the source and sink. To do this, we want to couple only our light quarks in spinor space to specify the quantum numbers of the state while allowing the heavy quarks to act only as color sources. Our general HLHL operator is then given by:

$$O^{(I, I_z, |J_z|, P, P_i)}_{HLHL}(\vec{x}, \vec{r}) = \bar{Q}(\vec{x}, t)Q(\vec{x} + \vec{r}, t) \times [q(\vec{x}, t)q(\vec{x} + \vec{r}, t)]_{(I, I_z, |J_z|, P, P_i)}$$

(4.2)

where the light quark wavefunctions $[q(\vec{x}, t)q(\vec{x} + \vec{r}, t)]$ are combined in such a way as to achieve the set of quantum numbers $(I, I_z, |J_z|, P, P_i)$ of the system. The explicit construction of these wavefunctions is described in Appendix A.5. For simplicity we restrict ourselves to identical source and sink interpolating fields neglecting any cross correlators between states. Isospin is a good quantum number on the $2 + 1$ flavor lattices with which we work, and we choose our interpolating fields to be isospin eigenstates with $(I, I_z) = (1, 1)$ and $(I, I_z) = (0, 0)$. At large spatial
separations, we expect the energy of the four quark state to asymptotically approach the energy of its dominant two meson component\(^2\). States with \(p_1 = -1\) will tend towards the energy of a \(BB_1\) combination at large spatial separations. There are two possible combinations of the light quark parities that yield \(p_1 = +1\): \((p_1, p_2) = (+, +), (-, -)\). In light of the above discussion of parity content of single HL states, we project our \(P_1 = +1\) interpolating fields to contain only negative or positive parity spinor components and retain these as distinct interpolating fields. The expectation is that interpolating fields constructed from lower spinor components will exhibit a significantly higher ground state energy in relation to those constructed from upper components. The reason for this is that the \((-,-)\) interpolating field are constructed by the product of two \(B_1\) meson interpolating fields, thus should exhibit an asymptotic energy (as \(r \to \infty\)) near twice that of the single \(B_1\) energy. Similarly the \((+, +)\) interpolating field is constructed from the product of two \(B\) meson interpolating fields tending asymptotically as \(r \to \infty\) towards a ground state energy of twice that of a single \(B\) meson. We differentiate all interpolating fields by their dominant asymptotic content in the tabulation of interpolating fields in Table ??.

4.3 Details of the lattice calculation

We work with colorwave propagators (described below) calculated on \(n_f = 2 + 1\) anisotropic \((24^3 \times 128)\) lattices generated by the Hadron Spectrum Collaboration [89] with a pion mass of roughly 380 MeV. The fermion action used was the clover Wilson action with stout link smearing, not smeared in the temporal direction. The gauge action was Symanzik tree level tadpole-improved without a rectangle in the

\(^2\)Here we are referring to the dominant lowest energy contribution, as we expect excited states to contribute negligibly to the extracted HLHL ground state energies.
TABLE 4.1: HLHL interpolating operator basis and expected asymptotic values

<table>
<thead>
<tr>
<th>((I, I_1, J_2, P_1, P, P_i))</th>
<th>((I, I_2, J_2, P_1, P, P_i))</th>
<th>Dominant asymptotic content</th>
</tr>
</thead>
<tbody>
<tr>
<td>((1,1,1,-,-,+))</td>
<td>((0,0,1,-,+,+))</td>
<td>(BB)</td>
</tr>
<tr>
<td>((1,1,0,-,-,+)</td>
<td>((0,0,0,-,+,+))</td>
<td>(BB)</td>
</tr>
<tr>
<td>((1,1,0,+,+,+))</td>
<td>((0,0,0,+,+,+))</td>
<td>(BB)</td>
</tr>
<tr>
<td>((1,1,1,-,-,+))</td>
<td>((0,0,1,-,+,+))</td>
<td>(B_1 B_1)</td>
</tr>
<tr>
<td>((1,1,0,-,-,+))</td>
<td>((0,0,0,-,+,+))</td>
<td>(B_1 B_1)</td>
</tr>
<tr>
<td>((1,1,0,+,+,+))</td>
<td>((0,0,0,+,+,+))</td>
<td>(B_1 B_1)</td>
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<td>(B_1 B_1)</td>
</tr>
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<td>(B_1 B_1)</td>
</tr>
<tr>
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<td>(B_1 B_1)</td>
</tr>
<tr>
<td>((1,1,0,-,-,-))</td>
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<td>(B_1 B_1)</td>
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<td>(B_1 B_1)</td>
</tr>
<tr>
<td>((1,1,0,-,-,-))</td>
<td>((0,0,0,+,+,+))</td>
<td>(B_1 B_1)</td>
</tr>
</tbody>
</table>

4.4 Colorwaves for HL systems

The use of Colorwave propagators allows us to implement spatial smearing at the source and sink of our correlation functions. In the limit where all momenta are summed over in equation 2.131, all to all point-point propagators are recovered. However, introducing a maximum momentum cutoff \(p_{\text{cut}}^2\) we are able to introduce and control the effective amount of spatial smearing\(^3\). The effect of restricting

\(^3\)It should be noted that smearing is achieved only in fixed gauge. In our case we use the Coulomb gauge, which is a smooth gauge allowing to project out high energy modes if the cutoff
the plane wave basis to $|p|^2 \leq p_{cut}^2$ (summing over a momentum space volume) is illustrated in Fig. 4.1 where effective masses for single HL $B$ meson correlation functions\(^4\) are presented. It’s evident that the noise of the signal decreases by increasing the momentum space cutoff (as this increases the statistics contributing to the correlation function).

Each effective mass plateau appears to begin at roughly the same point independent of $p_{cut}^2$, and thus a common fit range of $17 - 30$ was chosen for all values of $p_{cut}^2$. In Fig. 4.1 we can see that as $p_{cut}^2$ increases the overlap with excited states drops resulting lower values for the effective mass at earlier times. This indicates that a small radial smearing of the quarks field results interpolating fields that have better overlap with the ground state of the system. Such behavior is likely due to the fact that the a non-relativistic HL meson in the static limit is a highly localized object whose wavefunction is confined to a small spatial region.

In light of this behavior and in order to reduce computational cost associated with increasing the momentum cutoff, a value of $p_{cut}^2 = 1$ was chosen for calculations of the HLHL system.

\(^{\text{p}}\)\(^{\text{cut}}\) is kept small. However, no gauge dependence is introduced to our correlation functions as they are gauge invariant by construction.

\(^{\text{4}}\)These HL correlation functions are defined in Appendix A.4, eq. A.15.
4.5 HLHL states with colorwaves

We begin with a correlation function for two heavy-light mesons separated by \( \vec{r} \) as described above:

\[
C_{HLHL}(t, \vec{r}) = \sum_x \langle O_{HLHL}(\vec{x}, \vec{r}, t) O_{HLHL}^\dagger(\vec{x}, \vec{r}, t_0) \rangle
\]

\[
= \sum_x \langle \bar{Q}(\vec{x}, t) \bar{Q}(\vec{x} + \vec{r}, t) q(\vec{x}, t) q(\vec{x} + \vec{r}, t) \rangle
\]

\[
q(\vec{x} + \vec{r}, t_0) q(\vec{x}, t_0) Q(\vec{x} + \vec{r}, t_0) Q(\vec{x}, t_0) \rangle
\]

Each heavy quark source can only be contracted with the sink at the same spatial location, and upon contraction we work only with the Wilson line portion of the heavy quark propagator, as we want the quantum numbers of the system to be determined entirely by the light degrees of freedom. There are two possible light quark contractions, one where the light quarks contract with source and sink at the same spatial location (direct), and one where the light quarks contract at the other spatial location (crossed). Performing these contractions, we have (omitting the overall color trace):

\[
C_{HLHL}(t, \vec{r}) = \sum_x \gamma_5 W^\dagger(\vec{x}; t, t_0) \gamma_5 \gamma_5 W^\dagger(\vec{x} + \vec{r}; t, t_0) \gamma_5
\]

\[
\times \text{tr}_d \left[ S(\vec{x} + \vec{r}; t; \vec{x} + \vec{r}, t_0) S(\vec{x}, t; \vec{x}, t_0) -
S(\vec{x} + \vec{r}, t; \vec{x}, t_0) S(\vec{x}, t; \vec{x} + \vec{r}, t_0) \right]
\]

Here, \( \text{tr}_d \) denotes the trace over Dirac space spinor indices and \( W \) is the Wilson line

\[
W(\vec{x}; t, t_0) = \prod_{t'=t_0}^t U_4^\dagger(\vec{x}, t')
\]
We now introduce our partially fourier transformed light quark propagators as:

$$S(x',t; x_1, t_0) = \sum_{p_1', p_1} e^{ip_1' x_1'} S(p_1', t; p_1, t_0) e^{-ip_1 x_1}$$

(4.6)

where sums over momenta $p_i$ have been restricted to $|p^2| \leq 1$ as described in the previous section.

Using this, the above correlator can be rewritten as:

$$C_{HLHL}(t, \tau) = \sum_{p_1 p_1' p_2 p_2'} \sum_{x} \gamma_5 W_{\uparrow}(\vec{x}; t, t_0) \gamma_5 \gamma_5 W_{\uparrow}(\vec{x} + \vec{\tau}; t, t_0) \gamma_5$$

$$\times e^{i(p_1' - p_1 + p_2' - p_2) x} e^{i(p_2' - p_2) \tau}$$

$$\times [S(p_2', t; p_2, t_0) S(p_1', t; p_1, t_0) -$$

$$S(p_2', t; p_1, t_0) S(p_1', t; p_2, t_0)]$$

(4.7)

Defining

$$D(\vec{\tau}, t, t_0, \omega) \equiv \sum_{x} \gamma_5 W_{\uparrow}(\vec{x}; t, t_0) \gamma_5 \gamma_5 W_{\uparrow}(\vec{x} + \vec{\tau}; t, t_0) \gamma_5 e^{i(\omega) x}$$

(4.8)

with $\omega \equiv p_1' - p_1 + p_2' - p_2$, our the final form of our HLHL correlation function becomes:

$$C_{HLHL}(t, \tau) = \sum_{p_1 p_1' p_2 p_2'} D(\vec{\tau}, t, t_0, \omega) \times e^{i(p_2' - p_2) \tau}$$

$$\times [S(p_2', t; p_2, t_0) S(p_1', t; p_1, t_0) -$$

$$S(p_2', t; p_1, t_0) S(p_1', t; p_2, t_0)]$$

(4.9)

With this method, we calculate the costly $D(\vec{\tau}, t, t_0, \omega)$ first using a parallel code (parallelization over space time) and then perform the far less expensive con-
tractions with the colorwave propagators for our complete operator basis on a scalar workstation class machine.

4.6 HLHL results

For \( q = \{ u, d \} \) we have 24 unique HLHL corresponding to the operators enumerated in Table ??, each potential curve is calculated by taking the jackknife difference between the energy of the HLHL state for various \( \tilde{r}' \) and the energy of the expected two meson asymptotic state:

\[
V (\tilde{r}') = E_{HLHL} (\tilde{r}') - E_{B_{(1)}} - E_{B_{(1)}}
\]  

(4.10)

The statistical uncertainty for each point is determined from jackknife statistical analysis. The systematic uncertainties are determined by adjusting the chosen fit range by one time slice in each direction and averaging the observed deviations in the energy. The systematic uncertainty for both \( E_{HLHL} \) and \( E_{B_{(1)}} \) are determined independently and then added in quadrature to determine the systematic uncertainty on \( V (r) \).

We find three different asymptotic values for the various states as illustrated in Fig. 4.2. The lowest lying asymptotic value corresponds to states with a positive intrinsic parity \( P_i \) with all spin components in the correlation function projected to the upper spin components, while the highest asymptotic value corresponds to states with positive intrinsic parity and all spins projected to the lower components. This asymptotic behavior is in line with our expectation that the spin projection of our positive intrinsic parity operators helps to increase the coupling to the lower energy \( BB \) state or the higher energy \( B_1 B_1 \) state. The energy difference between the highest and lowest asymptotic values is roughly twice the energy difference between
the single HL $B$ and $B_1$ states, indicating that they are both tending asymptotically towards their expected two meson asymptotic energies at long distances. The slight overshoot of the highest asymptotic state beyond its expected value of twice the $B_1$ energy for $d > 0.8$ fm may be indicative of contamination from mixing of the HL $B_1$ with a $\pi - B$ state. All $P_1 = (-)$ states exhibit an asymptotic tendency towards the sum of the single HL $B$ and $B_1$ energies as expected.

As the states with the lowest asymptotic energy values trend most cleanly towards their expected asymptotic value (indicating the least contamination from excited states), we will focus mainly on these states which we present in Fig. 4.3.

Several aspects of these potential curves should be noted: First, we find that the product of exchange parity $P$ and intrinsic parity $P_i$, which is the symmetry of the two meson spatial wavefunction under spatial inversion, directly corresponds to the attractiveness ($-$) or repulsiveness ($+$) of the state. This is in agreement with [85]. Second, the \((I, I_z, |J_z|, P_\perp, P, P_i) = (0, 0, 0, +, - , +)\) exhibits a significantly deeper and wider potential well when compared with the two other attractive channels. This qualitative difference was acknowledged in [85], and the quantum numbers of this channel are consistent with a bound state predicted in a phenomenological model in [78].

4.7 Bound States

As the HLHL system has been predicted to be an excellent candidate for bound tetraquark states, we seek a quantitative method for extracting such a bound state (if one exists) from our lattice calculation. Our method is as follows: We fit our lattice potential to a phenomenological quark model potential as described in [4]. We make the choice to focus on the \((I, I_z, |J_z|, P_\perp, P, P_i) = (0, 0, 0, +, - , +)\) channel, as previous work has hinted at the possibility of a bound state here. As a control,
we also perform the fit for the \((I, I_z, |J_z|, P_\perp, P, P_i) = (1, 1, 0, -,-,+\) channel as well. In our fit, we neglect the \(\vec{r} = 0\) points as the finite value of the potential at \(\vec{r} = 0\) is a lattice artifact stemming from the ultraviolet cut off introduced by the lattice discretization, leaving us with 7 data points for each potential curve, and two free parameters from the fit model. The model with the extracted fit parameters is then taken to be the interaction potential between two \(B\) mesons in the continuum limit. The two body (one-dimensional) Schrodinger equation is then solved numerically with this interaction potential to determine the existence of any negative energy (bound) states. It should be noted here that the solutions to the Schrodinger equation will converge to their continuum values as the continuum limit of the lattice calculation is taken. As we have only a single lattice spacing available to work with this continuum extrapolation is not an option, and it should be understood that the results presented in this section are at finite lattice spacing.

### 4.7.1 Potential Model

We have limited our displacements \(|\vec{r}| \leq 1.27\ \text{fm}\), therefore long range effective interactions due to meson exchange do not provide a good description of the HLHL system. In reference [4], a quark model picture of a two meson interaction was used to derive an interaction potential for the HLHL system, which included color Coulomb, spin-spin, linear confinement interactions. Details of the derivation of the potential model can be found in the aforementioned reference, and we will only highlight several modifications we make when fitting this potential model to our numerical results. The quark model HLHL potential has the form:

\[
V_{BBDS}(r) = C_I V_{cc}(\alpha_s, \beta, r) + C_{SS} V_{ss}(\alpha_s, \beta, \bar{m}, r) + C_I V_{lc}(b, \beta, r) \tag{4.11}
\]
with:

\[
V_{cc}(\alpha_s, \beta, r) = -\frac{4\alpha_s}{9r} \left[ 1 + \left( \frac{2}{\pi} \right)^{1/2} \beta r - 4\text{Erf} \left( \frac{\beta r}{2} \right) \right] e^{-\beta^2 r^2/2} \tag{4.12}
\]

\[
V_{ss}(\alpha_s, \beta, \bar{m}, r) = \frac{2}{27} \left( \frac{2}{\pi} \right)^{1/2} \frac{\alpha_s \beta^3}{\bar{m}^2} e^{-\beta^2 r^2/2} \tag{4.13}
\]

\[
V_c(b, \beta, r) = \frac{b}{3\beta} \left[ \beta r e^{-\beta^2 r^2/2} + 2 \left( \frac{2}{\pi} \right)^{1/2} e^{-\beta^2 r^2/2} \right.
\]

\[
- \left( \frac{\beta r}{2} \right) \text{Erf} \left( \frac{\beta r}{2} \right) e^{-\beta^2 r^2/2} - \frac{2}{\pi^{1/2}} e^{-3\beta^2 r^2/4} \right] \tag{4.14}
\]

Here, \( \alpha_s \) is the strong coupling constant, \( \beta \) is the spatial width of the quark model single HL meson wavefunction, \( \bar{m} \) is the mass of the light quark in the \( \overline{MS} \) scheme, and \( b \) is the QCD string tension. The coefficients \( C_I \) and \( C_{SS,SS} \), which contain the spin information of the HLHL state, are defined as matrix elements between initial (unprimed) and final (primed) two meson states and will be discussed further below. It should be noted that the above potential model acquires an overall minus sign if the isospin wavefunction of the two meson state is antisymmetric. Additionally, the potential is a function of \( |\vec{r}| \) and not \( \vec{r} \), as any tensor interaction terms are neglected in this model.

### 4.7.2 Fit Model

When applying the above model to our lattice data, we must make several modifications to the above quark model potential. Due to the use of periodic boundary conditions in the calculation, interactions with image "charges" lying past the boundary must be accounted for. We must also consider the possibility that there will be long range meson exchange interactions that were neglected in our choice of potential model. To account for these long range interactions, we extend the original...
model by adding a simple Yukawa like term for one pion exchange:

\[
V^{Yuk} (r) = V_{BBDS} (r) + g \frac{e^{-m_{\pi} r}}{r} \tag{4.15}
\]

Here we take \( m_{\pi} \) to be the mass of the pion on the gauge field configurations used in the calculation (\( \sim 390 \) GeV). The parameter \( g \) is discussed below.

In principle, interactions with each of the infinitely many image charges contribute to the potential and must be included. In practice however, we may restrict ourselves to contributions where the image of the first meson is \( \leq 3L/2 \) (\( \sim 4.5 \) fm) away from the second and vice versa. This approximation is valid as the contribution of these truncated images (at separations of \( r > 3L/2 \)) to the potential (with the choice of parameters outlined below) is \( \mathcal{O}(10^{-4}) \) MeV. With the inclusion of the image charges our potential model then becomes:

\[
V_{lm}^{Yuk} = V^{Yuk} (r) + 2 \sum_{r_i < 3L/2} V^{Yuk} (r_i) \tag{4.16}
\]

The addition of these image charges modify the potential at long distance as illustrated in Fig. 4.4

The final modification made to the potential model is a modification of the spin dependent coefficients \( C_I \) and \( C_{S_S} \). The original presentation of this phenomenological potential model in Ref. [4] sought to provide a comparison with the lattice calculations of the time, which had an incomplete classification of the HLHL states in terms of the total isospin \( I \) and spin \( S \) of the system, while also maintaining a connection with the physical \( B \) meson states. Because of this, classification of the various potentials was made in terms of the physical \( B \) and \( B^* \) (first angular excitation of the \( B \) meson) with respect to the quantum numbers \( I \) and \( S \).

The difference in angular momentum spaces of the non-static and static limit
prevents a direct interpretation of the lattice data from the present work in terms of physical $B$ and $B^*$ states, and our classification of states makes it difficult to reconcile the previous classification with ours. We therefore choose to recalculate the spin dependent coefficients of the potential model relevant for the static limit $BB$ system we study on the lattice, the results of which are presented in Table 4.2 (For details of the calculation, see Appendix A.6). The previous determination of these coefficients for the HLHL system included spin degrees of freedom for the heavy quarks in the two meson states $|M_iM_j>$ allowing for better classification of the potential in terms of non-static limit states. We choose to neglect the spin degrees of freedom of the heavy quarks in our determination, effectively fully implementing the static limit for the the potential model. Thus the spin degrees of freedom of our two meson kets $|M_iM_j>$ are just those of the spin of the light degrees of freedom of our HLHL state. The evaluation of these coefficients however requires knowledge of the total angular momentum of the two meson state, a point that has been neglected until now. As we seek to fit the $(I, I_z, |J_z|, P_\perp, P, P_i) = (0, 0, 0, +, - , +)$ and $(1, 1, 0, - , - , +)$ states, we need to determine if these particular states are in a symmetric angular momentum triplet, or an antisymmetric angular momentum singlet. In order to make this identification, we must rely on the overall symmetries of the state in question. We know that the parity $P$ of a given state is the product of the intrinsic parity $P_i$ and the symmetry of the spatial wavefunction. From this relationship, and with knowledge of the symmetry of the isospin spatial wavefunction, we can infer the symmetry of the angular momentum wavefunction:

$$Sym_J = (-) (Sym_I) (P_i) (P),$$

where $Sym_J$ and $Sym_I$ the symmetries of the angular momentum and isospin wavefunctions. The overall negative sign appears from exchanging fermions in the
parity operation. Using this we are able to identify the \((I, I_z, |J_z|, P_\perp, P, P_i) = (0, 0, 0, +, -, +)\) channel with \(Sym_J = -\) as a \(J = 0\) state, and the \((I, I_z, |J_z|, P_\perp, P, P_i) = (1, 1, 0, -, -, +)\) channel with \(Sym_J = +\) as a \(J = 1\) state. The spin dependent coefficients can then be recalculated for our states and are shown in Table [4.2].

### 4.7.3 Fitting Procedure and Bound State Determination

In fitting the potential model of eq. 4.15 to our lattice data, we use two free fit parameters: \(\beta\) and \(g\) and take the remaining parameters \(b\), \(\bar{m}\) and \(\alpha_s\) to be 0.18 GeV\(^2\), 0.33 GeV, and 0.5 respectively as in Ref. [4]. A fit is performed for each of 305 jackknife ensembles, allowing for an accurate way to estimate the error on the extracted fit parameters, shown in Table [4.2]. As we are ultimately interested in the energy levels allowed by the potential model, and not the model parameters themselves, we will only briefly comment on the fit parameters. It is immediately obvious that \(g\) is not well determined for the \(J = 1\) channel. It’s also interesting that the fit parameter \(\beta\) is significantly smaller for the \(J = 0\) channel, indicating a much narrower spatial distribution of the two meson wavefunction.

Once the fit parameters have been extracted they are then inserted into the two body radial Schrödinger equation to determine if any bound states exist. As we are restricting ourselves to \(L = 0\) states, the two body Schrödinger equation can be written as:

\[
\left[ -\frac{\hbar^2}{2\bar{m}} \frac{d^2}{dr^2} + V_{\text{Yuk}}(r) \right] u(r) = Eu(r)
\]

where \(\bar{m}\) is the reduced mass of a two B meson system (with the single meson mass taken from the Particle Data Group [90]), \(u(r) = r\psi(r)\) and \(V_{\text{Yuk}}(r)\) is the potential model presented in the preceding section excluding the image terms.

Eq. 4.18 is then solved numerically as an eigenvalue problem with a spatial
discretization of 0.01 fm and a spatial cutoff of 10 fm (corresponding to a sphere with \( r = 10 \) fm), and the boundary condition that \( \Psi (r) \rvert_{r=10} = 0 \). This spatial volume provides ample space for the potential to decay to zero. The eigenvalue spectrum is then analyzed for each of the two states discussed above. While the \( J = 1 \) channel exhibits a near continuum of positive eigenvalues (discrete only because of the numerical solution method), the \( J = 0 \) channel does admit a single bound state with energy \( E_0 = -50.0(5.1) \) MeV (with the uncertainty determined by carrying through the jackknife analysis from the fit parameters and solving eq. 4.18 for each of the 305 \((\beta, g)\) sets). Aside from the binding energy, we can also calculate the RMS radius for the two meson wavefunction \( \Psi (r) \) from the wavefunctions \( u(r) \) above:

\[
\langle r^2 \rangle^{1/2} = \left[ \frac{\sum_i r_i^2 |u(r_i)|^2}{\sum_i |u(r_i)|^2} \right]^{1/2}
\]

(4.19)

For the bound state wavefunction \( u_0 (r) \), we find an RMS radius of 0.383(6) fm, the error again estimated by jackknife analysis.

In comparing this result with [86] (in which a numerical solution to the Schrödinger equation was performed with a similar radial cutoff) we find our results to be consistent with all of the binding energies quoted in that work within confidence bounds. Additionally, Ref. [78] quote’s binding energies and RMS radii for a doubly bottom \( J^P (L, S, I) = 0^+ (0, 0, 0) \) channel which is consistent (in the static limit) with the quantum numbers of our static limit \((I, I_z, |J_z|, P_\perp, P, P_z) = (0, 0, 0, +, -, +)\) channel. This reference uses two different potential models to calculate binding energies: the constituent quark cluster model CQC and the the Bhaduri-Cohler-Nogami or BCN model. The BCN model includes the same interactions as those used in Ref. [4] to derive the potential used to fit our lattice results (namely, color
coulomb, linear confinement and spin-spin). Furthermore, the BCN parameters corresponding to string tension $b$, strong coupling $\alpha_s$, and constituent quark mass $m$ used in [78] are very similar to those used in our potential model (compare our $(b, \alpha_s, m) = (0.18 \text{ GeV}^2, 0.5, 0.33 \text{ GeV})$ to $(0.186 \text{ GeV}^2, 0.52, 0.337 \text{ GeV})$). These binding energies should provide a relevant point of comparison for our results provided our lattice discretization errors have minor effects on the extracted potential model fit parameters. In comparison, we find our values for the binding energy and RMS radius to be consistent with the values quoted in [78] from the BCN model $(E_0, r_{RMS}) = (-52 \text{ MeV}, 0.334 \text{ fm})$, providing a good cross check that our lattice calculation has identified a bound state in the static limit $(I, I_z, |J_z|, P_\perp, P, P_i) = (0, 0, 0, +, -, +)$ channel. The fact that the bound state identified in that work has an RMS radius that is smaller than the sum of the individual mesonic RMS radii is indicative of the compact nature of that bound state. Additionally, as illustrated in Ref. [88] (see eqns. 4), the static limit HLHL tetraquark state can be written as a linear combination of products of two single meson wavefunctions in different spin states. This is consistent with the idea that although the compact tetraquark state may have a complicated color space structure composed of color vectors, this state can always be decomposed into a linear combination of products of two single meson wavefunctions.

<table>
<thead>
<tr>
<th>$(J, J_z)$</th>
<th>$C_I$</th>
<th>$C_{SS}$</th>
<th>$\beta$ (GeV)</th>
<th>$g$</th>
<th>$\chi^2/d.o.f.$</th>
<th>$E_0$ (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0)</td>
<td>-1</td>
<td>3/4</td>
<td>0.274(14)</td>
<td>0.041(12)</td>
<td>0.9943</td>
<td>-50.0(5.1)</td>
</tr>
<tr>
<td>(1,0)</td>
<td>1</td>
<td>1/4</td>
<td>0.459(38)</td>
<td>0.016(20)</td>
<td>0.4119</td>
<td>N/A</td>
</tr>
</tbody>
</table>

TABLE 4.2: Spin dependent coefficients from reference [3] and fit parameters from fitting our lattice data to a modified version of the model presented in ref. [4]. Here $\beta$ corresponds to the spatial width of the HL meson wavefunction, and $g$ is the coupling strength of the additional Yukawa term introduced in this work. The uncertainties quoted for the fit parameters are jackknife estimates.
FIG. 4.1: Effective mass for HL $B$ for increasing $|p^2| \leq |p_{cut}^2|$
FIG. 4.2: Comparison of $BB$ vs. $BB_1$ (left) and $BB$ vs $B_1B_1$ (right) asymptotic states. Here we take the energy difference for the three potential curves with respect to twice the HL $B$ energy.
FIG. 4.3: Calculated HLHL $BB$ energies with expected asymptotic value (twice the calculated HL $B$ mass)
FIG. 4.4: Contribution of image charges to the potential (left) and contributions to the potential model $V_{H_{LUH}}$ from the individual terms in eq. 4.11.

FIG. 4.5: Fit of the potential model in eq. 4.15 to the $(I, I_z, |J_z|, P_{\perp}, P, P_i) = (0, 0, 0, +, -, +)$ channel. The colored band represents the uncertainty in the fit parameters $\beta$ and $g$ from jackknife analysis.
CHAPTER 5

Conclusions

The main theme of the current work has been the investigation of spectroscopy, interactions, and the existence of exotic states for hadronic systems containing one or more heavy quarks. The work began by introducing quantum field theory in the context of the strong force, with an aim at providing a historical perspective on the development of the field of quantum chromodynamics. The main conceptual pillars and framework of quantum chromodynamics were then introduced, followed by a discussion of effective theories for both light and heavy quarks. The framework of lattice quantum chromodynamics was then introduced in the following chapter as a prescription for performing numerical calculations in the low energy regime where perturbative calculations are not feasible for a non-Abelian gauge theory such as QCD. Numerical methods were presented for heavy quarks in the context of three frameworks, each suited for different types of calculations. In the chapters that followed, these frameworks were then applied in several lattice QCD calculations.

In the first calculation, the low-lying spectrum of baryons containing at least one bottom or charmed quark was calculated, producing the most comprehensive single calculation of this kind to date. For the charmed quark sector, a fully relativis-
tic fermion action was used. For the bottom quark sector, the quarks were treated non-relativistically. Baryon masses were computed using both a fine \((a \sim 0.08 \text{ fm})\) and course \((a \sim 0.11 \text{ fm})\) lattice spacing, allowing for extrapolations to the continuum limit (assuming a linear dependence on the square of the lattice spacing). The calculation was carried out using partial quenching, with eight distinct combinations of sea and valence light quark masses resulting in pion masses ranging from 227 MeV through 419 MeV in the valence sector. This wide range of pion masses allowed for chiral extrapolations to be carried out guided by partially quenched heavy hadron chiral perturbation theory. Both systematic and statistical uncertainties were estimated and propagated through to the final extrapolated results. These final results of the low-lying heavy baryon spectrum were presented in Tables 3.13 and 3.14. Results were found to be in good agreement with experiment, providing evidence that using a relativistic lattice action for the charmed quarks and a non-relativistic lattice action for the bottom quarks was a valid choice for this type of spectroscopy calculation.

Following the spectroscopy calculation, the interaction potential between two b-meson states in the limit of static b quarks was computed. With this lattice potential parametrized with a functional form motivated by the quark model description of the two b-meson interaction, the bound state energies in the heavy-light-heavy-light (HLHL) tetraquark system were determined. To perform this study, colorwave propagators were introduced for calculating meson correlation functions and the formalism was extended to the HLHL system in order to provide a novel way for an efficient calculation of HLHL correlation functions for several \((I, I_z, |J_z|, P_\perp, P, P_i)\) channels. The effect of limiting the colorwave plane wave basis on the ground state overlap of single HL correlation functions was explored, and a choice for the momentum cutoff \(p_{\text{cut}}^2\) was made to optimize the quality of the signal versus the computational cost. For a single HL meson, results indicated that a larger value of
\( p_{\text{cut}}^2 \) provided better overlap with the ground state.

HLHL potentials were calculated for 24 distinct \((I, I_z, |J_z|, P_\perp, P, P_i)\) channels, exhibiting three distinct asymptotic values as \( r \to \infty \) corresponding to the different ways \( B \) and \( B_1 \) mesons can be combined. The tendency of the HLHL energy to overshoot the expected asymptotic value of \( E_{B_1} + E_B \) and \( 2E_{B_1} \) may have been due to contamination from excited states and the possibility of \( B_1 \) mixing with a \( B - \pi \) state. It was determined that the attractiveness or repulsiveness of the HLHL potential corresponds directly to the symmetry of the two meson spatial wavefunction under spatial inversion, in agreement with Ref. [85]. The asymptotic behavior of the various HLHL states was shown to be dependent on the intrinsic parity of the state. While the \( P_i = - \) states have only one asymptotic value (corresponding to a single two meson \( B B_1 \) component), the \( P_i = + \) channels have two asymptotic values corresponding to both \( B B \) and \( B_1 B_1 \) two meson components. By examining the construction of single HL correlation functions, it was determined that we could increase overlap with the \( B B \) and \( B_1 B_1 \) two meson wavefunctions by projecting the correlation functions to include only positive or negative parity components of the Dirac basis quark spinors.

The existence of bound states was then explored for the \((I, I_z, |J_z|, P_\perp, P, P_i) = (0, 0, 0, +, -, +)\) channel as it exhibited a wider and deeper potential when compared with the other attractive potentials. Analysis was also carried out for the \((I, I_z, |J_z|, P_\perp, P, P_i) = (1, 1, 0, -, -, +)\) for the purposes of comparison. A modified version of the potential model described in Ref. [4] was used to fit the lattice data, and two fit parameters \( \beta \) (the gaussian width of the HL meson wavefunction) and \( g \) (the Yukawa interaction constant) were extracted from the fit. Inserting the potential with the extracted fit parameters into the two body Schrödinger equation, we then solved numerically for the eigenvalues of the hamiltonian, searching for any negative energy eigenstates. A single negative energy bound state was found.
in the (0, 0, 0, +, −, +) channel, with an energy of $E_0 = -50.0(5.1)$ MeV and RMS radius $r_{\text{RMS}} = 0.383(6)$ fm. These results were found to be consistent with results presented in Ref. [86] as well as phenomenological results presented in Ref. [78] for the state $J^P(L, S, I) = 0^+ (0, 0, 0)$ (which maps onto our (0, 0, 0, +, −, +) channel in the static limit). The errors quoted on these results are statistical only. One needs to account for several systematic errors such as $1/m_b$ corrections ($m_b$ the b quark mass), lattice spacing effects as well as dependence on the light quark mass.

In contrast to a common lattice method for calculating scattering phase shifts for two hadrons, working in the static limit allowed us to calculate hadronic interactions by way of an inter-meson potential. In this way, the static heavy quark action provided a starting point from which the existence of four quark bound states could be explored.

The two topics composing the main focus of this work may seem initially disparate at a superficial level. The main theme tying the projects together is the various ways in which heavy quarks, which introduce an energy scale that is traditionally impractical for lattice calculations, can be treated on the lattice using various formulations. We have shown that various frameworks for treating heavy quarks on the lattice can be used strategically to ones benefit, both to simplify the computational complexity of the calculation (in the case of static quarks and heavy quarks in NRQCD) as well to explore alternative avenues by which to study complex systems such as four quark states (utilizing static heavy quarks).

Extensions of this work that will be studied in the future include studying the HLHL spectra of systems with non-zero strangeness, studying the excited state charmed bottom baryon spectrum. For the latter calculation, the non-local baryon operators in the color wave formalism developed in this work could be utilized to achieve maximum overlap with the excited states of interest. These are just several possible extensions of the current work, and I look forward to the opportunity to
pursue these interests in future research!
APPENDIX A

Supporting Formulae for Chiral Extrapolations

A.1 Singly heavy chiral extrapolation loop contributions

The singly heavy baryon masses are of the form:

\[ M_B = M_0(\mu) + \Delta_{T,B}(\mu) + M_1^{(B)}(\mu) + M_{3/2}^{(B)}(\mu) \]  \hspace{1cm} (A.1)

The non analytic contributions the the baryon masses are given by

\[ M_{3/2}^{(B)}(\mu) = \frac{1}{12\pi^2 f^2} \sum_{\phi} \sum_{I} \delta_{s_B,s_I} \times \left[ A_{\phi,I}^{(B)} \mathcal{F}(m_\phi, \Delta_B, I, \mu) + A_{\phi^*,I}^{(B)} \mathcal{F}(m_\phi, m_\phi, \Delta_B, I, \mu) \right] \]  \hspace{1cm} (A.2)

where the sum over baryons runs over all \( B \in \{\Lambda_Q, \Xi_Q, \Sigma_Q, \Xi'_Q, \Omega_Q, \Sigma^*_Q, \Xi'^*_Q, \Omega^*_Q\} \) and that over mesons is over \( \phi = \pi, \phi_j, \eta_u \). The delta-function restricts the baryon...
sum to be over a fixed strangeness sector where the strangeness of the external state, \( S_B \), is the same as that of the state in chiral loops, \( S \). We impose isospin symmetry in both the sea and valence sectors and use the same \( f = 132 \text{ MeV} \) as in Ref. [22] as well as the same definitions of the non-analytic functions \( F(m_\phi, \Delta, \mu) \) and \( F(m_\phi, m_\phi, \Delta, \mu) \):

\[
F(m, \delta, \mu) = (m^2 - \delta^2) \left[ \sqrt{\delta^2 - m_\mu^2} \log \left( \frac{\delta - \sqrt{\delta^2 - m_\mu^2 + i\epsilon}}{\delta - \sqrt{\delta^2 - m_\mu^2 + i\epsilon}} \right) - \delta \log \left( \frac{m^2}{\mu^2} \right) \right] - \frac{1}{2} \delta m_\mu^2 \log \left( \frac{m^2}{\mu^2} \right), \tag{A.3}
\]

\[
F(m, m', \delta, \mu) \bigg|_{m' = m} = -\frac{1}{2} F(m, \delta, \mu) \tag{A.4}
\]

We define the splittings \( \Delta_{ST} = M_{\Sigma_b} - M_{\Lambda_b} \) and \( \Delta_* = M_{\Sigma_{b*}} - M_{\Sigma_b} \) and assume that there is no light quark mass dependence of these parameters.

The baryon dependent coefficient functions are as follows

\[
A_{\phi}^{(B \in T)} = -g_3^2 \left( \delta_{T \in S_{1/2}} + 2 \delta_{T \in S_{3/2}} \right) A_{\phi}^{(B)} \tag{A.5}
\]

\[
A_{\phi}^{(B \in S_{1/2})} = -g_3^2 \delta_{T \in T} A_{\phi}^{(B)} + \frac{g_2^2}{3} \left( \delta_{T \in S_{1/2}} + 2 \delta_{T \in S_{3/2}} \right) B_{\phi}^{(B)} \tag{A.6}
\]

\[
A_{\phi}^{(B \in S_{3/2})} = -g_3^2 \delta_{T \in T} A_{\phi}^{(B)} + \frac{g_2^2}{6} \left( \delta_{T \in S_{1/2}} + 5 \delta_{T \in S_{3/2}} \right) B_{\phi}^{(B)} \tag{A.7}
\]

with analogous relations between \( A_{\phi, \phi}^{(B)} \) and the \( A_{\phi}^{(B)} \) and \( B_{\phi}^{(B)} \).
TABLE A.1: The baryon mass splitting $\Delta_{B,I}$

<table>
<thead>
<tr>
<th>$\Delta_{E,I}$</th>
<th>internal</th>
</tr>
</thead>
<tbody>
<tr>
<td>external</td>
<td>$T$</td>
</tr>
<tr>
<td>$T$</td>
<td>0</td>
</tr>
<tr>
<td>$S_{1/2}$</td>
<td>$-\Delta_{ST}$</td>
</tr>
<tr>
<td>$S_{3/2}$</td>
<td>$(\Delta_{ST} + \Delta_s)$</td>
</tr>
</tbody>
</table>

TABLE A.2: The couplings $A^{(B)}_g$, $B^{(B)}_g$, $A^{(B)}_{\phi}$, and $B^{(B)}_{\phi}$ for the various baryons. For the sextet baryons, the coefficients are the same for the spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$ states.

<table>
<thead>
<tr>
<th>$B$</th>
<th>$A^{(B)}_g$</th>
<th>$A^{(B)}_{\phi}$</th>
<th>$A^{(B)}_{\eta_u\eta_u}$</th>
<th>$B^{(B)}_g$</th>
<th>$B^{(B)}_{\eta_u}$</th>
<th>$B^{(B)}_{\eta_u\eta_u}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Lambda_Q$</td>
<td>$\frac{1}{2}$</td>
<td>1</td>
<td>0</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
</tr>
<tr>
<td>$\Xi_Q$</td>
<td>0</td>
<td>$\frac{1}{2}$</td>
<td>$\frac{1}{4}$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
</tr>
<tr>
<td>$\Sigma^{(*)}_b$</td>
<td>$-\frac{1}{2}$</td>
<td>1</td>
<td>0</td>
<td>$\frac{1}{2}$</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$\Xi^{(*)}_b$</td>
<td>0</td>
<td>$\frac{1}{2}$</td>
<td>$\frac{1}{4}$</td>
<td>0</td>
<td>$\frac{1}{2}$</td>
<td>$\frac{1}{4}$</td>
</tr>
<tr>
<td>$\Omega^{(*)}_b$</td>
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<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

A.2 Doubly heavy chiral extrapolation loop contributions

The doubly heavy baryon masses with strangeness $S = 0$ are of the form:

$$M_{\Xi} = M_0 - (1/2)\Delta_H + M_{\Xi}^{(1)} + M_{\Xi}^{(3/2)}$$

$$M_{\Xi^*} = M_0 + (1/4)\Delta_H + M_{\Xi^*}^{(1)} + M_{\Xi^*}^{(3/2)},$$

(A.8)

Here, $\Delta_H$ is the mass splitting in the chiral limit and $M_0$ is the mass of the spin doublet in the SU(2) Chiral limit. The terms $M_{\Xi}^{(1)} = M_{\Xi^*}^{(1)}$ comes from tree level counterterms in the chiral expansion, and are proportional the square of both the sea and valence pion masses. The terms $M_{\Xi}^{(3/2)}$ and $M_{\Xi^*}^{(3/2)}$ come from one loop diagrams, and are given in Eqns A.9 and A.10.
\[ M_{\Xi}^{(3/2)} = \frac{-4g^2}{(4\pi f)^2} \left[ \frac{5}{9} \mathcal{F}(m_{\pi\pi}, \Delta_{\Xi_0^0\Xi_0^-, \mu}) + \frac{4}{9} \mathcal{F}(m_{\pi\pi}, -\Delta_{\Xi_0^0\Xi_0^-, \mu}) \right] + \frac{g^2}{(4\pi f)^2} \left[ \frac{5}{9} \mathcal{F}(m_{\pi\pi}, 0, \mu) + \frac{4}{9} \mathcal{F}(m_{\pi\pi}, -\Delta_{\Xi_0^0\Xi_0^-, \mu}) \right] \] (A.9)

\[ M_{\Xi}^{(3/2)} = \frac{-4g^2}{(4\pi f)^2} \left[ \frac{1}{9} \mathcal{F}(m_{\pi\pi}, \Delta_{\Xi_0^0\Xi_0^-, \mu}) + \frac{8}{9} \mathcal{F}(m_{\pi\pi}, \Delta_{\Xi_0^0\Xi_0^-, \mu}) \right] + \frac{g^2}{(4\pi f)^2} \left[ \frac{1}{9} \mathcal{F}(m_{\pi\pi}, 0, \mu) + \frac{8}{9} \mathcal{F}(m_{\pi\pi}, \Delta_{\Xi_0^0\Xi_0^-, \mu}) \right] \] (A.10)

with \( \mathcal{F}(m, \delta, \mu) \) given in Eqn. A.3.

We assume the splittings \( \{\Delta_{\Xi_0^0\Xi_0^-, \Delta_{\Xi_0^0\Xi_0^-, \Delta_{\Xi_0^0\Xi_0^-, \Delta_{\Xi_0^0\Xi_0^-, \mu}}\} \) (here, v,s refers to baryons containing valence and sea light quarks respectively) to be independent of the pion mass and take their values to be the average of the measured splittings over the various ensembles.

### A.3 Finite volume corrections to extrapolation formulae

In order to account for the effects of the finite volume on the baryon masses, we use the expressions presented in Ref. [73].

The finite volume corrections to the function \( \mathcal{F}(m, \delta, \mu) \) are given by:

\[ \mathcal{F}_{FV}(m, \delta) = -m^2\pi \sum_{\delta \neq 0} e^{-umL} uL A \] (A.11)
where $\bar{u} = (u_1, u_2, u_3)$ with $u_i \in \mathbb{Z}$, $u \equiv |\bar{u}|$ and

$$
\mathcal{A} = e^{(z^2)}[1 - \text{Erf}(z)]
+ \left( \frac{1}{umL} \right) \left[ \frac{1}{\sqrt{\pi}} \left( \frac{9z}{4} - \frac{z^3}{2} \right) + \left( \frac{z^4}{2} - 2z^2 \right) e^{(z^2)}[1 - \text{Erf}(z)] \right]
- \left( \frac{1}{umL} \right)^2 \left[ \frac{1}{\sqrt{\pi}} \left( -\frac{39z}{64} + \frac{11z^3}{32} - \frac{9z^5}{16} + \frac{z^7}{8} \right) - \left( -\frac{z^6}{2} + \frac{z^8}{8} \right) e^{(z^2)}[1 - \text{Erf}(z)] \right]
+ O\left( \frac{1}{(umL)^3} \right),
$$

with

$$
z = \left( \frac{\Delta}{m} \right) \sqrt{umL}.
$$

In determining the chiral loop contributions from Appendices A.1 and A.2, we must include these finite volume corrections as:

$$
\tilde{\mathcal{F}}(m, \delta, \mu) = \mathcal{F}_{IV}(m, \delta, \mu) + \mathcal{F}_{FV}(m, \delta)
$$

where $\mathcal{F}_{IV}(m, \delta, \mu)$ is given by Eqn. A.3. In evaluating the extrapolation expressions presented in Section ?? at the physical point, the finite volume contributions to the chiral function $\mathcal{F}(m, \delta, \mu)$ are set to zero in order to take the infinite volume limit.

### A.4 Parity content of HL interpolating operators

Here we show that correlation functions for our $B(B_1)$ states are composed entirely of upper(lower) components of the Dirac basis components of the light quark flavors. We begin with a general HL correlation function with arbitrary source and sink operators (neglecting color indices and working in the Dirac basis):
\[
C_{HL}(t)_{i,j} = \sum_{\bar{x}} \left\langle \mathcal{O}_{B_i}(\bar{x},t) \mathcal{O}_{B_j}^\dagger(\bar{x},0) \right\rangle \\
= \sum_{\bar{x}} \left\langle \tilde{Q}(\bar{x},t) \Gamma_i q(\bar{x},t) \tilde{q}(\bar{x},0) \Gamma_j Q(\bar{x},0) \right\rangle \\
= \sum_{\bar{x}} tr \left( \gamma_5 (S_H(\bar{x},t;0))^\dagger \gamma_5 \Gamma_i S_L(\bar{x},t;0) \Gamma_j \right) 
\]

(A.15)

\[S_H\] is a heavy quark propagator given by:

\[
S_H(\bar{x},t;0) = \left(\frac{1 + \gamma_4}{2}\right) W(\bar{x},t;t_0) = P_+ W(\bar{x},t;t_0) 
\]

(A.16)

where \(W(\bar{x},t;t_0)\) is a Wilson line from \(t_0\) to \(t\). Substituting this, we have:

\[
C_{HL}(t) = \sum_{\bar{x}} tr \left( \gamma_5 (P_+ W^\dagger(\bar{x},t;0)) \gamma_5 \Gamma_i S_L(\bar{x},t;0) \Gamma_j \right) \\
= \sum_{\bar{x}} tr_c \left( W^\dagger(\bar{x},t;0) tr_d (\Gamma_i P_- \Gamma_j S_L(\bar{x},t;0)) \right) 
\]

(A.17)

where we have used \(\gamma_5 P_+ \gamma_5 = P_-\). For \(\Gamma_i = \Gamma_j = 1\), we project to only the lower components of the Dirac basis light quark propagator, while for \(\Gamma_i = \Gamma_j = \gamma_5\) we project only to the upper components of the Dirac propagator.

### A.5 Construction of light quark wavefunctions

To determine two quark wavefunctions in spin and flavor space yielding the quantum numbers \((I, I_z, |J_z|, P_\perp, P, P_i)\), we begin with states of definite \((I, I_z, J, J_z, P_i)\):

\[
[q_1(p_1) q_2(p_2)]_{(I, I_z, |J_z|, P_\perp, P, P_i)} = \sum_{m_1, m_2} \sum_{t_1, t_2} W_{m_1, m_2}^{J, J_z} W_{t_1, t_2}^{I, I_z} q_1(m_1, t_1, p_1) q_2(m_2, t_2, p_2) 
\]

(A.18)
where \(m, t, p\) are the projections of spin and isospin along the \(z\)-axis and the intrinsic parities of the light quarks, and the \(W_{m_1,m_2}^{J_1,J_2} = \langle 1/2, m_1, 1/2, m_2 | J_z \rangle\), \(W_{t_1,t_2}^{I_1,I_2} = \langle 1/2, t_1, 1/2, t_2 | I_z \rangle\) are the Clebsch-Gordon for angular momentum and isospin. From these operators, we average over \(J_z = \pm 1\) states and determine \(P_\perp\) from the quantum numbers \(P_i\) and \(P\) and the spatial symmetry of the operator. It should be noted here that there are two combinations of \((p_1, p_2)\) that contribute to the \(P_i = +1\) HLHL states, and we make the decision to keep these as distinct operators.

Linear combinations of the above operators are then taken to produce states of definite exchange parity \(P\), the necessary combinations determined by summing over sets of the above operators that map onto each other under \(P\) with the appropriate weight \(W_{p_1,p_2} = \pm 1\)

\[
[q_1 q_2]_{(I_1 J_1, J_z, P_\perp, P, P_i)} = \sum_{p_1,p_2} W_{p_1,p_2}^{P} \left[ q_1 (p_1) q_2 (p_2) \right]_{(I_1 J_1, J_z, P_\perp, P, P_i)}
\]  

(A.19)

### A.6 Determination of spin coefficients for potential model

Here we present our derivation of the spin coefficients \(C_I\) and \(C_{S,S}\) presented in Table 4.2. In Ref. [3], an interaction potential for two meson states is calculated by including spin-spin, color coulomb and linear confinement interactions in a two quark interaction hamiltonian. By considering these interactions between each of the quark quark pairs in a 4 quark (2 meson) scattering state, transfer matrix elements are calculated and then Fourier transformed to give a corresponding position space potential. In Ref. [4], this method was applied to the HLHL system. When calculating the spin dependent portion of the potential, all but one of the interaction diagrams (referred to as “Transfer 2”) can be neglected because the spin of the
heavy quarks is neglected in the static approximation. This diagram includes an insertion of the interaction hamiltonian between the two light quarks, as illustrated in Fig. A.1. The spin dependent contribution of this diagram to the potential can be factorized such that all the dependence enters through two coefficients, which are defined as matrix elements between the initial and final two meson states:

\[ C_I = \langle CD|I|AB \rangle \] \hspace{1cm} (A.20)

\[ C_{S \cdot S} = \langle C_i D_j|S_i \cdot S_j|A_i B_j \rangle \] \hspace{1cm} (A.21)

Where \( I \) here is understood to be the identity operator in spinor space. Upon inspection of the diagram, it’s clear that the matrix element of \( I \) will not always trivially be unity due to the quark interchange between the initial and final two meson state.

With respect to Fig. A.1, these matrix elements as outlined in [3] are defined explicitly as:

\[ C_I = \langle CD|I|AB \rangle = \chi_{s_c,s_d}^{\lambda C} \chi_{\delta_a,\delta_b}^{\lambda D} \left[ < s_c, s_d|I|s_a, s_b > \delta_{s_a,s_c} \delta_{s_b,s_d} \right] \chi_{\delta_a,\delta_b}^{\lambda A} \chi_{s_a,s_b}^{\lambda B} \] \hspace{1cm} (A.22)

\[ C_{S \cdot S} = \langle C_i D_j|S_i \cdot S_j|A_i B_j \rangle = \chi_{s_c,s_d}^{\lambda C} \chi_{\delta_a,\delta_b}^{\lambda D} \left[ < s_c, s_d|S_i \cdot S_j|s_a, s_b > \delta_{s_a,s_c} \delta_{s_b,s_d} \right] \chi_{\delta_a,\delta_b}^{\lambda A} \chi_{s_a,s_b}^{\lambda B} \] \hspace{1cm} (A.23)

For our purposes, we wish to entirely neglect the spin of the heavy quarks in the above matrix elements. Because of this, the Clebsch-Gordan coefficients \( \chi_{s_c,s_d}^{\lambda C} \) etc. (relating the spin of the two quark state to the meson state) are all unity. The states between which we wish to calculate these matrix elements are two particle angular
momentum eigenstates $|J, J_z\rangle_{a,b} \equiv |s_a, s_b\rangle$ of which we are only interested in $|1,0\rangle$ and $|0,0\rangle$. To account the light quark exchange in Fig. A.1, we note the following relations:

$$|s_a, s_b\rangle_{J=0, J_z=0} = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) = \frac{1}{\sqrt{2}} (|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle) = - |s_c, s_d\rangle_{J=0, J_z=0}$$

(A.24)

and

$$|s_a, s_b\rangle_{J=1, J_z=0} = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) = \frac{1}{\sqrt{2}} (|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle) = |s_c, s_d\rangle_{J=1, J_z=0}$$

(A.25)

From the above relations, it is easy to calculate the matrix elements of interest for our problem (for the states $|1,0\rangle \rightarrow |1,0\rangle$ and $|0,0\rangle \rightarrow |0,0\rangle$):

$$\langle 1,0|_{c,d} I |1,0\rangle_{a,b} = \langle 1,0|_{a,b} I |1,0\rangle_{a,b} = 1$$

(A.26)

$$\langle 0,0|_{c,d} I |0,0\rangle_{a,b} = (-) \langle 0,0|_{a,b} I |0,0\rangle_{a,b} = -1$$

(A.27)

and

$$\langle 1,0|_{c,d} S_i \cdot S_j |1,0\rangle_{a,b} = \langle 1,0|_{a,b} S_i \cdot S_j |1,0\rangle_{a,b} = 1/4$$

(A.28)

$$\langle 0,0|_{c,d} S_i \cdot S_j |0,0\rangle_{a,b} = (-) \langle 0,0|_{a,b} S_i \cdot S_j |0,0\rangle_{a,b} = -(-3/4)$$

(A.29)
FIG. A.1: Transfer 2 diagram from Ref. [4]
BIBLIOGRAPHY


Zachary S. Brown was born on the 2nd of August, 1984 in Oak Harbor Washington. Shortly thereafter his family relocated to Western New York. He attended Attica Elementary, Middle and Senior High Schools in Attica, NY. During his senior year, he developed a keen interest in physics. In 2003, he began study at the State University of New York College at Fredonia in pursuit of a degree in Sound Recording Technology. After taking several university level physics courses, he rediscovered his interest in physics and decided to add it as a second major. He graduated from Fredonia Magna Cum Laude in 2008 with a Bachelor of Science degree in both Physics and Sound Recording Technology, and a minor in applied mathematics. Zachary entered the College of William & Mary in the fall of 2008, and began work with Dr. Konstantinos Orginos in early 2010 working on applications of the framework of Lattice Quantum Chromodynamics in studying the interactions and energy spectra of heavy hadrons. He received a Master of Science in 2010.