Heavy Semileptonic Form Factors from Lattice Quantum Chromodynamics

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Abstract:

I did some lattice

Declaration of originality

This thesis is my own work, except where explicit attribution to others is made. In particular Chapters ... are based on the following publications:
All results and figures presented in these chapters are my own, except for ...

please help i am trapped in this computer

Acknowledgments

I claim sole credit for everything in this thesis.

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Chapter 1

Background and Motivation

1.1 Testing the Standard Model

1.2 Flavour Physics

1.2.1 The CKM Matrix

1.2.2 Weak Decays

The key motivations for studying decays like the $B_s \to D_s l\nu$ are:

- Determination of CKM matrix elements. Specifically, by combining the theoretical prediction and an observed brancing fraction of $B_s \to D_s l\nu$, $|V_{cb}|$ can be extracted.
- Precision tests of the standard model. There are currently a number of tensons between experiment and the standard model predictions of B decays, some closely related to $B_s \to D_s l\nu$ [1].

We will first discuss the general ideas in computing semileptonic decays. Semileptonic decays are useful for studying the sector of the standard model (SM) which couples quarks to the weak force [2]:

$$\mathscr{L}_W = \frac{g}{\sqrt{2}} \left[\quad V_{ij} J^{\mu}_{ij} W^{+}_{\mu} + V^{\dagger}_{ij} J^{\mu\dagger}_{ij} W^{-}_{\mu} \quad \right] \tag{1.1}$$

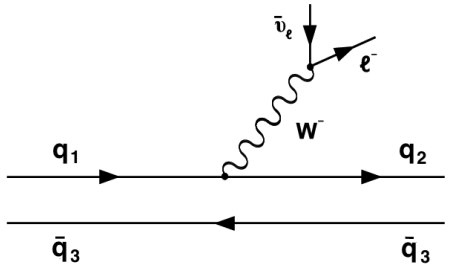

Figure 1.1: Semileptonic decay at tree level

$J^{ij}_{\mu} = \bar{u}_i \gamma_\mu \frac{1}{2}(1 - \gamma_5) d_j$ are the weak currents, $\underline{u} = (u, c, t)$ and $\underline{d} = (d, s, b)$ are the quark fields, g is the weak coupling constant, $W^{\pm}$ are the charged weak bosons, and V is the (unitary) Cabibbo-Kobayashi-Maskawa (CKM) matrix. V_{ij} can be thought of as a matrix of couplings which dictate the probability

of mixing between two quark flavours, for example the amplitude of a b decaying to a u (and emitting a W) is proportional to $V_{13} \equiv V_{ub}$.

A semileptonic decay is any $hardon \to hadron + leptons$ process. Fig. 2.1 shows the tree level (in weak coupling) contribution to a semileptonic decay. We denote a meson with valence quark content q and q' as $M_{qq'}$. The $M_{q_1\bar{q}_3} \to M_{q_2\bar{q}_3} l\bar{\nu}_l$ decay (l is some charged lepton and $\bar{\nu}_l$ is it's neutrino) is proportional to $V_{q_1q_2}$ at tree level.

This is given by

$$\mathcal{M} = \left(\frac{ig}{\sqrt{2}}\right)^2 V_{q_1q_2} \langle M_{q_2\bar{q}_3}, l\bar{\nu}| J_\alpha^{q_1\bar{q}_2} D_W^{\alpha\beta}(p^2) J_\beta^{l\bar{\nu}} |M_{q_2\bar{q}_3}\rangle \tag{1.2}$$

$J^{l\bar{\nu}}$ is the analog of the quark currents $J^{q_1\bar{q}_2}$, since the W couples in the same way to leptons (with V replaced by a unit matrix). If the external momenta of the process p^2 are much smaller than the W mass, one can remove the W propagator from the tree level amplitude [3];

$$\left(\frac{ig}{\sqrt{2}}\right)^2 D_W^{\mu\nu}(p^2) = \left(\frac{ig}{\sqrt{2}}\right)^2 \left(\frac{-ig^{\mu\nu}}{p^2 - M_W^2}\right) = \underbrace{\frac{i}{M_W^2}\left(\frac{ig}{\sqrt{2}}\right)^2}_{\equiv -2\sqrt{2}G_F} g^{\mu\nu} + \mathcal{O}\left(\frac{p^2}{M_W^4}\right) \tag{1.3}$$

Then $\mathcal{M}$ can be factorised;

$$\begin{aligned}
\mathcal{M} &\simeq -2\sqrt{2}G_F V_{q_1q_2} \langle M_{q_1\bar{q}_3}, l\bar{\nu}| J_\mu^{q_1\bar{q}_2} J^{l\bar{\nu}\mu} |M_{q_2\bar{q}_3}\rangle \\
&= -2\sqrt{2}G_F V_{q_1q_2} \langle l\bar{\nu}| J^{l\bar{\nu}\mu} |0\rangle \langle M_{q_1\bar{q}_3}| J_\mu^{q_1\bar{q}_2} |M_{q_2\bar{q}_2}\rangle \\
&\equiv -2\sqrt{2} V_{q_1q_2} G_F L^\mu H_\mu.
\end{aligned} \tag{1.4}$$

L_μ can be computed in perturbation theory. The hadronic matrix element H_μ however, due to the non-perturbative nature of QCD at low energies, cannot be computed analytically. It is quantities such as H_μ that we wish to calculate in lattice QCD.

Speaking heuristically, if one can calculate the quantity $G_F L^\mu H_\mu$ from theory, and measures the amplitude of the process $\mathcal{M}$, they could then rearrange equation (1.4) to deduce $V_{q_1q_2}$. Speaking more practically, the relevant equation is, for example, for the $B_s \to D_s l\nu$ decay [1]:

$$\frac{d\Gamma}{dq^2} = \eta_{\mathrm{EW}} \frac{G_F^2 |V_{cb}|^2}{24\pi^3 M_{B_s}^2} \left(1 - \frac{m_l^2}{q^2}\right)^2 |\underline{p}| \tag{1.5}$$

$$\times \left[\left(1 + \frac{m_l^2}{2q^2}\right) M_{B_s}^2 |\underline{p}| f_+^2(q^2) + \frac{3m_l^2}{8q^2}(M_{B_s}^2 - M_{D_s}^2)^2 f_0^2(q^2)\right] \tag{1.6}$$

where m_l is the mass of the charged lepton, η_{EW} is an electroweak correction factor, q^2 is the momentum transfer, $d\Gamma/dq^2$ is the branching fraction, and $f_{0,+}(q^2)$ are the form factors associated with the decay, to be defined in **??**. Given experimental data for $d\Gamma/dq^2$ and theoretical data for $f_{0,+}(q^2)$, one can deduce $|V_{cb}|$.

What is the value of determining CKM elements? Firstly, uncertainty in CKM elements are the dominant error in many standard model predictions. V elements can also test the standard model. V is unitary by definition. However, if there were more than 3 generations of quark, requiring V to be 4x4 or larger, the 3x3 submatrix which couples the 3 known generations would not itself be unitary in general ([4] ch. 29). Therefore, if one can deduce the elements of the 3x3 V to high enough precision to show it is not unitary, this would be indirect evidence for new physics.

Unitarity imposes a constraint on each row of V. The current status of the unitarity of V can be read off from below (each quantity should be zero for unitarity to hold) [5]:

$$\begin{aligned} |V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2 - 1 &= -0.020(9) \\ |V_{cd}|^2 + |V_{cs}|^2 + |V_{cb}|^2 - 1 &= 0.06(3) \end{aligned} \tag{1.7}$$

both of the above relations display a $\sim 2\sigma$ deviation from unitarity. More precise values of these parameters are needed to discover if CKM is infact non-unitary.

Now we consider $|V_{cb}|$ specifically. $|V_{cb}|$ is the dominant uncertainty in many standard model predictions of rare decays, such as $B_s \to \mu^+\mu^-$,$K \to \pi\nu\bar{\nu}$, and the CP violation parameter ϵ_K [1]. The FLAG working group quotes their average $|V_{cb}|$ to currently be [5]:

$$|V_{cb}| = 0.04085(95) \tag{1.8}$$

However, the water is slightly muddied by the presence of tensions between different determinations of $|V_{cb}|$, namely between that deduced from studying $B \to D^* l\nu$, and an inclusive analysis of $B \to X_c l\nu$ where X_c is any meson containing a c quark [1]:

$$|V_{cb}|_{\text{inclusive}} = 0.04221(78) \ , \ |V_{cb}|^{B\to D^* l\nu} = 0.03904(49)_{\text{expt.}}(53)_{\text{QCD}}(19)_{\text{QED}} \tag{1.9}$$

A recent review of $|V_{cb}|$ determinations from the lattice is given in [6]. This issue would benefit from a $|V_{cb}|$ determination from annother channel, like $B_s \to D_s l\nu$,

to flesh out the landscape of $|V_{cb}|$ values and pinpoint the source of the tension, if there is any.

1.2.3 Flavour Anomalies

There are a number of tensions currently between theory and experiment in B decays, who's true nature can be eludicated by our $B_s \to D_s l\nu$ study, and eventual $B \to Dl\nu$ study.

Define the ratios

$$R(X) = \frac{\mathcal{B}(B \to X\tau\nu_\tau)}{\mathcal{B}(B \to Xl\nu_l)} \tag{1.10}$$

where $l = e$ or μ. These can be computed either purely from a lattice calculation, or purely from experimental data, independantly of the associated CKM element. It therefore can be used for comparison between experiment and the standard model. $R(D^*)$ contains a 2.1σ discrepancy [7]:

$$R(D^*)|_{\text{SM}} = 0.252(3)\ ,\ R(D^*)|_{\text{LHCb}} = 0.336(27)_{sys}(30)_{stat} \tag{1.11}$$

The issue is similarly present for $R(D)$ [8]:

$$R(D)|_{\text{SM}} = 0.299(7)\ ,\ R(D)|_{\text{exp}} = 0.391(28)_{sys}(41)_{stat} \tag{1.12}$$

where in this case $R(D)|_{\text{expt}}$ is a world average of experimental values. Our eventual study of $B \to Dl\nu$ will produce a new standard model determination of $R(D)$, helping shed light on the issue.

Besides these, there are also tensions in the quantitites [9]:

$$R'(K^{(*)}) = \frac{\mathcal{B}(B \to K^{(*)}\mu^+\mu^-)}{\mathcal{B}(B \to K^{(*)}e^+e^-)} \tag{1.13}$$

All of the above anomalies are suggestive of lepton flavour violating effects. Various BSM models have been suggested; hot topics include Leptoquarks, Z' models, and partial compositeness [9].

1.2.4 Lepton Flavour Violation

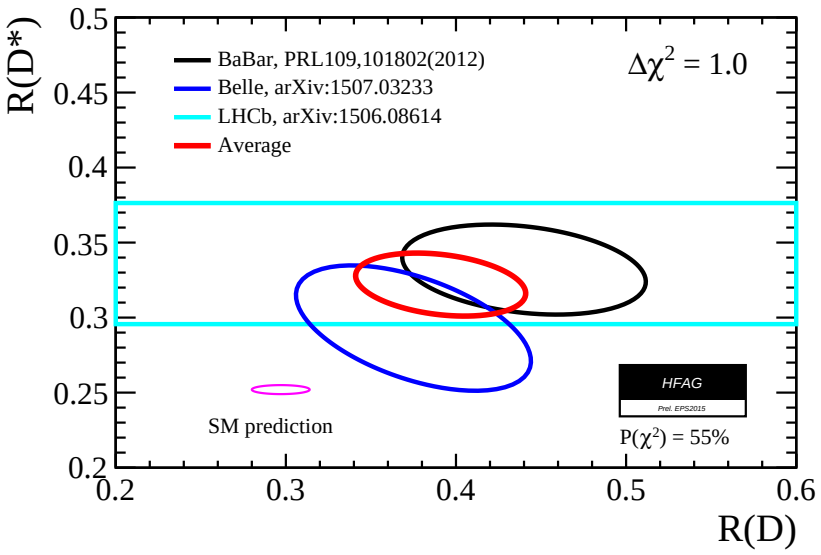

Figure 1.2: $R(D)/R(D^*)$ determinations from standard model and experiment [**?**]

Chapter 2

Heavy Semileptonic Decays

In this chapter we will review the key physical principles and theoretical machenery one needs to understand semileptonic decays involving heavy quarks. The presence of hadrons in these processes neccessitates an introduction to strong interaction physics. The presence of heavy quarks offers us extra theoretical leverage to divide and conquer the different relevant scales of the decays.

2.1 Form Factors

The goal of this work is to compute the transition amplitudes that make up the non-perturbative part of semileptonic decays, i.e. $H_\mu = \langle H_2|J_\mu|H_1\rangle$, where $H_{1,2}$ are initial and final meson states and J_μ is a current representing the emission of a $W^\pm$.

We will refer to the 4-momenta and mass of the initial and final states as $p_{1,2}, M_{1,2}$ respectively, and define the 4-momentum taken away by the $W^\pm$ boson as $q \equiv p_2 - p_1$. We work in the rest frame of the initial meson, in which

$$q^2 = M_1^2 + M_2^2 - 2M_1E_2. \tag{2.1}$$

There is a physically allowed range of values for an on-shell q^2. The minimum is when all of the 3-momentum of the initial state is taken by the final meson, $q^2_{\text{min}} = 0$. q^2 is maximised when all of the 3-momentum is taken by the boson, $\underline{p}_2^2 = 0 \rightarrow E_2 = \sqrt{M_2^2 + \underline{p}_2^2} = M_2 \rightarrow q^2_{\text{max}} = M_1^2 - M_2^2 - 2M_1M_2 = (M_2 - M_1)^2$. So

$$0 \leq q^2 \leq (M_2 - M_1)^2 \tag{2.2}$$

This also creates an allowed range for the final meson 3-momentum:

$$0 < \underline{p}_2^2 < \left(\frac{M_1^2 + M_2^2}{2M_1}\right)^2 - M_2^2 \tag{2.3}$$

To make the connection with experiment, H_μ must be expressed in terms of Lorentz-invariant factors, known as *form factors*. The current operator between between the states is a conserved current, so then the matrix element must be proportional to only conserved quantities, namely, elements of the stress-energy tensor. Lorentz invariance requires indices on either side of such a relation match, so a matrix element with a single Lorentz index can only be proportional to 4-momenta.

There are two cases of interest: the pseudoscalar $\to$ pseudoscalar and pseudoscalar $\to$ vector. Let us consider the first case first, with a the insertion of a left-handed current representing an emission of a $W^\pm$. From eq. (weak decays section), the coupling of quarks q_1 and q_2 to the $W^\pm$ is given by $L_\mu = \bar{q_2}\gamma_\mu \frac{1}{2}(1-\gamma_5)q_1$. This can be written as $L_\mu = V_\mu - A_\mu$, these are the vector and axial vector currents.

The axial vector evaluated between two pseudoscalar states must vanish because the combination is not parity invariant thus does not contribute in pure QCD, leaving just the vector current. The most common parameterisation used in the experiment community is:

$$\langle P_2(p_2)|V^\mu|P_1(p_1)\rangle = f_+(q^2)\left[p_1^\mu + p_2^\mu - \frac{M_1^2 - M_2^2}{q^2}q^\mu\right] + f_0(q^2)\frac{M_1^2 - M_2^2}{q^2}q^\mu \quad (2.4)$$

Where $|P_i(p_i)\rangle$ is a pseudoscalar meson state with momentum p_i.

2.1.1 Analyticity

2.1.2 z-Expansion

2.2 Strong Interaction Physics

It has been pretty much established that the strong interaction, and the observed pattern of hadrons, can be explained with a non-abelian Yang-Mills field and a number of flavours of fermions (quarks) that interact with it [SO MUCH EVIDENCE]. In this section we review the main features of the fundemental theory, along with a useful effective theory for describing dynamics at the hadron level.

2.2.1 Quantum Chromodynamics

Quantum Chromodynamics (QCD) is defined to be the $SU(3)$ Yang-Mills gauge theory. The Lagrangian is derived by requiring:

- N_f fermion fields transforming in the fundemental representation of an $SU(3)$ gauge group.
- Invariance under that gauge group.
- Renormalizability of all interactions.

From these we find [4]

$$\mathscr{L}_{\text{QCD}} = \sum_f \bar{q}_f(i\not{D} - m_f)q_f - \frac{1}{4}\text{Tr}G_{\mu\nu}G^{\mu\nu} - g\frac{\bar{\theta}}{64\pi^2}\epsilon^{\mu\nu\rho\sigma}\text{Tr}G_{\mu\nu}G_{\rho\sigma} \tag{2.5}$$

$$D_\mu = \partial_\mu - igG_\mu \tag{2.6}$$

$$G_{\mu\nu} = [D_\mu, D_\nu] \tag{2.7}$$

$q_f = (q_{f,r}, q_{f,b}, q_{f,g})$ are the N_f fermions, transforming under $q_f(x) \to U(x)q_f(x)$, $\bar{q}_f(x) \to \bar{q}_f(x)U^\dagger(x)$ where $U(x)$ is an $SU(3)$ matrix. G_μ are the $\mathfrak{su}(3)$-valued gluon fields, transforming under $G_\mu(x) \to U(x)G_\mu(x)U^\dagger(x) - i/g[\partial_\mu U(x)]U^\dagger(x)$. g is the coupling constant of the theory, often expressed instead as $\alpha_s = (g/4\pi)^2$. $\bar{\theta}$ has strong experimental bounds on it's size, to the extent for our purposes it can be neglected [10].

The most notable feature of QCD is due to the running of the QCD coupling α_s [11]. In contrast with the electroweak force, the coupling of the strong force diverges at low energies. This is referred to as *asymptotic freedom*. At energies at and below $\Lambda_{\text{QCD}} \sim 0.3\text{GeV}$, α_s becomes too large to be a good expansion parameter, and perturbation theory becomes unreliable for making predictions.

At large α_s, quarks and gluons become strongly interacting, this is beleived to be the source of confinement, the mechanism that bounds quarks together into hadrons. A common assumption then is that all of the dynamics that occurs inside hadrons have energies on the scale of Λ_{QCD}.

We arrive at the conclusion that processes involving hadrons cannot be understood using the traditional method of perturbation theory. Broadly speaking there are two alternative approaches:

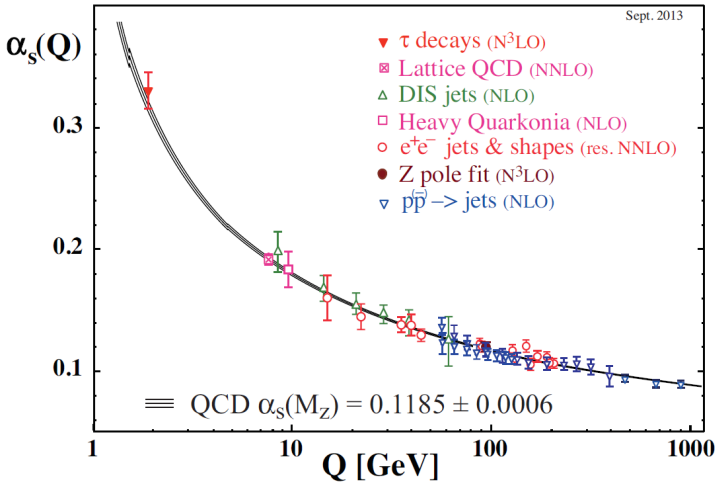

Figure 2.1: The relationship between scale Q and the strong coupling constant α_s, from the Particle Data Group [**?**]

1. Chiral Perturbation theory - an effective theory of hadrons with the same symmetry properties as QCD. This will be introduced in the next section.

2. Lattice simulations - solve the path integral by brute force, eliminating the need for an expansion in α_s. This is covered in sections 3 and 4, since it is the method used in the work presented in this thesis.

2.2.2 Chiral Symmetry

In the limit of $m_f \to 0, \forall f$, QCD develops two new global symmetries between the flavours;

$$q_f(x) \to \exp(i\theta_a \lambda_a^{ff'}) q_{f'}(x) \tag{2.8}$$

$$q_f(x) \to \exp(i\gamma_5 \theta_a \lambda_a^{ff'}) q_{f'}(x) \tag{2.9}$$

where λ_a are $U(N_f)$ matrices. They are labelled $U(N_f)_V$ and $U(N_f)_A$ respectively, standing for vector and axial. Each of these groups can be decomposed into $U(1)_{V/A} \times SU(N_f)_{V/A}$, the $U(1)$ contains the single element corresponding to $\lambda_a = 1$, and $SU(N_f)$ contains the elements where λ_a are $SU(N_f)$ generators. Neccesary? In the below we will take $N_f = 3$ when discussing physical aspects of the symmetry, since in the regeime where chiral symmetry is important, the heavier three quarks do not effect the dynamics.

Via Noether's theorem, these symmetries imply currents that are conserved in the massless limit [?];

$$V_\mu^a = \bar{q}\gamma_\mu\lambda_a q \quad , \quad \partial^\mu V_\mu^a = i\bar{q}[M,\lambda_a]q \tag{2.10}$$

$$A_\mu^a = \bar{q}\gamma_\mu\gamma_5\lambda_a q \quad , \quad \partial^\mu A_\mu^a = i\bar{q}\{M,\lambda_a\}\gamma_5 q \tag{2.11}$$

where $M = \text{diag}(m_u, m_d, m_s, ...)$ acts on flavour. Since one can connect any two flavours via the $U(N_f)$ generators, one can build such currents charged with any combination of flavours from linear combinations of (2.10),(2.11), i.e.

$$V_\mu^{ff'} = \bar{q}_f\gamma_\mu q_{f'} \quad , \quad \partial^\mu V_\mu^{ff'} = i(m_f - m_{f'})S_{ff'} \tag{2.12}$$

$$A_\mu^{ff'} = \bar{q}_f\gamma_\mu\gamma_5 q_j \quad , \quad \partial^\mu A_\mu^{ff'} = i(m_f + m_{f'})P_{ff'} \tag{2.13}$$

where $S_{ff'} = \bar{q}_f q_{f'}$, $P_{ff'} = \bar{q}_f\gamma_5 q_{f'}$ are the scalar and pseudoscalar densities. The non-conservation equations in (2.12),(2.13) are examples of Ward identities.

A useful theorem [?] is that partially conserved currents (currents that become conserved when some parameter in the theory vanishes, like $V_\mu^{ff'}$ and $A_\mu^{ff'}$) require no renormalization. This comes in useful when matching operators between regularization schemes, and will be used in chapter N.

Spontanious Chiral Symmetry Breaking

Besides the explicit breaking of chiral symmetry by the quark masses, the $U(N_f)_A$ symmetry is also *spontaniously broken* by the QCD dynamics. This is to say that, while the Lagrangian still holds this symmetry, the ground state of the theory is not invariant under such transformations;

$$Q_A^a|0\rangle \neq 0 \tag{2.14}$$

where $Q_A^a = \int d^3x A_0^a(x)$ is the conserved charge associated with the axial symmetry, and therefore also the generator of that symmetry acting on the Hilbert space [?].

There are three pieces of evidence for this claim.

- Scalar quark condensate. Using the comutation relations of $U(N_f)_A$, and assuming $Q_V^a|0\rangle = 0$, one can show that (2.14) implies

$$\langle 0|\bar{u}u|0\rangle = \langle 0|\bar{d}d|0\rangle = \langle 0|\bar{s}s|0\rangle \neq 0 \tag{2.15}$$

  This value has been calculated in [?] to be ~ 290GeV.

- Lack of Parity Doubling. Q_A^a transforms states to states with opposite parity. If Q_A^a was unbroken we could say that $[Q_A^a, H] = 0$ (H is the Hamiltonian), and from this demonstrate a degeneracy between states of opposite parity that interact with the strong force, for example a degeneracy between scalar and pseudoscalar particles. However, Pseudoscalar particles are not even approximately degenerate to scalar particles [?].

- The Light Pseudoscalar Octet. Goldstone's theorem says that for every spontaniously broken generator, there should be a massless spin-zero excitation with the same quantum numbers as that generator (Goldstone boson). In the case of $N_f = 3$, 8 the broken Q_A^a's would lead to an octet of massless pseudoscalar particles. In the presence of explicit symmetry breaking by the quark masses, these pseudoscalars would not be massless but have small masses proportional to the quark masses (pseudo-Goldstone bosons). This is exactly what is observed: there is an octet of pions, kaons and η particles that have masses ($\sim$ 200MeV) much lower than any other states in QCD (e.g. the ρ meson, with mass $\sim$ 1GeV) ref!.

Chiral Perturbation Theory (χPT)

Chiral Perturbation Theory is an effective theory of the pseudo-Goldstone bosons in the massless limit. It is useful for lattice calculations as it gives us information about how observables in strongly interacting systems should vary with light quark mass. This can be used when extrapolations in light quark masses are performed. It is also a useful language for understanding finite volume effects in lattice simulations, since a finite volume will effect the lightest degrees of freedom in the system.

Terms in χPT are organized by number of derivatives acting on the fields, since we assume the excitations to have small masses (proportional to light quark masses), and are approximately on-shell.

Goldstone's theorem tells us that the (pseudo-)Goldstone bosons should have the same transformation properties under the chiral symmetry as the broken generators, in our case those of $SU(3)_A$. Using this, and the requirement that the theory should be $SU(3)_V$ invariant, we can write down the leading order Lagrangian (minimal number of derivatives):

$$\mathscr{L}_2 = \frac{f^2}{4}\mathrm{Tr}[\partial_\mu U \partial^\mu U^\dagger] \tag{2.16}$$

$$U = \exp\left(\frac{i}{f}\sum_{a=1}^{8}\lambda_a\phi_a\right) \tag{2.17}$$

λ_a are $SU(3)$ generators and ϕ_a are the eight Goldstone bosons.

Connections between χPT and QCD can be found by considering how external fields interact with either of the theories. For example, one can consider the quark masses in QCD as external scalar fields which couple to scalar currents $\bar{q}_f q_f$ and obtain a vev. One then asks: how would this field have to transform under the chiral symmetry for QCD to be $SU(3)_V$ invariant? So we are imagining $M = \mathrm{diag}(m_u, m_d, m_s, ...)$ is a field that transforms like

$$M \to \exp(i(1-\gamma_5)\theta_a\lambda_a) M \exp(-i(1+\gamma_5)\theta_b\lambda_b) \tag{2.18}$$

One then transitions into χPT and asks: what interactions between the Goldstone fields and M are allowed by $SU(3)_V$? The answer is

$$\mathscr{L}_M = \frac{f^2 B_0}{2}\mathrm{Tr}[MU^\dagger + UM^\dagger] \tag{2.19}$$

where B_0 is a new parameter of the theory. By comparing ground state energies of the two theories, i.e. $\langle 0|H_{\mathrm{QCD}}|0\rangle = \langle 0|H_{\chi\mathrm{PT}}|0\rangle$, one can identify $B_0 = \langle \bar{u}u\rangle/f^2$. By expanding $\mathscr{L}_M$ in powers of quark masses and $1/f$, one can find mass terms for the Goldstones. Three of the goldstones are mass eigenstates, with masses given by

$$M_{\pi^0}^2 = B_0(m_u + m_d) \tag{2.20}$$

$$M_{K^0}^2 = B_0\left(\frac{1}{2}m_u + \frac{1}{2}m_d + m_s\right) \tag{2.21}$$

$$M_\eta^2 = \frac{2}{3}B_0\left(\frac{1}{2}m_u + \frac{1}{2}m_d + 2m_s\right) \tag{2.22}$$

where π,K, and η correspond to the physical mesons π, K, η, since their masses approximately respect these relations. Other terms that come out of expanding

$\mathscr{L}_M$ become mixing terms between the ϕ_a's, via these we can identify the rest of the fields with physical mesons, resulting in

$$\begin{aligned} &\pi^0 = \phi_3 \qquad K^0/\bar{K}^0 = (\phi_6 \pm i\phi_7)/\sqrt{2} \qquad \eta = \phi_8 \\ &\pi^\pm = (\phi_1 \pm i\phi_2)/\sqrt{2} \qquad K^\pm = (\phi_4 \pm i\phi_5)/\sqrt{2} \end{aligned} \tag{2.23}$$

By a similar process one can deduce the Chiral currents in χPT, for example the axial current is given by $A^a_\mu = if^2\mathrm{Tr}[\lambda_a(U^\dagger\partial_\mu U - (\partial_\mu U)U^\dagger)]/4$. By computing $\langle 0|A^3_\mu|\pi^0\rangle = M_{\pi^0}f_{\pi^0}$, one can identify the parameter f to be equal to the Pion decay constant f_{π^0} at leading order in χPT.

Predictions in χPT can be systematically improved by including terms with more derivatives in $\mathscr{L}_{\chi\mathrm{PT}}$.

2.3 Heavy Quark Physics

Quarks with mass $m_Q >> \Lambda_{\mathrm{QCD}}$ are referred to as heavy quarks. Charm and bottom quarks are considered heavy: $\Lambda_{\mathrm{QCD}}/m_c \sim 1/4$, $\Lambda_{\mathrm{QCD}}/m_b \sim 1/14$. This separation of scales can come in very useful. They mean one can integrate out the degrees of freedom at m_Q, and still have a good description of the dynamics at Λ_{QCD}. As will be demonstrated, this does not mean totally removing the heavy quark from the theory.

The physical picture of a meson containing a heavy quark is very similar to that of a hydrogen atom. In the hydrogen atom, the nucleus has a mass much greater than the charactoristic energies of the electron and photons. One can treat the nucleus as a static source of electric charge, and solve to high precision the dynamics of the electron. The electron's behaviour is not affected by the mass or the spin of the nucleus. Similarly, one can consider a heavy quark in a meson to be a static source of color charge, and solve the Λ_{QCD} dynamics in it's presence. The mass and spin of the heavy quark does not effect the light degrees of freedom, this is the well understood *heavy quark symmetries*. The effective field theories introduced in this section gives us a framework to take this approximation and systematically correct for it.

2.3.1 HQET

Heavy Quark Effective Theory (HQET) is an effective field theory with the cutoff at the heavy quark mass m_Q, and terms organized in a series in $\Lambda_{\rm QCD}/m_Q$. Since at the b (and c) mass QCD is perturbative ($\alpha_s(m_Q) << 1$), one can match HQET to perturbative QCD at m_Q, then run the couplings of HQET down to produce useful predictions at the confinement scale.

It is a useful tool for when we perform extrapolations in heavy quark mass, as it supplies us with explicit expressions for the heavy quark mass dependance on various phenomenological quantities.

HQET Lagrangian

As a simple example, we will derive HQET for a single heavy quark interacting with gluons. The fermion part of the Lagrangian is

$$\mathscr{L}_{\rm QCD} = \bar{Q}(i\not{D} - m_Q)Q, \tag{2.24}$$

where Q is the heavy quark field. Define the heavy quark velocity v according to

$$v = \frac{p_Q}{m_Q}. \tag{2.25}$$

Now split Q into "heavy" and "light" components:

$$Q = h + H \quad : \quad h = \frac{1}{2}e^{-im_Q v\cdot x}(1+\not{v})Q \tag{2.26}$$

$$H = \frac{1}{2}e^{-im_Q v\cdot x}(1-\not{v})Q \tag{2.27}$$

with the important property

$$\not{v}h = h \quad \not{v}H = -H. \tag{2.28}$$

In terms of these new fields the Lagrangian becomes

$$\mathscr{L}_{\rm QCD} = i\bar{h}(v\cdot D)h - \bar{H}(i(v\cdot D) - 2m_Q)H + i\bar{h}\not{D}^{\perp}H + i\bar{H}\not{D}^{\perp}h. \tag{2.29}$$

where $v_\mu(v\cdot D)$ is the covariant derivative projected along the direction of v, and $D^\perp = D - v_\mu(v\cdot D)$ is the components perpendicular to v. In the rest frame of the heavy quark, $v = (1,0,0,0)$ so $v_\mu(v\cdot D)$ becomes the temporal derivative and $D^\perp$ the spacial. The physical interpretation of the above definition can be seen by

acting a spacial derivative on the definition of h, and by recognising $\partial Q = -ip_Q$, $\partial h = -ip_h$, we find that

$$p_Q = m_Q v + p_h \tag{2.30}$$

Since $p_h << p_Q$, we see that the quark's momentum is dominated by it's mass (the quark is close to on-shell), and the h field represents perturbations around on-shell due to interactions with the lighter degrees of freedom at Λ_{QCD}.

From (2.29), we see that h is a massless field and H has a mass of $2m_Q$. From this Lagrangian we can derive an equation of motion for H:

$$(i(v \cdot D) + 2m_Q)H = i\not{D}^{\perp} h, \tag{2.31}$$

with the solution

$$H = \frac{1}{i(v \cdot D) + 2m_Q} i\not{D}^{\perp} h = \frac{1}{2m_Q} \sum_{n=0}^{\infty} \frac{(-i(v \cdot D))^n}{2m_Q} \not{D}^{\perp} h. \tag{2.32}$$

By substituting this into the Lagrangian we arrive at

$$\mathscr{L}_{\text{HQET}} = i\bar{h}(v \cdot D)h - \bar{h}\not{D}^{\perp} \frac{1}{2m_Q} \sum_{n=0}^{\infty} \frac{(-i(v \cdot D))^n}{2m_Q} \not{D}^{\perp} h. \tag{2.33}$$

This can be found by a more rigorous proof by performing the Gaussian integration over the H field in the path integral ref!. Since we expect $v \cdot D \sim \Lambda_{\text{QCD}}$, we can interpret the infinite sum as a series in Λ_{QCD}/m_Q, and truncate it at some order. For example to $\mathcal{O}(\Lambda_{\text{QCD}}/m_Q)$, we have

$$\mathcal{L}_{\text{HQET}^1} = i\bar{h}(v \cdot D)h - \frac{1}{2m_Q} \bar{h}\not{D}^{\perp 2} h \tag{2.34}$$

Leading order HQET exhibits new symmetries not present in full QCD, known as the heavy quark symmetries. Since m_Q is not present in the leading order Lagrangian, there is a flavour symmetry - a set of N heavy quarks with the same v can be mixed via an $SU(N)$ symmetry. Similarly due to the absense of spin mixing matrices, a heavy quark has an $SU(2)$ spin symmetry. This builds up a physical picture of a heavy quark in a meson being a static colour charge, the dynamics at Λ_{QCD} is not effected by it's mass or spin.

Isgur-Wise Function

A consequence of heavy quark symmetry relevant to semileptonic decays are the Wigner-Eckart theorems. Consider a transition amplitude between two heavy pseudoscalar mesons:

$$\langle M(v)|\bar{h}\Gamma h|M(v')\rangle \tag{2.35}$$

The spin structure of $|M(v)\rangle$ is $\gamma_5(1-\not{v})$, this can be shown with the following argument. The state can be generally written as $|M(v)\rangle = \int d^4x d^4y f(x,y)\bar{h}(x)\gamma_5 q(y)|\Omega\rangle$ which, using $\not{v}h = h$, can be reexpressed as $|M(v)\rangle = \int d^4x d^4y f(x,y)\bar{h}(x)\gamma_5(1-\not{v})q(y)|\Omega\rangle/2$. Then via the spin symmetry, one can always rotate the h spin in the meson state such that it matches the spin of the current, i.e. $h_\alpha \bar{h}_\beta \to 1_{\alpha\beta} f(h,\bar{h})$. Then the amplitude can be written as

$$\langle M(v)|\bar{h}\Gamma h|M(v')\rangle = m_M Tr[\frac{1}{2}\gamma_5(1-\not{v})\Gamma\frac{1}{2}\gamma_5(1-\not{v}')\mathcal{M}(v,v')] \tag{2.36}$$

where $\mathcal{M}(v,v')$ can be any gamma-matrix valued function. The m_M factor comes from the relativistic normalization of the states. A general spin decomposition of this is

$$\mathcal{M}(v,v') = \xi_0(v\cdot v') + \not{v}\xi_1(v\cdot v') + \not{v}'\xi_2(v\cdot v') + \not{v}\not{v}'\xi_4(v\cdot v'). \tag{2.37}$$

Plugging this into (2.36), we can then write the amplitude in terms of a single function:

$$\langle M(v)|\bar{h}\Gamma h|M(v')\rangle = m_M Tr[\frac{1}{2}\gamma_5(1-\not{v})\Gamma\frac{1}{2}\gamma_5(1-\not{v}')]\xi(v\cdot v') \tag{2.38}$$

where $\xi(v\cdot v') = \xi_0(v\cdot v') + \xi_1(v\cdot v') - \xi_3(v\cdot v') - \xi_4(v\cdot v')$ is known as the Isgur-Wise function. For a general pair of mesons with spin structure $\mathcal{H}$,$\mathcal{H}'$, a transition amplitude between them with a heavy current insertion can always be written as

$$\langle \mathcal{H}|\bar{h}\Gamma h|\mathcal{H}'\rangle = \xi(v\cdot v')Tr[\bar{\mathcal{H}}\Gamma\mathcal{H}] + \mathcal{O}\left(\frac{\Lambda_{\rm QCD}}{m_Q}\right) \tag{2.39}$$

So all heavy semileptonic decays involving any combination of masses or spins are described by a single non-perturbative function, $\xi(v\cdot v')$. A couple of relevant examples are:

$$\langle D(v')|\bar{c_{v'}}\gamma^\mu b_v|\bar{B}(v)\rangle = \sqrt{m_B m_D}(v+v')^\mu\xi(v\cdot v') \tag{2.40}$$

$$\langle D^*(v')|\bar{c_{v'}}\gamma^\mu b_v|\bar{B}(v)\rangle = i\sqrt{m_B m_{D^*}}\epsilon^{\mu\nu\alpha\beta}\varepsilon^*_\nu v'_\alpha v_\beta\xi(v\cdot v') \tag{2.41}$$

$$\langle D^*(v')|\bar{c_{v'}}\gamma^\mu\gamma_5 b_v|\bar{B}(v)\rangle = \sqrt{m_B m_{D^*}}[\varepsilon^{*\mu}(v\cdot v'+1) - v'^\mu\varepsilon^*\cdot v]\xi(v\cdot v'). \tag{2.42}$$

Here we have subscripted the fields $c_{v'}$,b_v to specify the velocity used to separate those fields from the heavy components e.g. in eq. (2.26).

AG and Luke's Theorem

Luke's theorem, which can be derived from the Ademollo-Gatto (AG) theorem, tells us the leading order heavy quark mass dependance of form factors. First we will derive the AG theorem. We will follow the proof given in [12].

Consider the transition amplitude

$$\langle\alpha|Q_a|\beta\rangle \tag{2.43}$$

where Q_a is a conserved charge associated with some global symmetry $\mathcal{G}$, and $|\alpha\rangle$ and $|\beta\rangle$ belong to an irrep of $\mathcal{G}$. Imagine explicitly breaking the symmetry with a term like $\mathscr{L}_{\text{break}} = \lambda\mathcal{O}_{\text{break}}$. The states in the broken theory can be expressed as

$$|\beta\rangle = c_{\beta\beta}|\beta'\rangle + \sum_m c_{\beta m}|m'\rangle \tag{2.44}$$

$$\langle\alpha| = c^*_{\alpha\alpha}\langle\alpha'| + \sum_n c^*_{\alpha n}\langle n'|. \tag{2.45}$$

where primed states are states belonging to irreps of $\mathcal{G}$. Here $|m'\rangle$ can only be states that can be mixed with $|\beta\rangle$ by $\mathcal{O}_{\text{break}}$ via the broken dynamics of the theory, and similarly for $\langle n'|$ and $\langle\alpha|$. The transition amplitude becomes

$$\begin{aligned}\langle\alpha|Q_a|\beta\rangle = {} & c^*_{\alpha\alpha}c_{\beta\beta}\langle\alpha'|Q_a|\beta'\rangle \\ & + \sum_m c^*_{\alpha\alpha}c_{\beta m}\langle\alpha'|Q_a|m'\rangle \\ & + \sum_n c^*_{\alpha n}c_{\beta\beta}\langle n'|Q_a|\beta\rangle \\ & + \sum_m\sum_n c^*_{\alpha n}c_{\beta m}\langle n'|Q_a|m'\rangle\end{aligned} \tag{2.46}$$

The theorem applies to the situation where $|n'\rangle$ and $|m'\rangle$ live in different $\mathcal{G}$ irreps to $|\alpha\rangle$ and $|\beta\rangle$ (we assume $|\alpha\rangle$ and $|\beta\rangle$ to be in the same irrep otherwise the transition amplitude will always be zero). In this case the amplitudes in the second and third terms vanish. Now consider the order of the coefficients c_{nm}. We can assume that $c_{nm} = \mathcal{O}(\lambda)$ for arbitrary $n, m \neq \alpha, \beta$, since switching off the symmetry breaking by setting $\lambda = 0$ should cause $|\alpha\rangle$ and $|\alpha'\rangle$ to coencide. Then, using the normalization of the states $\sum_n |c_{\alpha n}|^2 = 1$, we find $c_{\alpha\alpha} = \sqrt{1 - \mathcal{O}(\lambda)^2} = 1 + \mathcal{O}(\lambda^2)$, and similarly for $c_{\beta\beta}$. Applying this to the two surviving terms in (2.46), we end up with

$$\langle\alpha|Q_a|\beta\rangle = 1 + \mathcal{O}(\lambda^2) \tag{2.47}$$

This is the AG theorem: if the current Q_a and the symmetry breaking therm $mathcalO$ act orthogonally on the states, the transition amplitude can have at most a second order correction in the symmetry breaking parameter.

Now we will apply this to HQET to produce Luke's theorem. Consider a transition including two heavy quarks (b and c). Then, the heavy quark symmetry is a spin symmetry for each flavour, and a flavour symmetry between them. The leading order spin symmetry breaking terms can be found from (2.34) to be

$$\frac{1}{4m_Q}\bar{h}\gamma^\mu\gamma^\nu F_{\mu\nu}h \tag{2.48}$$

for both $h = b$ and $h = c$. The leading order flavour breaking term is

$$\left(\frac{1}{2m_b} - \frac{1}{2m_c}\right)\frac{1}{2}\bar{h}\sigma_z \not{D}^{\perp 2}h \tag{2.49}$$

where now $h = (b, c)$ and the σ_z is the third pauli matrix acting on flavour. These terms cause states, for example $|B\rangle$ to mix with states $|n'\rangle$, each being of the order of at least one of the following: $1/2m_b$,$1/2m_c$, and $(1/2m_b - 1/2m_c)$. It can be shown ([12]) that the leading order symmetry breaking terms can only mix pseudoscalar and vector mesons with other irreps of the heavy quark symmetries. Hence, for example the example of the $B \to D$ transition, where

$$\langle D|\bar{c}\gamma_\mu b|B\rangle = 1 + \mathcal{O}\left(\epsilon_b^2\right) + \mathcal{O}\left(\epsilon_c^2\right) \tag{2.50}$$

$$+ \mathcal{O}\left((\epsilon_b - \epsilon_c)^2\right). \tag{2.51}$$

where we have now defined $\epsilon_h = 1/2m_h$. This implies the Isgur-Wise function ξ also has corrections of this order. As we move away from the infinite-mass limit, ξ becomes h_+, and h_- becomes non-zero. In this case we see that

$$h_+(q^2_{\text{max}}) = (1 + \mathcal{O}\left(\epsilon_b^2\right) + \mathcal{O}\left(\epsilon_c^2\right) \tag{2.52}$$

$$+ \mathcal{O}\left((\epsilon_b - \epsilon_c)^2\right)) \tag{2.53}$$

$$h_-(q^2_{\text{max}}) = (\mathcal{O}\left(\epsilon_b\right) + \mathcal{O}\left(\epsilon_c\right) + \mathcal{O}\left(\epsilon_b - \epsilon_c\right)) \tag{2.54}$$

Away from q^2_{max}, the velocities for the b and c quarks become different, resulting in a new flavour breaking term in the effective Lagrangian;

$$i\bar{c}(v - v') \cdot Dc \sim \mathcal{O}\left(1 - \frac{E_D}{M_D}\right) + \mathcal{O}\left(\frac{\not{p}_D}{M_D}\right) \tag{2.55}$$

where to deduce the orders we took the rest frame of the B meson. This results in extra corrections of these orders (raised to the second power) in the form factors.

Second Order Form Factors

The process in 2.3.1 of decomposing matrix elements into general expressions parameterized by non-perturbative functions can be extended beyond leading order in HQET. In [13] this process was continued to second order in $1/m_b$ and $1/m_c$ for $B \to D^{(*)}$ transitions. The form factors for general v, v' that are relevant to our work, were found to have the forms

$$h_+ = \xi + (\epsilon_b + \epsilon_c)L_1 + (\epsilon_b^2 + \epsilon_c^2)l_1 + \epsilon_b\epsilon_c\phi_1 \tag{2.56}$$

$$h_- = (\epsilon_c - \epsilon_b)L_4 + (\epsilon_c^2 - \epsilon_b^2)l_4 \tag{2.57}$$

$$h_{A_1} = \xi + \epsilon_c L_{25} + \epsilon_b L_{14} + \epsilon_c^2 l_{25} + \epsilon_b^2 l_{14} + \epsilon_c\epsilon_b\phi_2 \tag{2.58}$$

where, due to the normalization of the form factors for $m_c = m_b$ at q^2_{max};

$$L_1(q^2_{\text{max}}) = L_{25}(q^2_{\text{max}}) = L_{14}(q^2_{\text{max}}) = 0 \tag{2.59}$$

A calculation using the non-relativistic constituent quark model [**?**] estimates the factor $l_1(q^2_{\text{max}}) = -3m_q^2$ where q is the spectator of the decay.

Decay Constants

questions that still need answered:
1) how come the $\sqrt{m_b}$ from state normalizations don't appear in h_+ etc? 2) how much does the above stuff apply away from continuum limit?

2.3.2 NRQCD

An effective field theory closely related to HQET is Non-Relativistic QCD (NRQCD). This differs from HQET only by the power couting; instead of organizing terms in the Lagrangian according to their order in Λ_{QCD}/m, the terms are organized in terms of orders of the heavy quark's spacial velocity $v \sim p/m$ (where now $p = |\underline{p}|$). NRQCD is derived with the following process:

- Separate the quark and antiquark components of the heavy quark Q. Define the antiquark-free 2-component spinor h via $Q = e^{\underline{\gamma}\cdot\underline{\nabla}/2m}\begin{pmatrix} h \\ 0 \end{pmatrix}$ [14].
- Define power-counting by considering the expected expectation values of operators for heavy mesons [15]. The three relevant scales concerning the heavy meson are M,$p \sim Mv$ and $E_K \sim Mv^2$, where M is the meson mass, p the

spacial momentum and E_K the kinetic energy. By relating operators to these three scales, we deduce their order in v. Start with the normalization of a scalar current:

$$\langle M| \int d^3x h^\dagger(x) h(x) |M\rangle \sim 1 \tag{2.60}$$

where $|M\rangle$ is some heavy meson state. Since we expect the meson state to be localized in a region of size $1/p$, we can assert that

$$\int d^3x \sim \frac{1}{p^3} \tag{2.61}$$

from this and (2.60), we find $h \sim p^{3/2} \sim v^{3/2}$. The order of the derivative operator can be deduced from

$$E_K = \langle M| \int d^3x h^\dagger(x) \frac{\underline{D}^2}{2M} h(x) |M\rangle \tag{2.62}$$

to be $D \sim v$. Following such a chain of arguments, we can deduce the order in v of any operator.

- The Lagrangian to $\mathcal{O}(v^n)$ is then simply all of the operators satisfying the symmetries of QCD of orders below v^n, with some Wilson coefficients [15]. To $\mathcal{O}(v^6)$:

$$\begin{aligned}
\mathscr{L}_{\text{NRQCD}} = h^\dagger \Bigg(& iD_0 + \frac{\underline{D}^2}{2m} + c_1 \frac{\underline{D}^4}{m^3} + c_2 g \frac{\underline{D}\cdot\underline{E} - \underline{E}\cdot\underline{D}}{m^2} \\
& + c_3 ig \frac{\underline{\sigma}\cdot(\underline{D}\times\underline{E} - \underline{E}\times\underline{D})}{m^2} + c_4 g \frac{\underline{\sigma}\cdot\underline{B}}{m} \\
& f_1 g \frac{\{\underline{D}^2, \underline{\sigma}\cdot\underline{B}\}}{m^3} + f_2 ig \frac{\{\underline{D}^2, \underline{\sigma}\cdot(\underline{D}\times\underline{E} - \underline{E}\times\underline{D})\}}{m^4} + f_3 ig^2 \frac{\underline{\sigma}\cdot\underline{E}\times\underline{E}}{m^3} \Bigg) h \\
& + d_1 \frac{(h^\dagger H)(H^\dagger h)}{m^2} + d_2 \frac{(h^\dagger \underline{\sigma} H)\cdot(H^\dagger \underline{\sigma} h)}{m^2} \\
& + d_3 \sum_a \frac{(h^\dagger T^a H)(H^\dagger T^a h)}{m^2} + d_4 \sum_a \frac{(h^\dagger T^a \underline{\sigma} H)\cdot(H^\dagger T^a \underline{\sigma} h)}{m^2}
\end{aligned} \tag{2.63}$$

$\underline{E}$ and $\underline{B}$ are the chromoelectric and chromomagnetic fields, T^a are $SU(3)$ color generators, and H is the antiquark components of the heavy quark. The Wilson coefficients are fixed by perturbative matching to full QCD at the cutoff (the heavy quark mass, where QCD is perturbative), then the coefficients can be run down to the scale of interest.

Chapter 3

Lattice Quantum Chromodynamics

At low energies (∼200MeV and below), QCD becomes non-perturbative, in other words, the coupling α_s becomes $\mathcal{O}(1)$, and an expansion in α_s (as in perturbation theory) will not be dominated by the leading orders [4]. We require an alternative.

The expectation value of an observable $\mathcal{O}$ in a Yang-Mills theory can be expressed as a Euclidean path integral [16];

$$\langle \mathcal{O} \rangle = \int \mathcal{D}A\mathcal{D}\psi\mathcal{D}\bar{\psi}\mathcal{O}e^{-S[A,\psi,\bar{\psi}]}, \tag{3.1}$$

where A is a gauge field, $\psi(\bar{\psi})$ is an (anti)fermion field, S is the Euclideanised classical action, and $\mathcal{D}$ denotes integration over all configurations of a field. "Euclideanised" refers to a Wick rotation $t \to it$ in S. In the perturbative approach, we would expand exp(−interacting part of S) resulting in a power series in the gauge coupling populated by Feynman diagrams.

The other option is to instead carry out the integral directly. This can only be done numerically. Since it's not numerically feasible to carry out an infinite number of integrals, one must approximate spacetime as a discrete 4 dimensional lattice with spacing "a" between lattice sites, finite spacial volume L_x^3 and finite temporal extent L_t. The functional integral becomes

$$\int \mathcal{D}A\mathcal{D}\psi\mathcal{D}\bar{\psi} = \prod_n \int dU(x_n)d\psi(x_n)d\bar{\psi}(x_n), \tag{3.2}$$

where n is a 4-vector with integer components labelling the sites, and $x_n^\mu = an^\mu$. This has a second benefit which is to naturally regularize the theory with a momentum cutoff $\Lambda \sim 1/a$ [16]. The gauge field has been replaced with the gauge "link":

$$U_\mu(x) \equiv \exp\left(igaA_\mu\left(x + \frac{a\hat{\mu}}{2}\right)\right) \in SU(N_c), \tag{3.3}$$

g is the gauge coupling, $\hat{\mu}$ is a unit vector in the μ direction. Parameterizing the gauge fields this way is motivated by the geometrical interpretation of Yang-Mills theories on discrete spacetime and the requirement of exact gauge symmetry [17].

3.1 Lattice Gauge Fields

3.1.1 The Wilson Gauge Action

3.1.2 Improvements

3.2 Lattice Fermions

The interacting Dirac action is most naively discretised with

$$S_F = \sum_{x,\mu} \bar{\psi}(x)\gamma_\mu \nabla_\mu \psi(x) + m \sum_x \bar{\psi}(x)\psi(x), \tag{3.4}$$

where ∇_μ is the gauge covariant finite difference operator,

$$\nabla_\mu \psi(x) = \frac{1}{2a}(U_\mu(x)\psi(x+a\hat{\mu}) - U_\mu^\dagger(x-a\hat{\mu})\psi(x-a\hat{\mu})). \tag{3.5}$$

In appendix **??** we describe the doubling problem. This is the observation that the propagator for a fermion obeying (3.7), $M^{-1}(k)$ has the property

$$M^{-1}(k + \frac{\pi}{a}\zeta) = \gamma_{5\mu} M^{-1}(k) \gamma_{5\mu} \tag{3.6}$$

For 16 4-vectors $\zeta_\mu \in \mathbb{Z}_2$. This leads to 16 poles in the fermion specturm, therefore 16 distinct excitations (called *tastes*). We require a way of removing the 15 unphysical excitations.

3.2.1 The Doubling Problem

The interacting Dirac action is most naively discretised with

$$S_F = \sum_{x,\mu} \bar{\psi}(x)\gamma_\mu \nabla_\mu \psi(x) + m \sum_x \bar{\psi}(x)\psi(x), \tag{3.7}$$

where ∇_μ is the gauge covariant finite difference operator,

$$\nabla_\mu \psi(x) = \frac{1}{2a}(U_\mu(x)\psi(x+a\hat{\mu}) - U_\mu^\dagger(x-a\hat{\mu})\psi(x-a\hat{\mu})). \tag{3.8}$$

An issue arises with fermions on the lattice, known as the doubling problem. S_F is invariant under a so-called "doubling symmetry", which is generated by

$$\psi(x) \to \mathcal{B}_\mu \psi(x) \equiv (-1)^{x_\mu/a} \gamma_{5\mu} \psi(x) \tag{3.9}$$

$$\bar{\psi}(x) \to \psi(\bar{x}) \mathcal{B}_\mu^\dagger \equiv (-1)^{x_\mu/a} \bar{\psi}(x) \gamma_{5\mu}^\dagger \tag{3.10}$$

where $\gamma_{5\mu} = i\gamma_\mu\gamma_5$. The product space of these form a group of 16 elements $\{\mathcal{B}_\zeta\}$, labeled by vectors ζ with $\zeta_\mu \in \mathbb{Z}_2$ (e.g.the element $\mathcal{B}_0\mathcal{B}_1$ is labeled by $\zeta = (1,1,0,0)$).

The physical signifiance of this symmetry can be seen when we study it's effect on the action. First, notice that

$$\mathcal{B}_\mu \psi(x) = \gamma_{5\mu} \sum_k \tilde{\psi}(k) e^{i(k + \frac{\pi}{a}\hat{\mu})\cdot x} \tag{3.11}$$

$$= \gamma_{5\mu} \sum_k \tilde{\psi}(k - \frac{\pi}{a}\hat{\mu}) e^{ik\cdot x} \tag{3.12}$$

where k is a set of discrete 4-momenta. The action in momentum space can be written as

$$S = \sum_k \bar{\tilde{\psi}}(k) M(k) \tilde{\psi}(k) \tag{3.13}$$

after the operation of $\mathcal{B}_\mu$ it becomes

$$S \to \sum_k \bar{\tilde{\psi}}(x)(k) \gamma_{5\mu} M(k + \frac{\pi}{a}\hat{\mu}) \gamma_{5\mu} \tilde{\psi}(k) \tag{3.14}$$

Since we know S is invariant under this transformation, it must be true that $\gamma_{5\mu} M(k + \frac{\pi}{a}\hat{\mu}) \gamma_{5\mu} = M(k)$, and therefore

$$M^{-1}(k + \frac{\pi}{a}\hat{\mu}) = \gamma_{5\mu} M^{-1}(k) \gamma_{5\mu} \tag{3.15}$$

M^{-1} is the propagator for the fermion field, so 3.15 shows that the spectrum of the fermion is periodic, with a period of π/a. We expect a pole in $M^{-1}(k)$ where $k \sim m$, where m is the pole mass of the fermion, but there will now be a second pole at $m + \pi/a$. This will be around the natural cutoff imposed by the lattice $1/a$, and any higher poles like $m + 2\pi/a$ is far above the cutoff so will not contribute.

Generalizing this argument to all elements of the doubling symmetry, we see that

$$M^{-1}(k + \frac{\pi}{a}\zeta) = \gamma_{5\mu} M^{-1}(k) \gamma_{5\mu} \tag{3.16}$$

leading to 16 poles in the fermion specturm, therefore 16 distinct excitations (called *tastes*).

We now show that there are only 4 tastes in the staggered quark formalism. One can isolate a single taste by a block-scaling procedure:

$$\psi^{(\zeta)}(x_B) = \sum_{\delta x_\mu \in \mathbb{Z}_2} \mathcal{B}_\zeta \psi(x_B + \delta x) \tag{3.17}$$

For example, for $\zeta = 0$, it would only contain the original non-doubler taste, since all other poles at $|k| \sim \psi/a$ have been integrated out. For $\zeta \neq 0$, the $\mathcal{B}_\zeta$ operator pushes the ζ doubler to where the $\zeta = 0$ taste originally was in k space, then the blocking procedure integrates out the rest. Now writing this isolated taste in terms of χ we arrive at:

$$\psi^{(\zeta)}(x_B) = \sum_{\delta x_\mu \in \mathbb{Z}_2} \Omega(\delta x)\mathcal{B}_\zeta(0)\chi(x + \delta x) \tag{3.18}$$

Recall we set $\chi(x) = (\chi_1(x), 0, 0, 0)$. The product $\Omega(\delta x)\mathcal{B}_\zeta(0)$ is simply a product of gamma matrices, so can only serve to "scramble" the elements of χ. Then, in the staggered formalism, all 16 tastes $\psi^{(\zeta)}$ amount to only 4 distinguishable fermions: $(\chi_1, 0, 0, 0)$, $(0, \chi_1, 0, 0)$, $(0, 0, \chi_1, 0)$, $(0, 0, 0, \chi_1)$ (with factors of (-1) and i).

3.2.2 Staggered Quarks

There are a number of solutions to this problem. The most straightforward is to modify the action to push the mass of the unwanted tastes above the momentum cutoff, preventing it from effecting the dynamics ("*Wilson fermions*")([18] ch.6.2). However, actions of this type explicity break Chiral symmetry. Among other issues, this causes additive renormalization of the fermion mass, immensely complicating the renormalization procedure.

Annother approach, known as *staggered quarks*([18] ch.6.3), partially resolves the doubling issue while retaining chiral symmetry. This is the method we use in our study. Other notable approaches besides Wilson and staggered quarks include *domain wall* [19] and *overlap* [20] fermions.

The general idea of staggered fermions is the following. Redefine the fields

according to

$$\psi(x) = \prod_{\mu} (\gamma_\mu)^{x_\mu/a} \chi(x) \equiv \Omega(x)\chi(x) \tag{3.19}$$

In terms of the new spinor variables $\chi(x)$, the naive action (3.7) becomes

$$S_F = \bar{\chi}(x)[\alpha_\mu(x)\nabla_\mu + m]\chi(x) \tag{3.20}$$

where $\alpha_\mu(x) = (-1)^{\sum_{\nu<\mu} x^\mu/a}$. The action is now diagonal in spin, leading to 4 decoupled grassman variables with identicle actions and identicle coupling to the gauge field. As a result, χ propagators (on fixed gauge backgrounds) are spin diagonal:

$$M_\chi^{-1}(x,y)[U] = s(x,y)[U]\ 1_{\text{spin}} \tag{3.21}$$

One need only to include a single component of χ in a simulation (i.e. fix $\chi = (\chi_1, 0, 0, 0)$). Then they can compute $M_\chi^{-1}(x,y)[U]$ to obtain $s(x,y)$. Then, using the inverse of (3.19), $s(x,y)$ can be transformed to a propagator of the original spinors:

$$M_\psi^{-1}(x,y)[U] = s(x,y)[U]\Omega(x)\Omega^\dagger(y) \tag{3.22}$$

This is clearly computationally beneficial. But also, by shaving off the other spinor components, one reduces the number propagating degrees of freedom by a factor of 4. This cuts the number of tastes from 16 down to 4 (this is shown in appendix **??**).

The remaining multipilcity is tacked in 3 steps:

1. Ensure only one taste is created and destroyed in the propagator.
2. Minimize the interaction between tastes by modifying the action.
3. Remove contributions of extra tastes in the sea by taking $\det M \to \sqrt[4]{\det M}$ in (4.3).

Step 3 can be justified by the following - in the $a \to 0$ limit, $\det M$ tends to $(\det M^{(0)})^4$, where $M^{(0)}$ is the Dirac oprator for a single taste. Then, taking the 4th root (in principle) reduces the determinant to that of a sea containing 1 taste.

3.2.3 Highly Improved Staggered Quarks

Step 2 above is the guiding principle for the action we use in our study, the Highly Improved Staggered Quark action (HISQ).

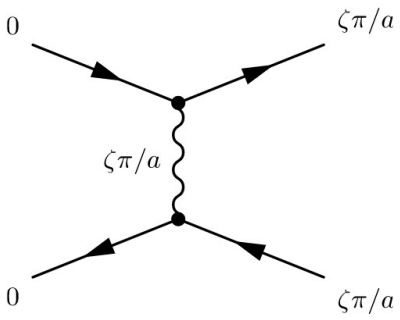

Figure 3.1: Taste mixing at tree level.

Interaction between different tastes ("taste mixing") is dominated by the process in fig. 3.1. In HISQ, this is suppressed by modifying the gauge fields in such a way as to minimize the coupling between a gluon with momentum π/a and the fermions, in other words, minimize the vertices in fig. 3.1. To this end, one can change the action so that fermions only couple to *smeared* gauge links, in which high frequency exitations have been removed.

Define the first and second covariant derivative operators:

$$\begin{aligned}\delta_\rho U_\mu(x) \equiv \frac{1}{a}\big(&U_\rho(x)U_\mu(x+a\hat{\rho})U_\rho^\dagger(x+a\hat{\mu}) \\ &- U_\rho^\dagger(x-a\hat{\rho})U_\mu(x-a\hat{\rho})U_\rho(x-a\hat{\rho}+a\hat{\mu})\big) \qquad (3.23)\\ \delta_\rho^{(2)} U_\mu(x) \equiv \frac{1}{a^2}\big(&U_\rho(x+a\hat{\rho})U_\rho^\dagger(x+a\hat{\mu}) \\ &- 2U_\mu(x) \\ &+ U_\rho^\dagger(x-a\hat{\rho})U_\mu(x-a\hat{\rho})U_\rho(x-a\hat{\rho}+a\hat{\mu})\big) \qquad (3.24)\end{aligned}$$

With this we can define the smearing operator;

$$\mathcal{F}_\mu = \prod_{\rho\neq\mu}\left(1+\frac{a^2\delta_\rho^{(2)}}{4}\right) \qquad (3.25)$$

HISQ uses two different smeared gauge fields defined by;

$$X_\mu(x) \equiv \mathcal{U}\mathcal{F}_\mu U_\mu(x) \qquad (3.26)$$

$$W_\mu(x) \equiv \left(\mathcal{F}_\mu - \sum_{\rho\neq\mu}\frac{a^2(\delta_\rho)^2}{2}\right)\mathcal{U}\mathcal{F}_\mu U_\mu(x) \qquad (3.27)$$

where $\mathcal{U}$ is a re-unitarization operator. The HISQ action can then be written as:

$$S_{\text{HISQ}} = \sum_x \bar{\psi}(x) \left(\gamma \cdot \left(\nabla_\mu(W) - \frac{a^2}{6}(1 + \epsilon_{\text{Naik}}) \nabla_\mu^3(X) \right) + m \right) \psi(x) \tag{3.28}$$

Where $\nabla_\mu(Z)$ is the covariant derivative (3.8) with gauge links repaced with Z. This action in fact not only removes tree level interactions like fig. 3.1, but also all taste mixing interactions at 1-loop. The ∇_μ^3 term is introduced to remove "lattice artifacts", i.e. it reduces the size of $\mathcal{O}(a)$ terms in the $a \to 0$ limit of the action. In the same spirit, ϵ_{Naik} is fixed according to the constraint

$$\lim_{\underline{p} \to 0} \frac{E^2(\underline{p}) - m^2}{\underline{p}^2} = 1 \tag{3.29}$$

where $E(\underline{p})$ obeys the dispersion relation from HISQ. The motivation for the specific smearing of the gauge fields (3.27), and more details on HISQ in general, are given in [21].

Chapter 4

Lattice Calculations

4.1 Correlation Functions from Lattice Simulations

A typical quantity that is computed on the lattice is a meson correlation function, i.e. when $\mathcal{O} = \Phi(x)\Phi^\dagger(y)$ and Φ is a meson creation operator. This is a good working example for showing the steps in a lattice calculation.

A creation operator for a meson in this context can be any operator containing the same quantum numbers as the meson one is trying to create. For example, the neutral B meson is a pseudoscalar charged with a d and $\bar{b}$ quark, so a suitable operator is $\Phi(x) = \bar{b}(x)\gamma_5 d(x)$. The path integral can then be written as

$$C(x,y) = \int \mathcal{D}\psi\mathcal{D}\bar{\psi}\mathcal{D}U \left(\bar{b}(x)\gamma_5 d(x)\bar{d}(y)\gamma_5 b(y) \right) e^{-S_G[U] - \sum_{w,z}\bar{\psi}(w)M(w,z)[U]\psi(z)} \tag{4.1}$$

where we have now broken the action up into a gauge part $S_G[U]$, and a fermion part. $M(x,y)[U]$ is the Dirac operator, and can be seen as a matrix in lattice site, flavor, color and spin. ψ is a vector of quark flavours.

The integral over fermions can be preformed analytically, since the fermion fields are Grassman valued. In our example, the result is [22],

$$C(x,y) = \int \mathcal{D}U \ \mathrm{Tr}\left[M_b^{-1}(y,x)[U]\gamma_5 M_d^{-1}(x,y)[U]\gamma_5 \right] e^{-S_G[U]}\det(M[U]) \tag{4.2}$$

The quantinties $M_f^{-1}(x,y)[U]$ are propagators of a quark of flavour f on a fixed gauge background U. The integration over gauge fields is generally carried out by an importance sampling method. A finite *ensemble* of gauge configurations $\{U_i\}$ is generated by a Monte Carlo Markov chain (MCMC), where the probability of a gauge configuration U_j being added to the ensemble is proportional to

$$e^{-S_G[U_j]}\det(M[U]) \tag{4.3}$$

See [18] ch. 7 for examples of such algorithms. In the case of our work, we use ensembles generated by the MILC collaboration [23].

Once the ensemble is created, the path integral can be approximated by simply

$$C(x,y) \simeq \frac{1}{N}\sum_i \text{ Tr } [\ M_b^{-1}(y,x)[U_i]\gamma_5 M_d^{-1}(x,y)[U_i]\gamma_5\ ] \tag{4.4}$$

where N is the size of the ensemble. The calculation of the correlation function then is split into 3 steps:

1. Generate an ensemble of Gauge configurations $\{U_i\}$ by MCMC.
2. Compute quark propagators $M_f^{-1}(x,y)[U]$ on each Gauge configuration. This requires inverting the matrix M each time, this is typically done by conjugate gradient method.
3. Construct trace as in (4.4), and average over the ensemble.

We now turn to the issue of choosing lattice actions.

4.1.1 Path Integral

4.1.2 Dirac Operator Inversion

4.1.3 Random Wall Sources

The full set of spin-mixing matrices can be labelled according to

$$\gamma_n = \prod_\mu (\gamma_\mu)^{n_\mu} \quad n_\mu = \mathbb{Z}_2 \tag{4.5}$$

There are 16 such matrices representing corners of the hypercube. As $\gamma_\mu^2 = 1$, one can also use a general site vector x_μ to label the matrix, then $\gamma_x = \gamma_n$ where $n_\mu = x_\mu \mod 2$. One can show that for any x; $\gamma_x^\dagger \gamma_x = 1$.

Naive quarks $\psi(x)$ can be transformed into staggered quarks $\chi(x)$ via $\psi(x) = \gamma_x \chi(x)$. Then, Naive quark propagators (inverse Dirac operators) become

$$G_\psi(x,y) = \gamma_x \gamma_y^\dagger G_\psi(x,y) \tag{4.6}$$

By conjugating both sides and using γ_5-hermiticity $G^\dagger_\psi(y,x) = \gamma_5 G_\psi(y,x)\gamma_5$ it can be shown that

$$G_\psi(x,y) = \phi_5(x)\phi_5(y)G^\dagger_\psi(y,x) \tag{4.7}$$

where $\phi_5(x) = (-1)^{\sum_\mu x_\mu}$.

2pt correlation functions

We will break down the correlation function to see what quantities must be computed by the simulation. Consider the generic 2-point correlator:

$$C(x,y) = \langle \Phi^\dagger_X(x)\Phi_Y(y)\rangle_{\psi,U} \quad , \quad \Phi_X(x) = \frac{1}{4}\bar{\psi}_a(x)\gamma_X\psi_b(x) \tag{4.8}$$

$$= \frac{1}{16}\langle tr_{c,s}\gamma_X G_{a,\psi}(x,y)\gamma_Y G_{b,\psi}(y,x)\rangle_U \tag{4.9}$$

$$= \frac{1}{16} tr_s\left(\gamma^\dagger_x\gamma_X\gamma_x\gamma^\dagger_y\gamma_Y\gamma_y\right)\langle tr_c\left(G_{a,\chi}(x,y)G_{b,\chi}(y,x)\right)\rangle_U \tag{4.10}$$

tr_s is a trace over spin and tr_c is over colour. To deal with the spin trace, define the family of phases $\{\phi_X(x)\}$ according to

$$\gamma^\dagger_x\gamma_X\gamma_x = \phi_X(x)\gamma_X \tag{4.11}$$

for example, if $X = 5$, then $\gamma^\dagger_x\gamma_5\gamma_x = (-1)^{\sum_\mu x_\mu}\gamma^\dagger_x\gamma_x\gamma_5 = \phi_5(x)\gamma_5$. The map from X to ϕ_X is structure preserving, i.e. if $\gamma_X = \gamma_A\gamma_B$, then $\phi_X(x) = \phi_A(x)\phi_B(x)$. The spin trace becomes $\phi_X(x)\phi_Y(y)tr_s\left(\gamma_X\gamma_Y\right)$. The will vanish unless $Y = X$, as one would expect physically for the correlation function. We end up with

$$C(x,y) = \frac{1}{4}\phi_X(x)\phi_X(y)\langle tr_c G_{a,\chi}(x,y)G_{b,\chi}(y,x)\rangle_U \tag{4.12}$$

It is useful in the simulation to replace $G_{b,\chi}(y,x)$ with it's conjugate via (4.7), resulting in

$$C(x,y) = \frac{1}{4}\phi_{5X}(x)\phi_{5X}(y)\langle tr_c G_{a,\chi}(x,y)G^\dagger_{b,\chi}(y,x)\rangle_U \tag{4.13}$$

where $\phi_{5X}(x) = \phi_5(x)\phi_X(x)$. To obtain the correlation function of a meson in an eigenstate with momentum $\underline{p}$, the above must be replaced with

$$C_{\underline{p}}(t_0,t) = \frac{1}{L^3}\sum_{\underline{x},\underline{y}} e^{i\underline{p}\cdot(\underline{x}-\underline{y})}C(\underline{x},t_0;\underline{y},t) \tag{4.14}$$

$$= \frac{1}{4L^3}\sum_{\underline{x},\underline{y}} e^{i\underline{p}\cdot(\underline{x}-\underline{y})}\phi_{5X}(x)\phi_{5X}(y)\langle tr_c G_{a,\chi}(x,y)G^\dagger_{b,\chi}(y,x)\rangle_U, \tag{4.15}$$

where it is understood that $x_0 = t_0$ and $y_0 = t$. In order to evaluate this function, the simulation must perform inversions to create $G_{a/b,\chi}(x,y)$ for each x and y, so 2·Vol^2 operations. This is prohibitively expensive. The number of inversions can be reduced using *random wall sources*. Define

$$P^{t_0}_{a,\underline{p},X}(y) \equiv \frac{1}{\sqrt{L^3}} \sum_{\underline{x}} e^{i\underline{p}\cdot(\underline{x}-\underline{y})} \phi_{5X}(\underline{x},t_0)\xi(\underline{x})G_{a,\chi}(\underline{x},t_0;y), \tag{4.16}$$

where $\xi(\underline{x})$ is a random field of colour vectors, varying with U. This has the property

$$\langle f(\underline{x},\underline{x}')\xi^*(\underline{x}')\xi(\underline{x})\rangle_U = \delta_{\underline{x},\underline{y}}\langle f(\underline{x},\underline{y})\rangle_U. \tag{4.17}$$

Using this property it can be shown that the correlator can be build instead according to

$$C(\underline{x},t_0;\underline{y},t) \simeq \frac{1}{4}\sum_{\underline{y}} \phi_{5X}(y)\langle tr_c P^{t_0}_{a,\underline{p},X}(\underline{y},t)P^{t_0,\dagger}_{b,\underline{0},1}(\underline{y},t)\rangle_U \tag{4.18}$$

Now all the simulation has to do is compute $P^{t_0}_{a/b}(y)$ for general y, so 2·Vol operations, a reduction by a factor of Vol.

In the MILC code, "sources" are first created (the fields $\phi_{5X}(\underline{x},t_0)\xi(\underline{x})$), then the objects $P^{t_0}(y)$ (referred to as "propagators") are generated from them. Any extra factors dependant on y (this is useful for "smeared" propagators, see ?) can be multiplied in. The resulting object $f(y)\cdot P^{t_0}(y)$ is referred to as a "quark". Finally, two of these quarks can be "tied together" according to (4.18), to produce correlation functions. The sources are chosen to be on some single timeslice t_0, resulting in a value for $C(t_0,t)$ at each t.

The above discussion can be generalized to 3−(or N−)point correlation functions using *extended sources*. Consider a 3-pt correlator encoding the form-factors of a semileptonic decay from meson X to meson Z, via a current J. We start by evaluating

$$C(x,y,z) = \langle \Phi^\dagger_X(x)J(y)\Phi_Z(z)\rangle_{\psi,U} \quad , \quad \begin{aligned} \Phi_X(x) &= \frac{1}{4}\bar{\psi}_b(x)\gamma_X\psi_s(x) \\ J(y) &= \bar{\psi}_b(y)\gamma_J\psi_a(y) \\ \Phi_Z(z) &= \frac{1}{4}\bar{\psi}_a(z)\gamma_Z\psi_s(z) \end{aligned} \tag{4.19}$$

in the same way as before:

$$C(x,y,z) = \frac{1}{16} tr_s \left(\gamma_x^\dagger \gamma_X \gamma_x \gamma_y^\dagger \gamma_J \gamma_y \gamma_z^\dagger \gamma_Z \gamma_z \right) \langle tr_c G_{b,\chi}(x,y) G_{a,\chi}(y,z) G_{s,\chi}(z,x) \rangle_U \tag{4.20}$$

$$= \frac{1}{4} \phi_{5X}(x) \phi_J(y) \phi_{5Z}(z) \langle tr_c G_{b,\chi}(x,y) G_{a,\chi}(y,z) G^\dagger_{s,\chi}(z,x) \rangle_U \tag{4.21}$$

We have assumed that $tr_s \gamma_X \gamma_J \gamma_Z = 4$, requiring that each gamma matrix in this combination has a partner and therefore cancels. In any other situation the trace would vanish. For example, if the current is a temporal vector $J = 0$, and the two mesons represent pseudoscalars, one of the meson operators must have a γ_0, i.e. one could choose $\gamma_X = \gamma_0 \gamma_5, \gamma_Z = \gamma_5$. why is it ok to have a non-goldstone for X?

Putting X into an eigenstate of zero momentum, and Y into an eigenstate of momentum $\underline{p}$, we get

$$C_{\underline{p}}(t_0,t,T) = \frac{1}{4L^3} \sum_{\underline{x},\underline{y},\underline{z}} e^{i\underline{p}\cdot(\underline{y}-\underline{z})} \phi_{5X}(x) \phi_J(y) \phi_{5Z}(z) \langle tr_c G_{b,\chi}(\underline{x},t_0;\underline{y},t) G_{a,\chi}(\underline{y},t,\underline{z},T) G^\dagger_{s,\chi}(\underline{z},T;\underline{x},t_0) \rangle_U \tag{4.22}$$

This can be built by first creating propagators for the b and s quarks: $P^{t_0}_{b,\underline{0},X}(y)$,$P^{t_0}_{s,\underline{0},1}(z)$. Then, build the a propagator using an extended source, i.e.:

$$P^T_{a,\underline{p},ext}(y) = \sum_{\underline{z}} P^{t_0}_{s,\underline{0},1}(\underline{z},T) \phi_{5Z}(\underline{z},T) G_{a,\chi}(\underline{z},T;y) \tag{4.23}$$

Then, by plugging $P^{t_0}_{b,\underline{0},X}(y)$ and $P^T_{a,\underline{p},ext}(y)$ into the MILC tie-together defined by (4.18),one ends up evaluating (4.22).

4.2 Analysis of Correlation Functions

4.2.1 Non-Linear Regression

Once a correlation function like the in **??** has been computed, we can extract physics from it, namely the mass and decay constant of the meson we are studying. In practice the meson creation operators defined above are fourier transformed

$$\Phi(\underline{k},t) = \sum_{\underline{x}} e^{-i\underline{k}\cdot\underline{x}} \Phi(\underline{x},t) \tag{4.24}$$

which serves to change (4.4) into

$$C_{\underline{k}}(t) = \frac{1}{N}\sum_{i}\sum_{\underline{x},\underline{y}} e^{-i\underline{k}\cdot(\underline{x}-\underline{y})}\ \mathrm{Tr}\left[\ M_b^{-1}(\underline{y},t;\underline{x},0)[U_i]\gamma_5 M_d^{-1}(\underline{x},0;\underline{y},t)[U_i]\gamma_5\ \right] \tag{4.25}$$

(4.25) is computed for many t values with a lattice calculation following the principles detailed above. One performs a least-squares fit of this to a theoretically motivated function of t. To derive such a function, first construct a complete set of momentum $\underline{k}$ states with quantum numbers matching the meson:

$$1 = \sum_{n=0}\frac{1}{2E_n^r}|\lambda_n\rangle\langle\lambda_n|. \tag{4.26}$$

Where $E_n^r = \sqrt{M_n^2 + \underline{k}^2}$ are the relativistic energies of each state. Inserting this into the correlation function, and moving from the Heisenberg to Schroedinger picture;

$$\begin{aligned} C_{\underline{k}}(t) &= \sum_{n=0}\frac{1}{2E_n^r}\langle 0|e^{Ht}\Phi(\underline{k},0)e^{-Ht}|\lambda_n\rangle\langle\lambda_n|\Phi^\dagger(\underline{k},0)|0\rangle \\ &= \sum_{n=0}\left(\frac{\langle 0|\Phi(\underline{k},0)|\lambda_n\rangle}{\sqrt{2E_n^r}}\right)\left(\frac{\langle\lambda_n|\Phi^\dagger(\underline{k},0)|0\rangle}{\sqrt{2E_n^r}}\right)e^{-E_n^l t} \\ &\equiv \sum_{n=0}|a_n|^2 e^{-E_n^l t}. \end{aligned} \tag{4.27}$$

The fit results in a determination of the parameters a_n, and E_n^l. Since the lowest energies dominate the function at late times, one can afford to truncate the sum over n to some tractable range, in our case $n \in [1,6]$. We interpret $|\lambda_0\rangle$ to be the ground state of the meson we are studying. The exponential decays mean the fit function is dominated by the ground state at large t, and subsequent excited states become less important as E_n^l increases. Hence by only including $C_{\underline{k}}(t)$ at suitably large t values, we can affort to truncate the sum in n. In our fits we chose $n = 6$.

We maintain a distinction between E^l and E^r, since for example in simulations involving NRQCD quarks these differ. If this is not an issue, as is the case with HISQ, one can compute the correlation function at zero momentum $C_{\underline{0}}(t)$, then fit it to find the parameter E_0^l, which will equal the meson's mass M. Noting the definition of a meson decay constant f: $\langle 0|J_0|\mathrm{Meson}(\underline{k}=0)\rangle = Mf$, where J_0 is a temporal current with the same quantum numbers as the meson, we can see that the fit parameters a_n at zero momentum are related to the meson's decay constant

via

$$f = \sqrt{\frac{2}{M}} a_0 \tag{4.28}$$

Hence the fit can also be used to extract decay constants.

The above discussion can be straightforwardly generalized to 3-point correlation functions, from which we are able to extract quantities like the hadronic transition amplitudes $H_\mu = \langle M_{q_1\bar{q}_3}|J_\mu^{q_1\bar{q}_2}|M_{q_2\bar{q}_2}\rangle$ from sec. **??**. Specifically the quantity we require in order to deduce the $B_s \to D_s l\nu$ form factors is $\langle D_s|V_\mu|B_s\rangle$, where $V_\mu = \bar{c}\gamma_\mu b$.

The generalization of the above for 3pt functions is summarized here:

$$C_3(t,T) = \int \mathcal{D}\psi\mathcal{D}\bar{\psi}\mathcal{D}U \left(\Phi_{D_s}(\underline{0},0) V_\mu(-\underline{p},t) \Phi^\dagger_{B_s}(\underline{p},T) \right) e^{-S[\psi,\bar{\psi},U]} \tag{4.29}$$

$$\simeq \frac{1}{N}\sum_i \sum_{\underline{x},\underline{y},\underline{z}} e^{-i\underline{p}\cdot(\underline{y}-\underline{z})} \text{ Tr}\left[M_b^{-1}(\underline{x},0;\underline{y},t)[U_i]\gamma_\mu M_c^{-1}(\underline{y},t;\underline{z},T)[U_i]\gamma_5\gamma_5 M_s^{-1\dagger}(\underline{z},T;\underline{x},0)[U_i] \right] \tag{4.30}$$

$$= \sum_{n,m} \left(\frac{\langle 0|\Phi_{D_s}|\lambda_n\rangle}{\sqrt{2E_n^r}} \right) \left(\frac{\langle \lambda_n|V_\mu|\lambda_m\rangle}{2\sqrt{E_n^r E_m^r}} \right) \left(\frac{\langle \lambda_m|\Phi^\dagger_{B_s}|0\rangle}{\sqrt{2E_n^r}} \right) e^{-E_m^l(T-t)} e^{-E_n^l t} \tag{4.31}$$

$$\equiv \sum_{n,m} a_{D_s,n} V_{nm} a^*_{B_s,m} e^{-E_m^l(T-t)} e^{-E_n^l t}.$$

$C(t,T)$ is computed at different values of t and T, then a least-squares fit is performed to the fit function (4.32). a_n will vanish for states $|\lambda_n\rangle$ which have different quantum numbers to Φ_{B_s}, and similarly for b_m and Φ_{D_s}. Non-zero a_n's will match the analagous parameters extracted from fitting a 2pt function $\langle \Phi^\dagger_{B_s}\Phi_{B_s}\rangle$, similarly for b_n's and Φ_{D_s}. This carries on to the energies, $\{E_n^l\}$ is the spectrum for the D_s meson, and $\{E_m^l\}$ is the spectrum for the B_s. Therefore, we compute and fit the appropriate 2pt functions to deduce the parameters $\{a_n\}$,$\{b_m\}$,$\{E_n^l\}$. Then, fitting $C_3(t,T)$ results in an accurate determination of the remaining free parameters, V_{nm}. This set contains the quantity we need, recoginising that:

$$V_{00} = \frac{\langle D_s|V_\mu|B_s\rangle}{2\sqrt{E^{B_s}E^{D_s}}} \tag{4.32}$$

2-point correlation functions are then fitted as in sec. **??**. The fit function we use

is modified a little from (4.27), we use:

$$C^{\alpha\beta}(t) = \sum_n a_n^{\alpha *} a_n^{\beta} (e^{-E_n^l t} - s e^{-E_n^l (T-t)}) + \sum_n a_n^{'\alpha *} a_n^{'\beta} (-1)^t (e^{-E_n^{'l} t} - s e^{-E_n^{'l} (T-t)}) \quad (4.33)$$

Firstly, the parameters $\{a_n\}$ must vary between source and sink to account for the different operators. Secondly, the periodicity of the lattice in the time direction means an extra exponential term is required, but not in the case of the B_s since NRQCD quarks do not experience the periodicity of the lattice. Hence s is set to 0 for the B_s correlator and 1 for the D_s. T is the time extent of the lattice. The second term is to account for the so-called "oscillating state", which is in fact the $\zeta = (1,0,0,0)$ doubler fermion appearing due to the doubling in the HISQ action (see sec. 3.15). No other doublers contribute, since $\Phi_{\underline{k}}$ has a 3-momentum fixed at $\underline{k}$, which we always take to be small relative to π/a, hence does not couple to the states at $k \sim (0, \pi/a, 0, 0)$, $k \sim (0, 0, \pi/a, 0)$ etc. However, $\Phi_{\underline{k}}$ can couple to arbitrarily high energy states, so the $k \sim (\pi/a, 0, 0, 0)$ doubler contributes. The second term in (4.33) is justified by performing the doubling operation $\mathcal{B}_0$ defined in (4.27), the quark fields in $\Phi_{\underline{k}}$ which obey the HISQ action. See appendix G of [21] for details.

We use the *CorrFitter* package [24] for performing Baysian least-squares fitting to the correlation functions. The package employs the trust region method of least-squares fitting. The fits require priors for each of the fit parameters. The "amplitude" parameters $a^{\alpha}_{n,B_s/D_s}$ are given priors of 0.1(1.0), thus inserting only the assumption that they are of $\mathcal{O}(1)$. The ground state energies are given priors motivated by the meson masses, and excited state energies are given loose, evenly spaced priors with 600MeV between each level.

2-point correlation functions for B_s and D_s are fit to (4.33), resulting in $a^{\alpha}_{n,B_s/D_s}$,$E^l_{n,B_s/D_s}$. Since the HISQ action is fully relativitstic, E^l_{0,D_s} at $\underline{k} = 0$ can be interpreted as the D_s meson mass. The same cannot be done for the B_s. The decay constants for B_s and D_s can be deduced from a^0_{0,B_s} and a^0_{0,D_s}, since $\Phi^0_{B_s,D_s}$ are also temporal axial currents. This is a good avenue for consistency checks, we compared $M_{D,s}$,f_{D_s} and f_{B_s} to those computed in [25], [8] amongst others, and found them to be consistent (modulo small shifts we can reasonably expect due to differing choices of bare quark masses).

We now discuss fitting the 3-point correlation functions. The same considerations as those that went into (4.33) lead us to our 3-point fit function:

$$\begin{aligned} C_3^{\alpha\beta}(t,T) = \sum_{k,m} \big(& a^{\alpha}_{k,D_s} V^{nn}_{km} a^{*\beta}_{m,B_s} e^{-E^l_m t} e^{-E^l_k (T-t)} \\ & + a^{\alpha}_{k,D_s} V^{no}_{km} a^{'*\beta}_{m,B_s} e^{-E'^l_m t} e^{-E^l_k (T-t)} \\ & + a^{'\alpha}_{k,D_s} V^{on}_{km} a^{*\beta}_{m,B_s} e^{-E^l_m t} e^{-E'^l_k (T-t)} \\ & + a^{'\alpha}_{k,D_s} V^{oo}_{km} a^{'*\beta}_{m,B_s} e^{-E'^l_m t} e^{-E'^l_k (T-t)} \big) \end{aligned} \tag{4.34}$$

The 2-point and 3-point correlators are fit simultaniously, according to fit functions (4.33) and (4.34). The parameters involved in the 2pt fits are mostly fixed by the data in the 2pt correlation functions, so the fit can use most of the data in the 3pt correlation functions to determine the transition amplitudes V^{ab}_{km}. This is carried out for each B_s and D_s smearing, each direction μ and each current correction i of the vector current $V^{(i)}_{\mu}$.

In this large 2pt/3pt fit, there is a huge χ^2 manifold with many local minema, and it is crucial to impose strong priors in order to ensure the fit finds the true minemum. Priors for ground state 2-point amplitudes and energies $a^{\alpha}_{0,B_s/D_s}$,$E^l_{0,B_s/D_s}$ are taken to be the results from individual fits of the 2-point functions, with the errors expanded by a factor of 2. The excited state amplitudes and energies are given the same priors as in the 2-point fits. The transition amplitueds V^{ab}_{km} are given the prior 0.1(1.0), assuming it to be $\mathcal{O}(1)$.

Finally, we end up with the sought-after parameters V^{nn}_{00} representing $V^{(i)}_{\mu}$, via the relation

$$\langle D_s | V^{(i)}_{\mu} | B_s \rangle = 2\sqrt{M^{B_s} E^{D_s}} V^{nn}_{00}|_{V = V^{(i)}_{\mu} \text{in simulation}} \tag{4.35}$$

We have asserted the ground state of B_s to be it's mass, but not the D_s, as we give D_s spacial momenta in the calculation (to be expanded on in the next section). Then, the full vector currents $\langle D_s | V^{(i)}_{\mu} | B_s \rangle$ can be build from a linear combination of these according to **??**.

4.2.2 Signal/Noise Ratio

One of the main obstacles in our calculation is the *signal degredation* of correlation functions computed on the lattice.

A random variable x has mean and standard deviation

$$\hat{x} = \langle x \rangle \tag{4.36}$$

$$\sigma^2 = \frac{1}{N}(\langle x^2 \rangle - \langle x \rangle^2), \tag{4.37}$$

where N is the size of the sample. So the (square of) the signal/noise ratio is

$$\frac{\hat{x}^2}{\sigma^2} = N \left(\frac{\langle x^2 \rangle}{\langle x \rangle^2} - 1 \right)^{-1}. \tag{4.38}$$

Consider 2 point correlators where $x = \Phi^\dagger(t)\Phi(0)$, where Φ is a meson operator with zero spacial momentum.

$\langle x^2 \rangle$ and $\langle x \rangle$ can be written as

$$\langle x \rangle = \sum_k \frac{1}{2E_n} \langle 0|\Phi^\dagger(t)|\lambda_n\rangle\langle\lambda_n|\Phi(0)|0\rangle e^{-E_n t} \simeq_{t\to\infty} e^{-E_0 t} \tag{4.39}$$

$$\langle x^2 \rangle = \sum_n \frac{1}{2E_n} \langle 0|\Phi^{\dagger 2}(t)|\lambda_n\rangle\langle\lambda_n|\Phi^2(0)|0\rangle e^{-E_n t} \simeq_{t\to\infty} e^{-E'_0 t} \tag{4.40}$$

where we have assumed the ratio of matrix elements and energies are $\mathcal{O}(1)$. The two ground state energies E_0 and E'_0 need not be the same, since the lowest states for which $\langle\lambda_n|\Phi(0)|0\rangle \neq 0$ and $\langle\lambda_n|\Phi^2(0)|0\rangle \neq 0$ may differ.

The operator Φ^2 will contain two quark and two antiquark operators, connected by some matrices in spin space. Φ^2 can create a combination of all possible 2 meson states where the mesons are made of the available quark species, and quantum numbers. For example, If Φ is a pion, Φ^2 is a 2 pion state, and $E'_0 = 2m_\pi$. If Φ is a D_s meson, then $E'_0 = m_{\tilde{\pi}} + m_{\eta_c}$ ($\tilde{\pi}$ is a pseudoscalar $s\bar{s}$ state).

Define $\mu_0 = E'_0/2$. Then

$$\frac{\hat{x}^2}{\sigma^2} \simeq N \left(e^{-2(\mu_0 - m_\Phi)t} - 1 \right)^{-1} \tag{4.41}$$

In the case of pions, $\mu_0 = m_\Phi$, the ratio becomes simply $\sim N$. For mesons heavier than the pion, $\mu_0 < m_\Phi$, so at large times $e^{-2(\mu_0 - m_\Phi)t} >> 1$, and upon taylor expanding the inverse of this phase we arrive at

$$\frac{\hat{x}}{\sigma} \simeq \sqrt{N} e^{-(m_\varphi - \mu_0)t} \tag{4.42}$$

From this we see there are 3 variables which effect the quality of the signal:

1. The size of the sample N.
2. At large t, the correlators undergo *signal degredation*, i..e, become dominated by noise.
3. The degree of signal degradation is decided by $m_\varphi - \mu_0$. Heavier mesons will tend to experience more signal degredation.

Relevant to our calculation is how giving mesons non-zero spacial momenta $\underline{p}$ can exaserbate this problem. In this case, m_Φ in (4.42) is replaced with $\sqrt{m_\Phi^2 + \underline{p}^2}$. As $\underline{p}$ increases, the signal/noise ratio will degrade more and more and statistics will suffer.

In the $B_s \to D_s l\nu$ calculation, to deduce form factors over the whole range of q^2 values, we need to simulate the process with the D_s having a range of momenta $0 < |\underline{p}| < 2.32$GeV, as discussed in sec. **??**. Correlation functions at the higher end of this range may be too noisy for any meanigful results to be extracted. We are investigating ways of taming this problem, see sec. **??**.

4.3 Dealing with Heavy Quarks

4.3.1 Heavy HISQ

4.3.2 Lattice NRQCD

4.4 Renormalization of Currents

Once one has computed a matrix element from a lattice calculation, it needs to be translated into a continuum regularization scheme. Suppose we have some bare operator $\mathcal{O}_0$, we expect this to be related to the renormalized operator in $\overline{MS}$ at scale μ, $\mathcal{O}^{\overline{MS}}(\mu)$, via

$$\mathcal{O}^{\overline{MS}}(\mu) = Z^{\overline{MS}}(\mu)\mathcal{O}_0. \tag{4.43}$$

Similarly, in a lattice regularization,

$$\mathcal{O}^{\text{lat}}(1/a) = Z^{\text{lat}}(1/a)\mathcal{O}_0. \tag{4.44}$$

Hence we expect a multiplicative factor between the lattice matrix elements, and the continuum $\overline{MS}$ ones:

$$\langle\mathcal{O}\rangle^{\overline{MS}} = \mathcal{Z}(\mu, 1/a)\langle\mathcal{O}\rangle^{\text{lat}} \tag{4.45}$$

where $\mathcal{Z}(\mu, 1/a) = Z^{\overline{MS}}(\mu)/Z^{\text{lat}}(1/a)$. These "matching factors" $\mathcal{Z}$ can be deduced by equating observables calculated in both lattice QCD and continuum (appropriately regularized) QCD, producing equations which can be solved for $\mathcal{Z}$. The lattice side of the calculation can be done either through lattice perturbation theory ("perturbative matching"), or through a simulation ("non-perturbative matching").

It is a well-known result that conserved (or partially conserved) currents do not receive any renormalization in any scheme, i.e. $Z^{\text{any}} = 1$ ("absolutely normalized").

In principle this is of great help, since the currents we are calculating, namely V_μ, are partially conserved, so we are not required to include any matching factors. However in practice, this is complicated by the fact that the conserved current in the lattice theory is often computationally difficult or impossible to compute. For example, in NRQCD, the partially conserved current corresponding to $SU(N)_V$ is an infinite sum in $1/m_b$ where m_b is the bottom mass. The corresponding current in HISQ is also the sum of a large number of operators. This can be interpreted as a mixing in the renormalization:

$$\langle \mathcal{O}_i \rangle^{\overline{MS}} = \mathcal{Z}_{i,j} \langle \mathcal{O}_j \rangle^{\text{lat}} \tag{4.46}$$

In practice, lattice calculations often use only the dominant operators that contribute to the conserved current. Since these will be "close" to the conserved current, one can expect the matching factor to only be a small deviation from unity, and the more sub-dominant operators you add, the overall matching factor should tend towards one.

4.4.1 Non-perturbative Renormalization of HISQ Currents

4.4.2 Matching NRQCD currents to $\overline{MS}$

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