

YETI 2023

How to use Lattice QCD to compute hadronic form factors

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Outline

- 1 – Lattice Preliminaries
- 2 – Naïvely Discretising the action
- 3 – Improved actions, Fermions and the Doubling Problem
- 4 – Computing and Fitting correlation functions
- 5 – Extracting Form Factors
- 6 – Getting to the physical Form Factors
- 7 – Checks of Stability

General introductory texts that I have found useful:

- Quantum Chromodynamics on the Lattice – Gattringer, Lang. Lecture Notes in Physics 788
- Quantum Fields on a Lattice - Montvay, Münster. Cambridge Monographs on Mathematical Physics
- Please also feel free to email me with any questions: judd.harrison@glasgow.ac.uk

Lattice Preliminaries

The two essential ingredients to lattice calculations.

The first relates the trace of a product of Euclidean operators to a sum over states:

$$Z_T = \text{tr}[e^{-T\hat{H}}] = \sum_M \langle M | e^{-T\hat{H}} | M \rangle = \sum_M e^{-TE_M}$$

$$\lim_{T \rightarrow \infty} \frac{1}{Z_T} \text{tr}[e^{-T\hat{H}} e^{t_n \hat{H}} \hat{O}_n e^{-t_n \hat{H}} \dots e^{t_1 \hat{H}} \hat{O}_1 e^{-t_1 \hat{H}}]$$

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Extract matrix elements, energies, from multi-exponential fits

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Naïvely Discretising the Fermion Action

In continuum QCD, the purely fermionic portion of the Euclidean action is

$$S_E^{Fermi}[\psi, \bar{\psi}] = \int dx^4 \bar{\psi}(x)(\gamma_E^\mu \partial_\mu + m)\psi(x), \quad \{\gamma_E^\mu, \gamma_E^\nu\} = 2 \delta^{\mu\nu}$$

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$$x \rightarrow ax_n, \quad x_n = (n_x, n_y, n_z, n_t); \quad n_{x,y,z} \in [0, N-1]; \quad n_t \in [0, N_T-1],$$

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$$S_E^{Fermi}[\psi, \bar{\psi}] \rightarrow S_E^{F, \text{latt}}[\psi_n, \bar{\psi}_n] = \sum_{x_n} a^4 \bar{\psi}(x_n) \left(\sum_{\mu} \gamma_E^\mu \left(\frac{\psi(x_n + \hat{\mu}) - \psi(x_n - \hat{\mu})}{2a} \right) + m\psi(x_n) \right)$$

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The gluonic portion of the continuum Euclidean action is

$$S_E^{g, \text{int}}[\psi, \bar{\psi}, A] = \int d^4x \frac{1}{2g^2} \text{tr}[F_{\mu\nu} F^{\mu\nu}] + \bar{\psi}(x) \gamma_E^\mu A_\mu \psi(x)$$

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$$\psi(x_n) \rightarrow \Omega(x_n) \psi(x_n), \quad \bar{\psi}(x_n) \rightarrow \bar{\psi}(x_n) \Omega^\dagger(x_n), \quad \Omega \in SU(3)$$

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The most straightforward way to do this is by adding in gauge links $U \in SU(3)$

$$D_\mu \psi(x) \rightarrow \nabla_\mu \psi(x_n) = \frac{U_\mu(x_n) \psi(x_n + \hat{\mu}) - U_\mu^\dagger(x_n - \hat{\mu}) \psi(x_n - \hat{\mu})}{2a},$$

transforming as

$$U_\mu(x_n) \rightarrow \Omega(x_n) U_\mu(x_n) \Omega^\dagger(x_n + \hat{\mu})$$

Naïvely Discretising the Gluon Action

The “gauge links” U_μ are related to Wilson lines,

$$G(x, y) = P \exp \left(i \int_{C_{x \rightarrow y}} A \cdot ds \right)$$

that act as gauge transporters

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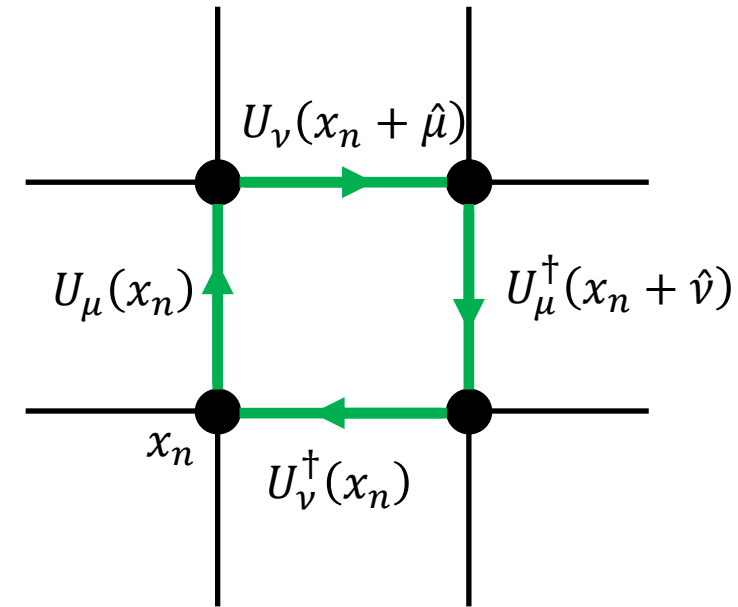
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The gauge action is built from gauge invariant traces of loops of gauge links, the simplest of which is the “plaquette”

$$U_{\mu\nu}(x_n) = U_\mu(x_n) U_\nu(x_n + \hat{\mu}) U_\mu^\dagger(x_n + \hat{\nu}) U_\nu^\dagger(x_n) = \exp(i a^2 F_{\mu\nu}^i + O(a^3))$$

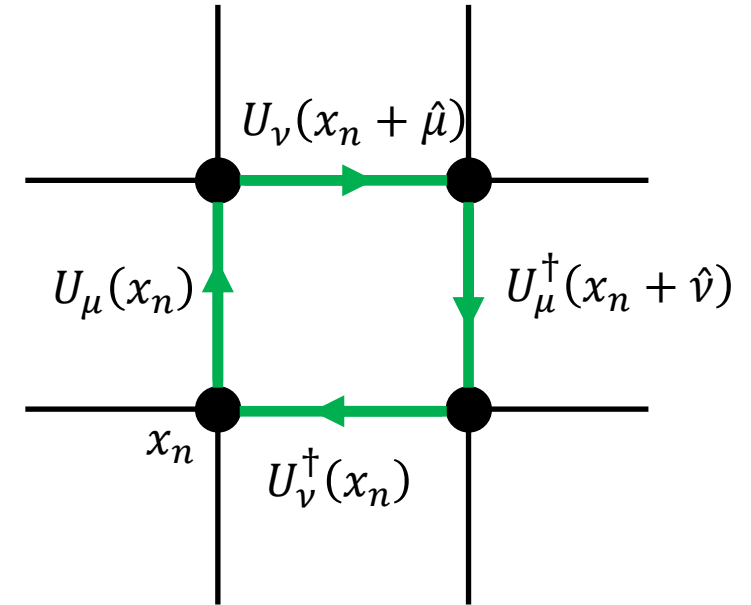
Naïvely Discretising the Gluon Action

Using the plaquette we can build a simple gluon action, called the “Wilson action”, that we expect to reproduce the continuum action in the limit $a \rightarrow 0$

$$\begin{aligned} S_U[U] &= \frac{2}{g^2} \sum_{x_n} \sum_{\mu < \nu} \text{Re}(\text{tr}[1 - U_{\mu\nu}(x_n)]) \\ &= \frac{a^4}{2g^2} \sum_{x_n} \sum_{\mu, \nu} \text{tr}[F_{\mu\nu}(x_n)^2] + O(a^2) \end{aligned}$$

Usual to identify $\beta = \frac{6}{g^2}$, so that

$$S_U[U] = \frac{\beta}{3} \sum_{x_n} \sum_{\mu < \nu} \text{Re tr}[1 - U_{\mu\nu}(x_n)]$$



Improving the Gluon Action

- Tadpole Improvement, [hep-lat/9507010](https://arxiv.org/abs/hep-lat/9507010)

In the quantum field theory, the expansion of the gauge links in powers of a

$$U_\mu(x_n) = \exp\left(iaA_\mu(x_n)\right) \approx 1 + iaA_\mu(x_n) - \left(aA_\mu(x_n)\right)^2 + i\left(aA_\mu(x_n)\right)^3 \dots$$

is complicated by the fact that loop integrals contribute divergences going as powers of $1/a^2$. As such a term which naively is of $O(\alpha_s^n a^{2n} a^m)$ can generate contributions $O(\alpha_s^n a^m)$.

Fortunately, these effects are process independent, and can be removed by taking

$$U_\mu \rightarrow U_\mu/u_0$$

where u_0 is the tadpole improvement factor.

Improving the Gluon Action

- Symanzik Improvement

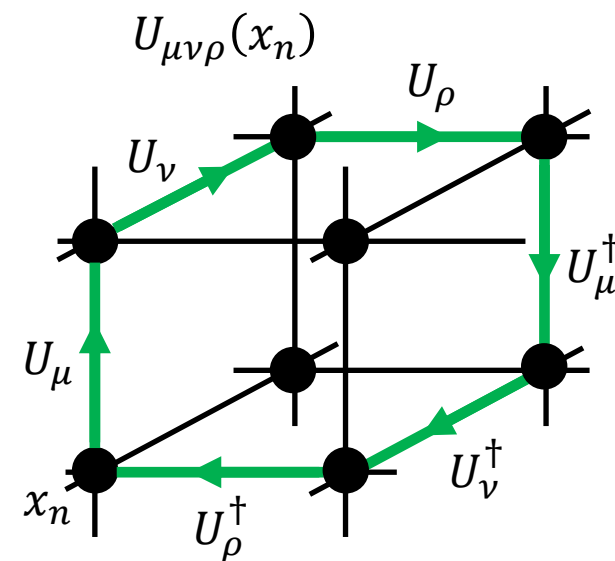
$O(a^2)$ corrections may be removed from the gluon action by including additional higher dimension gauge-invariant operators, e.g.

$$S_U[U] = \beta \sum_{x_n} [c_0 P_0 + c_1 P_1 + c_2 P_2]$$

$$P_0 = \sum_{\mu < \nu} \left[1 - \frac{1}{3} \text{Re tr}[U_{\mu\nu}(x_n)] \right]$$

$$P_1 = \sum_{\mu < \nu} \left[1 - \frac{1}{3} \text{Re tr}[U_{\mu\mu\nu}(x_n) + U_{\mu\nu\nu}(x_n)] \right]$$

$$P_2 = \sum_{\mu < \nu < \rho} \left[1 - \frac{1}{3} \text{Re tr}[U_{\mu\nu\rho}(x_n) + U_{\mu\rho\nu}(x_n) + U_{\rho\mu\nu}(x_n) + U_{\rho-\mu\nu}(x_n)] \right]$$



The coefficients c_i have been computed for a variety of improved fermion actions (as we will discuss momentarily) at 1-loop, e.g. [arXiv:0812.0503](https://arxiv.org/abs/0812.0503).

The Fermion Doubling Problem

Unfortunately, life is not so straightforward for our naïvely discretised fermions. The tree-level massless propagator in momentum space is

$$\begin{aligned} G(p) &= \left(\frac{i}{a} \gamma_E^\mu \sin(ap_\mu) \right)^{-1} \\ &= \frac{ia^{-1} \gamma_E^\mu \sin(ap_\mu)}{a^{-2} |\sin(ap_\mu)|^2} \end{aligned}$$

This has the desired pole at $p = (0,0,0,0)$, unfortunately it also has 15 additional poles at $p_\mu = (\pi/a, 0,0,0), (0, \pi/a, 0,0) \dots (\pi/a, \pi/a, \pi/a, \pi/a)$.

This is the fermion doubling problem - that for a single naïve fermion flavour our naïve lattice action describes 16 “tastes”.

The Fermion Doubling Problem

There are many ways to get around this problem, each with their own benefits and drawbacks.

In this lecture, we will use staggered quarks.

The reasoning behind using staggered quarks is simple:

- The different tastes live at different corners of the Brillouin zone, so interactions between them involve gluons with large momenta $p \sim \pi/a$.
- If we modify the gauge links in the fermion action to remove high momentum gluons, the different tastes can be treated as non-interacting and can be accounted for.

Staggered Quarks

To cut down the number of tastes from 16 to 4, in the staggered quark formalism we first diagonalise the action by taking

$$\psi(x_n) \rightarrow S(x_n)\chi(x_n), \quad \bar{\psi}(x_n) \rightarrow \bar{\chi}(x_n)S^\dagger(x_n), \quad S(x_n) = (\gamma_E^3)^{x_n^3}(\gamma_E^2)^{x_n^2}(\gamma_E^1)^{x_n^1}(\gamma_E^0)^{x_n^0}$$

With this the fermion action becomes diagonal in Dirac indices:

$$a^4 \sum_{x_n} \bar{\psi}(x_n)(\gamma_E^\mu \nabla_\mu + m)\psi(x_n) = a^4 \sum_{x_n} \bar{\chi}(x_n)(\alpha^\mu(x_n)\nabla_\mu + m)\chi(x_n),$$

$$\alpha^\mu(x_n) = (-1)^{\sum_{\nu < \mu} x_\nu}.$$

With the action diagonal we can drop all but 1 of the components of $\chi(x_n)$ and $\bar{\chi}(x_n)$ to go from 16 flavours to 4. Finally, we make use of the equivalence of the different tastes (up to discretisation effects) and take the 4th root of the fermion determinant appearing in the path integral.

Highly Improved Staggered Quarks (HISQ)

[hep-lat/0610092](https://arxiv.org/abs/hep-lat/0610092)

Staggered quark formalisms rely on removing discretisation effects that violate taste symmetry. For HISQ this is done by smearing the gauge fields entering the covariant derivative.

Extensive testing of the size of different possible taste exchange interactions has demonstrated that HISQ has taste exchange effects 3-4 times smaller than previous improved staggered actions.

For clarity, in the remainder of this lecture I will work with the naïve quark fields $\psi(x)$ and $\bar{\psi}(x)$, which are formally equivalent to the staggered expressions following the procedure described on the previous slide.

Highly Improved Staggered Quarks (HISQ)

- Symanzik Improvement

Our naïve fermion action was based on a simple finite difference

$$D_\mu \psi(x) \rightarrow \nabla_\mu \psi(x_n) = \frac{U_\mu(x_n)\psi(x_n + \hat{\mu}) - U_\mu^\dagger(x_n - \hat{\mu})\psi(x_n - \hat{\mu})}{2a}$$

However, this approximation receives tree level corrections at $O(a^2)$.

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We can do better by adding in a cubic “Naik term”,

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However, this approximation receives tree level corrections at $O(a^2)$.

We can do better by adding in a cubic “Naik term”,

$$D_\mu \psi(x) \rightarrow \left(\nabla_\mu - \frac{a^2}{6} (1 + \epsilon) \nabla_\mu^3 \right) \psi(x_n),$$

HISQ also includes an additional “Naik- ϵ ” term, that corrects the tree level dispersion relation for massive quarks

so that tree level corrections now appear at $O(a^4)$.

$$\epsilon = -\frac{27}{40} (am)^2 + \frac{327}{1120} (am)^4 + \dots$$

Computing Correlation Functions

With improved actions for the quark and gluon fields on the lattice in hand, can compute correlation functions.

Remember, we want to evaluate:

$$= \lim_{T \rightarrow \infty} \frac{1}{Z_T} \int \mathcal{D}[\bar{\psi}_f, \psi_f, U] e^{-\sum_{x,f} \bar{\psi}_f D_f[U] \psi_f} e^{-S_U[U]} O_1(t_1) O_2(t_2) \dots, \quad f \in [u, d, s, c \dots]$$

numerically, then extract matrix elements, energies, from

$$\sum_{N_{n+1}, \dots, N_1} \langle 0 | \hat{O}_n | N_n \rangle e^{-(t_n - t_{n-1}) E_{N_n}} \langle N_n | \hat{O}_{n-1} | N_{n-1} \rangle \dots e^{-(t_2 - t_1) E_{N_1}} \langle N_1 | \hat{O}_1 | 0 \rangle$$

The first nonzero energy state is the pion, and on modern lattices typically we have $M_\pi aL_t \approx 10$ which is sufficient to approximate the $aL_t = T \rightarrow \infty$ limit

Note: it is typical to take $u = d \equiv l$, hence you will often see phrases like “2+1+1 flavours” in the literature, 2 meaning the up and down quark masses are equal.

Computing Correlation Functions

To evaluate the Euclidean path-integral numerically, first factor out the gauge part

$$\int \mathcal{D}[\bar{\psi}, \psi, U] e^{-\Sigma \bar{\psi}_f D_f[U] \psi_f - S_U} O_1(t_1) O_2(t_2) \dots$$

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where in $\langle O_1(t_1) O_2(t_2) \dots \rangle_U$, we wick contract the fermion fields using the inverse of the full Dirac operator $D_f[U]$ including gauge fields. For example, for a pseudoscalar D_s -meson interpolating operator

$$O_1(t) = \bar{c}(x, t) \gamma^5 s(x, t), \quad O_2(0) = O_1^\dagger(0) = \bar{s}(y, 0) \gamma^5 c(y, 0)$$

we have

$$\langle \bar{c}(x, t) \gamma^5 s(x, t) \bar{s}(y, 0) \gamma^5 c(y, 0) \rangle_U = \text{tr}[D_s^{-1}[U](x, t; y, 0) \gamma^5 D_c^{-1}[U](y, 0; x, t) \gamma^5].$$

Computing Correlation Functions

Now, we can generate and store general purpose “ensembles” of gauge field configurations, with probability distribution

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We compute the average on the left to get an estimate for the quantity on the right, together with a variance.

Example 2-point correlation function

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When we do calculations in practice, it is typical to project onto a state with definite spatial momentum. Again, using a D_s -meson interpolating operator as an example we have.

$$O_1(t) = \frac{1}{V} \sum_x \bar{c}(x, t) \gamma^5 s(x, t) e^{ip \cdot x}, \quad O_2(0) = O_1^\dagger(0) = \frac{1}{V} \sum_y \bar{s}(y, t) \gamma^5 c(y, t) e^{-ip \cdot y}$$

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So that, with relativistic normalisation of states, we have

$$\begin{aligned} \overline{\frac{1}{N_{\text{cfg}}} \sum_i^{N_{\text{cfg}}} \langle O_1(t) O_2(0) \rangle_{U_i}} &= \sum_N \langle 0 | \hat{c}(0) \gamma^5 \hat{s}(0) | N, p \rangle \frac{1}{2E_N(p)} \langle N, p | \hat{s}(0) \gamma^5 \hat{c}(0) | 0 \rangle e^{-tE_N(p)} \\ &= \sum_N |A_N|^2 e^{-tE_N}, \quad A_N = \frac{\langle 0 | \hat{c}(0) \gamma^5 \hat{s}(0) | N, p \rangle}{\sqrt{2E_N(p)}} \end{aligned}$$

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So, on the computer, we want to evaluate

$$\frac{1}{N_{\text{cfg}}} \sum_i^{N_{\text{cfg}}} \langle O_1(t) O_2(0) \rangle_{U_i} = \frac{1}{N_{\text{cfg}}} \sum_i^{N_{\text{cfg}}} \sum_{x,y} \text{tr}[D_s^{-1}[U_i](x, t; y, 0) \gamma^5 D_c^{-1}[U_i](y, 0; x, t) \gamma^5]$$

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→ impractical to compute $D^{-1}[U](x, y) \sim 10$ petabytes in even single precision.

Fortunately, it's easier to solve $Dx = b$ for $x = D^{-1}b$ numerically.

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A few generic tricks allow us to project onto momentum correctly. Use γ^5 hermicity and “colour random walls,” $\xi_i^{ab}(x)$, satisfying

$$\overline{\xi_i^{bc}(y) \left(\xi_i^{dc}(y') \right)^*} = \delta^{bd} \delta(y, y').$$

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Example 2-point correlation function

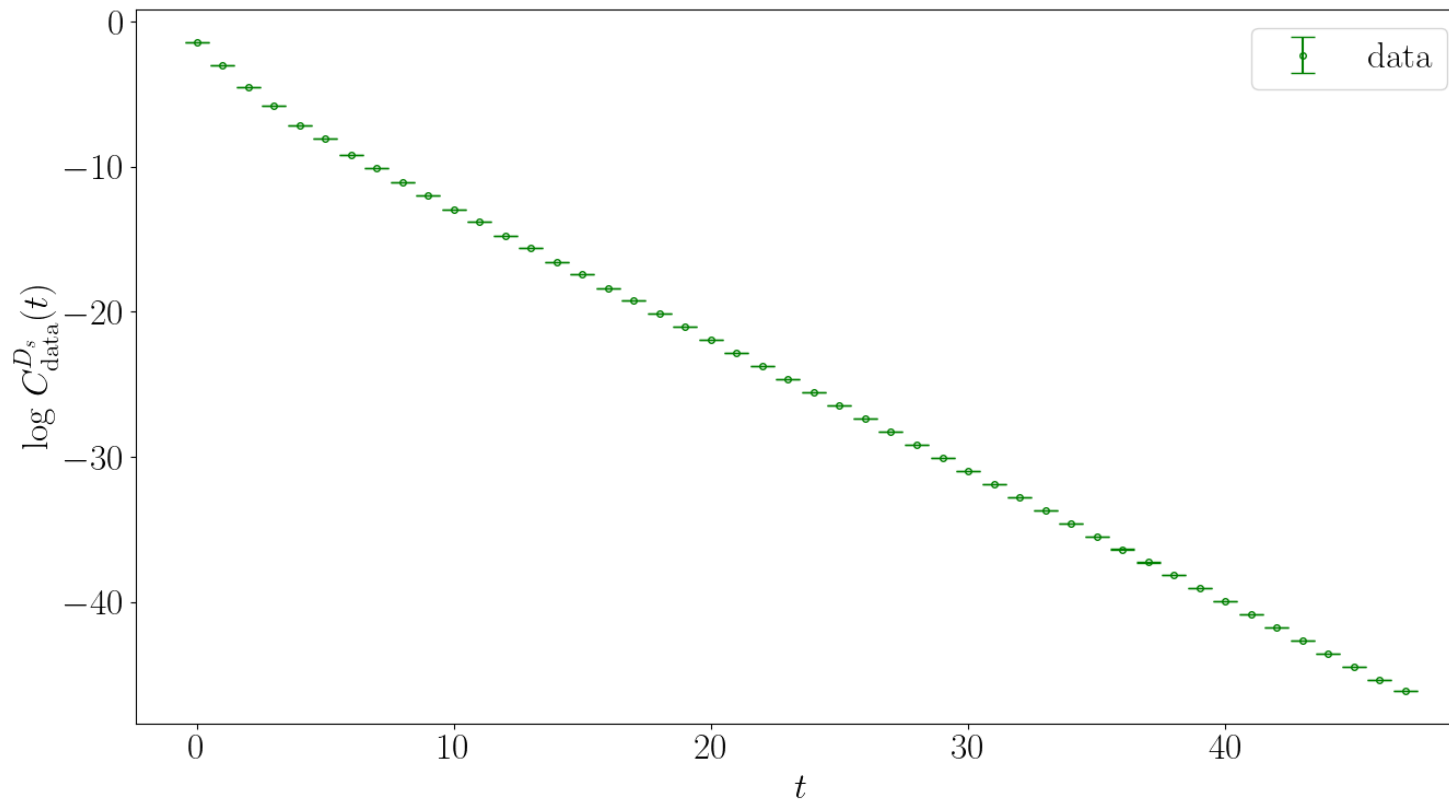
Practically speaking, the calculation of a 2-point is broken up in the following way

$$\frac{1}{N_{\text{cfg}}} \sum_i^{N_{\text{cfg}}} \langle O_1(t) O_2(0) \rangle_{U_i} = \frac{1}{N_{\text{cfg}}} \sum_i^{N_{\text{cfg}}} \sum_x \left(\sum_y D_s^{-1}[U_i]_{a\alpha;b\beta}(x, t; y, 0) \xi_i^{bc}(y) \right) \left(\sum_{y'} D_c^{-1}[U_i]_{a\alpha;d\beta}(x, t; y', 0) \xi_i^{dc}(y') \right)^*$$

we will denote the resultant data points $C^{D_s}(t)$.

Example 2-point correlation function

Here is some example data



$$\begin{aligned} N_{\text{cfg}} &= 1000 \\ a &\approx 0.09\text{fm} \\ L_x &= 32, \quad L_t = 96 \end{aligned}$$

Note that:

- Periodic boundary conditions, so average opposite halves of time extent
- Very precise

Example 2-point correlation function

We want to fit our data to a truncated sum over exponentials

$$C^{D_s}(t) \approx \sum_{N=0}^{n_{\text{exp}}-1} |A_N|^2 e^{-tE_N}$$

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$$C^{Ds}(t) \approx \sum_{N=0}^{n_{\text{exp}}-1} |A_N|^2 e^{-tE_N}$$

We follow the constrained fit approach, choosing priors for A_N and E_N and minimising

$$\chi_{\text{aug}}^2 = \sum_{t,t'} \Delta C(t) \sigma_{t,t'}^{-2} \Delta C(t') + \sum_N \frac{(A_N - \tilde{A}_N)^2}{\tilde{\sigma}_{A_n}^2} + \sum_N \frac{(E_N - \tilde{E}_N)^2}{\tilde{\sigma}_{E_n}^2}$$

where we take priors $\tilde{A}_N \pm \tilde{\sigma}_{A_n}$ and $\tilde{E}_N \pm \tilde{\sigma}_{E_n}$ and

$$\Delta C(t) = \overline{C(t)} - C(t, A_N, E_N),$$

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$$C^{D_s}(t) \approx \sum_{N=0}^{n_{\text{exp}}-1} |A_N|^2 e^{-tE_N}$$

Easy to show using T-symmetry and parity, that the A_N are real for our choice of interpolating operators.

To make fitting easier, it is typical to cut out the first few data points near $t = 0$, so that we only include data points where the ground state amplitude is the dominant contribution

Example 2-point correlation function

The choice of priors for A_N and E_N is important – we must allow sufficiently wide priors as to not constrain the fit, but equally they must not be so wide that they cause instability.

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Typical priors for the ground state can be chosen based on the observed D_S mass and decay constant, which is related to A_0 (in lattice units) by

$$A_0 = \frac{M_{D_S}^{\frac{3}{2}}}{\sqrt{2}(m_c + m_s)} f_{D_S}$$

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We can then take, e.g. $\pm 50\%$ for uncertainties on the ground state.

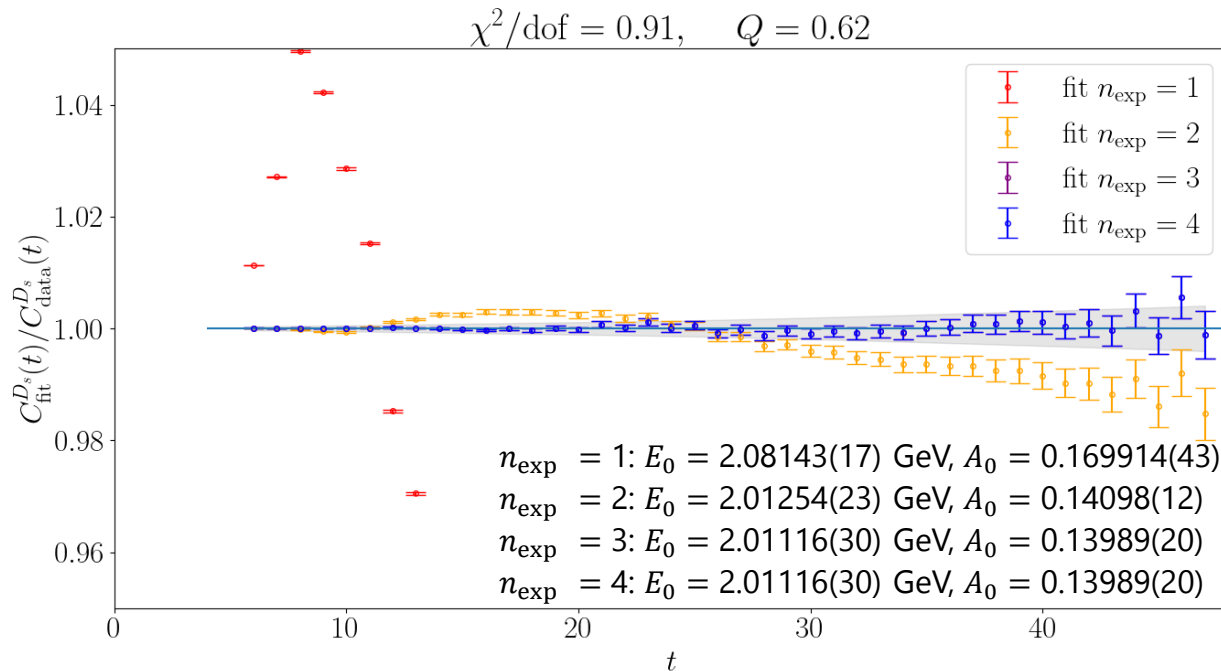
For excited state amplitudes, we typically take something like $A_0 \pm 1.5 A_0$.

For excited state energies we typically take $E_N - E_{N-1} = \Lambda_{\text{QCD}} \pm \Lambda_{\text{QCD}}/2$.

Example 2-point correlation function

In practice, we only need a few exponentials to get a good fit, e.g.

$$C^{D_s}(t) \approx \sum_{N=0}^3 |A_N|^2 e^{-tE_N}$$



Here is an example fit for D_s 2-point data.

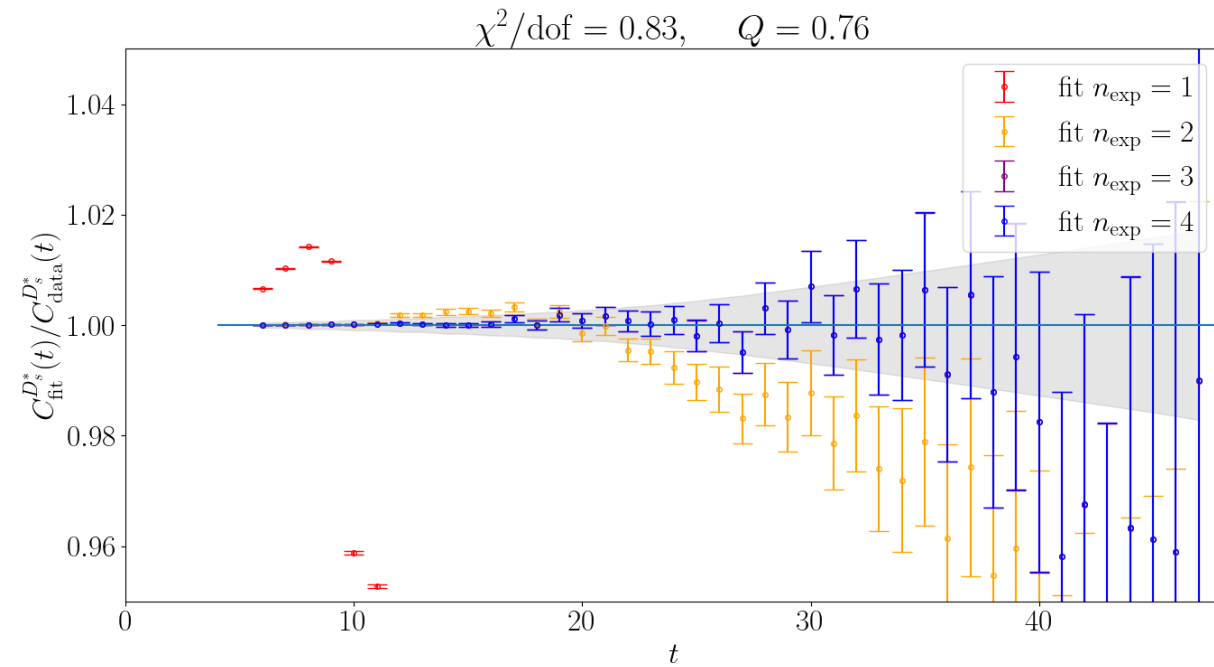
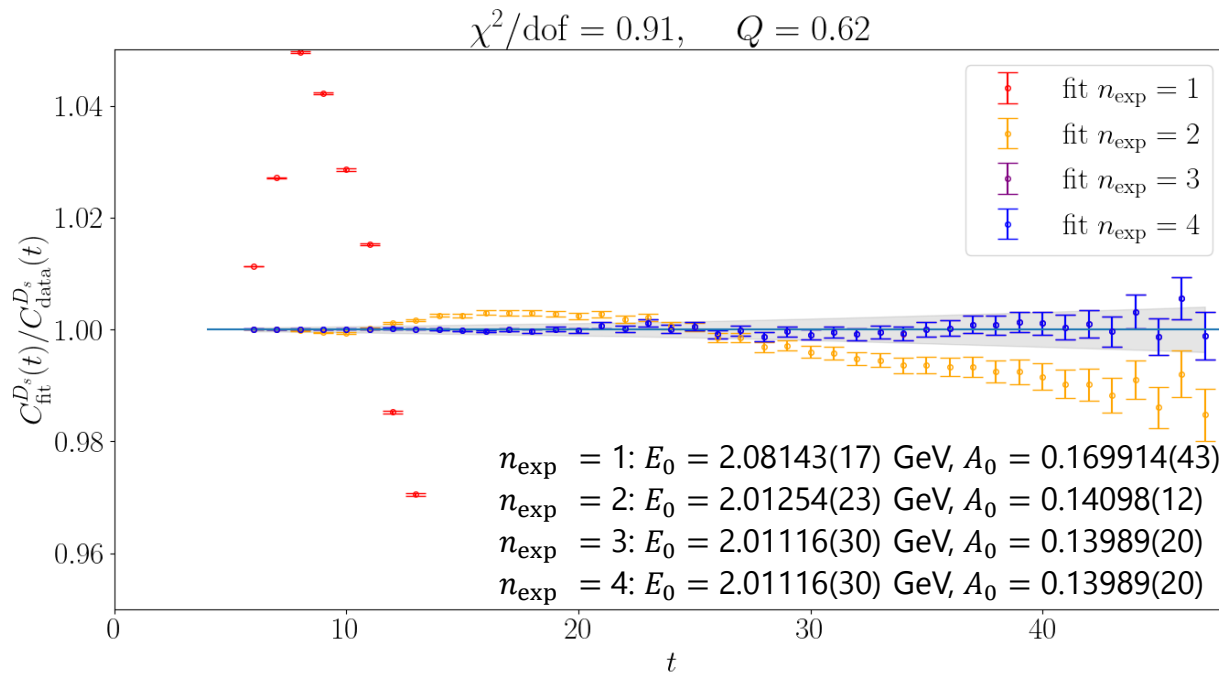
Note that:

- We don't include data near $t = 0$, where excited states are not well controlled.
- 3 exponentials is typically adequate to describe our data.

Fits were done using G. P. Lepage's `corrfit` python package, based around the constrained fitting methods described in [hep-lat/0110175](https://arxiv.org/abs/hep-lat/0110175).

Example 2-point correlation function

Now here is some D_s^* data – notice that the signal/noise deteriorates much more quickly with t .



Signal to Noise

This growth in signal to noise can be understood in terms of the physical states. The variance is given by, for the 2-point correlation function for a generic meson operator

$$\sigma^2(t) = \overline{\left(\langle O_M(t) O_M^\dagger(0) \rangle_U \right)^2} - \left(\overline{\langle O_M(t) O_M^\dagger(0) \rangle_U} \right)^2$$

where the expectation value is now understood as an integral over the gauge field probability density.

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where the expectation value is now understood as an integral over the gauge field probability density. However, notice that

$$\left(\langle O_M(t) O_M^\dagger(0) \rangle_U \right)^2 \in \left\langle \left(O_M(t) O_M^\dagger(0) \right)^2 \right\rangle_U$$

and

$$\overline{\left\langle \left(O_M(t) O_M^\dagger(0) \right)^2 \right\rangle_U} = \sum_N \langle 0 | \hat{O}_M \hat{O}_M | N \rangle \langle N | \hat{O}_M^\dagger \hat{O}_M^\dagger | 0 \rangle e^{-t E_N^{MM}(p)}$$

so that the variance contains a piece decreasing as $e^{-t E_0^{MM}(p)}$, where E_0^{MM} is the energy of the lowest energy state interpolated by $(\hat{O}_M^\dagger)^2$

Signal to Noise

$(\hat{O}_M^\dagger)^2$ clearly interpolates a two-particle state, with two copies of the original meson, but it is not generally the case that this is the lowest energy state.

In the case of the D_S^* for instance, our interpolating operator has charm, anti-strange flavour, and spin-1, so the lowest energy multiparticle state the squared operator couples to may be some combination of $\bar{c}c\bar{s}s$ states, with spin = 0, 1, 2. e.g. a $D_S^- D_S^+$, which clearly has lower energy than a $D_S^{*-} D_S^{*+}$ state.

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So, the ratio of noise to signal then goes like, for large t ,

$$\frac{|A_0^{MM}| e^{-tE_0^{MM}/2}}{|A_0^M|^2 e^{-tE_0^M}} \sim e^{t(E_0^M - E_0^{MM}/2)}$$

Side note: Spin on the lattice e.g. 1203.6041

- Because we break rotational symmetry, the irreps of the little group for massive particles on the lattice are not the usual irreps of the double cover of $SO(3)$
- Instead, the little group for massive particles at rest is the double cover of the octahedral symmetry group, O_h^D . For particles with momentum, O_h^D is broken even further.

It turns out there are only a finite number of irreps for these little groups.

They “subduce” into an infinite tower of continuum spin states. e.g. for a particle at rest, O_h^D , has an irrep labelled A_1^- . This subduces into a tower of continuum J^P states like

$$A_1^- \rightarrow 0^-, 4^-, \dots$$

A_1^- is the only lattice irrep which subduces into a continuum $J^P = 0^-$ state.

For our purposes this means we can use the continuum $\bar{\psi}\gamma^5\psi$ pseudoscalar operator, and not end up accidentally interpolating the wrong ground state.

This is also true for the $J^P = 1^-$ vector interpolating operator $\bar{\psi}\gamma^i\psi$.

3-point Functions and Matrix Elements

Now we can get on to computing matrix elements, and ultimately hadronic form factors. Here we want to use 2 interpolating operators and a current, for $B \rightarrow D^*$ this looks like

$$O_{D^*}^\nu(T) = \frac{1}{V} \sum_y \bar{u}(y, T) \gamma^\nu c(y, T) e^{ip \cdot y}, \quad J^\Gamma(t) = \frac{Z_J^\Gamma}{V} \sum_z e^{-ip \cdot z} \bar{c}(z, t) \Gamma b(z, t),$$
$$O_B^\dagger(0) = \frac{1}{V} \sum_y \bar{b}(x, 0) \gamma^5 u(x, 0)$$

where $\Gamma = \gamma^\mu, \gamma^5 \gamma^\mu, \sigma^{\mu\nu}$ for the vector, axial vector and tensor currents respectively. Z_J is a renormalisation factor matching the lattice current to the continuum current.

3-point Functions and Matrix Elements

This can be computed for the vector and axial vector currents using the PCAC and PCVC relations as renormalisation conditions. e.g. by requiring

$$\begin{aligned} Z_A (M_B - M_{D^*}) \langle \bar{c} \gamma^0 \gamma^5 b \rangle &= (m_b + m_c) \langle \bar{c} \gamma^5 b \rangle, \\ Z_V (M_B - M_{D^*}) \langle \bar{c} \gamma^0 b \rangle &= (m_b - m_c) \langle \bar{c} b \rangle \end{aligned}$$

For some appropriately chosen matrix elements.

For the tensor, need another approach, e.g. RI-SMOM.

Both approaches non-perturbative, small uncertainties compared to statistics.

3-point Functions and Matrix Elements

For matrix elements need both 2-point functions, as well as 3-point functions:

$$\langle O_{D^*}^{\nu}(T) \hat{f}^{\Gamma}(t) O_B^{\dagger}(0) \rangle = \sum_{N,M} \langle 0 | \hat{O}_{D^*}^{\nu} | N \rangle \frac{1}{2E_N(p)} \langle N | \hat{f}^{\Gamma} | M \rangle \frac{1}{2E_M} \langle M | \hat{O}_B^{\dagger} | 0 \rangle e^{-(T-t)E_N} e^{-tE_M}$$

$$\langle O_{D^*}^{\nu}(t) O_{D^*}^{\nu\dagger}(0) \rangle = \sum_N \langle 0 | \hat{O}_{D^*}^{\nu} | N, p \rangle \frac{1}{2E_N(p)} \langle N, p | \hat{O}_{D^*}^{\nu\dagger} | 0 \rangle e^{-tE_N(p)}$$

$$\langle O_B(t) O_B^{\dagger}(0) \rangle = \sum_M \langle 0 | \hat{O}_B | M, p \rangle \frac{1}{2E_M(p)} \langle M, p | \hat{O}_B^{\dagger} | 0 \rangle e^{-tE_M(p)}$$

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Which we can then fit to

$$\sum_{N,M=0}^{n_{\text{exp}}-1} A_N B_M M_{NM}^{J^{\Gamma}} e^{-(T-t)E_N} e^{-tE_M}, \quad \sum_{N=0}^{n_{\text{exp}}-1} |A_N|^2 e^{-tE_N}, \quad \sum_{M=0}^{n_{\text{exp}}-1} |B_M|^2 e^{-tE_M}$$

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For D^* we have $\langle 0 | \hat{O}_{D^*}^\nu | D^*(\lambda, p) \rangle = N_{D^*} \epsilon_\lambda^\nu(p)$, $\sum_\lambda \epsilon_\lambda^\mu(p) \epsilon_\lambda^\nu(p)^* = -g^{\mu\nu} + v^\mu v^\nu$

$$\Rightarrow A_0 = \frac{N_{D^*}}{\sqrt{2E_{D^*}(p)}} (1 + (v^\nu)^2)^{\frac{1}{2}}$$

3-point Functions and Matrix Elements

Putting the 2-point amplitudes and energies together with the 3-point function gives

$$A_0 = \frac{N_{D^*}}{\sqrt{2E_{D^*}(p)}} (1 + (v^v)^2)^{\frac{1}{2}}, \quad B_0 = \frac{\langle M | \hat{O}_B^+ | 0 \rangle}{\sqrt{2M_B}},$$

$$M_{00}^{J^\Gamma} = \frac{\sum_\lambda \epsilon_\lambda^v(p) \langle D^*(\lambda, p) | \hat{J}^\Gamma | B \rangle}{\sqrt{(1 + (v^v)^2) 2E_{D^*}(p)} \sqrt{2M_B}}$$

3-point Functions and Matrix Elements

Extracting $M_{00}^{J^\Gamma}$ from our 3-point fits. This gives us access to the matrix elements of interest,

$$\sum_{\lambda} \epsilon_{\lambda}^{\nu}(p) \langle D^*(\lambda, p) | \hat{j}^{\Gamma} | B \rangle = \sqrt{(1 + (v^{\nu})^2) 2E_{D^*}(p)} \sqrt{2M_B} M_{00}^{J^\Gamma}.$$

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So far, we've worked with generic choices of ν and Γ , but we need to pick some specific values for our numerical calculation.

We insert expressions for the matrix elements parameterised in terms of form factors,

$$\langle D^* | \bar{c} \gamma^{\mu} b | B \rangle = i \sqrt{M_B M_{D^*}} h_V(w) \epsilon^{\mu\nu\alpha\beta} \epsilon_{\nu}^* v'_{\alpha} v_{\beta},$$

$$\langle D^* | \bar{c} \gamma^{\mu} \gamma^5 b | B \rangle = \sqrt{M_B M_{D^*}} [h_{A_1}(w)(w+1) \epsilon^{*\mu} - h_{A_2}(w)(\epsilon^{*\mu} \cdot v) v^{\mu} - h_{A_3}(w)(\epsilon^{*\mu} \cdot v) v'^{\mu}],$$

$$\langle D^* | \bar{c} \sigma^{\mu\nu} b | B \rangle = -\sqrt{M_B M_{D^*}} \epsilon^{\mu\nu\alpha\beta} [h_{T_1}(w) \epsilon_{\alpha}^* (v + v')_{\beta} + h_{T_2}(w) \epsilon_{\alpha}^* (v - v')_{\beta} + h_{T_3}(w) (\epsilon^* \cdot v) v_{\alpha} v'_{\beta}],$$

so that we can choose appropriate combinations of Γ and ν in order to isolate linearly independent combinations of form factors.

3-point Functions and Matrix Elements

For example, for h_{A_1} , this choice is easy. We can choose $\vec{p} = (k, k, 0)$, $\Gamma = \gamma^3 \gamma^5$, $v = 3$ for some momentum k , then we have

$$\sum_{\lambda} \epsilon_{\lambda}^3(p) \left\langle D^*(\lambda, v') | \bar{c} \gamma^3 \gamma^5 b | B(v) \right\rangle = \sqrt{M_B M_{D^*}} \sum_{\lambda} \epsilon_{\lambda}^3(p) [h_{A_1}(w)(w+1)\epsilon^{*3} - h_{A_2}(w)(\epsilon^* \cdot v)v^3 - h_{A_3}(w)(\epsilon^* \cdot v)v'^3]$$

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$$\sqrt{M_B M_{D^*}} h_{A_1}(w)(w+1) = \sqrt{2E_{D^*}(p)} \sqrt{2M_B} M_{00}^{J^{\gamma^3 \gamma^5}}$$

$$h_{A_1}(w) = \frac{2\sqrt{w}}{w+1} M_{00}^{J^{\gamma^3 \gamma^5}}$$

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Also easy for h_V and h_{T_1} . For other form factors, we tend to pull out combinations, and it gets a bit messy.

Here, I'll focus on h_{A_1} , but ultimately the full set of combinations are fit and extracted simultaneously, fully preserving correlations.

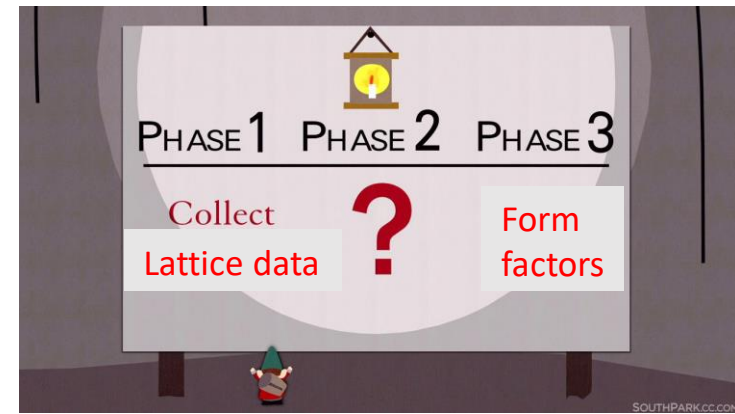
Side note: b -quarks are Expensive to Simulate

- We want $am_b \ll 1$ so that discretisation effects are small.
- Ideally take volume $\rightarrow \infty$ but too expensive. Instead keep the volume roughly fixed, at a large enough value that finite volume (FV) effects are negligible.
- For matrix elements involving stable, 1-meson states, FV effects $\sim e^{-M_\pi a L_x}$, so we want $M_\pi a L_x \gg 1$.
- This means that as we make a small so that $am_b \ll 1$, we also need to increase L_x to keep $M_\pi a L_x$ roughly fixed.

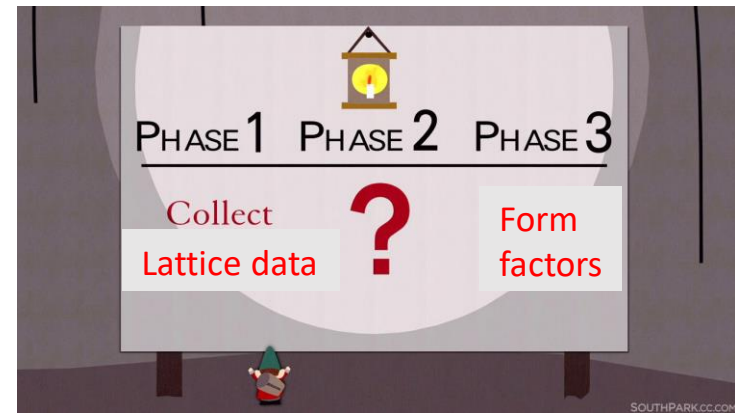
Lattices with small enough a for realistic b -quarks are very computationally expensive.

e.g. for HISQ lattices with $am_b \approx 0.625$, need $L_x \times L_T = 96^3 \times 288$,
 $\Rightarrow 250,000,000$ lattice sites

Getting to the Continuum

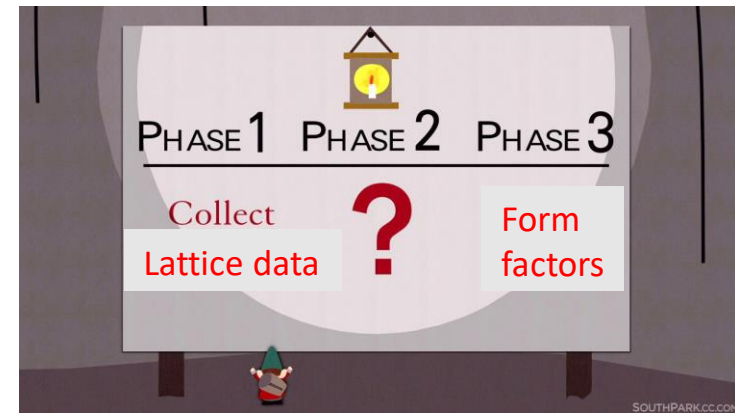


Getting to the Continuum



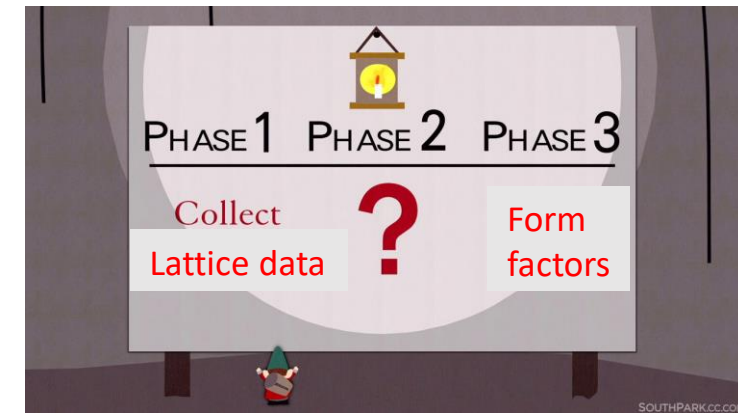
- Repeat calculation with different lattice spacings, momenta

Getting to the Continuum



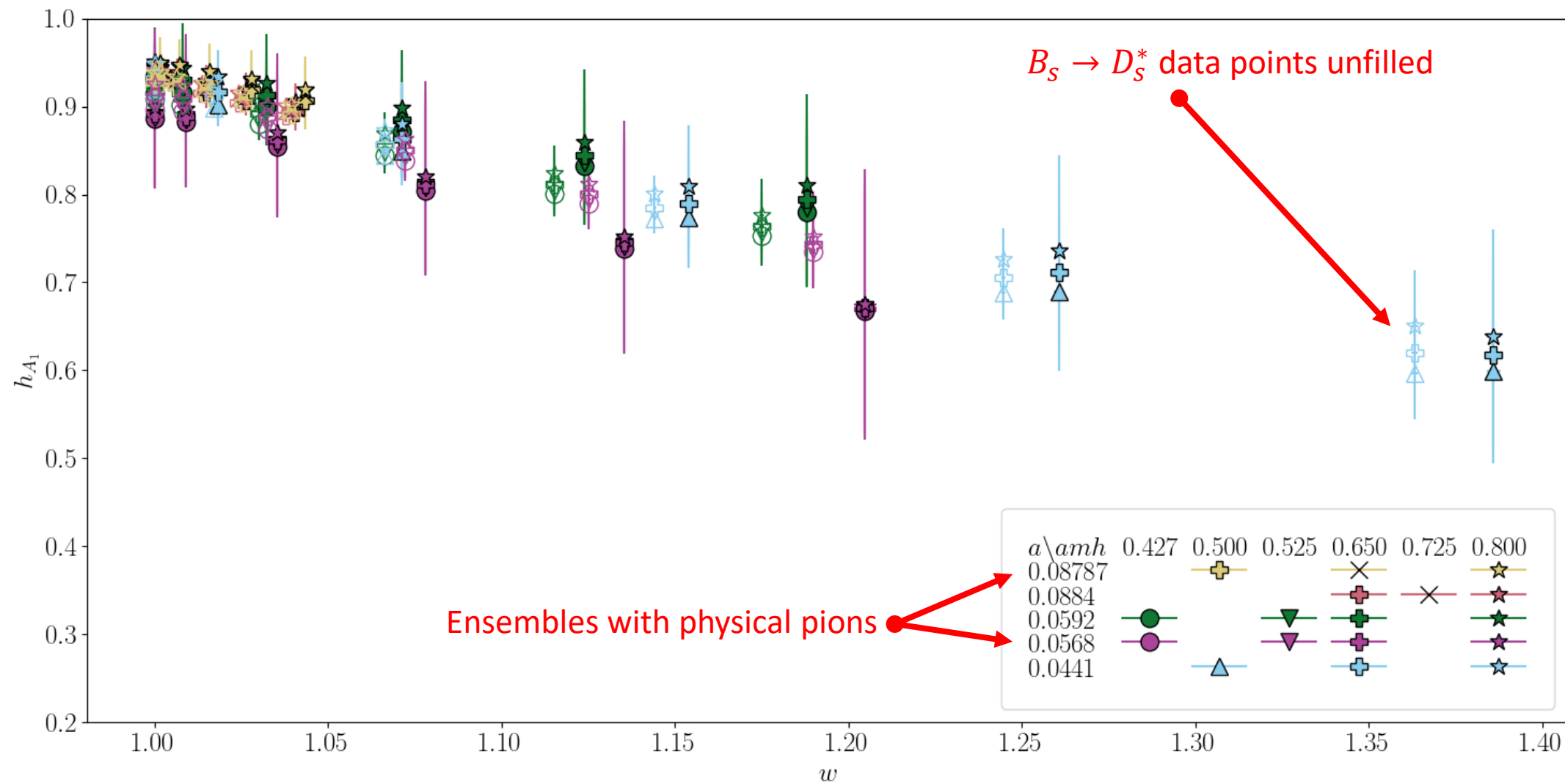
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Getting to the Continuum



- Repeat calculation with different lattice spacings, momenta
- To control am_b discretisation effects we also work with a heavy-quark ' h ' in place of the b -quark, with results at several h -quark masses, m_h ranging up to m_b
- $D^* \rightarrow D\pi$ threshold effects in the final state, so we also use different unphysical $m_{u/d}$ for the spectator quark, as well as doing $B_s \rightarrow D_s^*$ in parallel.

Getting to the Continuum



Chiral Continuum Extrapolation for $B \rightarrow D^*$

Need a parameterisation that can describe:

m_h dependence

- Use a polynomial in Λ_{QCD}/M_{H_S} motivated by HQET, using the easily computed H_S mass as proxy for m_h

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- Avoids mixing m_h dependence into our kinematics

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am_h discretisation effects

- Polynomial in $(am_h/\pi)^{2n}$

Other discretisation effects

- The next most significant discretisation effects come from the charm, going like $(am_c/\pi)^{2n}$

Chiral Continuum Extrapolation for $B \rightarrow D^*$

$$h_{A_1^{(s)}}^{\text{latt}}(w) = \sum_{n=0}^{N_{\text{max}}} a_n^{(s)} (w-1)^n \left(1 + \delta_{m_{\text{val}}}^{(s)} + \delta_{m_{\text{sea}}}\right) + \left[\text{logs}_{SU_f(3)}^{h_{A_1^{(s)}}} - \text{logs}_{SU_f(3) \text{ phys}}^{h_{A_1}} \right]$$

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Quark mass mistuning effects

Chiral Continuum Extrapolation for $B \rightarrow D^*$

Logarithms from 1-loop staggered chiral perturbation theory

$$h_{A_1^{(s)}}^{\text{latt}}(w) = \sum_{n=0}^{N_{\text{max}}} a_n^{(s)} (w-1)^n \underbrace{\left(1 + \delta_{m_{\text{val}}}^{(s)} + \delta_{m_{\text{sea}}}\right)}_{\text{Quark mass mistuning effects}} + \underbrace{\left[\text{logs}_{SU_f(3)}^{h_{A_1^{(s)}}} - \text{logs}_{SU_f(3) \text{ phys}}^{h_{A_1}} \right]}_{\text{Logarithms from 1-loop staggered chiral perturbation theory}}$$

Quark mass mistuning effects

The logs vary very little with w . Subtract off the physical $B \rightarrow D^*$ log, so that our physical result is a simple polynomial in $(w-1)$.

Chiral Continuum Extrapolation for $B \rightarrow D^*$

Different for $B \rightarrow D^*$ and $B_s \rightarrow D_s^*$

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These coefficients are what we allow to vary with am_h , am_c , M_{H_s} , and $M_{\pi(K)}$. We take

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$$a_n^{(s)} = \alpha_n \times \left(1 + \sum_{i,j,k \neq 0}^3 b_n^{ijk} \left(\frac{am_c}{\pi} \right)^{2i} \left(\frac{am_h}{\pi} \right)^{2j} \Delta_{H_s}^k + \sum_{i,j,k}^3 \delta_\chi^{(s)} \tilde{b}_n^{ijk} \left(\frac{am_c}{\pi} \right)^{2i} \left(\frac{am_h}{\pi} \right)^{2j} \Delta_{H_s}^k \right)$$

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Discretisation effects depend on the momentum cut-off π/a , with scale set by the masses

Chiral Continuum Extrapolation for $B \rightarrow D^*$

Different for $B \rightarrow D^*$ and $B_s \rightarrow D_s^*$

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This way, our continuum $B \rightarrow D^*$ form factor is just
$$h_{A_1}^{\text{phys}}(w) = \sum_{n=0}^{N_{\text{max}}} \alpha_n (w-1)^n$$

Chiral Continuum Extrapolation for $B \rightarrow D^*$

$$h_{A_1}^{\text{latt}(s)}(w) = \sum_{n=0}^{N_{\text{max}}} a_n^{(s)} (w-1)^n \left(1 + \delta_{m_{\text{val}}}^{(s)} + \delta_{m_{\text{sea}}}^{(s)}\right) + \left[\text{logs}_{SU_f(3)}^{h_{A_1}^{(s)}} - \text{logs}_{SU_f(3) \text{ phys}}^{h_{A_1}}\right]$$

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What priors should we choose?

Chiral Continuum Extrapolation for $B \rightarrow D^*$

$$h_{A_1}^{\text{latt}(s)}(w) = \sum_{n=0}^{N_{\text{max}}} a_n^{(s)} (w-1)^n \left(1 + \delta_{m_{\text{val}}}^{(s)} + \delta_{m_{\text{sea}}}^{(s)}\right) + \left[\text{logs}_{SU_f(3)}^{h_{A_1}^{(s)}} - \text{logs}_{SU_f(3) \text{ phys}}^{h_{A_1}}\right]$$

$$a_n^{(s)} = \alpha_n \times \left(1 + \sum_{i,j,k \neq 0}^3 b_n^{ijk} \left(\frac{am_c}{\pi}\right)^{2i} \left(\frac{am_h}{\pi}\right)^{2j} \Delta_{H_s}^k + \sum_{i,j,k}^3 \delta_\chi^{(s)} \tilde{b}_n^{ijk} \left(\frac{am_c}{\pi}\right)^{2i} \left(\frac{am_h}{\pi}\right)^{2j} \Delta_{H_s}^k\right),$$

$$\delta_\chi^{(s)} = \left(\frac{M_\pi^{\text{phys}^2}}{\Lambda_\chi^2} - \frac{M_{\pi(K)}^2}{\Lambda_\chi^2}\right), \quad \Delta_{H_s}^{k \neq 0} = \left(\frac{\Lambda_{\text{QCD}}}{M_{H_s}}\right)^k - \left(\frac{\Lambda_{\text{QCD}}}{M_{B_s}}\right)^k, \quad \Delta_{H_s}^0 = 1$$

What priors should we choose?

- The α_n are the physical $B \rightarrow D^*$ coefficients, so we can use the unitarity of the BGL parameters to construct conservative priors for these.
- Alternatively, can use generic priors wide enough that BGL parameters are not biased to values < 1

Chiral Continuum Extrapolation for $B \rightarrow D^*$

$$h_{A_1}^{\text{latt}(s)}(w) = \sum_{n=0}^{N_{\text{max}}} a_n^{(s)} (w-1)^n \left(1 + \delta_{m_{\text{val}}}^{(s)} + \delta_{m_{\text{sea}}}^{(s)}\right) + \left[\text{logs}_{SU_f(3)}^{h_{A_1}^{(s)}} - \text{logs}_{SU_f(3) \text{ phys}}^{h_{A_1}}\right]$$

$$a_n^{(s)} = \alpha_n \times \left(1 + \sum_{i,j,k \neq 0}^3 \tilde{b}_n^{ijk} \left(\frac{am_c}{\pi}\right)^{2i} \left(\frac{am_h}{\pi}\right)^{2j} \Delta_{H_s}^k + \sum_{i,j,k}^3 \delta_\chi^{(s)} \tilde{b}_n^{ijk} \left(\frac{am_c}{\pi}\right)^{2i} \left(\frac{am_h}{\pi}\right)^{2j} \Delta_{H_s}^k\right),$$

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What priors should we choose?

- Discretisation effects suppressed by improvement of HISQ action: no tree level a^2 errors, no tree level $(am)^4$ errors to leading order in quark velocity.
- Expect mild $(\Lambda_{\text{QCD}}/M_{H_s})$ dependence from e.g. QCD sum rule calculations of sub-leading Isgur-Wise function.

\Rightarrow using priors of $b_n^{ijk} = 0 \pm 1$ conservative

Chiral Continuum Extrapolation for $B \rightarrow D^*$

$$h_{A_1}^{\text{latt}(s)}(w) = \sum_{n=0}^{N_{\text{max}}} a_n^{(s)} (w-1)^n \left(1 + \delta_{m_{\text{val}}}^{(s)} + \delta_{m_{\text{sea}}}^{(s)}\right) + \left[\text{logs}_{SU_f(3)}^{h_{A_1}^{(s)}} - \text{logs}_{SU_f(3) \text{ phys}}^{h_{A_1}}\right]$$

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What priors should we choose?

- Taking equal central values and widths for b_n^{ijk} and \tilde{b}_n^{ijk} allows for $B_s \rightarrow D_s^*$ to vary by $\approx 25\%$ relative to $B \rightarrow D^*$, as well as capturing analytic dependence on M_π for $B \rightarrow D^*$
- Luke's theorem tells us that $h_{A_1}^{\text{latt}(s)}(1)$ has no $\frac{\Lambda_{\text{QCD}}}{M_{H_s}}$ term, so we can set $b_0^{001} = \tilde{b}_0^{001} = 0$

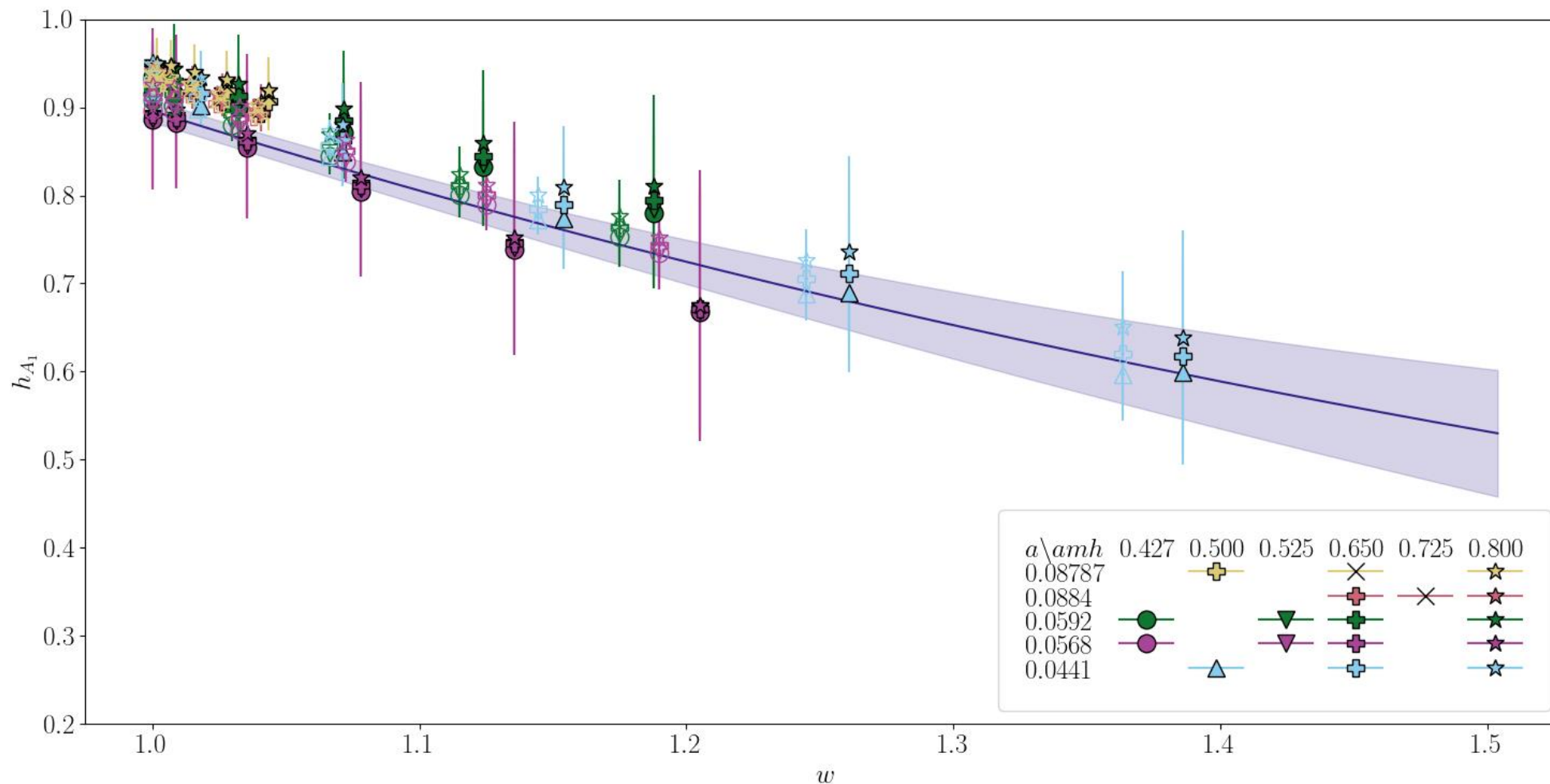
Chiral Continuum Extrapolation for $B \rightarrow D^*$

$$h_{A_1}^{\text{latt}(s)}(w) = \sum_{n=0}^{N_{\text{max}}} a_n^{(s)} (w-1)^n \left(1 + \delta_{m_{\text{val}}}^{(s)} + \delta_{m_{\text{sea}}}^{(s)}\right) + \left[\text{logs}_{SU_f(3)}^{h_{A_1}^{(s)}} - \text{logs}_{SU_f(3) \text{ phys}}^{h_{A_1}}\right]$$
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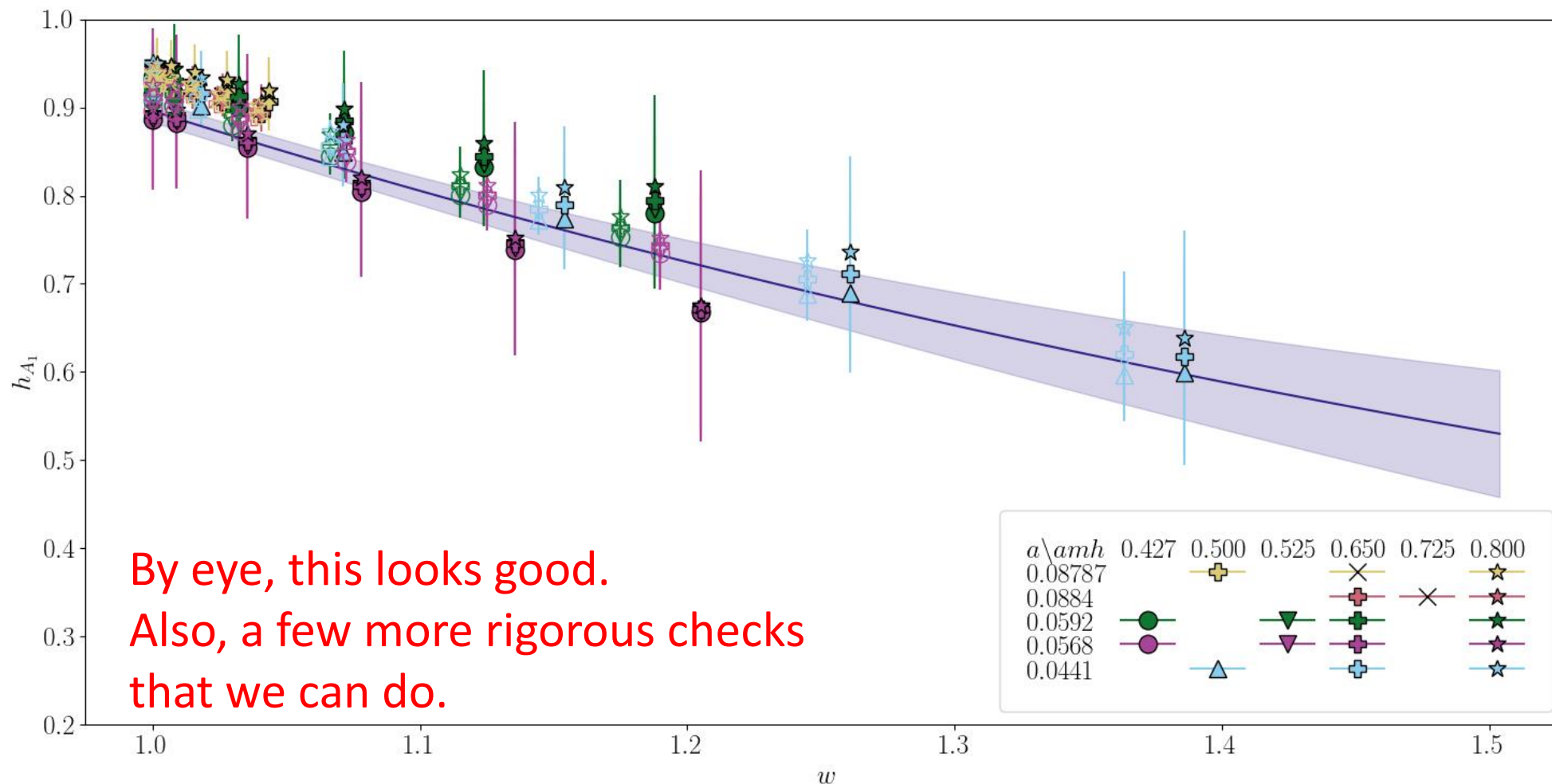
What priors should we choose?

We use the python packages 'lsqfit' and 'gvar' to perform the constrained fit to our fit function.

Chiral Continuum Extrapolation for $B \rightarrow D^*$



Chiral Continuum Extrapolation for $B \rightarrow D^*$



Checks of Stability

An important final step of any lattice calculation is to check that our results are insensitive to reasonable changes to our analysis.

This starts with changes to our correlator fits. In doing them we made choices about:

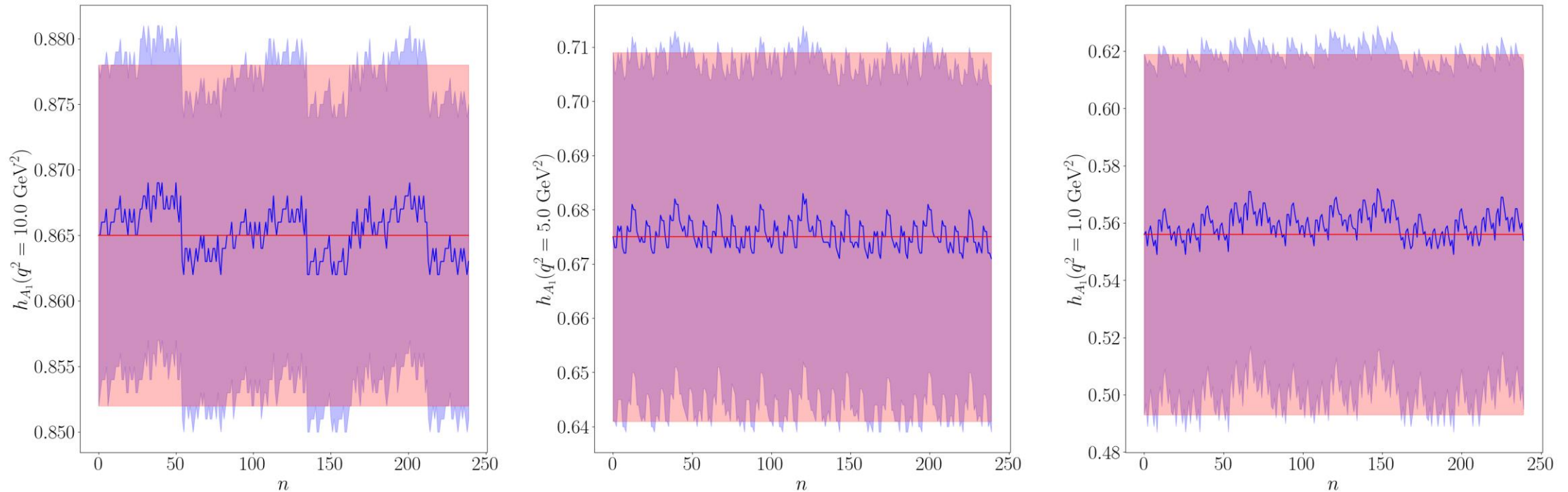
- Cutting off data near $t = 0$
- The number of exponentials to include, n_{exp}
- Size of SVD cut – necessary when fitting many correlation functions simultaneously.

To investigate if any of these has an effect, we perform correlator fits on each ensemble with larger t_{min} , increasing n_{exp} by 1 and decreasing the SVD cut by roughly an order of magnitude.

Then we feed all possible combinations of those fits through the chiral continuum extrapolation and check if our form factors change.

Checks of Stability

Check the form factors for different combinations of correlator fits, labelled by n , at different values of q^2 across the range, e.g. $q^2 = 1\text{GeV}^2$, 5GeV^2 , 10GeV^2 .



Checks of Stability

We also want to check if our chiral-continuum extrapolation was sensible.

Empirical Bayes Analysis

- Pick a set of prior widths, e.g. the widths of all the parameters b_n^{ijk} and \tilde{b}_n^{ijk} and multiply them by a variable η .
- Maximise the Gaussian-Bayes factor, to find the value of η for which $P(\text{data}|\text{priors})$ is greatest.
- Check that the optimum value of $\eta < 1$, \Rightarrow our prior widths are not overly constraining our data.

Not useful for priors that encode systematic uncertainties, e.g. coefficients of higher order terms in our fit.

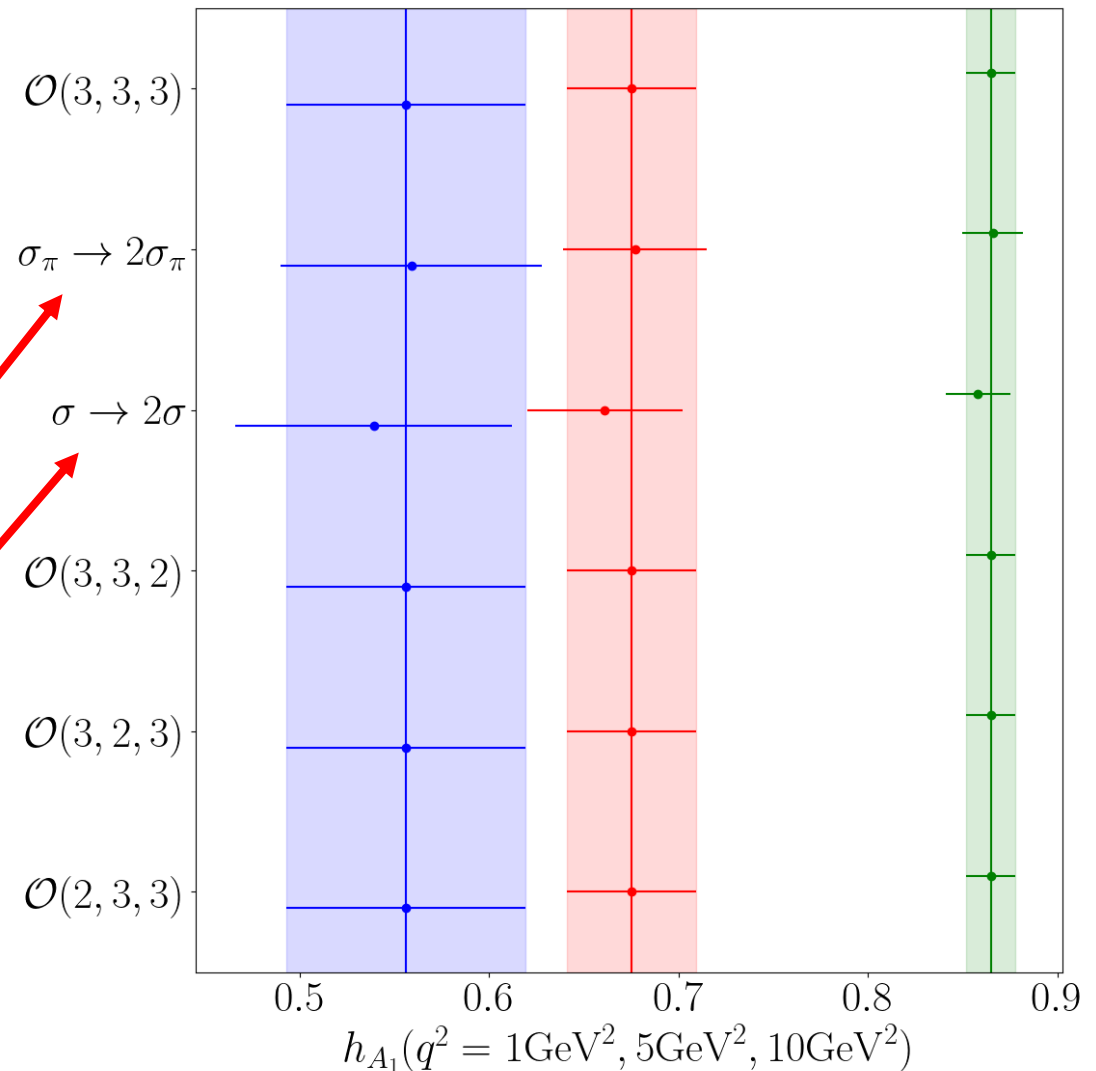
Checks of Stability

Can do the same thing for our chiral continuum extrapolation, checking we have gone to high enough order, and that our results are roughly insensitive to prior widths.

Double prior widths of \tilde{b}_n^{ijk}

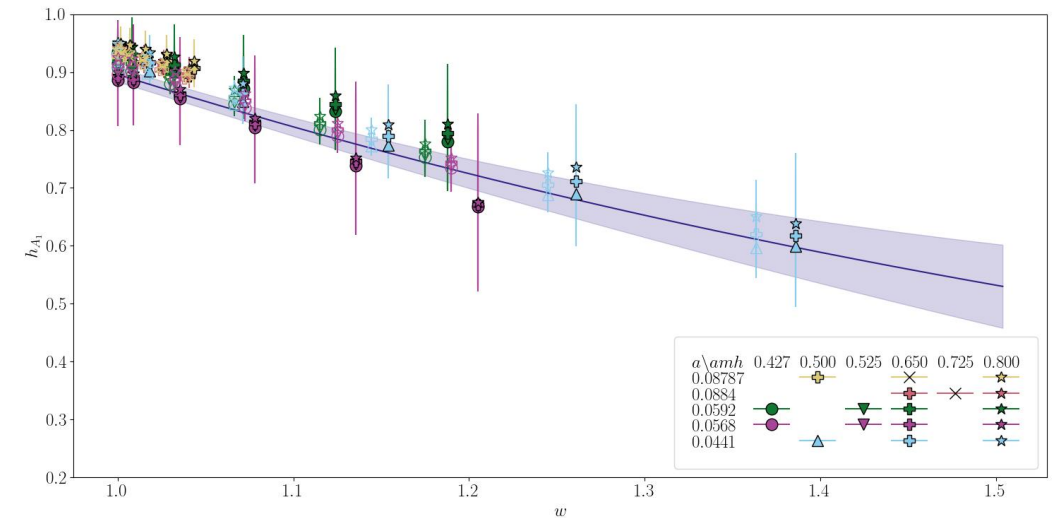
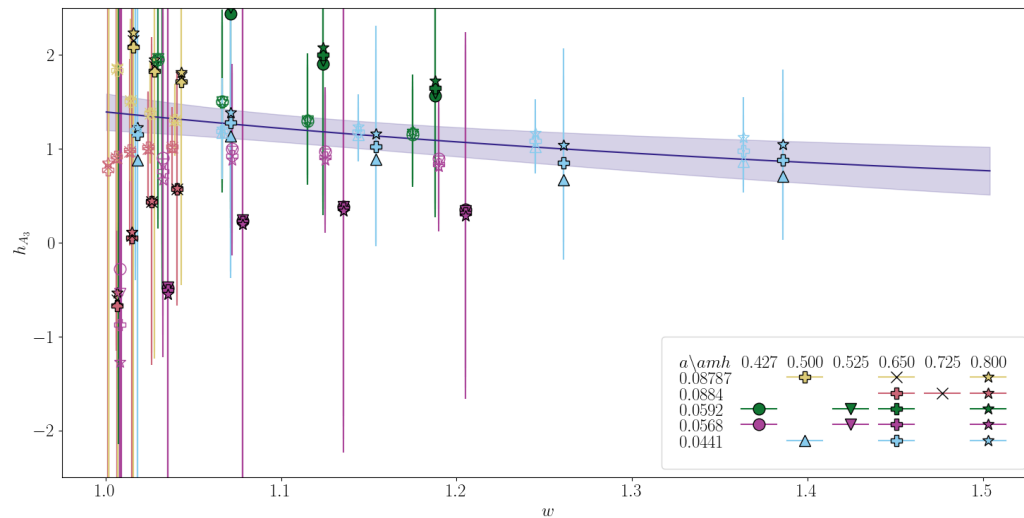
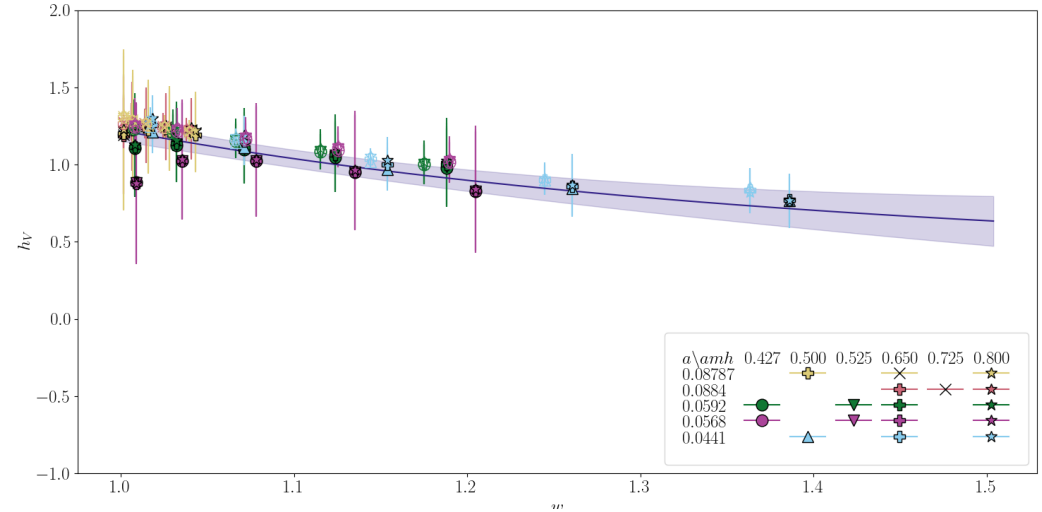
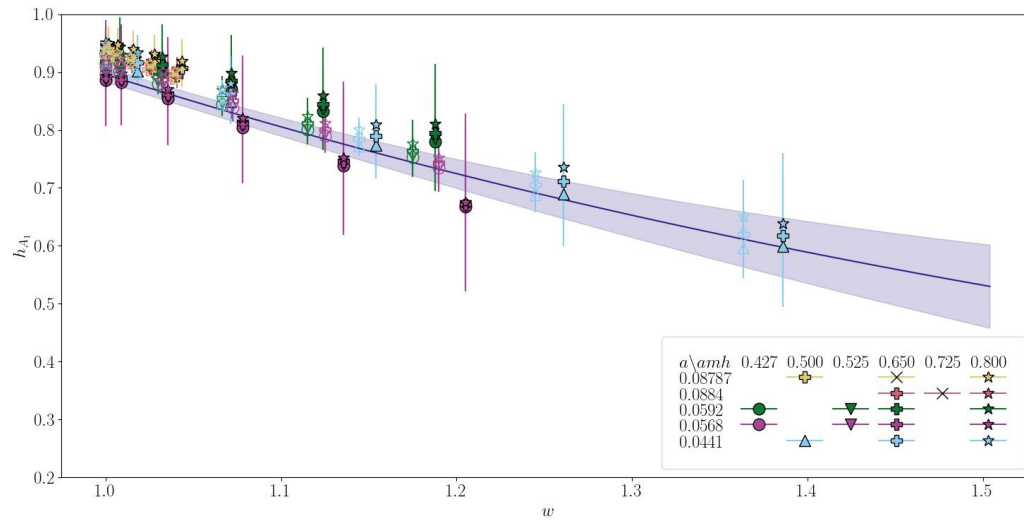
Double prior widths of b_n^{ijk}

$$O(N_i, N_j, N_k) \Rightarrow \sum_{i,j,k}^{N_i-1, N_j-1, N_k-1} \dots$$



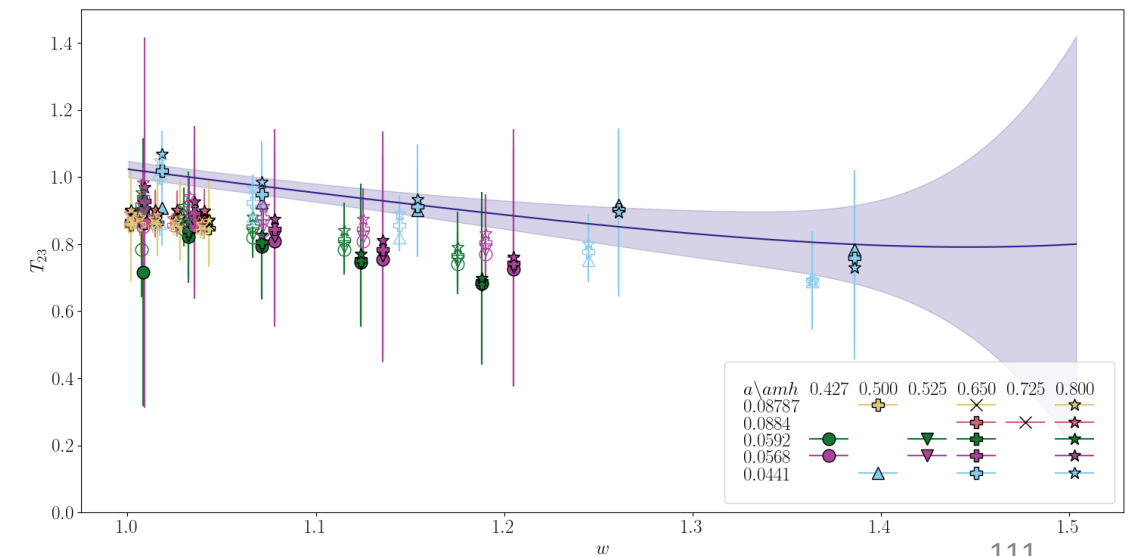
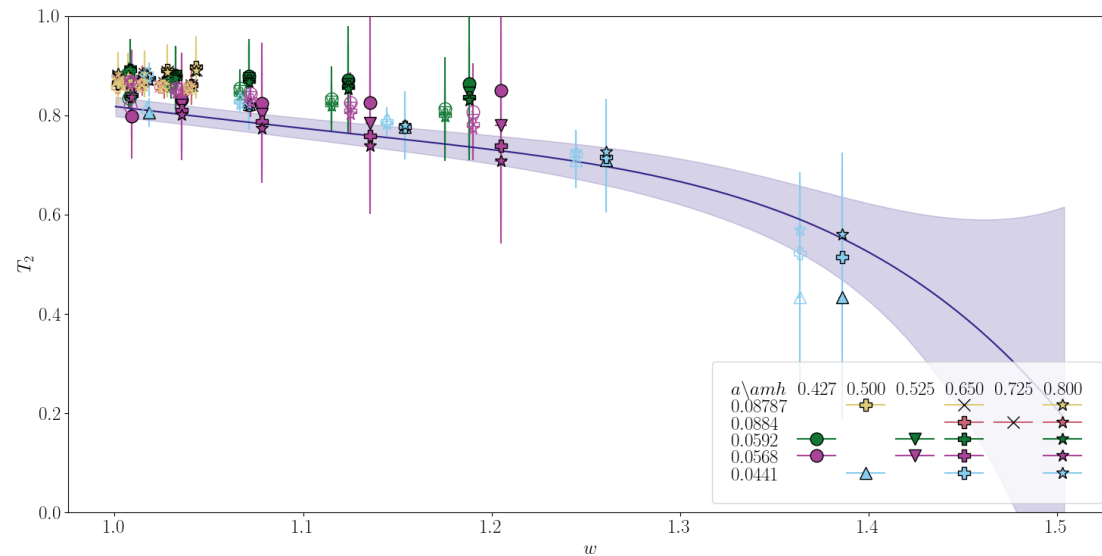
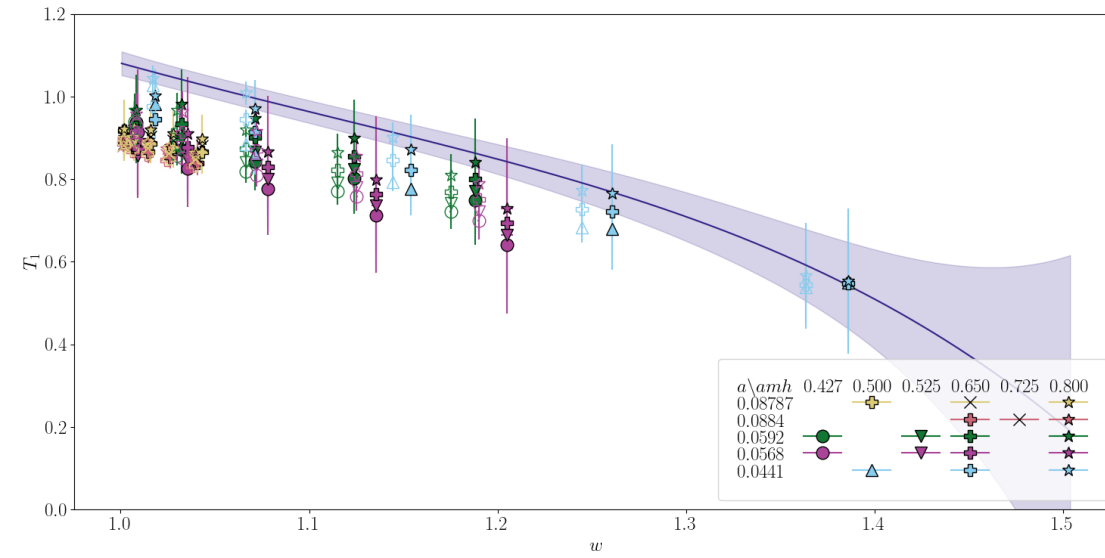
Full Set of Form Factors

We do this analysis simultaneously, using similar chiral-continuum fit functions for all the FFs: the SM ones...



Full Set of Form Factors

...and the tensor FFs.



Summary:

Saw how to:

- Compute correlation functions on the lattice
- Fit correlation functions to extract masses and matrix elements
- Choose operators to extract form factors for $B \rightarrow D^*$
- Use our lattice form factors to take the $m_h \rightarrow m_b$ chiral-continuum limit

We followed the HPQCD calculation in [2304.03137](#), using 2+1+1 Heavy-HISQ

Other modern lattice calculations:

- FNAL/MILC - [2105.14019](#), 2+1 asqtad, Fermilab heavy-quark action
- JLQCD - [2306.05657](#), 2+1 flavour relativistic Möbius domain-wall quarks