Non-perturbative step-scaling

and its application to heavy quark physics

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Hadronic physics and heavy quarks on the lattice
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Why should we do B-physics on the lattice?

- Search for BSM physics at the high-precision frontier: Deviations between Standard Model predictions and experiment in flavor physics observables.
- Several *B-anomalies*, e.g.,
  - Ratios testing lepton flavor universality.
  - Branching fractions of rare decays.
  - Tension between inclusive and exclusive determinations of $|V_{\mathrm{ub}}|$ and $|V_{\mathrm{cb}}|$.
- Need precise determinations of hadronic matrix elements and quark masses.

$\rightarrow$ *Ab initio* Standard Model predictions from lattice QCD.

Multi-scale problems in lattice QCD

- By discretizing QCD in a finite volume, we introduce two cutoffs:
  - Infrared cutoff: $\Lambda_{\mathrm{IR}} \sim 1/L$
  - Ultraviolet cutoff: $\Lambda_{\mathrm{UV}} \sim 1/a$

- Finite-volume effects vanish exponentially $\propto \exp(-m_\pi L)$

  $\rightarrow$ require $m_\pi L \geq 4$.

- Cutoff effects vanish polynomially $\propto c_1 a + c_2 a^2 + c_3 a^3 + c_4 a^4 \ldots$, possibly with logarithmic corrections [Husung et al., 1912.08498]

  $\rightarrow$ For energy scales q: fulfill $aq \ll 1$ for reliable continuum extrapolations.

$$L^{-1} \ll m_\pi \approx 135\,\mathrm{MeV} \ll q \ll a^{-1}$$

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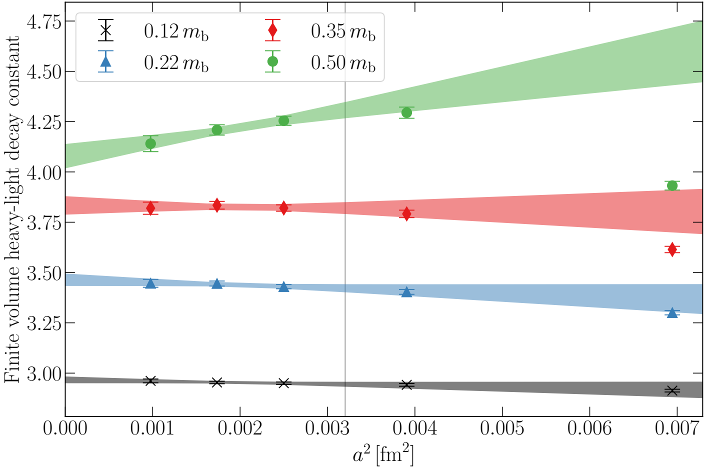
- The cost to generate ensembles scales at least with L^5.
- What are the energy scales that can be reached at physical pion mass?
  - $m_\pi^{\mathrm{phys}} L \geq 4$ implies $L \geq 6\,\mathrm{fm}$ (assume $T \gg L$ here).
  - State of the art: $L/a = 96$ at $a = 0.06\,\mathrm{fm} \to a^{-1} \sim 3.3\,\mathrm{GeV}^{-1}$.
  - Largest on the market: $L/a = 144$ at $a = 0.04\,\mathrm{fm} \to a^{-1} \sim 4.9\,\mathrm{GeV}^{-1}$.
- We are limited in view of the energy scales, e.g. quark masses, that we can simulate on large lattices.

Quark mass dependent cutoff effects



- Consider (finer than) conventional lattice spacings

$$0.031\,\mathrm{fm} \leq a \leq 0.083\,\mathrm{fm}$$

  in finite-volume.

- Continuum extrapolation of the pseudoscalar heavy-light decay constant at fixed (renormalized) quark masses.

- For illustration: Use three finest resolutions $\leq 0.05\,\mathrm{fm}$ to extrapolate with

$$f_{\mathrm{hl}}(a) = p_0 + p_1 \cdot a^2$$

Non-perturbative step-scaling

The running coupling of QCD

The case of the strong coupling constant

The computation of the strong coupling constant $\alpha_s(q)$ is a multi-scale problem:

- Define α_s from an Euclidean short-distance quantity $\mathcal{O}(q)$ with the perturbative expansion (see, e.g., [Dalla Brida, 2012.01232]),

$$\mathcal{O}(q) \overset{q\to\infty}{\approx} \sum_{n=1}^{N} c_n \alpha_{\overline{\rm MS}}^n(q) + \mathrm{O}(\alpha_{\overline{\rm MS}}^{N+1}) + \mathrm{O}\left(\frac{\Lambda^p}{q^p}\right) \qquad \to \qquad \boldsymbol{\alpha_{\mathcal{O}}(q) \equiv \frac{\mathcal{O}}{c_1}}\,,$$

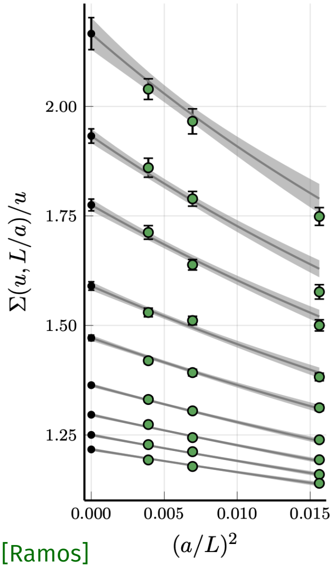
  up to truncation errors.

- Converges as $\alpha_{\mathcal{O}}(q) \overset{q\to\infty}{\propto} 1/\log(q/\Lambda_{\rm QCD}) \to$ have to reach high energy scales.

- Possible solution to the multi-scale problem [Lüscher, Weisz, Wolff]:
  Use finite-volume effects as part of the definition of $\alpha_{\mathcal{O}}(q)$,

$$\alpha_{\mathcal{O}}(q) \text{ with } q = L^{-1} \ll a^{-1}\,,$$

  and work with a series of lattices and physically small volumes.



[Ramos]

1. Given $\alpha_{\mathcal{O}}(q_{\text{had}} = L_{\text{had}}^{-1})$ determine $q_{\text{had}}/m_{\text{had}} \sim 1$
2. Measure the change in $\alpha_{\mathcal{O}}(q = L^{-1})$ as you change the volume $L \to L/2$: the step-scaling function

$$\sigma_{\mathcal{O}}(u) \equiv \alpha_{\mathcal{O}}(2q)|_{u=\alpha_{\mathcal{O}}(q)}$$

   with the implicit relation to the non-pert. β function,

$$\log(2) = -\int_{\sqrt{u}}^{\sqrt{\sigma(u)}} \frac{\mathrm{d}x}{\beta(x)}$$

3. Starting from $q_{\text{had}} \sim \Lambda_{\text{QCD}}$, perform $n \sim \mathrm{O}(10)$ steps to reach

$$q_{\text{PT}} = 2^n q_{\text{had}} \sim \mathrm{O}(100\,\text{GeV})$$

   where $\alpha_{\mathcal{O}}(q_{\text{PT}}) \sim 0.1$.

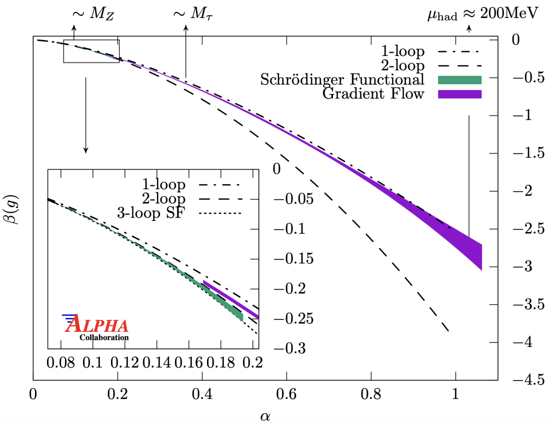
4. Extract $\alpha_{\overline{\rm MS}}(q_{\rm PT})$ from the perturbative expansion of $\alpha_{\mathcal{O}}$.

5. Compute $\Lambda_{\rm QCD}/m_{\rm had}$ by integrating the non-perturbative and perturbative β functions,

$$\Lambda = \mu\varphi(\alpha(\mu))\,,$$

$$\varphi(\alpha) = \ldots \exp\left\{-\int_0^{\alpha} \frac{{\rm d}x}{\beta(x)+\ldots}\right\}$$

from $\alpha_{\mathcal{O}}(q_{\rm had})$ to $\alpha_{\mathcal{O}}(q_{\rm PT})$ and from $\alpha_{\mathcal{O}}(q_{\rm PT})$ to 0.

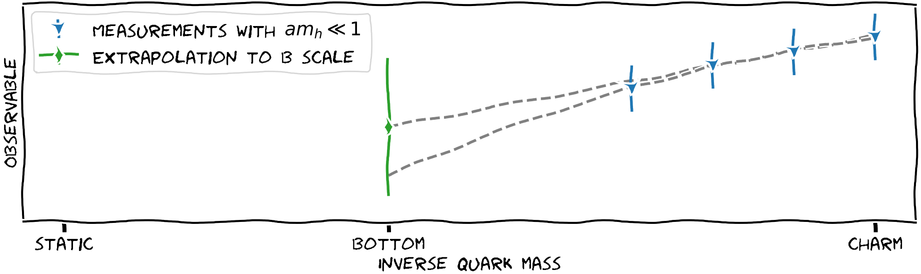


[Ramos][Bruno et al., 1706.03821]

Non-perturbative step-scaling

Heavy quark physics

- A heavy (e.g. bottom) quark introduces an energy scale m_h in addition to Λ_{QCD}.
- Simulating relativistic bottom quarks at several resolutions is not possible in large volumes!



- Extrapolation to the B scale is difficult, possibly mixing extra-/interpolations in a, m_h and q^2 for semi-leptonic form factors.

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- Simulating relativistic bottom quarks at several resolutions is not possible in large volumes!

Employ effective field theories for low-energy physics

$$a\,|\vec{p}| \ll 1\,, \qquad |\vec{p}| \ll m_{\mathrm{b}}$$

- here: Heavy Quark Effective Theory (HQET)
- Renormalizable effective theory $\leftrightarrow$ continuum limit.

Heavy Quark Effective Theory

- Integrate out heavy degrees of freedom of QCD Lagrangian for one heavy quark.
- Expand the Lagrangian in powers of $1/m_{\mathrm{h}}$.

→ Possible to describe bottom physics at next-to-leading order in HQET.

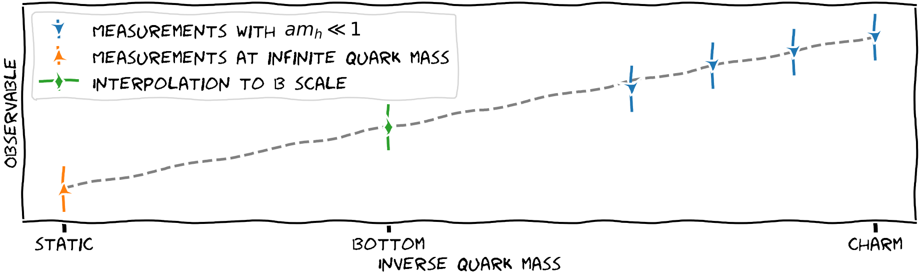
$$\mathcal{L}_{\text{heavy}} = \bar{h}_v D_0 h_v - \omega_{\text{kin}} \mathcal{O}_{\text{kin}} - \omega_{\text{spin}} \mathcal{O}_{\text{spin}} \,, \qquad \mathcal{O}_{\text{kin}} = \bar{h}_v \mathbf{D}^2 h_v \,, \quad \mathcal{O}_{\text{spin}} = \bar{h}_v \sigma \cdot \mathbf{B} h_v$$

- Perturbative matching at order g_0^{2l} leads to power divergences in the coefficients [Nucl.Phys.B 368 (1992) 281-292, Maiani et al.]

$$\Delta c_k \sim g_0^{2(l+1)} a^{-p} \sim a^{-p} \left[\ln(a\Lambda)\right]^{-(l+1)} \overset{a \to 0}{\longrightarrow} \infty$$

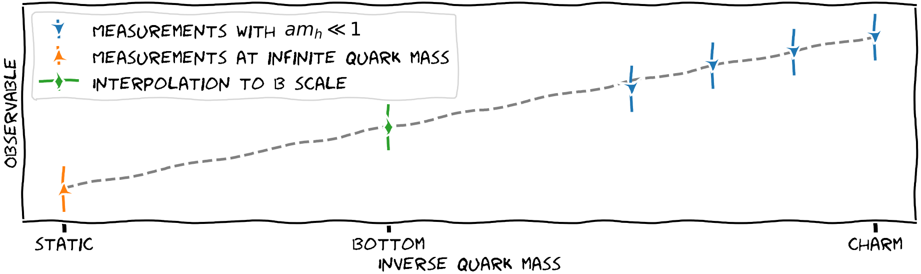
due to mixing of operators differing in dimensions by p.

(Non-perturbative) HQET



- Can we just perform an interpolation between results in static HQET and results in relativistic QCD below m_b where $am_h \ll 1$?

(Non-perturbative) HQET



- Can we just perform an interpolation between results in static HQET and results in relativistic QCD below m_b where $am_h \ll 1$?

$\rightarrow$ No! Even the static approximation requires non-trivial renormalisation and matching that would have to be **computed non-perturbatively**.

- Existing strategy to renormalize HQET non-perturbatively via step-scaling techniques [Heitger and Sommer, hep-lat/0310035].
  $\rightarrow$ Quite challenging since $1/m_\mathrm{b}$ effects are needed for precision.

The static theory

- Given the static action $\mathcal{L}^{\text{stat}} = \overline{\psi}_h D_0 \psi_h$, we have $E^{\text{stat}} \sim \frac{1}{a} g_0^2$.

  $\rightarrow$ E^{stat} divergent as $a \rightarrow 0$

- Renormalization $\rightarrow \delta m \sim \frac{1}{a} g_0^2$ and matching $\rightarrow m_b^{\text{finite}}$.

  $\rightarrow$ $E = E^{\text{stat}} + \delta m + m_b^{\text{finite}}$

- Heavy-light currents

$$V_k^{\text{stat}} = C_{V_k}(m_b) Z^{\text{stat}}(g_0) \overline{\psi}_h \gamma_k \psi_l$$
$$V_0^{\text{stat}} = C_{V_0}(m_b) Z^{\text{stat}}(g_0) \overline{\psi}_h \gamma_0 \psi_l$$

  $\rightarrow$ Matching coefficients $C_{V_{k(0)}}(m_b)$ log-divergent as $m_b \rightarrow \infty$ [Sommer, 1008.0710].

Our strategy, based on [Guazzini et al., 0710.2229]:

Cancel renormalization and matching [Sommer et al., 2312.09811].

- Phenomenologically relevant: the q^2 dependence of semi-leptonic form factors.
- Form factor decomposition in the B-meson rest frame

$$(\sqrt{2}p_k^\pi)^{-1}\langle\pi(p^\pi)|V_k(0)|B(\vec{p}=0)\rangle = h_\perp(E_\pi) = h_\perp^{\rm stat}(E_\pi) + O(1/m_{\rm b})$$

- Cancel matching and renormalization for $h_\perp^{\rm stat}$,

$$\frac{h_\perp(E_\pi)}{h_\perp(E_\pi^{\rm ref})} = \frac{h_\perp^{\rm stat}(E_\pi)}{h_\perp^{\rm stat}(E_\pi^{\rm ref})} + O(1/m_{\rm b})\,.$$

- Connection with $f_{B^\star}$: Normalize to the vector decay constant

$$h_\perp(E_\pi^{\rm ref}) = \hat{f}_{\rm V}\frac{h_\perp(E_\pi^{\rm ref})}{\hat{f}_{\rm V}} = \hat{f}_{\rm V}\left[\frac{h_\perp^{\rm stat}(E_\pi^{\rm ref})}{\hat{f}_{\rm V}^{\rm stat}} + {\rm O}(1/m_{\rm b})\right]$$

$\rightarrow$ Problem solved for $h_\perp$. How to compute $\hat{f}_{\rm V}$?

Step-scaling

We can make use of the step-scaling toolbox:

- Cancel matching and renormalization via ratios of observables $O(L_2)/O(L_1)$ or differences of logs computed in two volumes :

$$\sigma_{\rm V} = \left[\log[L_{\rm ref}^{3/2}\hat{f}_{\rm V}(L_2)] - \log[L_{\rm ref}^{3/2}\hat{f}_{\rm V}(L_1)]\right]$$

- Same ansatz to cancel the additive divergence in the static energy

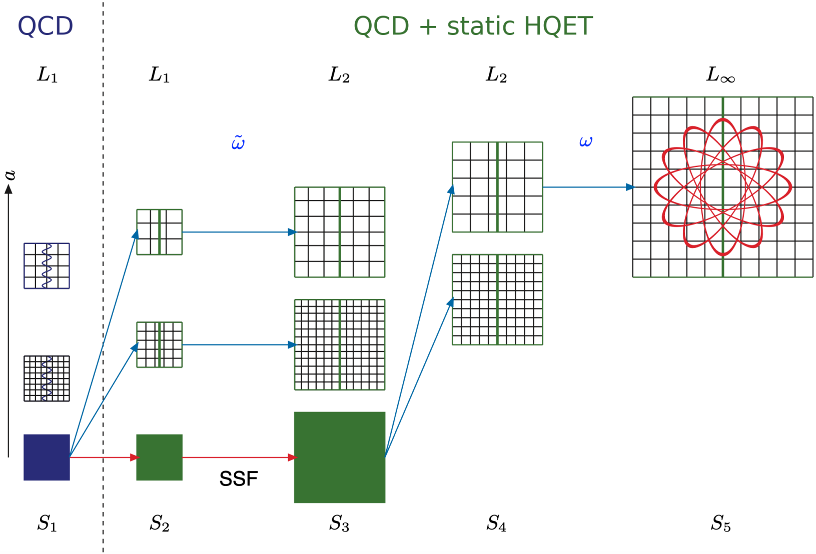
$$\sigma_m = L_{\rm ref}\left[m_{\rm PS}(L_2) - m_{\rm PS}(L_1)\right]$$

- Connect large-volume (CLS) ensembles with small volumes:

$$L_\infty \to L_2 = 1\,{\rm fm} \qquad \text{and} \qquad L_2 = 1\,{\rm fm} \to L_1 = 0.5\,{\rm fm}$$

- Small volume $L_1 = 0.5\,{\rm fm}$: Simulate relativistic b quarks.

B-PHYSICS FROM STEP-SCALING



- QCD observables with relativistic b quarks in finite volume at $L_1 = 0.5\,\text{fm}$ where $a^{-1} \in [9.5,\ 25]\,\text{GeV}^{-1}$.
- Step-scaling for observables with:
  - static quarks
  - relativistic quarks with $m_h < m_b$
- Contact with large-volume simulations.

- Vector meson decay constant $\hat{f}_V = f_V\sqrt{m_V}$,

$$\hat{f}_V = \sqrt{2}\langle 0|V_k(0)|V(\vec{p}=0,k)\rangle_{\mathrm{NR}} = \hat{f}_V^{\mathrm{stat}} + O(1/m_b)\,,$$

- For the step-scaling, we define

$$\Phi_{\vec{V}}(L) \equiv \ln\left(\frac{L_{\mathrm{ref}}^{3/2}\,\hat{f}_V(L)}{2}\right)$$

- Compute the large-volume (physical) quantity via

$$\Phi_{\vec{V}} = \Phi_{\vec{V}}(L_1) + [\Phi_{\vec{V}}(L_2) - \Phi_{\vec{V}}(L_1)] + [\Phi_{\vec{V}} - \Phi_{\vec{V}}(L_2)]$$

- Each observable is continuum extrapolated.

First results

for the vector decay constant

[2312.09811] [2312.10017]

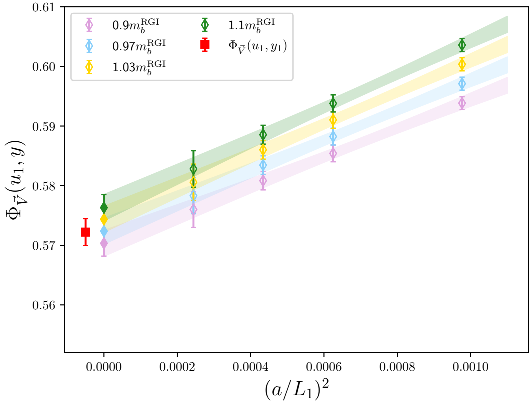
Recap: the strategy

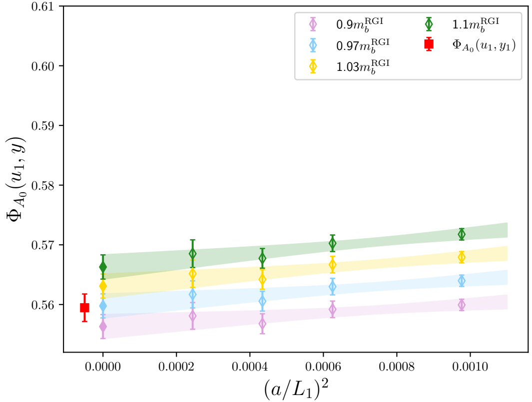
Interpolate observables to the B-scale:

- Interpolate between the static limit and $m_h \ll m_\mathrm{b}$:
  - In large volume: Ratios of observables like $h_\perp(E_\pi)/h_\perp(E_\pi^\mathrm{ref})$ or $h_\perp(E_\pi^\mathrm{ref})/\hat{f}_\mathrm{V}$.
  - Step-scaling functions such as σ_V, σ_m.
- Interpolate relativistic measurements around m_b:
  - In small volumes: Observables such as $\hat{f}_\mathrm{V}$, m_B/m_b.
- Interpolations in $1/m_h$ are performed in the continuum limit:
  - Continuum extrapolations at the B-scale only for $a^{-1} \in [9.5,\ 25]\,\mathrm{GeV}^{-1}$
  - Cutoff effects partially cancel in differences.

$$\Phi_{\vec{V}} = \Phi_{\vec{V}}(L_1) + [\Phi_{\vec{V}}(L_2) - \Phi_{\vec{V}}(L_1)] + [\Phi_{\vec{V}} - \Phi_{\vec{V}}(L_2)]$$

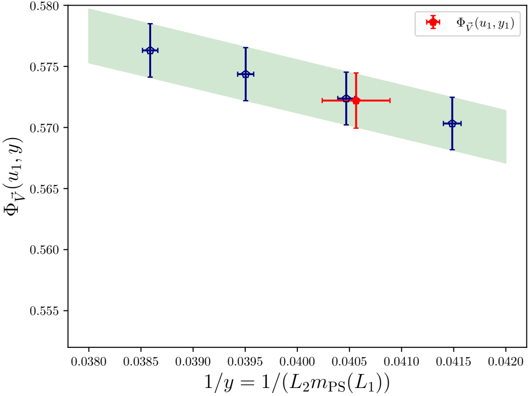
Continuum extrapolation at the bottom scale

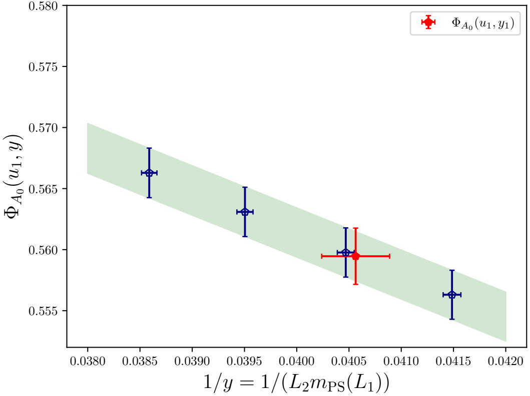




- B-physics on fine lattices in small volumes
- Continuum extrapolations for vector (left) and axial (right) decay constants.
- Four heavy valence quark masses encompass the bottom quark mass.

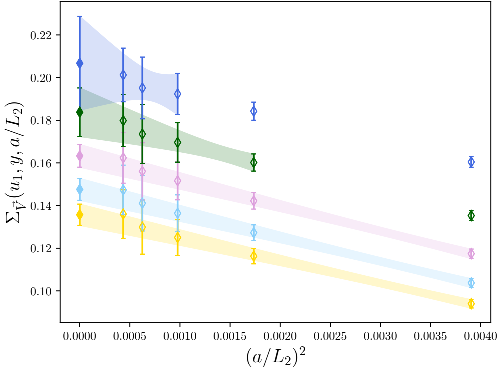
INTERPOLATION TO THE BOTTOM SCALE



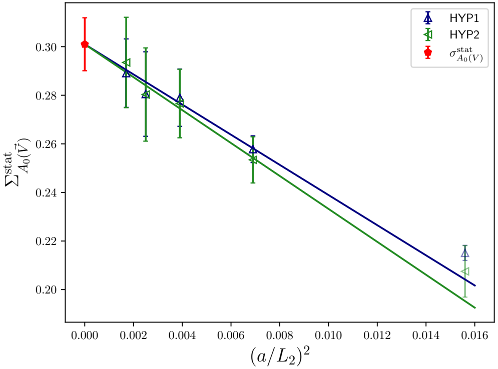


- B-physics on fine lattices in small volumes.
- Straight-forward interpolation to $m_h = m_{\rm b}$.
- Interpolate in inverse heavy-light meson mass $1/y = 1/(L_{\rm ref} m_{\rm PS}(L_1)) \propto 1/m_h$

- Continuum extrapolation of relativistic and static step-scaling functions for $\Phi_{\vec{V}}$.
- Vector and axial-vector decay constants are equal in the static theory.
- $L = 0.5\,\mathrm{fm}$ to $L = 1\,\mathrm{fm}$. Only include $am_h^{\mathrm{RGI}} < 0.8$.

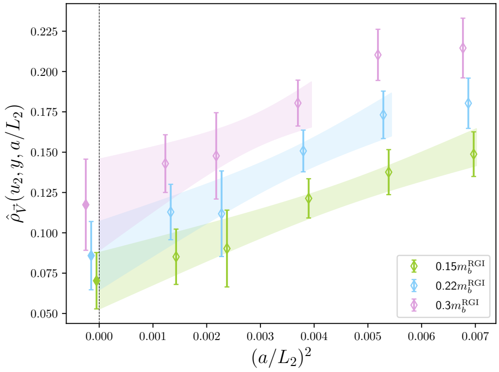


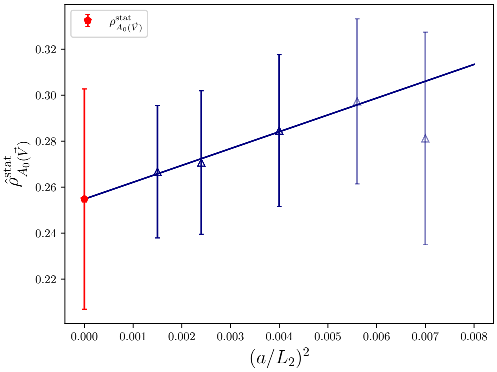
relativistic: valence masses $m_h^{\mathrm{RGI}} < 0.5\, m_b^{\mathrm{RGI}}$



static: two heavy quark actions

- Continuum extrapolation of relativistic and static step-scaling functions for $\Phi_{\vec{V}}$.
- $L = 1\,\mathrm{fm}$ to L_{CLS}. Only include $am_h^{\mathrm{RGI}} < 0.8$.

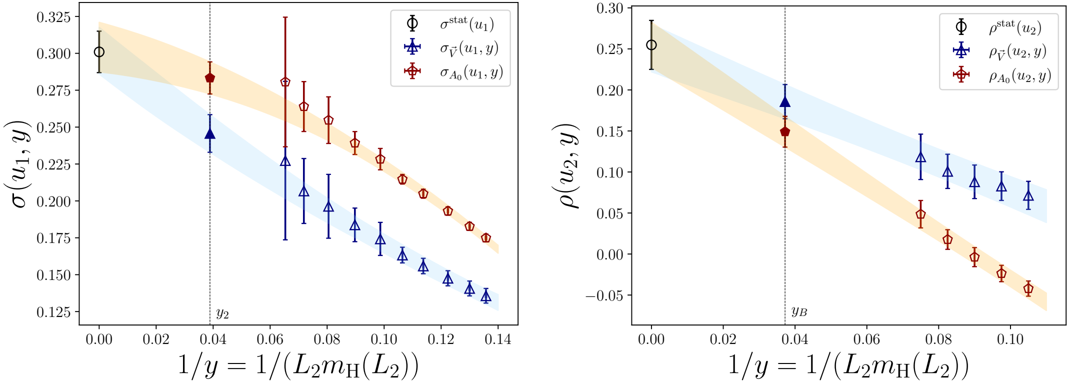




relativistic: valence masses $m_h^{\mathrm{RGI}} < 0.3\, m_b^{\mathrm{RGI}}$

static

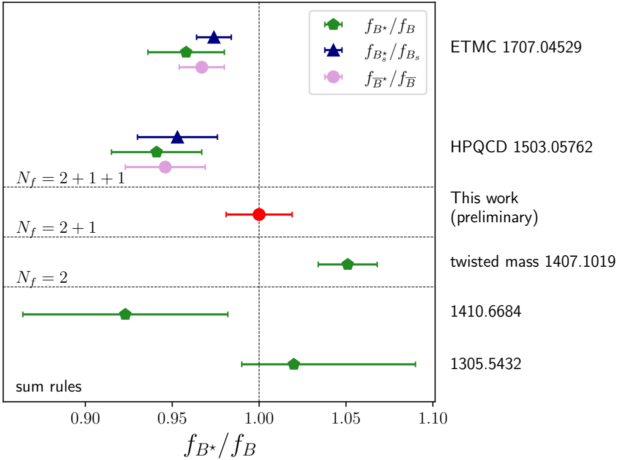
- Interpolation to $1/m_B$: highly constrained by the static result.
- Step-scaling functions of pseudoscalar Φ_{A_0} and vector $\Phi_{\vec{V}}$ decay constant have the same static limit (heavy quark symmetry).



$L_1 \to L_2$ $\qquad$ $L_2 \to L_{\text{CLS}}$

Results for $f_{B^\star}/f_B$

- Combine all pieces to arrive at the final result.
- N.b.: We (currently) work at the SU(3) symmetric point.
  Expect light quark dependence in the **ratio** $f_{B^\star}/f_B$ to be small.



- Puzzling situation for the ratios $f_{B_{(s)}}/f_{B^\star_{(s)}}$.
- Systematically improvable result with competitive uncertainties.

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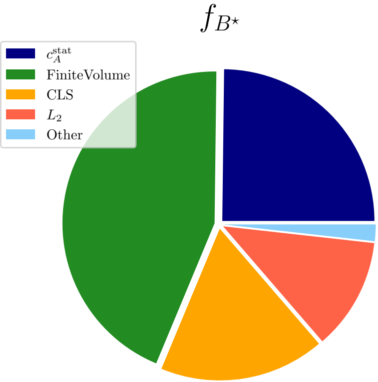
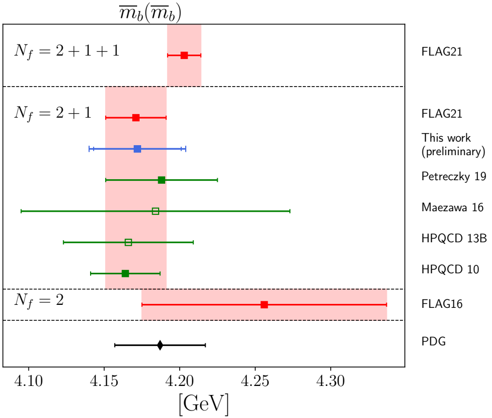
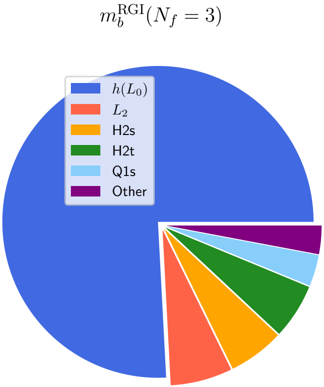


- Puzzling situation for the ratios $f_{B_{(\mathrm{s})}}/f_{B^\star_{(\mathrm{s})}}$.
- Systematically improvable result with competitive uncertainties.
- Decay constants currently at about 2.5% precision, dominated by finite-volume statistical uncertainties.

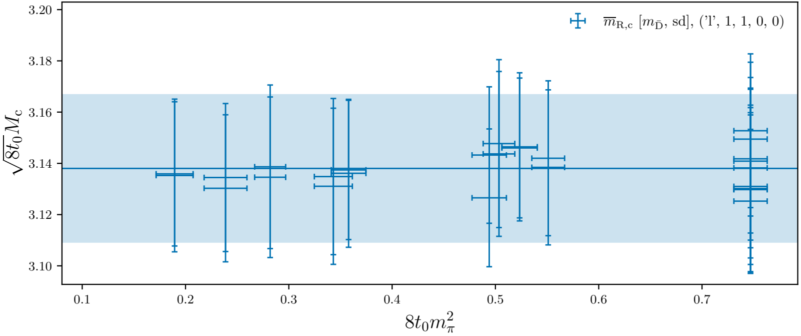
Full step-scaling for m_b

- Slightly more involved: Compute $m_b^{\mathrm{RGI}}(N_f = 3) = 6.605(61)\ \mathrm{GeV}\ [0.9\%]$.
- Uncertainty dominated by running to RGI $\rightarrow$ improvable external quantity.





- Slightly more involved: Compute $m_b^{\mathrm{RGI}}(N_f = 3) = 6.605(61)$ GeV $[0.9\%]$.
- Uncertainty dominated by running to RGI $\rightarrow$ improvable external quantity.
- Expect very mild light-quark dependence [Heitger, Joswig, SK, 2101.02694]:



Conclusions

- Step-scaling solves the multi-scale problem in lattice QCD: Standard Model predictions that are limited by statistical and not systematic uncertainties.
- This leads to the most precise predictions for α_s on the market.
- Prospects to remove the dominant systematic uncertainties in B-physics predictions from lattice QCD.
- Next step: Proceed from the proof of concept to phenomenologically semi-leptonic form factors.
- The step-scaling is performed in the continuum: Results can be used with **any discretization of large-volume QCD**.

Backup: more results

The mass of the bottom quark

[2312.09811] [2312.10017]

The bottom quark mass from step-scaling

- In small volume, compute

$$m_h^{\rm RGI} = \frac{M}{m_{\rm R}(1/L_0)} \frac{Z_{\rm A}}{Z_{\rm P}(L_0)} [1 + (b_{\rm A} - b_{\rm P}) a m_h] m_h^{\rm PCAC}(L_1) \quad \text{and} \quad \pi_m = \frac{m_{\rm PS}(L_1)}{m_h^{\rm RGI}}$$

with the running factor from [ALPHA, 1802.05243] and the renormalization and improvement from [Fritzsch, Heitger, SK].

- Compute the bottom quark mass via

$$L_{\rm ref} m_h^{\rm RGI} = \Big(L_{\rm ref} m_{\rm PS} - L_{\rm ref} [m_{\rm PS} - m_{\rm PS}(L_2)] - L_{\rm ref} [m_{\rm PS}(L_2) - m_{\rm PS}(L_1)] \Big) \frac{m_h^{\rm RGI}}{m_{\rm PS}(L_1)}$$

$$\equiv \frac{L_{\rm ref} m_{\rm PS} - \rho_m(L_2) - \sigma_m(L_1)}{\pi_m(L_1)}$$

with the physical input for $m_{\rm PS}$. We choose $m_{\rm PS} = m_{\overline{B}} \equiv \frac{2}{3} m_B + \frac{1}{3} m_{B_{\rm s}}$ for $h = {\rm b}$.

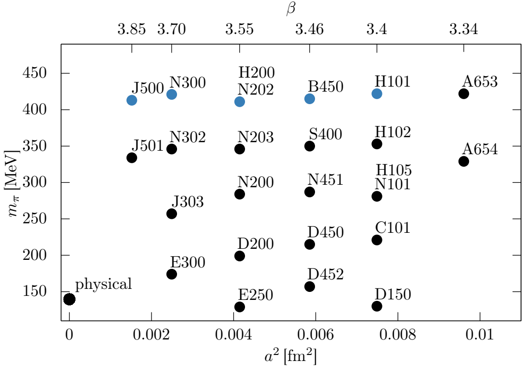
The bottom quark mass from step-scaling

- We have omitted the light quark dependence. Let's expand

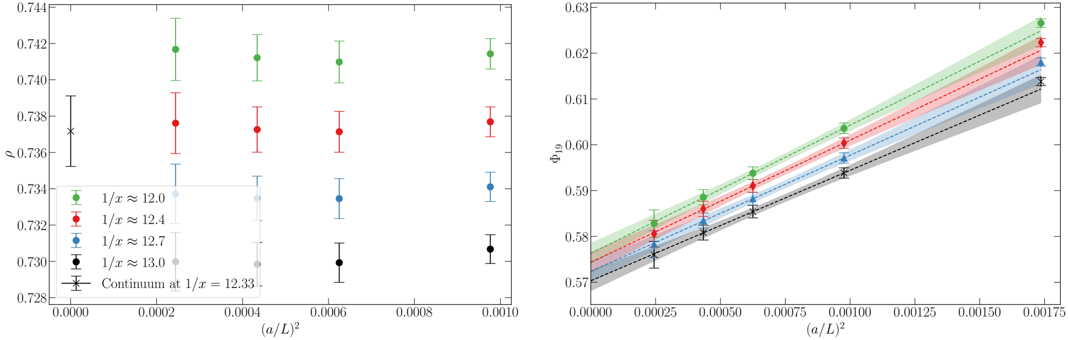
$$\rho_m(L_2) = L_{\mathrm{ref}}[m_{\mathrm{PS}} - m_{\mathrm{PS}}(L_2)]$$
$$= L_{\mathrm{ref}}\left[m_{\mathrm{PS}} - m_{\mathrm{PS}}^{\mathrm{SU(3)}}\right] - L_{\mathrm{ref}}\left[m_{\mathrm{PS}}^{\mathrm{SU(3)}} - m_{\mathrm{PS}}(L_2)\right]$$

where $m_{\mathrm{PS}}^{\mathrm{SU(3)}} \equiv m_{\mathrm{PS}}(m_\pi = m_K \approx 420\,\mathrm{MeV})$ is the heavy-light meson mass at the SU(3) symmetric point.

- Normalize step-scaling to the SU(3) symmetric point ($2+1$ flavor CLS).
- Compute $L_{\mathrm{ref}}[m_{\mathrm{PS}} - m_{\mathrm{PS}}^{\mathrm{SU(3)}}]$ for $m_\pi \to m_\pi^{\mathrm{phys}}$.
- Current status:
  Restrict to the SU(3) symmetric point.



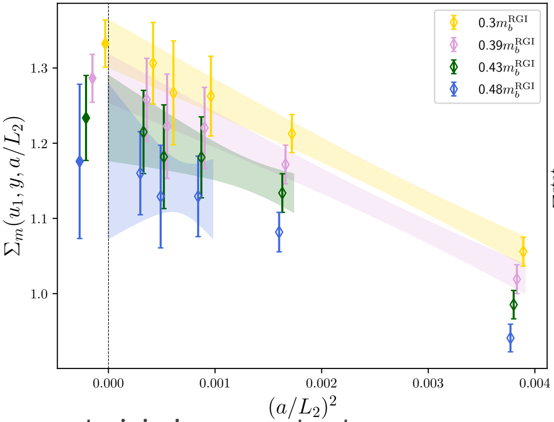
Continuum extrapolation at the bottom scale



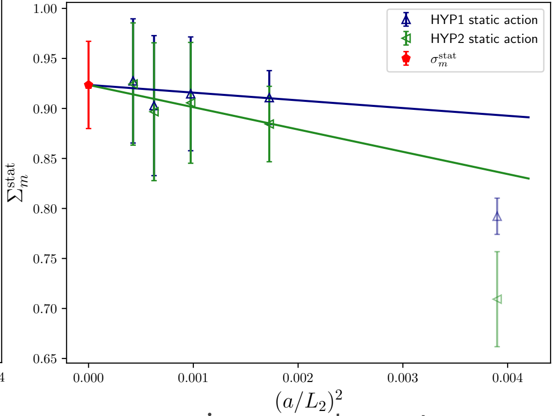
- Continuum extrapolations at the bottom scale for the step-scaling approach.
- Left: Ratio of heavy-light meson mass and heavy quark mass m_H/m_h^{RGI}.
- Right: Vector decay constant.

L_1 TO L_2: CONTINUUM LIMIT

- Continuum extrapolation of relativistic and static step-scaling functions for the quark mass $\Sigma_m = L_2\,[m_H(L_2) - m_H(L_1)]$ and $\Sigma_m^{\rm stat}$ from $L = 0.5\,{\rm fm}$ to $L = 1\,{\rm fm}$ with $m_h^{\rm RGI} < 0.5\,m_b^{\rm RGI}$.



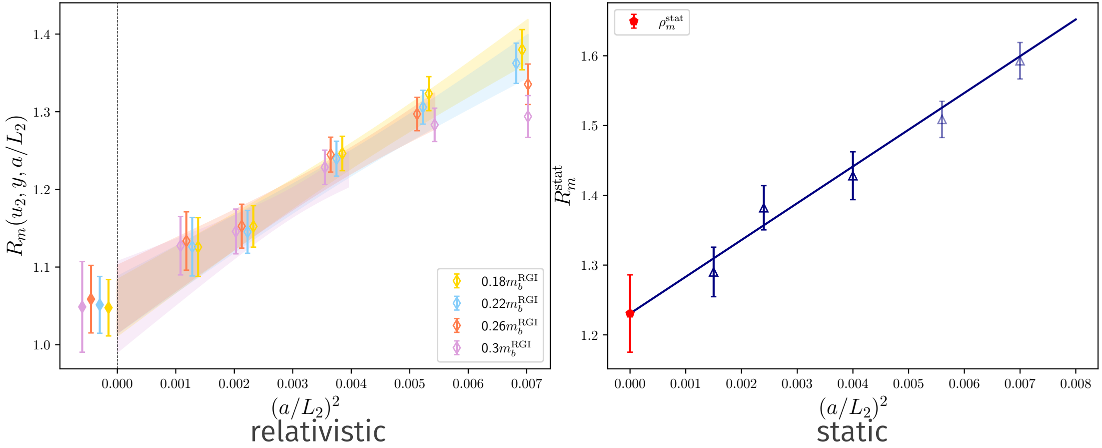
relativistic: several valence masses



static: $c_{\rm A}$ not known!

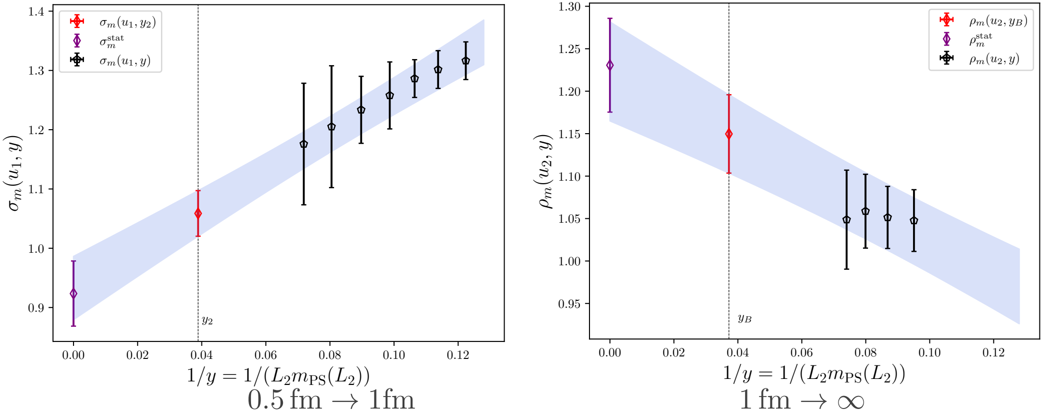
L_2 TO CLS: CONTINUUM LIMIT

- Continuum extrapolation of relativistic and static step-scaling functions for the quark mass $R_m = L_2\,[m_H - m_H(L_2)]$ and R_m^{stat} from $L = 1\,\mathrm{fm}$ to CLS with $m_h^{\mathrm{RGI}} < 0.3\, m_b^{\mathrm{RGI}}$.



SSFs in the continuum

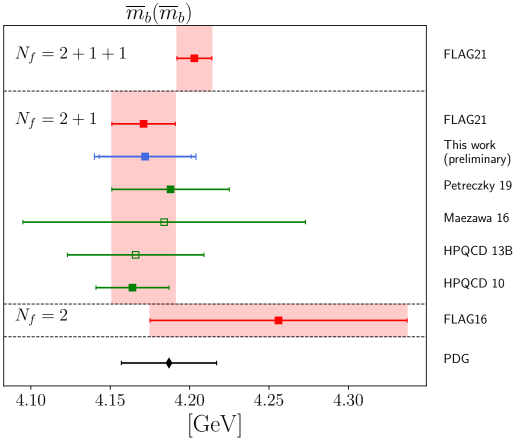
- Interpolate SSFs to the bottom scale in the continuum, where $\sigma_m = \lim_{a\to 0} \Sigma_m$ and $\rho_m = \lim_{a\to 0} R_m$.

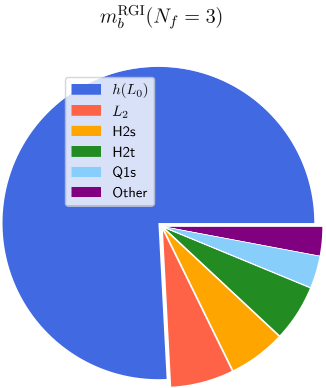


FULL STEP-SCALING FOR m_{b}

$$m_b^{\mathrm{RGI}}(N_f=3) = \frac{L_{\mathrm{ref}}m_{\mathrm{PS}} - \rho_m(L_2) - \sigma_m(L_1)}{L_{\mathrm{ref}}\pi_m(L_1)} = 6.605(61)\ \mathrm{GeV}\ [0.9\%]$$

- Uncertainty dominated by running to RGI $\to$ improvable external quantity.





Full step-scaling for m_b

$$m_b^{\mathrm{RGI}}(N_f = 3) = \frac{L_{\mathrm{ref}} m_{\mathrm{PS}} - \rho_m(L_2) - \sigma_m(L_1)}{L_{\mathrm{ref}} \pi_m(L_1)} = 6.605(61)\ \mathrm{GeV}\ [0.9\%]$$

- Uncertainty dominated by running to RGI $\rightarrow$ improvable external quantity.
- Expect very mild light-quark dependence [SK, Heitger, Joswig, 2101.02694]: