# Heavy flavor physics with O(a) improved Wilson quarks

SIMON KUBERSKI

FIRST LATTICENET WORKSHOP ON CHALLENGES IN LATTICE FIELD THEORY SEPTEMBER 13, 2022





#### THE SEARCH FOR NEW PHYSICS

- Indirect search via precision physics in the flavor sector.
- CKM matrix elements can be overconstrained to test the SM.
- **Discrepancy between exclusive and inclusive determination of**  $|V_{cb}|$ :

$$\left| V_{\rm cb}^{\rm excl} \right| = (39.1 \pm 0.5) \times 10^{-3}, \qquad \left| V_{\rm cb}^{\rm incl} \right| = (42.2 \pm 0.8) \times 10^{-3}$$

#### Lattice QCD provides input for both quantities

- Form factors of semi-leptonic *B* decays for  $|V_{cb}^{excl}|$ .
- Charm and bottom quark masses for  $|V_{cb}^{incl}|$ .

# LATTICE QCD - SCALES



Red marks: Pion, D- and B-meson masses

- $\Lambda_{\rm IR} = L^{-1}$ , inverse lattice extent. Typically  $L \gtrsim 4/m_\pi \approx 6$  fm
- $\Lambda_{\rm UV}=a^{-1}$ , inverse lattice spacing. Typically  $a\lesssim 1/(2m_{\rm D})pprox 0.05\,{\rm fm}$

Image taken from [1002.1807, Della Morte and Heitger]

- We work with three flavors of O(a) improved Wilson quarks in the sea.
- Renormalization and improvement pattern of flavor non-diagonal operators in a massless renormalization scheme [hep-lat/0511014, Bhattacharya et al.]:

$$(O^{ij})^{\mathrm{I}}_{\mathrm{R}}(x) = Z_{\mathrm{O}}(\tilde{g}_0^2, a\mu) \left[ 1 + ab_O(\tilde{g}_0^2)m_{\mathrm{q},ij} + a\bar{b}_O(\tilde{g}_0^2)\mathrm{Tr}[M_{\mathrm{q}}] \right] \left( O^{ij}(x) + a\delta O^{ij}(x) \right)$$

with the O(a) improved bare coupling  $\tilde{g}_0^2$  and a possible scale dependence  $a\mu$ .

- Valence  $am_{q,ij}$  and sea quark mass  $a Tr [M_q]$  dependent cutoff effects.
- Heavy flavor physics on  $N_{\rm f} = 2 + 1$  ensembles: Non-perturbative determination of  $b_O$  to cancel valence quark mass dependent cutoff effects  $O(am_{\rm q})$ .

# $2+1\ {\rm flavor}\ {\rm CLS}\ {\rm ensembles}$



- O(a) improved Wilson-clover fermions, Lüscher-Weisz gauge action.
- Five values of  $a \in [0.039, 0.087]$  fm, a factor of 5 in  $a^2$ .
- Open boundary conditions in temporal direction.

$$m_{\pi} \in [129, 422] \,\mathrm{MeV}$$

Trajectory in this work:  $\operatorname{Tr}[M_q] = 2m_1 + m_s = \text{const.}$  to keep improved coupling  $\tilde{g}_0^2 = g_0^2 \left(1 + \frac{1}{N_f} b_g a \operatorname{Tr}[M_q]\right)$  constant up to  $\mathcal{O}(a^2)$ .

# **CHARM PHYSICS**

- Charm quark mass is a basic parameter of the Standard Model.
- Meson and quark masses from axial  $A^{ij}_{\mu}$  and pseudoscalar  $P^{ij}$  quark bilinears.
- Bare quark masses from the PCAC relation:

 $\partial_0 \langle (A_{\rm I})_0^{ij} P^{ji} \rangle = 2m_{ij} \langle P^{ij} P^{ji} \rangle + \mathcal{O}(a^2) \,, \qquad \text{where} \quad (A_{\rm I})_\mu^{ij} = A_\mu^{ij} + ac_{\rm A} \partial_\mu P^{ij}$ 

- Measure at two heavy masses around the charm.
- Set the charm quark hopping parameter  $\kappa_c$  from the flavor averaged D-meson mass  $m_{\bar{D}} = \frac{2}{3}m_D + \frac{1}{3}m_{D_s}$  or the connected part of  $\eta_c$ .

<sup>&</sup>lt;sup>\*</sup>with J. Heitger and F. Joswig

## **RENORMALIZED QUARK MASS**

Compute the renormalized RGI charm quark mass from PCAC masses:

$$\begin{split} M_c^{\mathrm{RGI}} &= \frac{M}{\overline{m}(\mu_{\mathrm{had}})} m_{cc',\mathrm{R}} \\ &\equiv Z_{\mathrm{M}} m_{\mathrm{cc'}} \left[ 1 + \frac{(b_{\mathrm{A}} - b_{\mathrm{P}})}{Z} a m_{\mathrm{cc'}} + \left( \frac{(\overline{b}_{\mathrm{A}} - \overline{b}_{\mathrm{P}})}{Z r_{\mathrm{m}}} - \frac{(b_{\mathrm{A}} - b_{\mathrm{P}})}{Z} \frac{(r_{\mathrm{m}} - 1)}{r_{\mathrm{m}} N_{\mathrm{f}}} \right) a M_{\mathrm{sum}} \right] \end{split}$$

- ►  $Z_{\rm M} = M/\overline{m}(\mu_{\rm had}) \cdot Z_{\rm A}/Z_{\rm P}(\mu_{\rm had})$ : [1802.05243, Campos et al.], including  $Z_{\rm A}$  from [1808.09236, Dalla Brida et al.]
- ▶  $(b_{\rm A} b_{\rm P})$  and  $Z = Z_{\rm m} Z_{\rm P} / Z_{\rm A}$ : [1906.03445, de Divitiis et al.]
- $(r_{\rm m}-1)$ : [2101.10969, Heitger et al.]
- ▶  $(\overline{b}_{\rm A} \overline{b}_{\rm P}) \propto \mathcal{O}(g_0^4)$ , not known non-perturbatively

• 
$$aM_{sum} = am_{12} + am_{23} + am_{31} = Zr_{m}Tr[M_{q}] + O(a)$$

Alternative definitions via heavy-sea currents and the ratio-difference method [1011.2711, Dürr et al.]. Two definitions of discretized derivative  $\tilde{\partial}_0$  in PCAC mass.

# **CHARM PHYSICS**

Intermission: Non-perturbative improvement and renormalization

# THE SCHRÖDINGER FUNCTIONAL



■ ALPHA's tool of choice for renormalization and O(*a*) improvement [hep-lat/9207009, Lüscher et al.].

- Dirichlet boundary conditions in time direction. Suited for Monte Carlo simulations and perturbative calculations.
- Boundary conditions and finite volume allow the simulation of massless quarks [hep-lat/9312079, Sint].
- $\blacksquare$  Finite volume  $\rightarrow$  consider short-ranged quantities.
- Renormalization and improvement from Ward identities.

# Improvement and renormalization from the SF $^{\star}$



 $\blacksquare$  Non-perturbative determination of  $b_{\rm A} - b_{\rm P}$  and Z [1906.03445, de Divitiis et al.].

• Cut-off effects of  $O(am_{cc'})$  are canceled via  $\frac{(b_A - b_P)}{Z} am_{cc'}$ .

<sup>\*</sup>with G. M. de Divitiis, P. Fritzsch, J. Heitger, C. C. Koester, A. Vladikas

Simon Kuberski

# **CHARM PHYSICS**

Back to the quark mass

### MESON AND QUARK MASSES ON THE LATTICE



- Obtain bare quark masses with a relative error of  $O(10^{-3})$  to  $O(10^{-5})$ .
- Use distance preconditioning [1006.4028, de Divitiis et al.][1701.05502, Collins et al.] to prevent loss of numerical precision at large source-sink separation.

## CHIRAL-CONTINUUM EXTRAPOLATION

- Extrapolate to physical quark mass and vanishing lattice spacing.
- Measured on ensembles with  $m_{\pi} \ge 200 \,\mathrm{MeV}$ . No dependence on pion mass resolved.



# CONTINUUM EXTRAPOLATION

![](_page_14_Figure_1.jpeg)

- We find significant  $O(a^n)$ , n > 2 contributions for a > 0.06 fm.
- Different lattice definitions coincide in the continuum limit.

# CONTINUUM EXTRAPOLATION

![](_page_15_Figure_1.jpeg)

- Quantify systematic uncertainties in each data set via model averaging procedure [2008.01069, Jay and Neil].
- Combine results from all data sets for final result.

# Results for $m_{ m c}$

• Our final result is  $M_c(N_f = 3) = 1486(14)_{stat}(14)_{RGI}(6)_{sys} \text{ MeV} = 1486(21) \text{ MeV}.$ 

![](_page_16_Figure_2.jpeg)

Error dominated by external input.

- Convert to  $\bar{m}_c(\bar{m}_c)$  for comparison with other groups.
- Ongoing work on CLS ensembles:
  - RQCD with extended set of ensembles and different renormalization scheme [2206.04178, Bouma et al.].
  - Madrid group with twisted-mass on Wilson-clover  $\rightarrow$  automatic O(a)improvement of the charm.

# Outlook: Charmed decay constants \*

- Work with RQCD collaboration on the determination of  $f_{D_{(s)}^*}$  and  $f_{D_{(s)}^*}^{T}$ .
- **\blacksquare** Bare vector decay constants at 0.5% precision.
- Bare ratios  $f_{D_{(s)}^*}^T / f_{D_{(s)}^*}$  at sub permille precision, expect dominant contribution from  $Z_T(\mu)$  [1910.06759, Chimirri et al.][2111.15325, de Divitiis et al.].

![](_page_17_Figure_4.jpeg)

\*with G. Bali, S. Collins, J. Heitger, F. Joswig, W. Söldner

Simon Kuberski

# **BOTTOM PHYSICS**

# LATTICE QCD - SCALES

![](_page_19_Figure_1.jpeg)

- B-observables cannot be evaluated in large volume at several resolutions:  $L^{-1} \ll m_{\pi} \approx 140 \,\mathrm{MeV} \ll m_{\mathrm{B}} \approx 5 \,\mathrm{GeV} \ll a^{-1}$
- Bottom physics is a multi-scale problem!
- Employ non-perturbative Heavy Quark Effective Theory (HQET) to compute  $m_{\rm b}$ ,  $f_{B_{\rm (s)}}$ , form factors of semi-leptonic B-decays (everything is **preliminary**!).

Image taken from [1002.1807, Della Morte and Heitger]

# HQET AT ${ m O}(1/m_{ m h})$

#### Heavy Quark Effective Theory

- Integrate out heavy degrees of freedom of QCD Lagrangian for one heavy quark.
- Expand the Lagrangian in powers of  $1/m_{\rm h}$ .
- Describe bottom physics at next-to-leading order in HQET.

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

### HQET on the lattice

- Matrix elements in the effective theory can be computed in large volume.
- Renormalize the effective theory via **non-perturbative** matching to QCD.

# HQET AT ${ m O}(1/m_{ m h})$ on the lattice

- Cannot define the path integral from the HQET action at order  $1/m_h$  (contains dimension five operators  $\mathcal{O}_{kin}$  and  $\mathcal{O}_{spin}$ ).
- Expand the Boltzmann factor in the path integral in powers of the inverse heavy quark mass 1/m<sub>h</sub>.
- Expectation value of an operator:

$$\begin{split} \langle \mathcal{O} \rangle \approx &\frac{1}{Z} \int \mathcal{D}\phi \, \mathcal{O}\left(1 + a^4 \sum_{x} [\omega_{\rm kin} \mathcal{O}_{\rm kin}(x) + \omega_{\rm spin} \mathcal{O}_{\rm spin}(x)]\right) \mathrm{e}^{-(S_{\rm light} + S_{\rm HQET}^{\rm stat})} \\ = & \langle \mathcal{O} \rangle_{\rm stat} + \omega_{\rm kin} a^4 \sum_{x} \langle \mathcal{O} \mathcal{O}_{\rm kin} \rangle_{\rm stat} + \omega_{\rm spin} a^4 \sum_{x} \langle \mathcal{O} \mathcal{O}_{\rm spin} \rangle_{\rm stat} \,. \end{split}$$

 $\blacksquare$  O(1/m<sub>h</sub>) and O(a) mix on the lattice  $\rightarrow$  O(a) improvement is vital!

#### Simon Kuberski

### NON-PERTURBATIVE FINITE-VOLUME MATCHING

Perturbative matching at order g<sub>0</sub><sup>2l</sup> leads to power divergences in the coefficients [Nucl.Phys.B 368 (1992) 281-292, Maiani et al.]

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

due to mixing of operators differing in dimensions by p.  $\rightarrow$  Non-perturbative matching makes HQET well defined on the lattice.

- Hadronic input: Would loose predictivity of HQET.
- Finite-volume matching:
  - ► Match with continuum limit of lattice QCD observables.
  - Computation with fine resolutions in finite volume.
  - Assumption: Finite-volume effects only due to light degrees of freedom.

### NON-PERTURBATIVE FINITE-VOLUME MATCHING

- Finite volume  $L_1 = 0.5$  fm: Simulation of QCD with relativistic b-quarks and  $N_{\rm f} = 3$  massless sea quarks.
- Solve matching equations [hep-lat/0310035, Heitger and Sommer] [1312.1566, Della Morte et al.]:

 $\lim_{a \to 0} \phi_i^{\text{QCD}}(L_1, M, a) = \phi_i^{\text{HQET}}(L_1, M, a) = \eta_i(L_1, a) + \varphi_i^j(L_1, a)\omega(M, a) + O(1/m_h^2)$ 

for matching parameters  $\omega(M, a)$ .

■ 19 parameters → 19 equations to define Lagrangian and heavy-light axial and vector currents at  $O(1/m_h)$ .

■ Valence line of constant physics defined from fixed RGI quark mass,

$$z \equiv L_1 M = L_1 \frac{M}{\overline{m}(1/L_0)} \frac{Z(g_0^2) Z_{\rm A}(g_0^2)}{Z_{\rm P}(g_0^2, L_0)} (1 + b_{\rm m}(g_0^2) a m_{\rm q,h}) a m_{\rm q,h} \,,$$

based on the subtracted quark mass  $am_{q,h} = 1/2(1/\kappa_h - 1/\kappa_{cr})$  and  $L_0 = L_1/2$ .

- **Running factor known, dedicated computation of**  $Z_A$ ,  $Z_P$ , Z and  ${b_m}^*$ .
- Measure in a range of quark masses  $0.8z_{\rm c} < z_{\rm q,h} < 1.2z_{\rm b}$ .

<sup>&</sup>lt;sup>\*</sup>with P. Fritzsch and J. Heitger

# STEP-SCALING

- Need to know matching parameters in large volume!
- Step-scaling [Nucl. Phys. B359 (1991) 221, Lüscher et al.] offers an approach to multi-scale problems:
  - Determination of  $\Lambda_{\rm QCD}$  [1706.03821, ALPHA].
  - Running of quark masses up to RGI point [1802.05243, ALPHA].
  - **B-physics** [hep-lat/0310035, ALPHA].
- Introduce external scale via spatial lattice extent  $\mu = 1/L$ .
- Investigate scale evolution via step-scaling functions,

 $\sigma(O(L)) = O(sL)\,,$ 

where s = 2 is a conventional choice.

# NON-PERTURBATIVE FINITE-VOLUME MATCHING

![](_page_26_Figure_1.jpeg)

- QCD observables with relativistic b quarks in finite volume at  $L_1 = 0.5$  fm.
- Match with corresponding HQET observables.
- Evolve HQET parameters to large volumes via step-scaling  $L_1 \rightarrow 2L_1 \rightarrow L_{CLS}$ .
- Generated O(25) SF ensembles with volumes up to  $L^4 = 64^4$  and 100k MDU.

Image taken from [1001.4783, Blossier et al.] \*with P. Fritzsch, J. Heitger, H. Simma, R. Sommer

## FINITE-VOLUME MATCHING

![](_page_27_Figure_1.jpeg)

Look at matching observable

$$\phi_{V_0}^{\text{QCD}}(L_1) = \frac{F_{V_0}^{B \to \pi}(T/2)}{\sqrt{F_1^{\pi}(T)F_1^B(T)}},$$

needed to determine  $Z_{V_0}^{HQET}$ .

 $\leftarrow \mbox{ QCD results close to } z_{\rm b} \sim 17 \mbox{ at four } \\ \mbox{ lattice spacings } 0.0078 \mbox{ fm} < a < 0.0156 \mbox{ fm} \\ \mbox{ and mass-continuum fit.}$ 

Solve matching equations for matching parameters  $\omega(M, a)$ :

$$\lim_{a \to 0} \phi_i^{\text{QCD}}(L_1, M, a) = \phi_i^{\text{HQET}}(L_1, M, a) = \eta_i(L_1, a) + \varphi_i^j(L_1, a)\omega(M, a) + O(1/m_h^2)$$

## STEP-SCALING OF HQET

![](_page_28_Figure_1.jpeg)

- $\leftarrow \begin{array}{l} {\sf Step-scaling function of HQET observable} \\ \eta_{V_0} \mbox{ from } 0.5 \mbox{ fm to } 1 \mbox{ fm at five lattice} \\ {\sf spacings } 0.021 \mbox{ fm } < a < 0.063 \mbox{ fm} \end{array}$ 
  - Next step: contact with large-volume CLS ensembles.
  - Measurements done, analysis ongoing.

# Large-volume HQET with $N_{\mathrm{f}}=3$ \*

![](_page_29_Figure_1.jpeg)

- Measurements at O(1/m<sub>h</sub>) on CLS ensembles ongoing.
- HYP smeared static quark lines for exponential noise reduction [hep-lat/0307021, Della Morte et al.].
- Smeared quark fields and GEVP extraction of energies and matrix elements [0902.1265, Blossier et al.].

Extraction of static, as well as higher-order kinetic and spin contributions.

B-meson mass from large volume results and matching parameters:

$$m_B = m_{\text{bare}} + E^{\text{stat}} + \omega_{\text{kin}} E^{\text{kin}} + \omega_{\text{spin}} E^{\text{spin}} + O(1/m_{\text{h}}^2)$$

<sup>\*</sup>with A. Gérardin, J. Heitger, H. Simma, R. Sommer

# Large-volume HQET with $N_{ m f}=3$

![](_page_30_Figure_1.jpeg)

■ Splitting  $m_{B_s}^{\text{stat}} - m_B^{\text{stat}} = 82.2(1.9)_{\text{stat}}$  well defined without matching parameters.

■ PDG value  $m_{B_{\bullet}}^{\text{phys}} - m_{B}^{\text{phys}} = 87.42(14)$  allows estimate of  $O(1/m_{\text{h}})$  effects.

• Three resolutions  $a \ge 0.064 \text{ fm}$  so far: cutoff effects are small.

Simon Kuberski

# The $B^*B\pi$ coupling

![](_page_31_Figure_2.jpeg)

- Low energy constant  $\hat{g}$  of Heavy Meson  $\chi$ PT related to the  $B^*B\pi$  coupling with **static heavy** and **chiral light** quarks.
- Precision of lattice computations limited by chiral extrapolation (chiral log!).
- $\leftarrow \mbox{ Chiral-continuum extrapolation in} \\ y = \frac{m_\pi^2}{8\pi^2 f_\pi^2} \mbox{ and } a^2.$ 
  - Previous works at  $m_{\pi} \geq 270 \,\mathrm{MeV}$ .
- $\blacksquare$  Measurements are done, analysis to be finished. Aim at 2% precision.
- Will be of great use in (our) chiral extrapolations of lattice results and phenomenological calculations.

# Outlook: The step-scaling method for B-physics \*

There is an alternative route to employ step-scaling [hep-lat/0305018, de Divitiis et al.]: Scale finite-volume relativistic heavy quark observables with  $am_h \le am_b$ :

$$O(m_{\rm h}, L_{\infty}) = O(m_{\rm h}, L_1) \frac{O(m_{\rm h}, L_2)}{O(m_{\rm h}, L_1)} \dots \frac{O(m_{\rm h}, L_N)}{O(m_{\rm h}, L_{N-1})}$$

- As the lattice size is doubled:
  - ► The affordable lattice spacings increase.
  - The simulated maximal heavy quark mass decreases.
  - Need to extrapolate to obtain  $m_{\rm h} \rightarrow m_{\rm b}$  for  $L_2 \rightarrow L_{\rm CLS}$ .
- Combination with non-perturbative static HQET turns extrapolations to interpolations with enhanced precision [0710.2229, Guazzini et al.].

<sup>\*</sup>with A. Conigli, J. Frison, P. Fritzsch, A. Gérardin, J. Heitger, G. Herdoíza, C. Pena, H. Simma, R. Sommer

# PROOF OF CONCEPT IN THE QUENCHED APPROXIMATION

![](_page_33_Figure_1.jpeg)

- Quark mass dependence parameterized by  $x = 1/(L_1 m_{\rm PS}(m_{\rm h}, L))$ .
- Left: Step-scaling of the mass static constraint of the form  $1 + \sigma_m^{stat}x$ .
- **Right:** Step-scaling of decay constant static result at x = 0.

Image taken from [0710.2229, Guazzini et al.]

# **OUTLOOK: THE STEP-SCALING METHOD FOR B-PHYSICS**

![](_page_34_Figure_1.jpeg)

- Work in progress: Step-scaling and large-volume measurements (L<sub>2</sub> = L<sub>CLS</sub>).
- $\leftarrow \mbox{ Step scaling function} \\ \Sigma_{V_0}(L_1/a) = \frac{\phi_{V_0}(2L_1/a)}{\phi_{V_0}(L_1/a)} \\ \mbox{ for the time-component of the vector} \\ \mbox{ current from } 0.5 \mbox{ fm to } 1 \mbox{ fm at five lattice} \\ \mbox{ spacings } 0.021 \mbox{ fm } < a < 0.063 \mbox{ fm} \ \end{cases}$ 
  - Good parametrization up to  $1.2m_{\rm b}$ .
- **\blacksquare** Static HQET observables at x = 0 from the HQET project.
- CLS: Heavy quark measurements with  $m_c \le m_h \le 2.5m_c$  are on track at the  $SU(3)_f$ -symmetric point.

# Outlook

#### Charm physics

- Symanzik improvement allows reliable extraction of charm observables.
- Competitive determination of Standard Model parameters.
- $N_{\rm f} = 2 + 1 + 1$  non-trivial for O(a) improved Wilson [2002.02866, Höllwieser et al.].

#### Bottom physics

- Non-perturbative HQET on the lattice removes systematic uncertainties from large cutoff effects in B-physics observables.
- $\blacksquare$  High setup cost  $\rightarrow$  hope to have first results soon.
- Work on two approaches with different systematic effects.

![](_page_36_Picture_0.jpeg)

#### **TECHNICAL CHALLENGES WITH HEAVY QUARKS**

![](_page_37_Figure_1.jpeg)

- Quality of the solution deteriorates quickly for large source-sink separations (shown here: J501).
- Especially problematic if sources are placed close to the boundary.
- Charm-charm correlation functions: small but finite plateau regions.

# **DISTANCE PRECONDITIONING**

![](_page_38_Figure_1.jpeg)

- We employ Distance
   Preconditioning [1006.4028, de Divitiis et al.]
- SAP-preconditioned GCR solver [1701.05502, Collins et al.], [T. Korzec, mesons]
  - Figure: tuning for H400 at  $y_0/a = 84$

$$(PDP^{-1})(PS) = (P\eta), \quad P = \text{diag}(p_i), \quad p_i = \exp(\alpha |y_0 - x_0|)$$