Details of RQCD analyses on CLS ensembles

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High statistics results for quantities like the gradient flow scale, the quark masses, the lower lying baryon spectrum and the baryon octet sigma terms determined on CLS ensembles with $N_f = 2 + 1$ non-perturbatively $\mathcal{O}(a)$ improved Wilson dynamical fermions are presented at this conference by the RQCD collaboration. In this contribution, we provide further details of the analysis focusing on systematics associated with the extraction of the lattice data including autocorrelations and the continuum, quark mass and finite volume extrapolations, including the fit forms employed.

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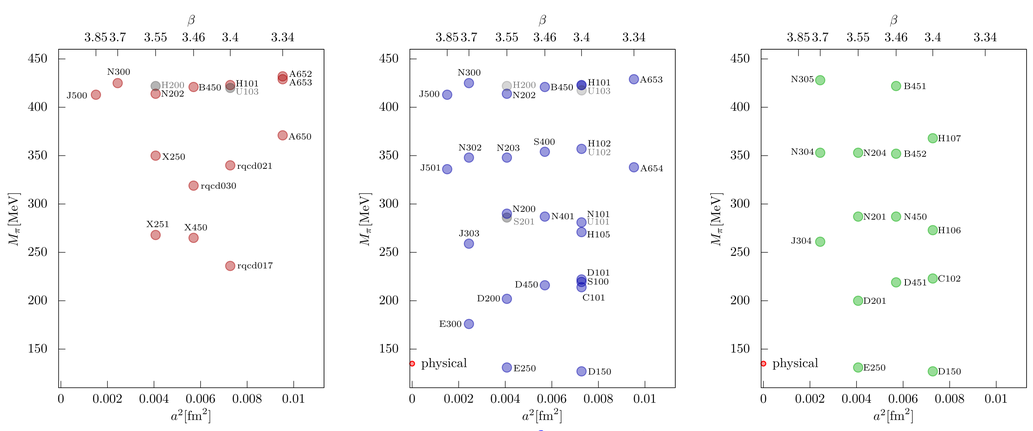
Ensemble overview



$m_s = m_\ell$ $m_s + 2m_\ell = \text{const.}$ $m_s = \text{const.}$

- Coordinated Lattice Simulations (CLS) ensembles
  - major effort to generate gauge field configurations (mostly with open boundary conditions)
  - aiming at large statistics/volumes and pion masses close to the physical point

  ⇒ main focus of this large scale project: performing a well controlled continuum limit
- Non-perturbatively improved Wilson fermions with $2 + 1$ flavour and tree-level Symmanzik-improved gauge action
- Open/Anti-periodic boundaries imposed in the time direction, periodic in spatial direction
- three different chiral trajectories: constant average quark mass: $m_s + 2m_\ell = \text{const.}$, constant physical strange quark mass: $m_s = const.$, symmetric line: $m_s = m_\ell$
- Lattice spacings $0.099\ \text{fm} - 0.04\ \text{fm}$, pion masses $700\ \text{MeV} - 135\ \text{MeV}$
- Large volumes with $M_\pi L \gtrsim 4$ (additional ensembles exist to check for finite volume effects)

Combining the systematics

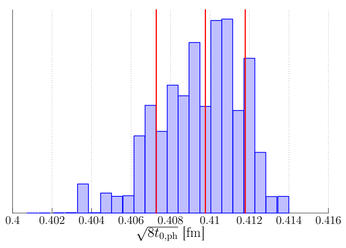
Two ways of including systematics

Approach for autocorrelations and determination of fit ranges

- fit ranges: excited states (and boundary effects) are estimated and fit ranges are chosen such that excited state (and boundary effect) contributions are negligible with respect to the statistical uncertainty → see mid-left panel
- autocorrelations: parameterize autocorrelations and take limit of vanishing autocorrelations → see mid-right panel

Approach for finite volume effects, chiral extrapolation, continuum extrapolation
→ vary systematics and assign individual weights based on the quality of the resulting fits (→ see AIC below)
→ perform average over the variations

- finite volume effects: include finite volume effects in fits + cuts on spatial extent L and LM_π
- chiral extrapolation: vary parametrization of mass dependence (BChPT, GMO, SSE,...) + cuts on the masses
- continuum extrapolation: vary lattice spacing dependence $(a^2, a^3, \bar{M}^2a^2, ...)$ + cuts on a → see lower two panels
- input parameters (like renormalization or improvement constants): errors included in the fit



histogram of the different weighted fits

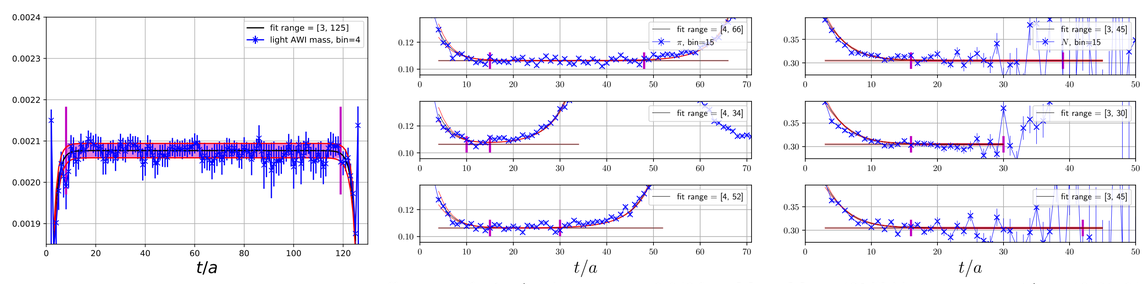
Akaike Information Criterion (AIC)

- we use a modified AIC [Akaike,(1998)] (following [BMWc,2002.12347])
- perform a weighted average of fit the results by weighting each fit j with $w_j = A \exp\left[-\frac{1}{2}\left(\chi^2_j - N_{DF,j} + p_j\right)\right]$
- standard AIC: fixed data, exponent $\chi^2_j + 2p_j$
  → favors fits with small χ^2/N_{DF} and a small number of parameters
- modification (subtract $n_{data,j} = N_{DF,j} + p_j$)
  → fix the parametrization and vary the data, favors small χ^2/N_{DF} and a large number of points

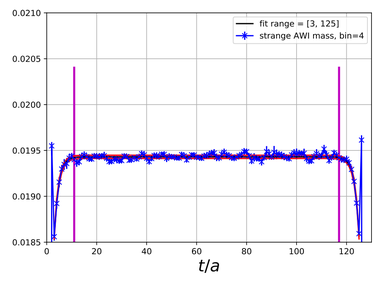
Example: calculation of Wilson flow parameter $t_{0,ph}$ → see talk by S. Collins

- fits to 18 differents cuts on the data, 18×100 bootstraps weighted with w_j
- final result: $\sqrt{8t_{0,ph}} = 0.4098^{(20)}_{(25)}$ fm (0.5% total uncertainty)
- dominated by fits with χ^2/N_{DF} of 0.94 ($N_{DF} = 80$) and 0.99 ($N_{DF} = 73$)

Extraction of hadron and AWI masses



eff. mass of pion/nucleon at $a = 0.049\,\text{fm}$, $M_\pi = M_K = 425\,\text{MeV}$, source pos. $t/a = 46, 81, 64$



light/strange AWI mass at $a = 0.075\,\text{fm}$ and $M_\pi = 216\,\text{MeV}$, $M_K = 480\,\text{MeV}$

Hadron masses: extraction of the ground state

- point-to-all correlators smeared at source and sink (rms smearing radius $r_{sm} \approx 0.60\,\text{fm}$ at $M_\pi \approx 420\,\text{MeV}$), number of sources: up to 32
- for pion/kaon additional one-end-trick data is available
- ground state is fitted within the range determined via this procedure:

  starting time slice:
  - estimate excited state contribution: fit to correlator by two-state fit
  - determine time slice where excited state contribution to correlator is smaller than 1/4 of statistical error of correlator

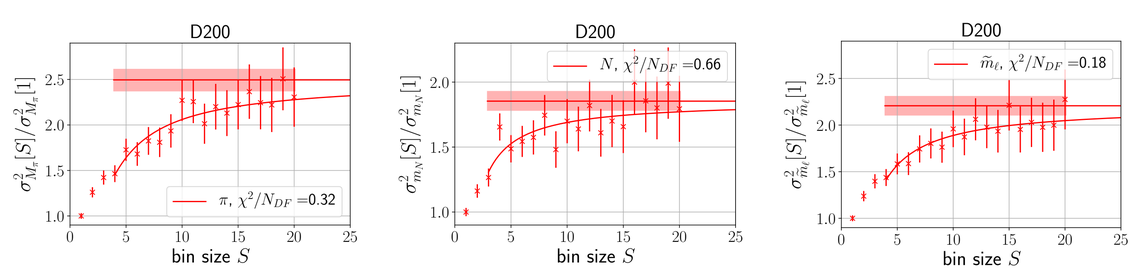
  ending time slice: similar procedure for estimating boundary effects
  → for baryons we stop fitting when signal becomes too noisy

⇒ determined fit range in above plot: indicated by the two red vertical bars

AWI masses

- parameterize boundary-/contact-terms by $\sim \mathrm{e}^{-m\,t}$
- determine time slice where the contribution of boundary-/contact-terms to AWI mass is smaller than 1/4 of statistical error of AWI mass
- fit AWI mass (to a constant) in the determined range → indicated by the two re vertical bars in the left plots

Autocorrelations



Bin size analysis

- HMC algorithm introduces autocorrelations
  → naive error determination underestimates statistical uncertainty
- utilize bin size analysis to account for autocorrelations → true errors are larger
- consider error $\sigma_A[S]$ of some quantity A at a bin size S
  → bin size dependence of σ_A is parameterized by:

  $\frac{\sigma^2_A[S]}{\sigma^2_A[1]} \approx 2\tau_{A,\text{int}}\left(1 - \frac{c_A}{S} + \frac{d_A}{S}e^{-S/\tau_{A,\text{int}}}\right)$ (with $c_A > d_A \geq 0$)

  → fit to data for $S \gtrsim 2\tau_{A,\text{int}}$

  → perform limit $S \to \infty$: $\sigma^2_A[S] \to 2\tau_{A,\text{int}}\,\sigma^2_A[1]$
- for coupling to only one mode one finds → $\frac{\sigma^2[S]}{\sigma^2[1]} \approx 2\tau\left[1 - \frac{\tau}{S}\left(1 - e^{-S/\tau}\right)\right]$
  → works very well for t_0
- also covariances σ_{AB} are extrapolated to infinite bin size using

  $\frac{\sigma_{AB}[S]}{\sigma_A[1]\sigma_B[1]} \approx 2\tau_{AB,\text{int}}\left(1 - \frac{c_{AB}}{S} + \frac{d_{AB}}{S}e^{-S/\tau_{AB,\text{int}}}\right)$
- plots: examples for pion mass M_π, nucleon mass m_N, AWI mass $\widetilde{m}_\ell$ (upper plots); Wilson flow parameter t_0 (mid-left) and σ_{M_π,M_K} (lower-left)

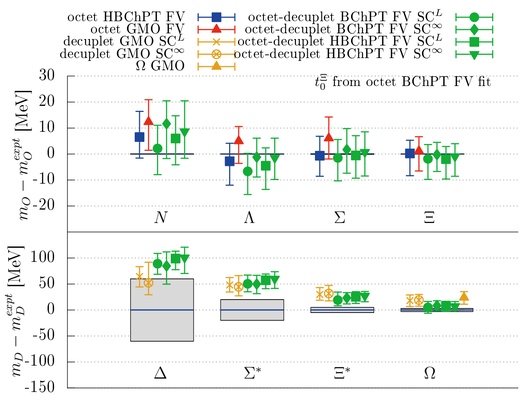
Continuum, finite volume and chiral extrapolation ← see talks by G. Bali/S. Collins

Quark mass dependence of observables parameterized through:

- $\overline{M}^2 := \frac{1}{3}(2M_K^2 + M_\pi^2) \approx 2B_0\overline{m} \sim \frac{1}{3}(2m_\ell + m_s)$ ← average quark mass (rescaled by $t_0 \to \phi_4 = 8t_0(M_K^2 + \frac{M_\pi^2}{2}) = 12t_0\overline{M}^2$)
- $\delta M^2 := 2(M_K^2 - M_\pi^2) \approx 2B_0\delta m \sim m_s - m_\ell$ ← flavor symmetry breaking parameter

Combined continuum, finite volume and chiral extrapolation of quantities (e.g. for baryon masses m_B)

- parametrization $m_B(M_\pi, M_K, L, a) = m_B(M_\pi, M_K, L, 0)\left[1 + c\,a^2 + \bar{c}\,a^2\overline{M}^2 + \delta c_B\,a^2\delta M^2 + c'\,a^3 + c''\,a^4 + \cdots\right]$
- continuum part $m_B \equiv m_B(M_\pi, M_K, L, a = 0)$ ← various fit ansätze including finite volume effects (see below)
- lattice artifacts part $\left[1 + c\,a^2 + \cdots\right]$ ← start at $\mathcal{O}(a^2)$ for m_B
  → we vary on $c, c', c'', \bar{c}, \delta c_N$ and on the cut in a wrt the coarsest lattice spacing

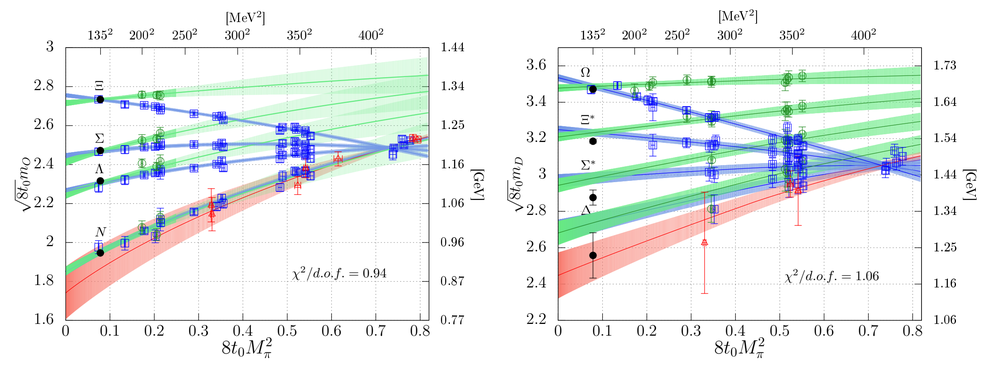


Chiral extrapolation of baryon masses m_B

- various parametrizations employed for the continuum part
  - NLO SU(3) Baryon ChPT (BChPT) (= linear in $M^2_{\pi,K}$), BChPT at order p^3 (NNLO), BChPT in the EOMS and HBChPT regularization
  - Taylor expansion a la Gell-Mann–Okubo (GMO)
  - small scale expansion (octet-decuplet (H)BChPT)
- finite size effects (FSE) included in fits by means of ChPT
- within our AIC procedure we perform cuts on
  - quark masses: $\phi_4 = 1.25, 1.4, 1.6$
  - FSE: $LM_\pi = 2.8, 3.5, 4.0$ and $L > 2.3\,\text{fm}$
- around 12 parameters to fit 4 baryon masses per ensemble (over 100 data points in total)

Plot: Comparison of the various fit results with the experimental values. Not shown are our main results from the BChPT fit to the octet baryon masses whose result on m_Ξ is used to set the scale in this comparison.

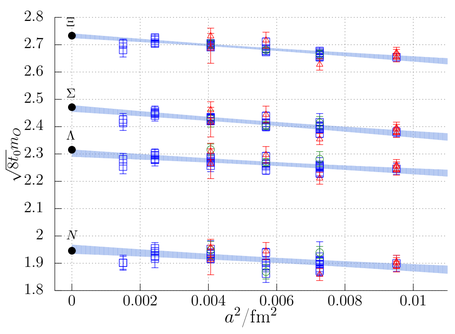
Examples of chiral fits for baryon octet and decuplet masses



three chiral trajectories: $\hat{m}_s \approx \hat{m}_{s,\text{ph}}$, $m_s + 2m_\ell \approx$ phys., $m_s = m_\ell$

Chiral fits with fit ansatz: order p^3 BChPT (upper plots)

- data points shifted to continuum + inf. volume limit according to fit
- upper left plot: fit to octet baryons with best χ^2/N_{DF}
  - cuts applied: $\phi_4 > 1.25$ and $LM_\pi > 4$
  - lighter part of the green error band indicates the region where data points have been discarded from the fit
- upper right plot: simultaneous fit to octet and decuplet baryons
  - fit with highest weight in AIC procedure
  - cuts applied: $\phi_4 < 1.6$, $a < 0.09\,\text{fm}$ and $LM_\pi > 4$
  - unstable decuplet baryons wrt strong decays (into a pion + octet baryon) in the infinite volume limit not included in the fit (also not shown)



Continuum limit extrapolation (right plot)

- lattice spacing dependence of masses from upper left fit in units of $\sqrt{8t_{0,\text{ph}}}$
- data are projected to infinite volume and the physical point in the quark mass plane