Towards the continuum limit with improved Wilson Fermions employing open boundary conditions –Part 1–

Wolfgang Söldner
for RQCD

Regensburg University

Lattice 2016
The 34rd International Symposium on Lattice Field Theory
July 29th, 2016

Motivation

Lattice QCD today

- more computing power and better algorithms $\rightarrow$ statistically more precise results
- increasingly important to control systematics

$\Rightarrow$ obviously, very important: controlled continuum limit

Problem when lattice spacing $a \rightarrow 0$

$\Rightarrow$ freezing of topology

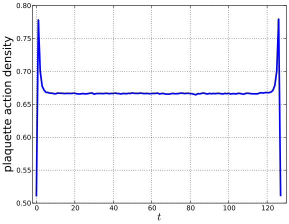
- lattice simulations get stuck in topological sectors
- problems start at $a \gtrsim 0.05\ \mathrm{fm}$

$\Rightarrow$ simple solution: lattice simulations with open boundary conditions

[Lüscher and Schaefer 2011]

$\rightarrow$ topology can flow in and out through the boundary

Lattice QCD with Open Boundaries



Open Boundaries

- $F_{0k}(x)|_{x_0=0} = F_{0k}(x)|_{x_0=T} = 0$
- $P_+\psi(x)|_{x_0=0} = P_-\psi(x)|_{x_0=T} = 0,$
- $\bar{\psi}(x)P_-|_{x_0=0} = \bar{\psi}(x)P_+|_{x_0=T} = 0$
- $P_\pm = \frac{1}{2}(1 \pm \gamma_0)$

Major $N_f = 2 + 1$ CLS effort

CLS: HU Berlin, CERN, TC Dublin, Mainz, UA Madrid, Milano Bicocca, Münster, Odense/CP3-Origins, Regensburg, Roma I, Roma II, Wuppertal, DESY Zeuthen

Simulation Overview

Lattice Action

- Two degenerate light quarks and one strange quark
- Non-perturbatively improved Wilson action (clover)
- Tree-level improved Symanzik gauge action

$\exists$ three different quark mass plane trajectories

(1) $\overline{m} = m_{\mathrm{symm}}$

$3\overline{m} = 2m_{(\ell)\text{ight}} + m_{(s)} = \text{const.} \leftrightarrow \frac{2}{\kappa_\ell} + \frac{1}{\kappa_s} = \text{const.} \rightarrow$ renormalized $2\widehat{m}_\ell + \widehat{m}_s = \text{const.} + \mathcal{O}(a)$.

(2) $\widetilde{m}_s = \widetilde{m}_{s,\mathrm{ph}}$

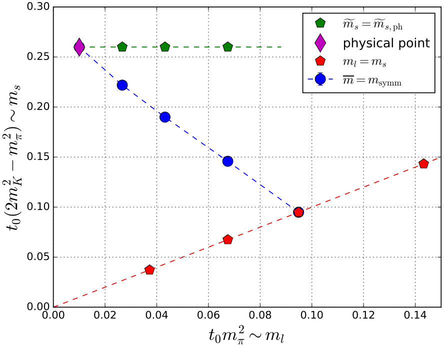
Strange AWI mass $\widetilde{m}_s = \text{const.} \rightarrow$ renormalized $\widehat{m}_s = \widehat{m}_{s,\mathrm{ph}}$, up to tiny $\mathcal{O}(a)$ effects.

(3) $m_s = m_\ell$ (Mainz/Regensburg)

For joint non-perturbative renormalization program

$\rightarrow$ simulations with anti-periodic boundary conditions (for $a > 0.05\,\mathrm{fm}$)

Overview of the simulation strategy → 1606.09039]



1. generate the $\overline{m} = m_{\mathrm{symm}}$ trajectory, starting from the $m_s = m_\ell$ point where $\overline{m} \approx \overline{m}_{\mathrm{ph}}$.
2. add points along the symmetric trajectory ($m_\ell = m_s$).
3. fit AWI masses (with $\mathrm{O}(a)$-improvement) to a known parametrization, using both trajectories.
4. determine the "physical" point on the $\overline{m} = m_{\mathrm{symm}}$ line, imposing $\widetilde{m}_s / \widetilde{m}_\ell = 27.46(44)$ [FLAG 2]
   $\rightarrow \widetilde{m}_{s,\mathrm{ph}}$
5. predict κ_ℓ, κ_s pairs for which $\widetilde{m}_s = \widetilde{m}_{s,\mathrm{ph}}$ from the parametrization in order to add $\widetilde{m}_s = \widetilde{m}_{s,\mathrm{ph}}$ simulation points.

How to predict κ_s as a function of κ_ℓ for $\widetilde{m}_s$ fixed I

$$\text{Average AWI masses:} \quad \frac{\widetilde{m}_j + \widetilde{m}_k}{2} = \widetilde{m}_{jk} = \frac{\partial_4 \langle 0|A_4^{jk}|\pi^{jk}\rangle}{2\langle 0|P^{jk}|\pi^{jk}\rangle}$$

$$\text{Lattice quark masses:} \quad m_j = \frac{1}{2a}\left(\frac{1}{\kappa_j} - \frac{1}{\kappa_{\text{crit}}}\right)$$

The Point along the symmetric line ($m_1 = m_2 = m_\ell = m_s = m_3$) where $\widetilde{m}_{jk} = 0$ defines $\kappa_j = \kappa_{\text{crit}}$.

Problem: Different renormalization of flavour-singlet and non-singlet quark mass combinations:

$$Z_m(m_s - m_\ell) = \frac{1}{2a}\left(\frac{1}{\kappa_s} - \frac{1}{\kappa_\ell}\right) = \widehat{m}_s - \widehat{m}_\ell = \frac{Z_A}{Z_P} 2\left(\widetilde{m}_{13} - \widetilde{m}_{12}\right)$$

$$\text{but:} \quad Z_m r_m \overline{m} = Z_m r_m \frac{2m_\ell + m_s}{3} = \frac{1}{6a}\left(\frac{2}{\kappa_\ell} + \frac{1}{\kappa_s} - \frac{3}{\kappa_{\text{crit}}}\right) = \frac{Z_A}{Z_P}\overline{\widetilde{m}}$$

NB: Due to $r_m > 1$ $m_\ell < m_s$ can become negative, away from the symmetric line.

How to predict κ_s as a function of κ_ℓ for $\widetilde{m}_s$ fixed II

$$3\widetilde{m}_s = 2\left(\widetilde{m}_s - \widetilde{m}_\ell\right) + 3\overline{\widetilde{m}} = \frac{Z}{2a}\left[2\left(\frac{1}{\kappa_s} - \frac{1}{\kappa_\ell}\right) + r_m\left(\frac{1}{\kappa_s} + \frac{2}{\kappa_\ell} - \frac{3}{\kappa_{\mathrm{crit}}}\right)\right],$$

where $Z = Z_m Z_P / Z_A$. Setting $\widetilde{m}_s = \widetilde{m}_{s,\mathrm{ph}}$ gives

$$\frac{1}{\kappa_s} = \frac{2}{2+r_m}\left(\frac{3a}{Z}\widetilde{m}_{s,\mathrm{ph}} + (1-r_m)\frac{1}{\kappa_\ell} + \frac{3r_m}{2}\frac{1}{\kappa_{\mathrm{crit}}}\right)$$

Subtracting the physical point result from both sides of the equation gives:

$$\frac{1}{\kappa_s} = \frac{1}{\kappa_{s,\mathrm{ph}}} + \frac{2(1-r_m)}{2+r_m}\left(\frac{1}{\kappa_\ell} - \frac{1}{\kappa_{\ell,\mathrm{ph}}}\right),$$

while the target κ_ℓ that corresponds to a given $\widetilde{m}_\ell$ value can be obtained through

$$\frac{1}{\kappa_\ell} = \frac{1}{\kappa_{\ell,\mathrm{ph}}} + \frac{2a(2+r_m)}{3Zr_m}(\widetilde{m}_\ell - \widetilde{m}_{\ell,\mathrm{ph}})$$

How to predict κ_s as a function of κ_ℓ for $\widetilde{m}_s$ fixed III

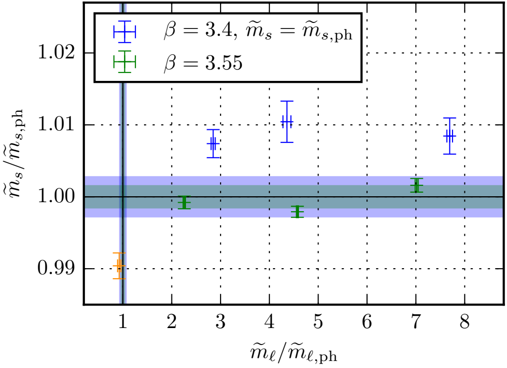
- Z and $\kappa_{\ell,\mathrm{ph}}$ can be obtained from $\widetilde{m}_{13} - \widetilde{m}_{12}$ as a function of κ_ℓ along the $\overline{m} =$ const. line. Then $\kappa_{s,\mathrm{ph}}$ is automatically determined too.
- Zr_m (and κ_{crit} if needed) can be obtained from $\widetilde{m}$ as a function of $1/\kappa$ along the symmetric $m = \overline{m} = m_s = m_\ell$ line.
- We carry out full order a improvement. In this case four combinations of improvement coefficients ($\mathcal{A}, \mathcal{B}_0, \mathcal{C}_0$ and $\mathcal{D}_0$) appear.

Does the κ_s prediction strategy work?

To be addressed later: Scale setting/tuning; we assumed that the physical point is on the $\overline{m} = m_{\mathrm{symm}}$ trajectory that we simulate (at least up to $\mathcal{O}(a^2)$ corrections). But is this true?

$m_s = \widetilde{m}_{s,\mathrm{ph}}$: prediction vs. simulation

Predicted and simulated value of physical $\widetilde{m}_{s,\mathrm{ph}}$ [hep-lat 1606.09039]



Mismatch at $\beta = 3.4$ due to shift of c_A value but still very constant!

$N_f = 2 + 1$ CLS simulations

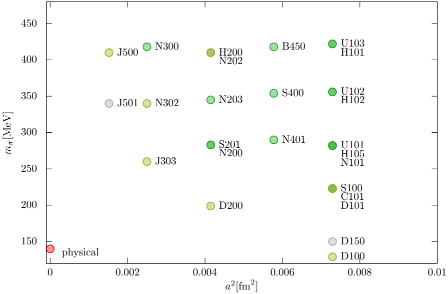
Great visibility at Lattice 2016 plenaries:

Coordinated Lattice Simulations: HU Berlin, CERN, TC Dublin, Mainz, UA Madrid, Milano Bicocca, Münster, Odense/CP3-Origins, Regensburg, Roma I, Roma II, Wuppertal, DESY Zeuthen

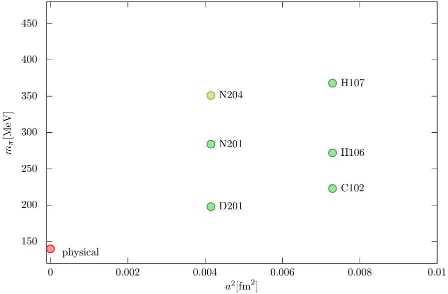
CLS ensemble overview

→ JHEP 1502 (2015) 043 [hep-lat 1411.3982]

$\overline{m} = m_{\text{symm}}$



$\widetilde{m}_s = \widetilde{m}_{s,\text{ph}}$



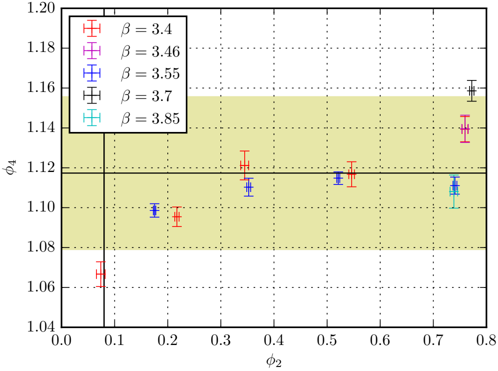
U: 128×24^3
B: 64×32^3
H: 96×32^3

S: 128×32^3
C: 96×48^3
N: 128×48^3

D: 128×64^3
J: 192×64^3

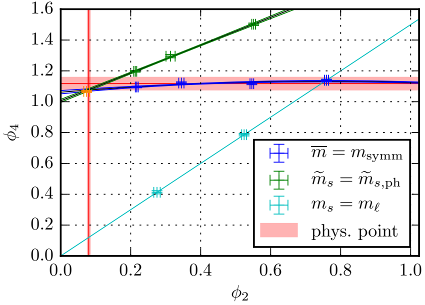
- Tuning details and results for the $\overline{m} = m_{\text{symm}}$ trajectory

Tuning strategy: $\overline{m} = m_{\text{symm}}$

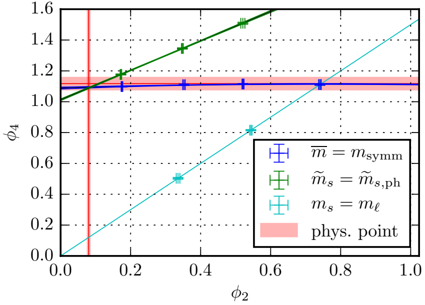


- $\phi_2 = t_0 m_\pi^2 \sim m_l, \quad \phi_4 = 8t_0(m_K^2 + m_\pi^2/2) \sim \overline{m}$
- At fixed β match lattices with different lattice spacings at flavor symmetric point (i.e. $m_{ud} = m_s \rightarrow m_\pi = m_{\mathrm{K}} \approx 415\ \mathrm{MeV}$)
- The (small) slope of ϕ_4 as a function of ϕ_2 was determined at $\beta = 3.4$ from a set of preliminary runs: $\phi_4\big|_{m_{ud}=m_s} = 1.15$
- Physical target (yellow bands): $\sqrt{t_0} = 0.1465(21)(13)$ fm [BMW], $m_\pi = 134.8(3)$ MeV, $m_K = 494.2(4)$ MeV [FLAG 2]

Chiral extrapolation: $\overline{m} = m_{\text{symm}}$ $\rightarrow$ hep-lat 1606.09039



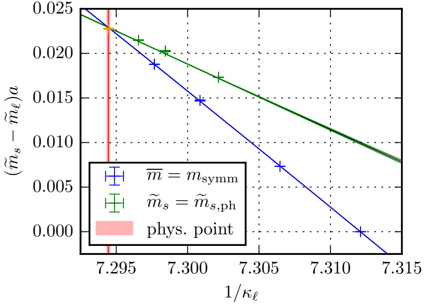
$\beta = 3.4$ $a \approx 0.085$ fm



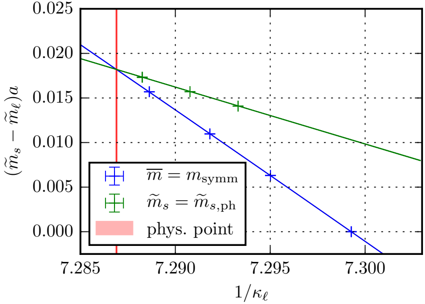
$\beta = 3.55$ $a \approx 0.064$ fm

- Combination shown is constant to NLO χPT along $\overline{m} = $ const. Corrections are of higher order or $\mathcal{O}(a)$.
- Dependence on ϕ_2 becomes weaker towards smaller $a \rightarrow$ mostly lattice artefact?
- At the physical point we are still within the target range!

AWI masses and O(a)-Improvement [hep-lat 1606.09039]



$\beta = 3.4$

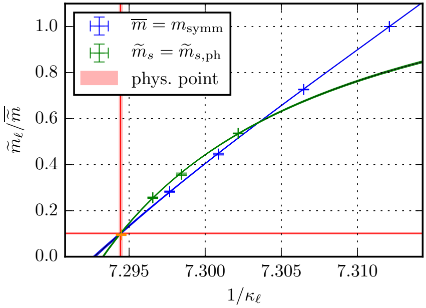


$\beta = 3.55$

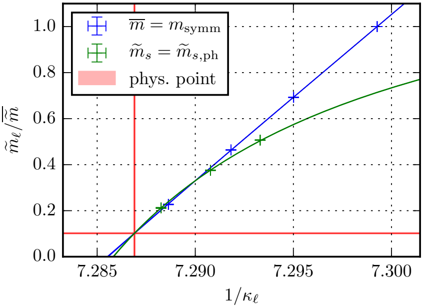
Simultaneous fit of light and strange AWI masses $\widetilde{m}_{(\ell,s)}(\kappa_\ell, \kappa_s)$ from $\overline{m} = m_{\mathrm{symm}}$ and $m_\ell = m_s$ trajectory

- Relevant parameters: $Z \equiv \frac{Z_P Z_m}{Z_A}$, $\mathcal{A}$, $\mathcal{B}_0$ ($\rightarrow$ slope is due to Z)
- use $\mathcal{A}$ from Ref. [Korcyl and Bali, arXiv:1607.07090] as input
- Sums of quark masses are sensitive to Zr_m, κ_{crit}, $\mathcal{C}_0$, ($\mathcal{D}_0$)
- $\mathcal{A}, \ldots, \mathcal{D}_0$ are combinations of r_m, b_P, b_A, b_m, d_m, $\tilde{b}_P$, $\tilde{b}_A$, $\tilde{b}_m$, $\tilde{d}_m$

Physical point [hep-lat 1606.09039]



$\beta = 3.4$



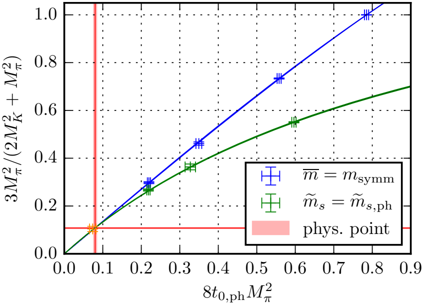
$\beta = 3.55$

$\widetilde{m}_s / \widetilde{m}_\ell$ along $\overline{m} = m_{\mathrm{symm}}$ determined from the global fit.

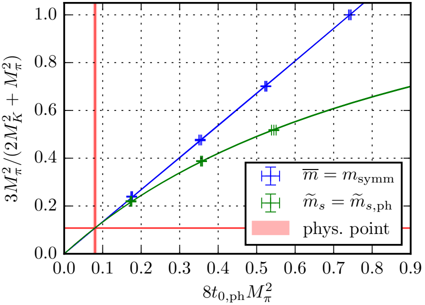
- physical value = 27.46(44) from [FLAG 2] used to define the physical point.

Physical Point II [hep-lat 1606.09039]

Is the FLAG value consistent with our results?



$\beta = 3.4$

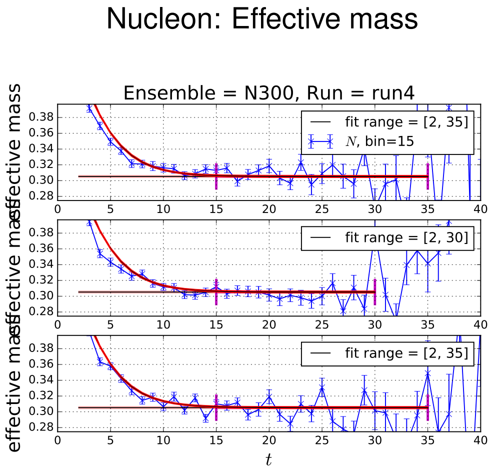


$\beta = 3.55$

We find consistency with experiment

- Predicting $\widehat{m}_s/\widehat{m}_\ell$ from the experimental pion masses would improve on the FLAG precision.
- However, we need to analyse additional lattice spacings to take the continuum limit.

Fitting Details



N300 Ensemble

- mass: $m_\pi = m_K \approx 420$ MeV
- lattice size: 128×48^3

Fitting: Two stage procedure

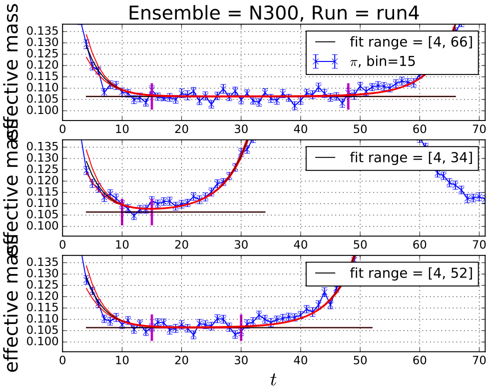
1. Determine actual fit range where excited state contribution is negligible by double exp fit
2. With determined fit range perform actual fit

Autocorrelations

$\rightarrow$ binning analysis, extrapolate error to infinite bin size

Fitting Details

Pion: Effective mass



N300 Ensemble

- mass: $m_\pi = m_K \approx 420$ MeV
- lattice size: 128×48^3

Fitting: Two stage procedure

1. Determine actual fit range where excited state contribution is negligible by double exp fit, boundary effects described by sinh
2. With determined fit range perform actual fit

Autocorrelations

$\rightarrow$ binning analysis, extrapolate error to infinite bin size

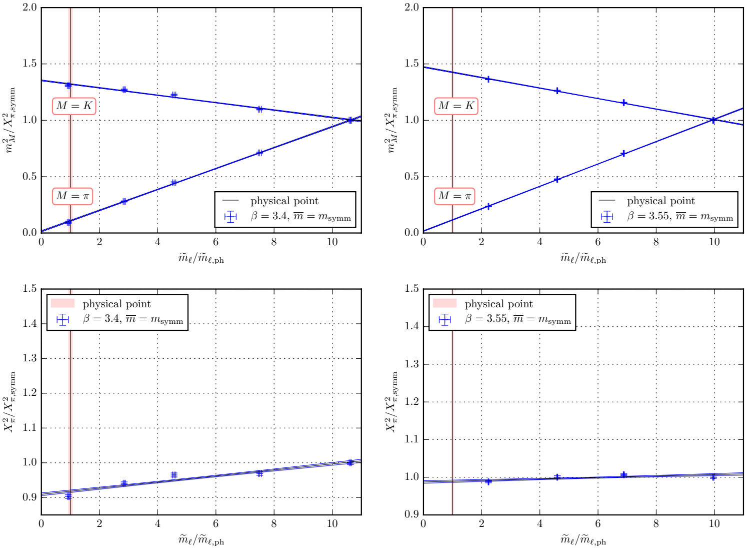
Comparing extrapolations $\overline{m} = m_{\mathrm{symm}}$ with $\widetilde{m}_s = \widetilde{m}_{s,\mathrm{ph}}$

Average Hadron Masses

- Average pion mass: $X_\pi^2 = (2M_K^2 + M_\pi^2)/3$
- Average octet baryon mass: $X_N = (M_\Xi + M_\Sigma + M_N)/3$ (no Σ_0 to circumvent Λ-Σ mixing)
- Average decuplet baryon mass: $X_\Delta = (2M_\Delta + M_\Omega)/3$
- For the experimental values we take the charge combinations of QCDSF: 1101.5300.
- All combinations scale in the Gell-Mann–Okubo expansion and NLO ChiPT $\propto \overline{m}$ and $\propto (m_s - m_\ell)^2$.

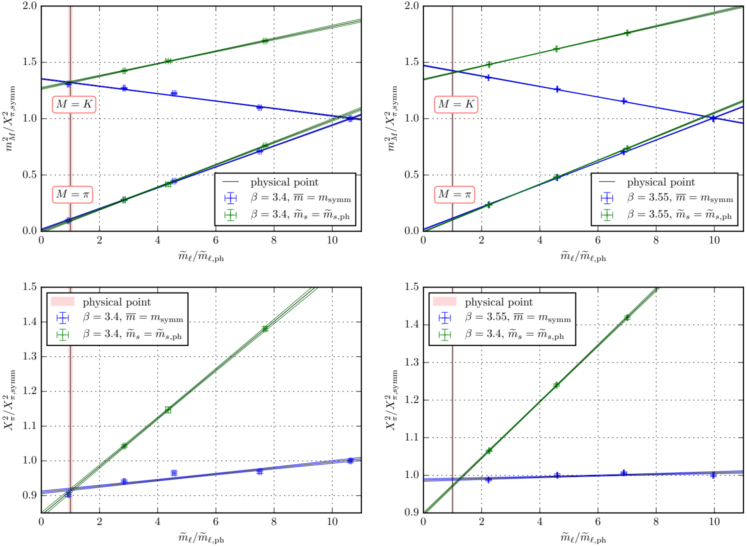
Pseudoscalar masses $\overline{m} = m_{\mathrm{symm}}$

preliminary



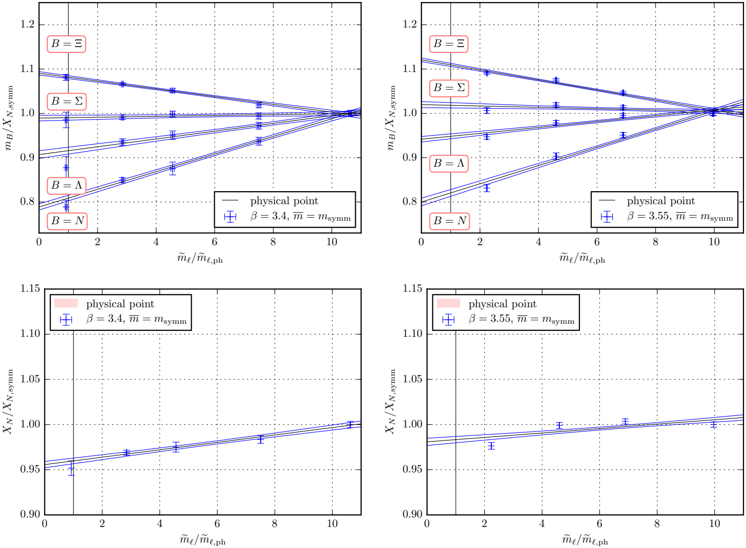
Pseudoscalar masses $\overline{m} = m_{\text{symm}}$ and $\widetilde{m}_s = \widetilde{m}_{s,\text{ph}}$

preliminary



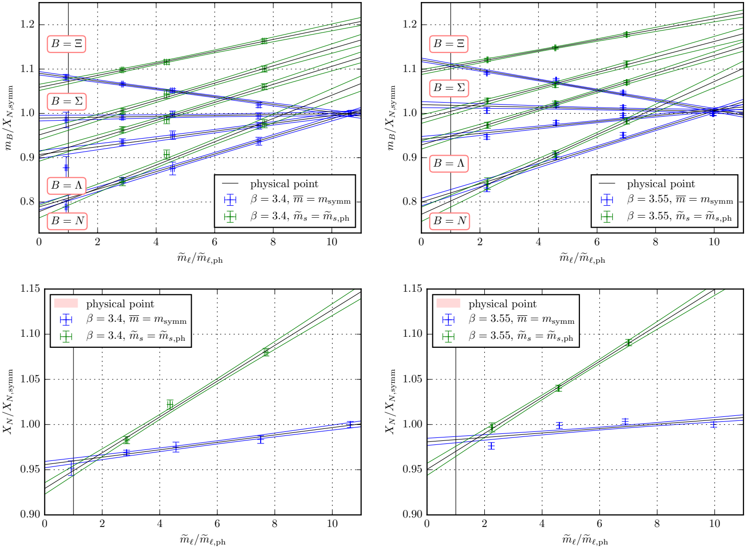
Octet baryons $\overline{m} = m_{\text{symm}}$

preliminary



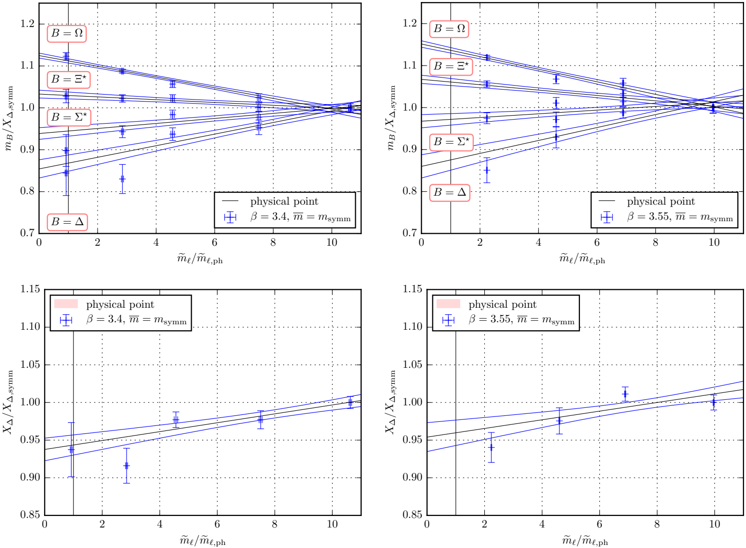
Octet baryons $\overline{m} = m_{\text{symm}}$ and $\widetilde{m}_s = \widetilde{m}_{s,\text{ph}}$

preliminary



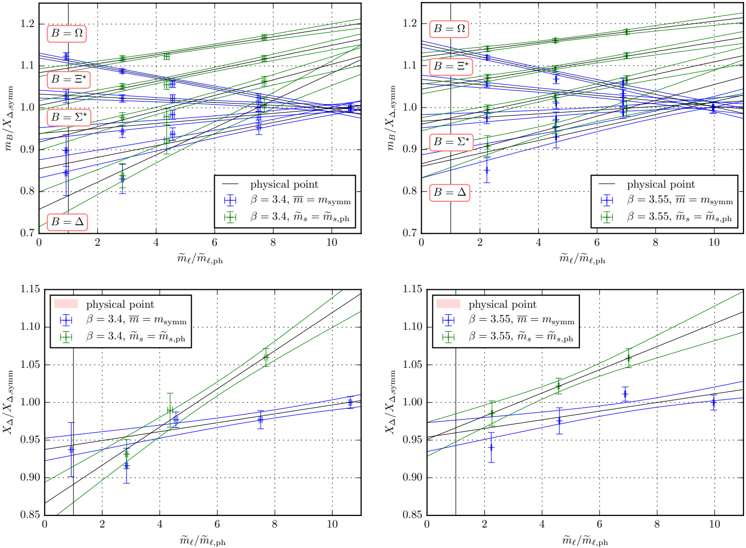
Decuplet baryons $\overline{m} = m_{\text{symm}}$

preliminary

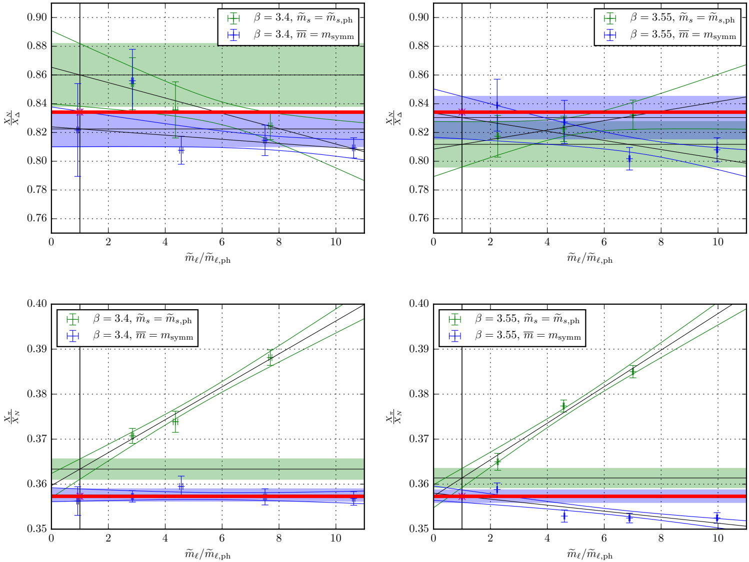


Decuplet baryons $\overline{m} = m_{\text{symm}}$ and $\widetilde{m}_s = \widetilde{m}_{s,\text{ph}}$

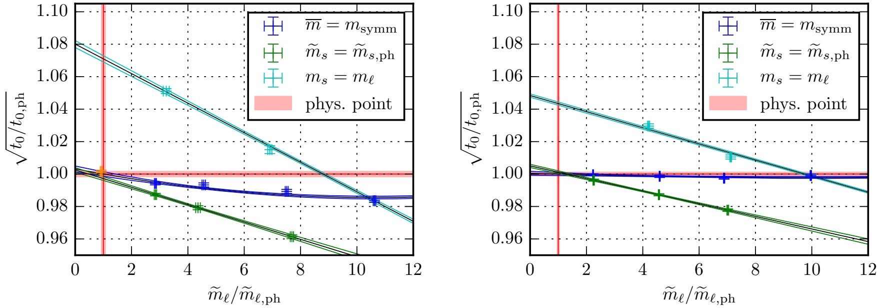
preliminary



preliminary



t_0 (preliminary)



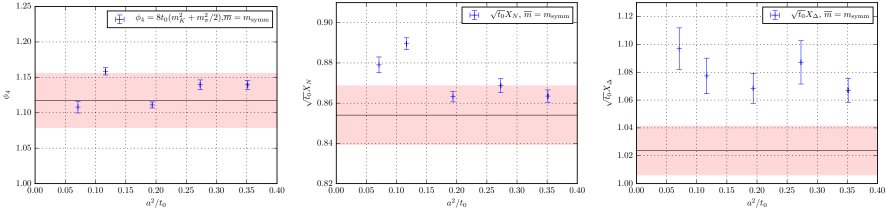
$\beta = 3.4$ RQCD(CLS) data

$\beta = 3.55$ RQCD(CLS) data

Compare scale setting

- relative error on a from $m_\Xi \approx 0.4\%$, $m_{\Xi^\star} \approx 0.9\%$, $m_\Omega \approx 0.7\%$, $X_N \approx 0.6\% \longleftrightarrow$ from BMW $t_0 \approx 1.7\%$
- a for $\beta = 3.40$: $a_{X_N} \approx 0.0833(4)$ fm $\longleftrightarrow$ from BMW $a_{t_0} = 0.0854(15)$ fm
- a for $\beta = 3.55$: $a_{X_N} \approx 0.0632(5)$ fm $\longleftrightarrow$ from BMW $a_{t_0} = 0.0644(11)$ fm

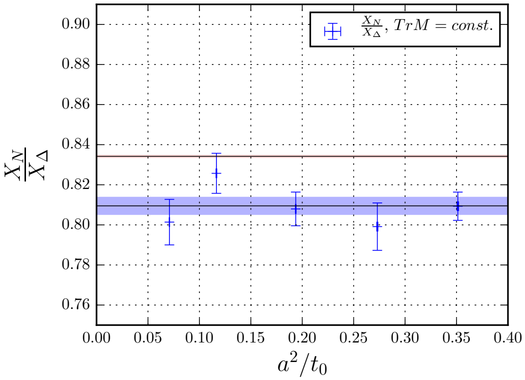
Continuum extrapolation along the symmetric line



- ϕ_4 (target $\phi_4 = 1.15$) was slightly mistuned
- This is reflected in other quantities
- As $\phi_{4,\rm ph}/\phi_{4,\rm symm}$ is subject to $\mathcal{O}(\overline{m}a)$ corrections this was fortunate in some cases, however:

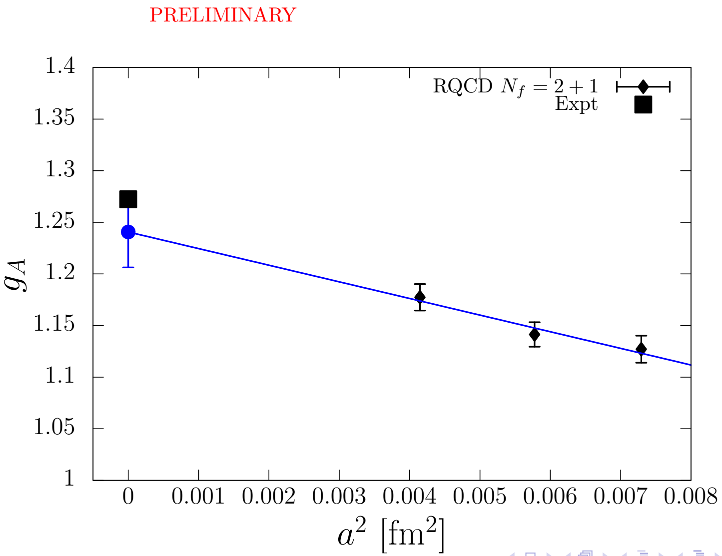
$\rightarrow$ need for correction (see also talk by Rainer Sommer)

Symmetric line continuum extrapolation

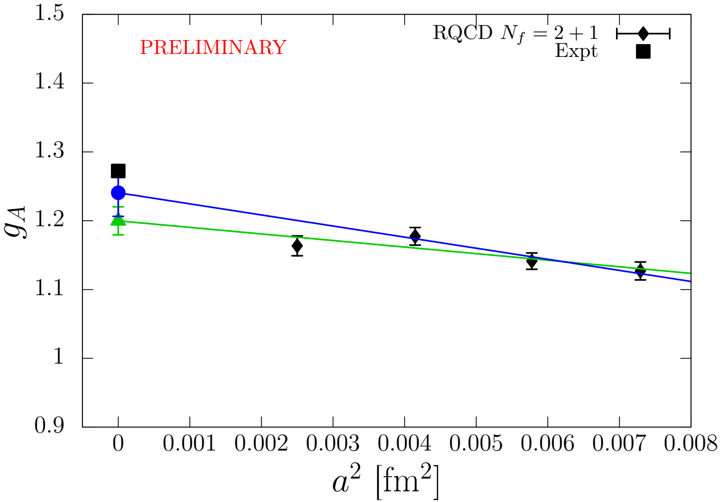


- weak dependence on $\overline{m}$ allows for a continuum extrapolation

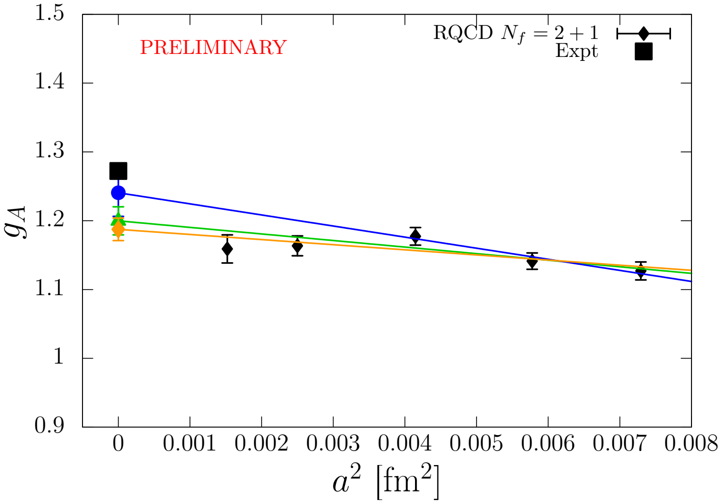
Continuum limit of g_A at $M_\pi \approx 415$ MeV



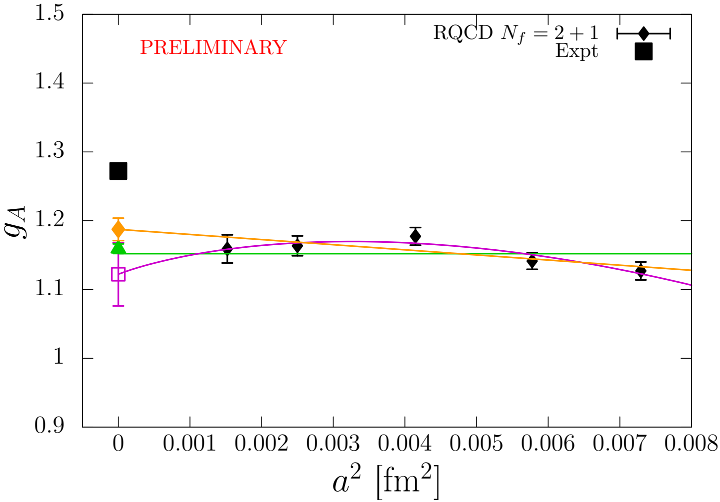
Continuum limit of g_A at $M_\pi \approx 415$ MeV



Continuum limit of g_A at $M_\pi \approx 415$ MeV



Continuum limit of g_A at $M_\pi \approx 415$ MeV



Disclaimer

The work presented was carried out in collaboration with

Sara Collins, Meinulf Göckeler, Fabian Hutzler, Rudolf Rödl, Andreas Schäfer, Enno Scholz, Jakob Simeth, André Sternbeck and Thomas Wurm

Code development and software support:

Benjamin Gläßle, Piotr Korcyl, Daniel Richtmann

Gauge configurations were generated using OPENQCD within CLS

We thank all other CLS colleagues who made this possible.

Summary

Lattice Simulations with Open Boundaries

- avoid topological freezing as $a \to 0$
- long term effort within CLS

$\overline{m} = m_{\rm symm}$ trajectory: Meson/Baryon Spectrum

- fitting to Gell-Mann–Okubo expansion and SU(3) ChiPT (combined within the other 2 trajectories) in progress

$\widetilde{m}_s = \widetilde{m}_{s,\rm ph}$ trajectory: Meson/Baryon Spectrum

- achieved a very constant strange quark mass
- reasonable overall agreement of quark and hadron masses at the physical point with $\overline{m} =$ const. trajectory
- fitting SU(2) and SU(3) ChiPT in progress

Strategy allows us

- to determine $\mathrm{SU}(2)$ as well as $\mathrm{SU}(3)$ low energy constants
- to safely extrapolate to the physical quark mass point

Outlook

- extend present study: continuum limit with $\geq$ 4 lattice spacings
- nucleon structure and other additional observables