

# Towards the continuum limit with improved Wilson Fermions employing open boundary conditions

## –Part 2–

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for RQCD

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# Motivation

## Lattice QCD today

- more computing power and better algorithms → statistically more precise results
  - increasingly important to control systematics
- ⇒ obviously, very important: controlled continuum limit

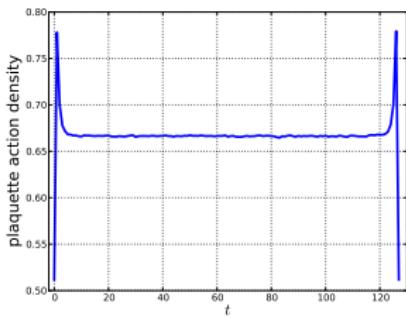
## Problem when lattice spacing $a \rightarrow 0$

- ⇒ freezing of topology
  - lattice simulations get stuck in topological sectors
  - problems start at  $a \gtrsim 0.05$  fm
- ⇒ simple solution: lattice simulations with open boundary conditions

[Lüscher and Schaefer 2011]

→ 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)  $\bar{m} = m_{\text{symm}}$

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

(2)  $\tilde{m}_s = \tilde{m}_{s,\text{ph}}$

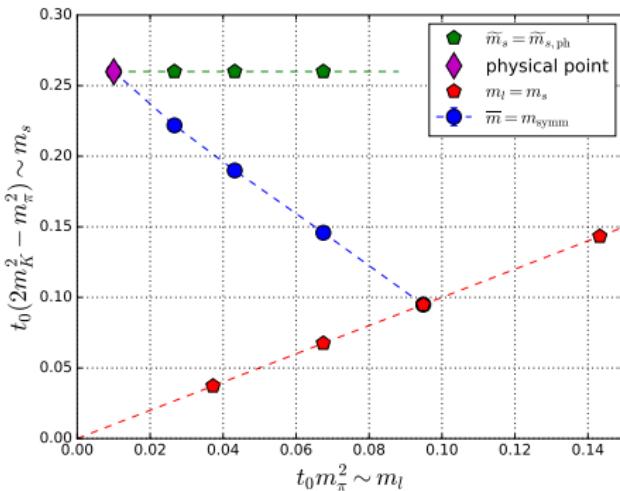
Strange AWI mass  $\tilde{m}_s = \text{const.} \rightarrow \text{renormalized } \hat{m}_s = \hat{m}_{s,\text{ph}}$ , up to tiny  $\mathcal{O}(a)$  effects.

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

For joint non-perturbative renormalization program

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

# Overview of the simulation strategy → 1606.09039



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

RQCD

# How to predict $\kappa_s$ as a function of $\kappa_\ell$ for $\tilde{m}_s$ fixed I

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

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

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

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

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

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

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



# How to predict $\kappa_s$ as a function of $\kappa_\ell$ for $\tilde{m}_s$ fixed II

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

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

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

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

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

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

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

# How to predict $\kappa_s$ as a function of $\kappa_\ell$ for $\tilde{m}_s$ fixed III

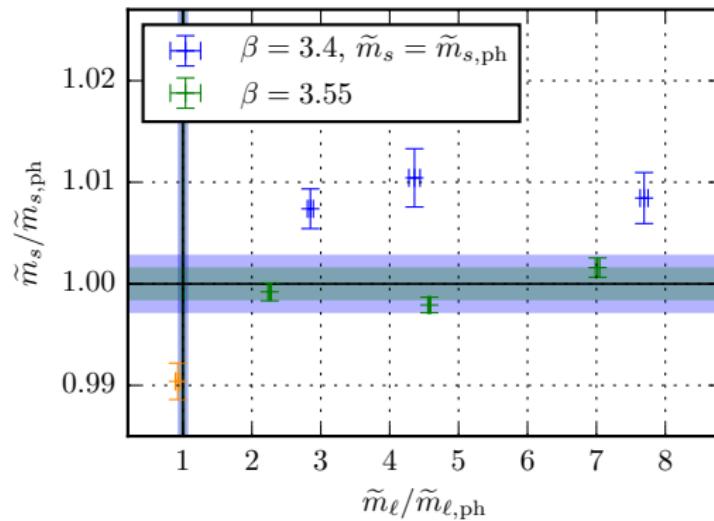
- $Z$  and  $\kappa_{\ell,\text{ph}}$  can be obtained from  $\tilde{m}_{13} - \tilde{m}_{12}$  as a function of  $\kappa_\ell$  along the  $\bar{m} = \text{const.}$  line. Then  $\kappa_{s,\text{ph}}$  is automatically determined too.
- $Zr_m$  (and  $\kappa_{\text{crit}}$  if needed) can be obtained from  $\tilde{m}$  as a function of  $1/\kappa$  along the symmetric  $m = \bar{m} = m_s = m_\ell$  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  $\kappa_s$  prediction strategy work?

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

# $m_s = \tilde{m}_{s,\text{ph}}$ : prediction vs. simulation

Predicted and simulated value of physical  $\tilde{m}_{s,\text{ph}}$  [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:



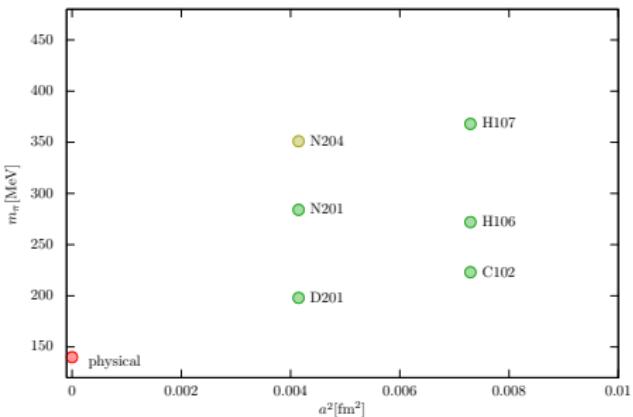
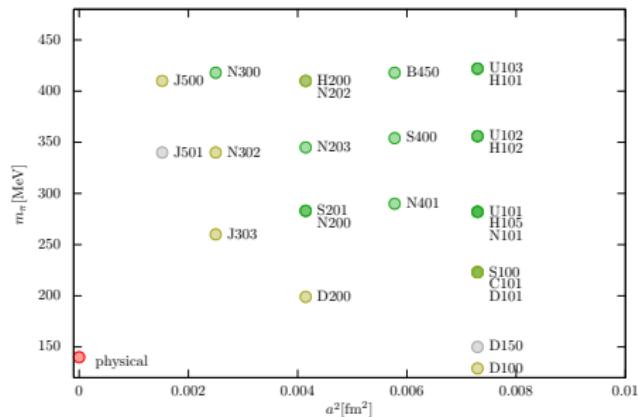
**Coordinated Lattice Simulations:** HU Berlin, CERN, TC Dublin, Mainz, UA  
Madrid, Milano Bicocca, Münster, Odense/CP3-Origins, Regensburg, Roma I,  
Roma II, Wuppertal, DESY Zeuthen

## CLS ensemble overview

 $\rightarrow$  JHEP 1502 (2015) 043 [hep-lat 1411.3982]

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

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

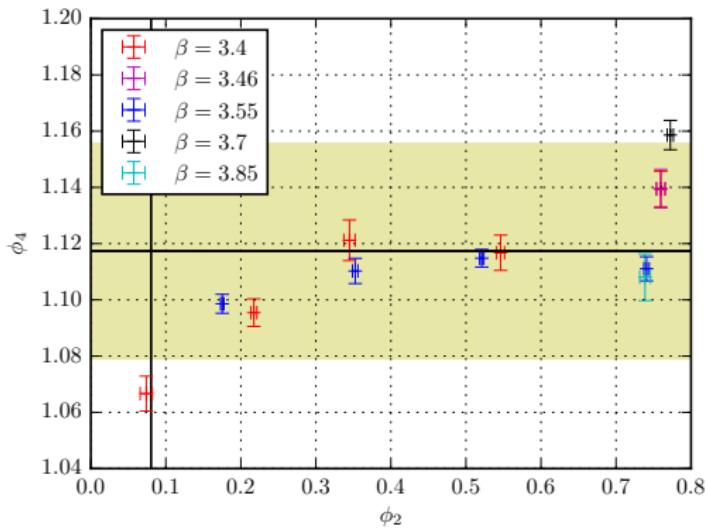


U:  $128 \times 24^3$   
 B:  $64 \times 32^3$   
 H:  $96 \times 32^3$

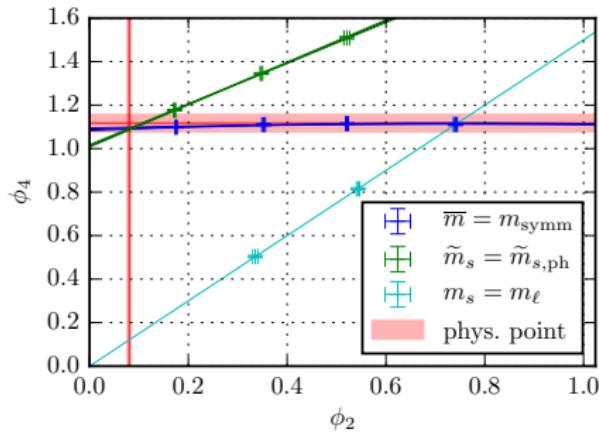
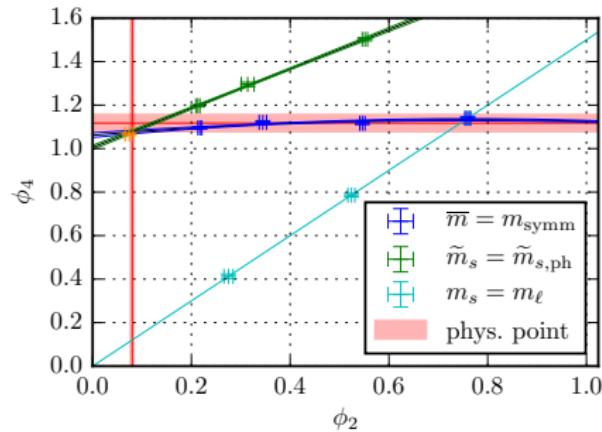
S:  $128 \times 32^3$   
 C:  $96 \times 48^3$   
 N:  $128 \times 48^3$

D:  $128 \times 64^3$   
 J:  $192 \times 64^3$

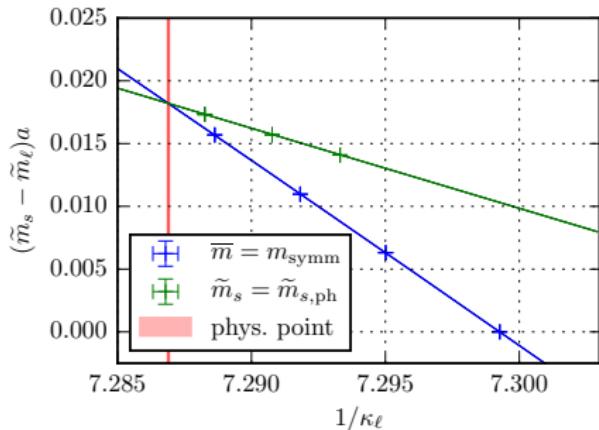
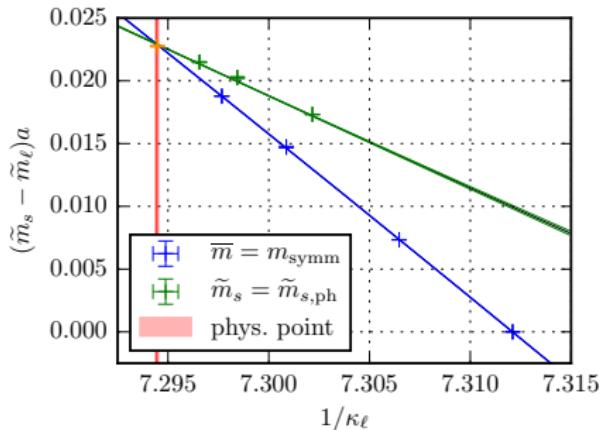
- Tuning details and results for the  $\overline{m} = m_{\text{symm}}$  trajectory

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

- $\phi_2 = t_0 m_\pi^2 \sim m_I$ ,  $\phi_4 = 8t_0(m_K^2 + m_\pi^2/2) \sim \overline{m}$
- At fixed  $\beta$  match lattices with different lattice spacings at flavor symmetric point (i.e.  $m_{ud} = m_s \rightarrow m_\pi = m_K \approx 415$  MeV)
- The (small) slope of  $\phi_4$  as a function of  $\phi_2$  was determined at  $\beta = 3.4$  from a set of preliminary runs:  $\phi_4|_{m_{ud}=m_s} = 1.15$
- 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:  $\bar{m} = m_{\text{symm}}$  $\rightarrow$  hep-lat 1606.09039

- Combination shown is constant to NLO  $\chi$ PT along  $\bar{m} = \text{const}$ . Corrections are of higher order or  $\mathcal{O}(a)$ .
- Dependence on  $\phi_2$  becomes weaker towards smaller  $a \rightarrow$  mostly lattice artefact?
- At the physical point we are still within the target range!

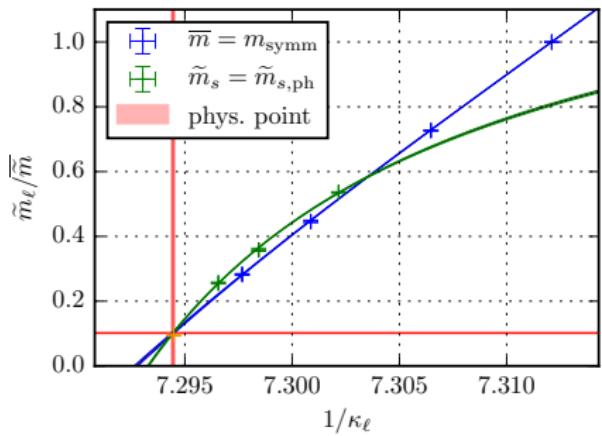
AWI masses and  $O(a)$ -Improvement [hep-lat 1606.09039]

$$\beta = 3.4$$

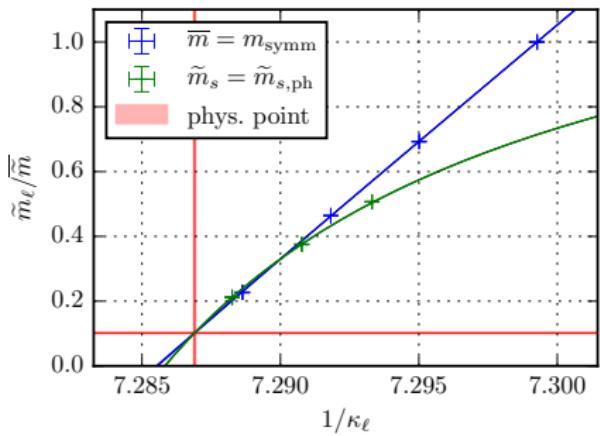
Simultaneous fit of light and strange AWI masses  $\tilde{m}_{(\ell,s)}(\kappa_\ell, \kappa_s)$  from  $\bar{m} = m_{\text{symm}}$  and  $m_\ell = m_s$  trajectory

- 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. [Korcy and Bali, arXiv:1607.07090] as input
- Sums of quark masses are sensitive to  $Zr_m, \kappa_{\text{crit}}, \mathcal{C}_0, (\mathcal{D}_0)$
- $\mathcal{A}, \dots, \mathcal{D}_0$  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]



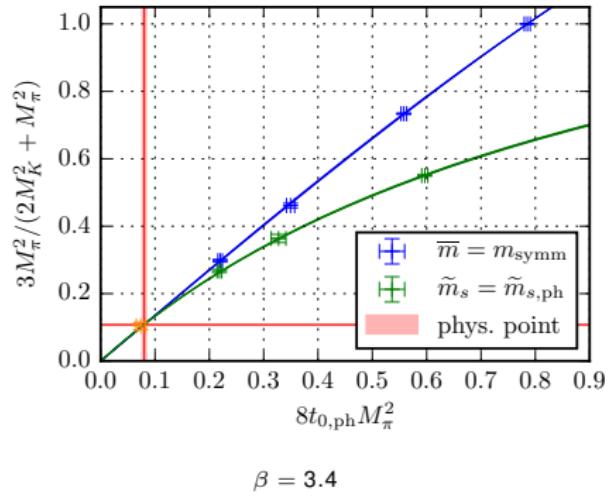
$\beta = 3.4$



$\beta = 3.55$

# Physical Point II [hep-lat 1606.09039]

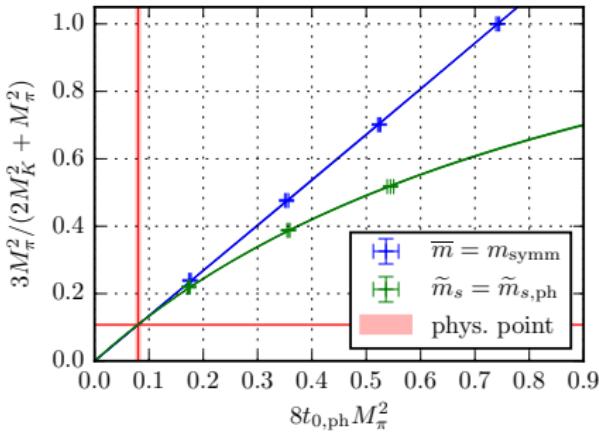
Is the FLAG value consistent with our results?



$$\beta = 3.4$$

We find consistency with experiment

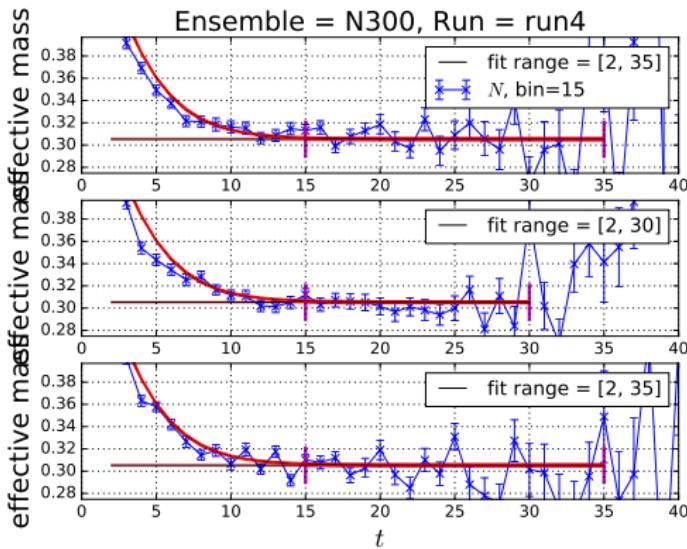
- Predicting  $\hat{m}_s/\hat{m}_\ell$  from the experimental pion masses would improve on the FLAG precision.
- However, we need to analyse additional lattice spacings to take the continuum limit.



$$\beta = 3.55$$

# Fitting Details

## Nucleon: Effective mass



### N300 Ensemble

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

### Fitting: Two stage procedure

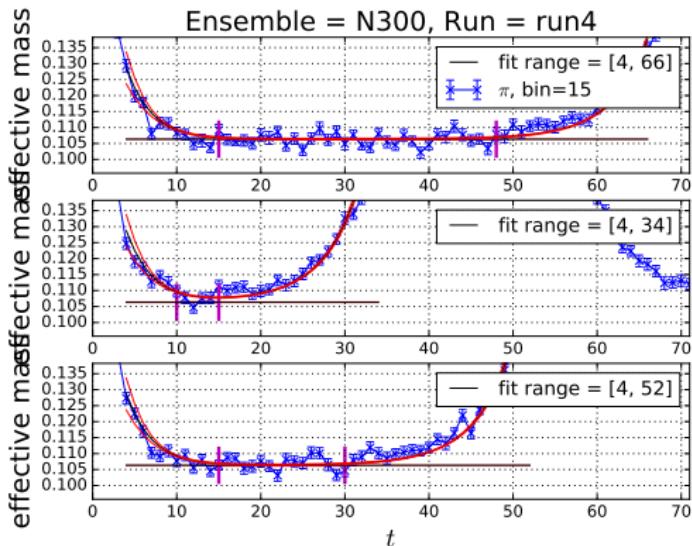
- Determine actual fit range where excited state contribution is negligible by double exp fit
- With determined fit range perform actual fit

### Autocorrelations

- 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:  $128 \times 48^3$

### Fitting: Two stage procedure

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

### Autocorrelations

- binning analysis, extrapolate error to infinite bin size

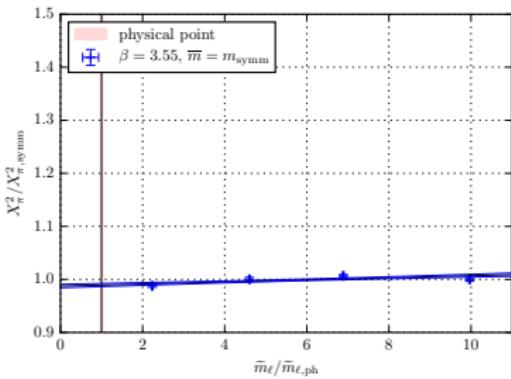
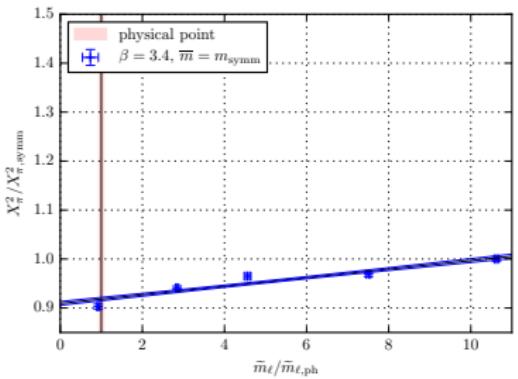
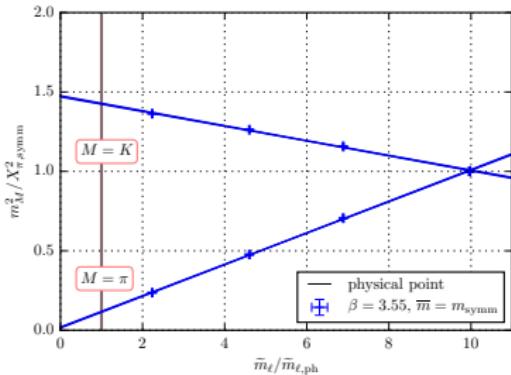
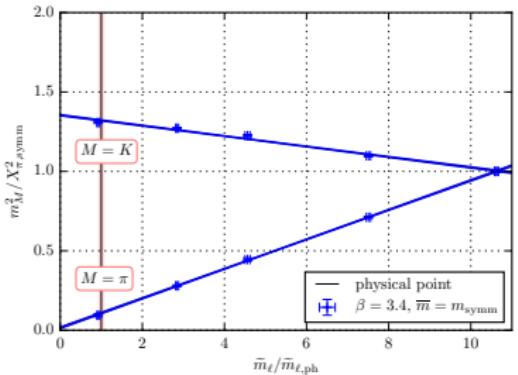
Comparing extrapolations  $\bar{m} = m_{\text{symm}}$  with  $\tilde{m}_s = \tilde{m}_{s,\text{ph}}$ 

## 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  $\Sigma_0$  to circumvent  $\Lambda$ - $\Sigma$  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 ChPT  $\propto \bar{m}$  and  $\propto (m_s - m_\ell)^2$ .

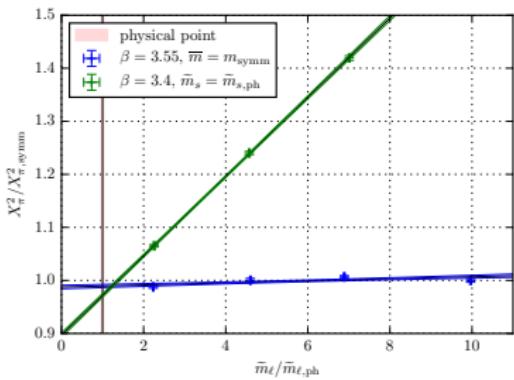
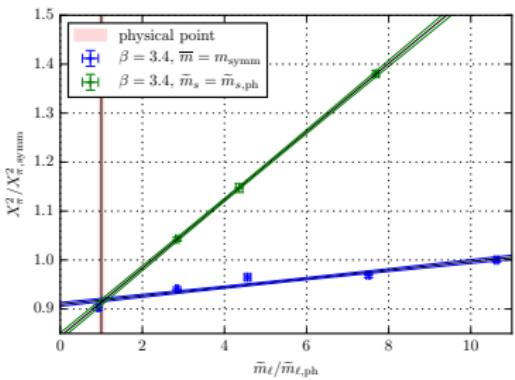
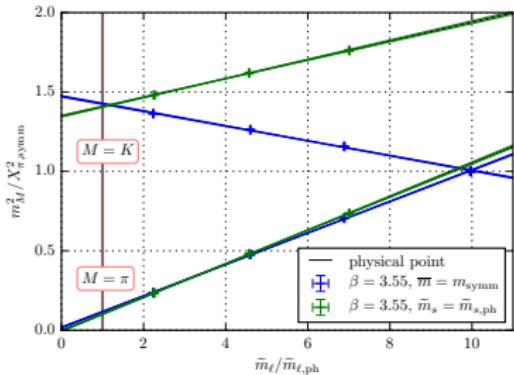
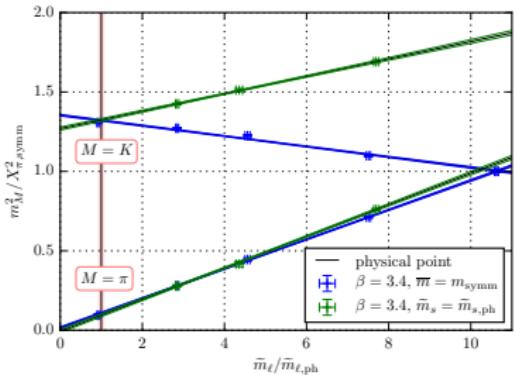
# Pseudoscalar masses $\bar{m} = m_{\text{symm}}$

preliminary



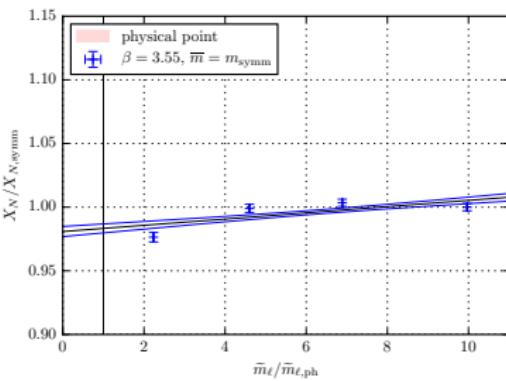
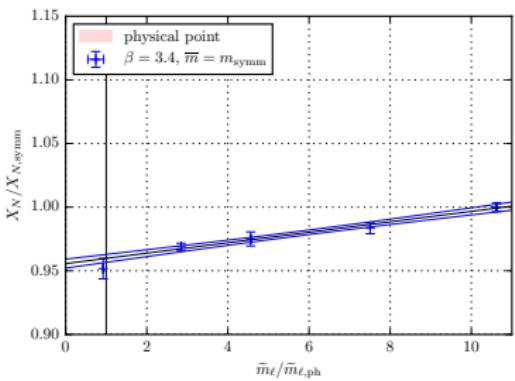
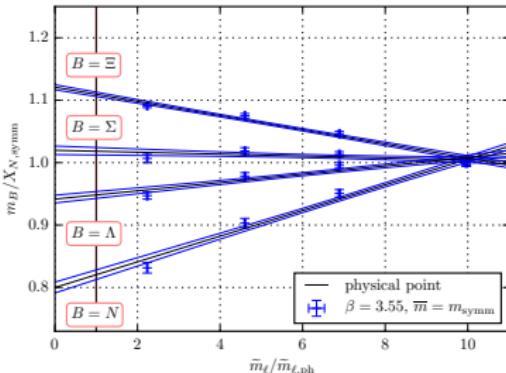
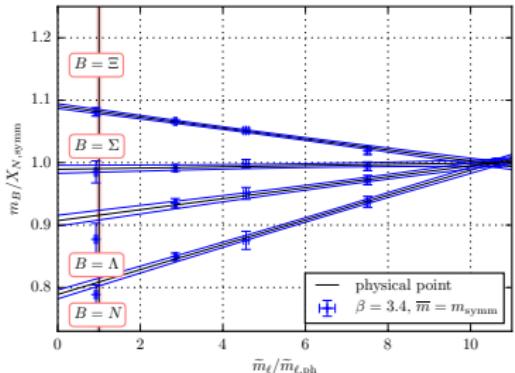
# Pseudoscalar masses $\bar{m} = m_{\text{symm}}$ and $\tilde{m}_s = \tilde{m}_{s,\text{ph}}$

preliminary



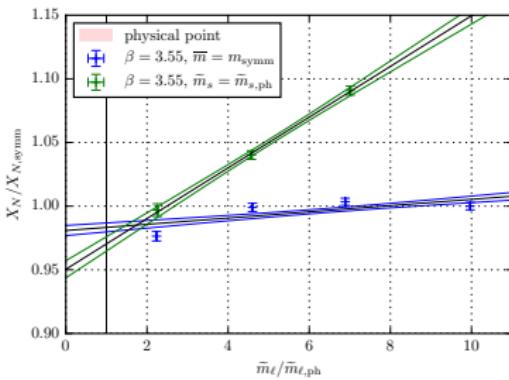
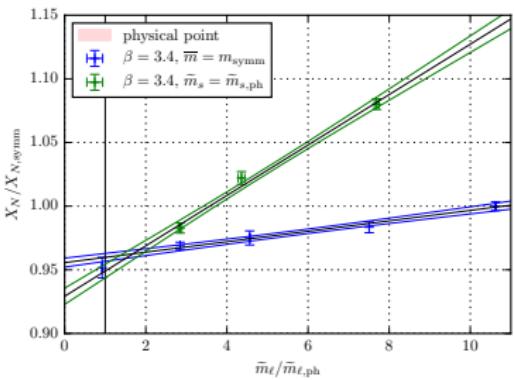
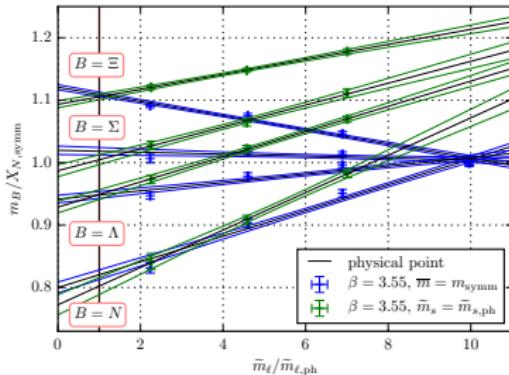
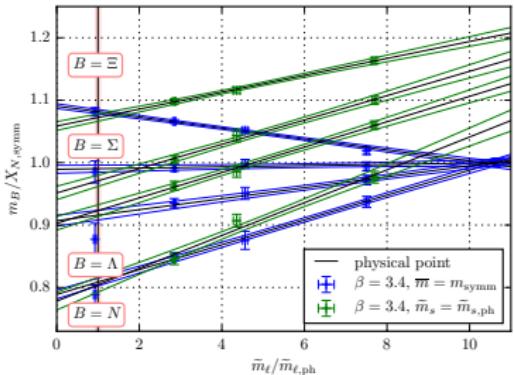
# Octet baryons $\bar{m} = m_{\text{symm}}$

preliminary



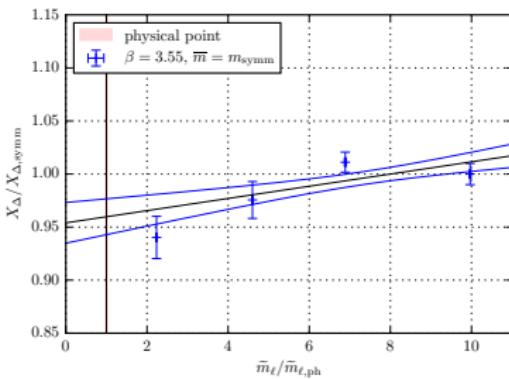
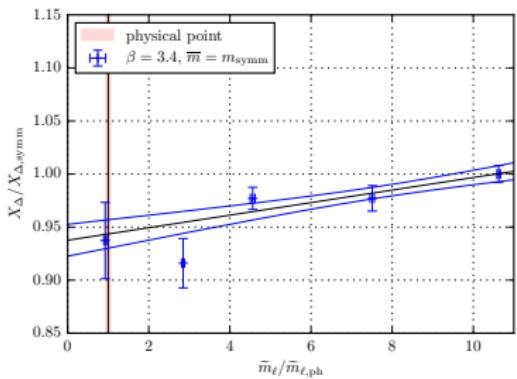
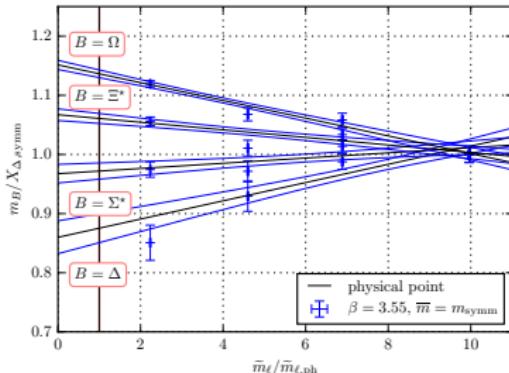
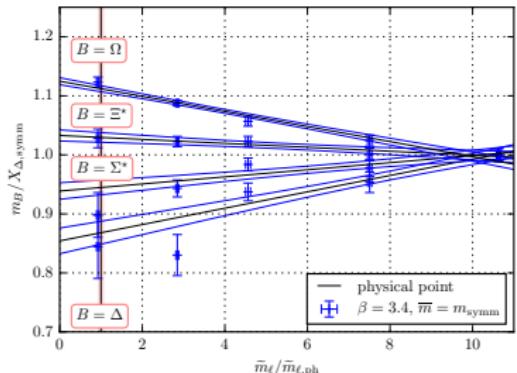
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preliminary



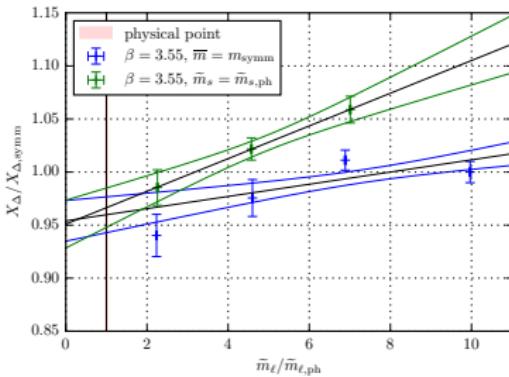
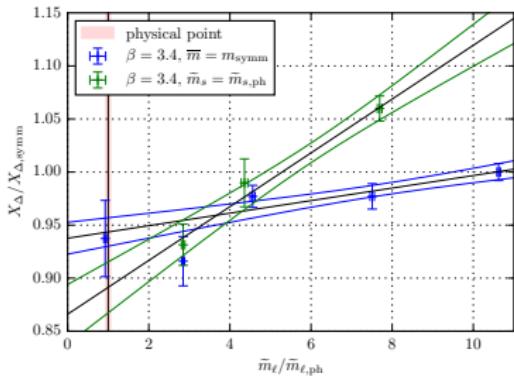
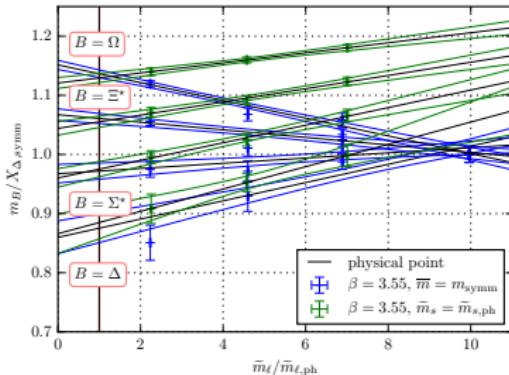
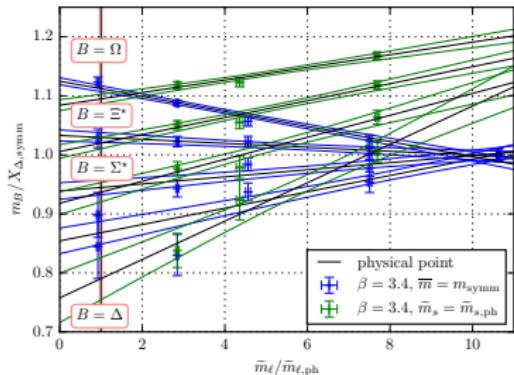
# Decuplet baryons $\bar{m} = m_{\text{symm}}$

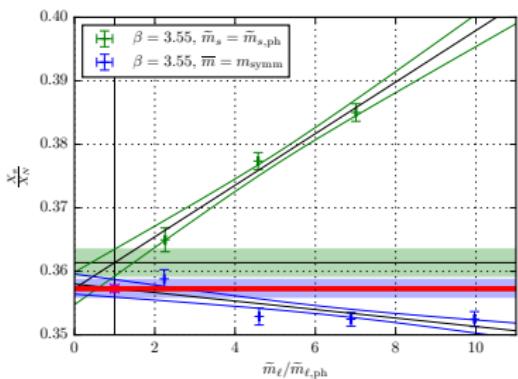
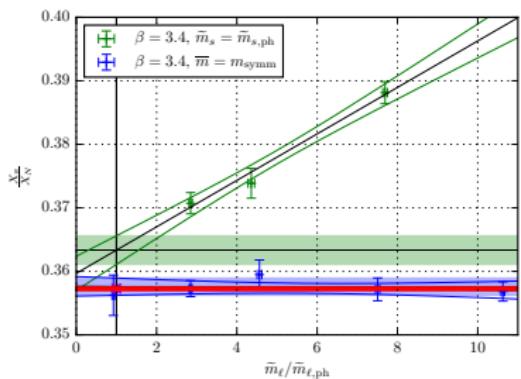
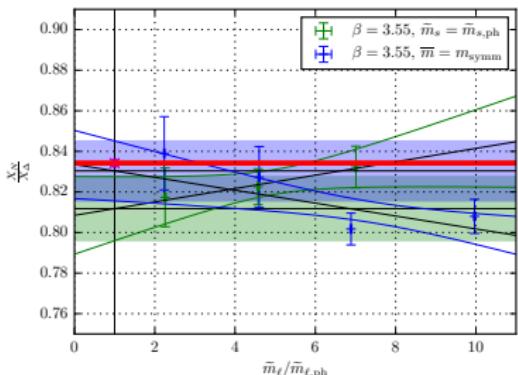
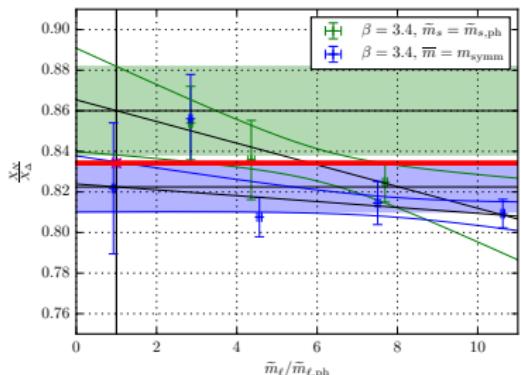
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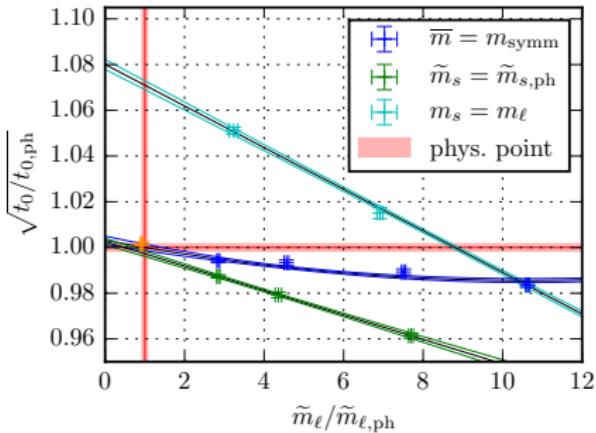
# Decuplet baryons $\bar{m} = m_{\text{symm}}$ and $\bar{m}_s = \bar{m}_{s,\text{ph}}$

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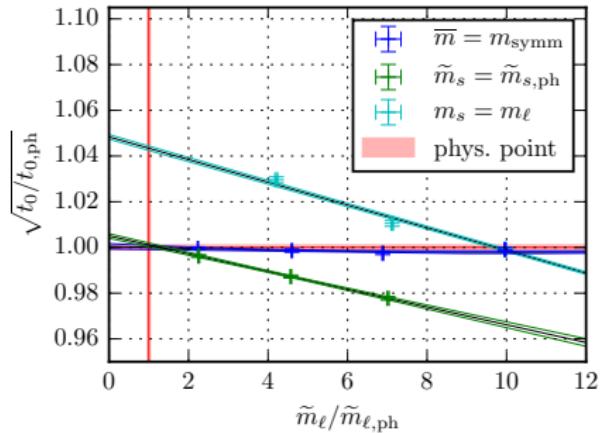




**t<sub>0</sub>** (preliminary)



$\beta = 3.4$  RQCD(CL) data

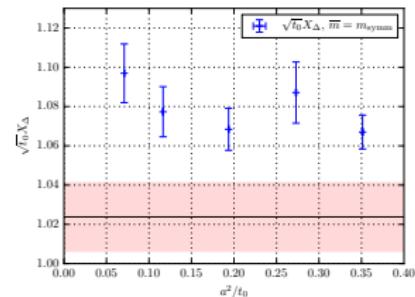
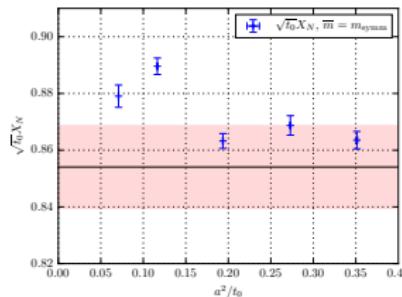
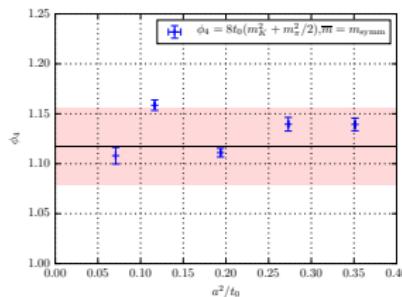


$\beta = 3.55$  RQCD(CL) data

### Compare scale setting

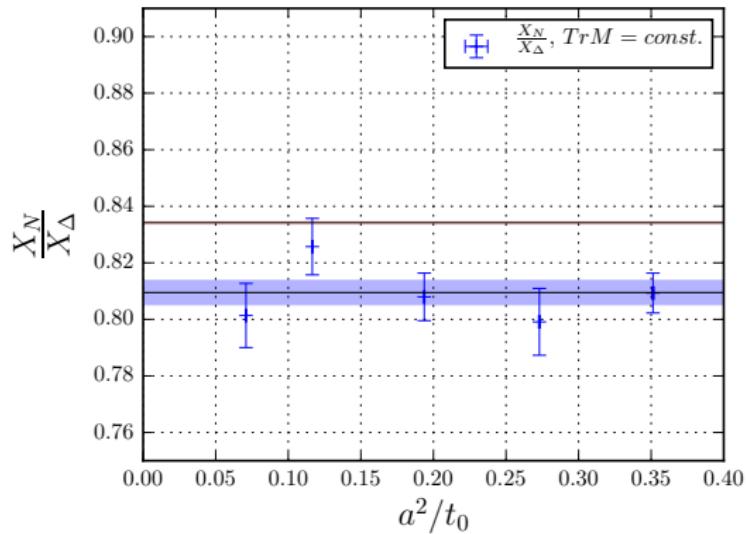
- relative error on  $a$  from  $m_{\Xi} \approx 0.4\%$ ,  $m_{\Xi^*} \approx 0.9\%$ ,  $m_\Omega \approx 0.7\%$ ,  $X_N \approx 0.6\% \longleftrightarrow$  from BMW  $t_0 \approx 1.7\%$
- $a$  for  $\beta = 3.40$ :  $a_{X_N} \approx 0.0833(4)$  fm  $\longleftrightarrow$  from BMW  $a_{t_0} = 0.0854(15)$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



- $\phi_4$  (target  $\phi_4 = 1.15$ ) was slightly mistuned
- This is reflected in other quantities
- As  $\phi_{4,\text{ph}}/\phi_{4,\text{symm}}$  is subject to  $\mathcal{O}(\bar{m}a)$  corrections this was fortunate in some cases, however:
  - need for correction (see also talk by Rainer Sommer)

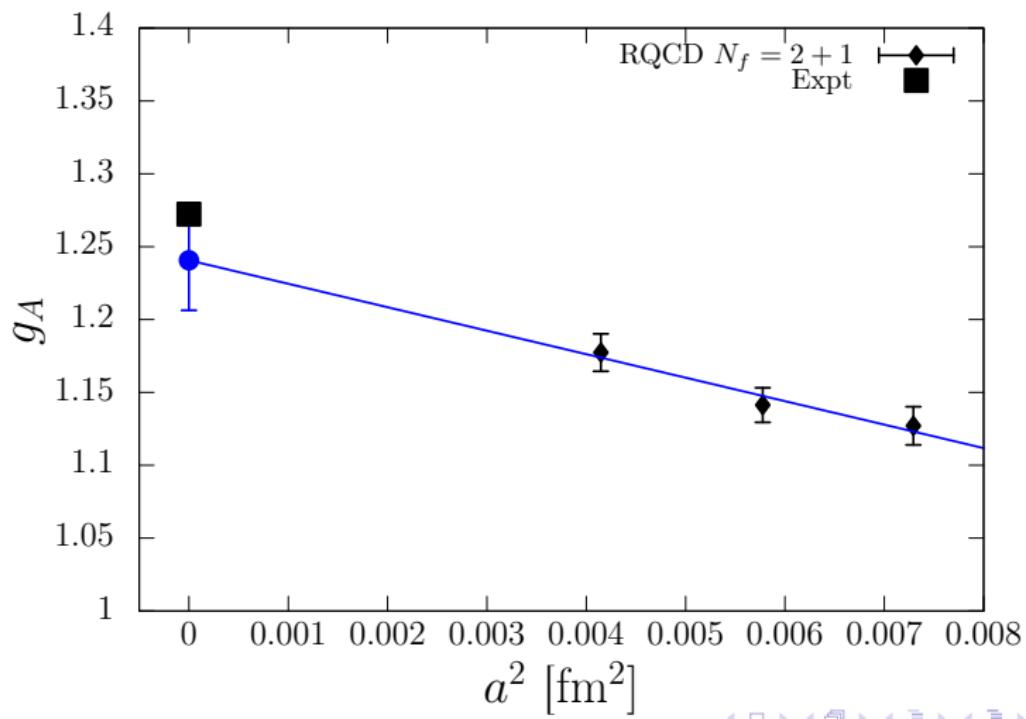
# Symmetric line continuum extrapolation



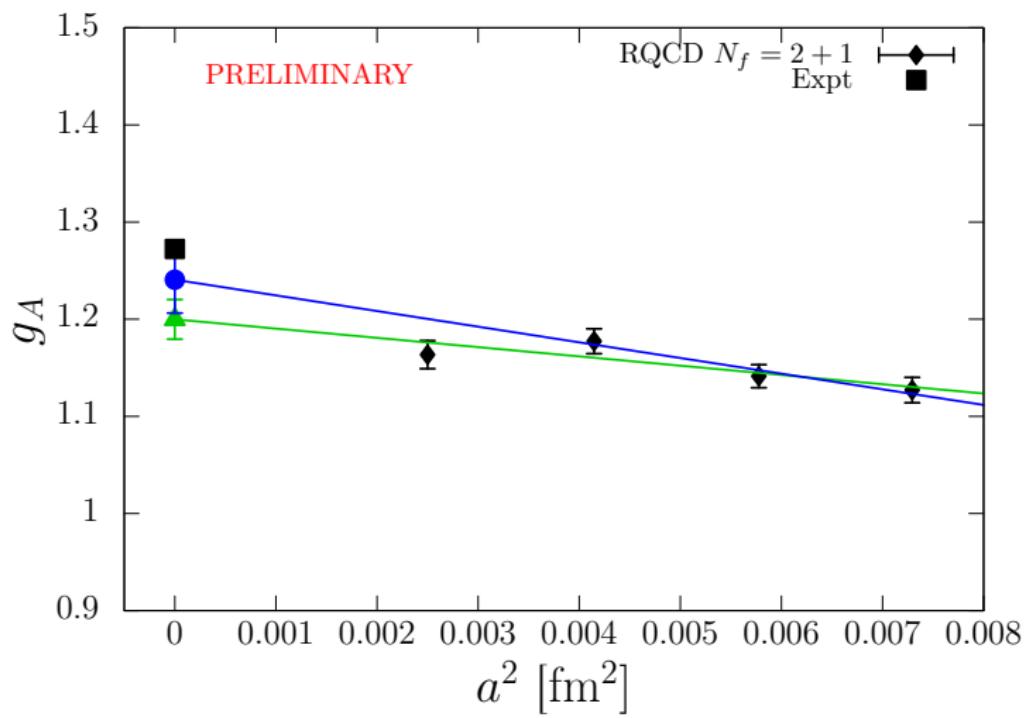
- weak dependence on  $\bar{m}$  allows for a continuum extrapolation

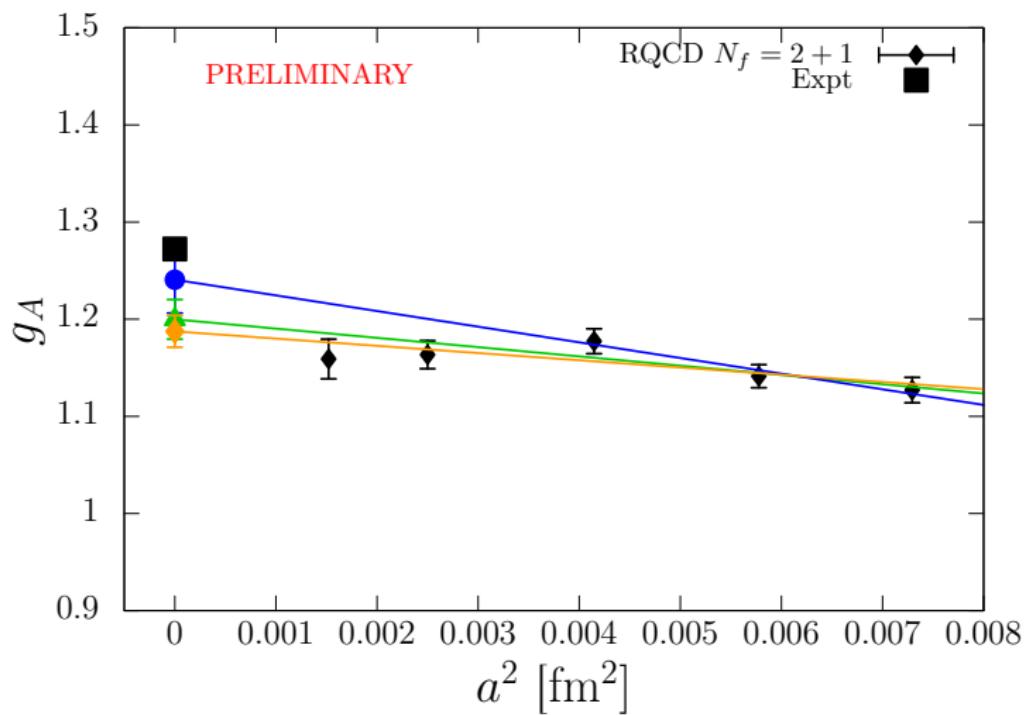
Continuum limit of  $g_A$  at  $M_\pi \approx 415$  MeV

PRELIMINARY

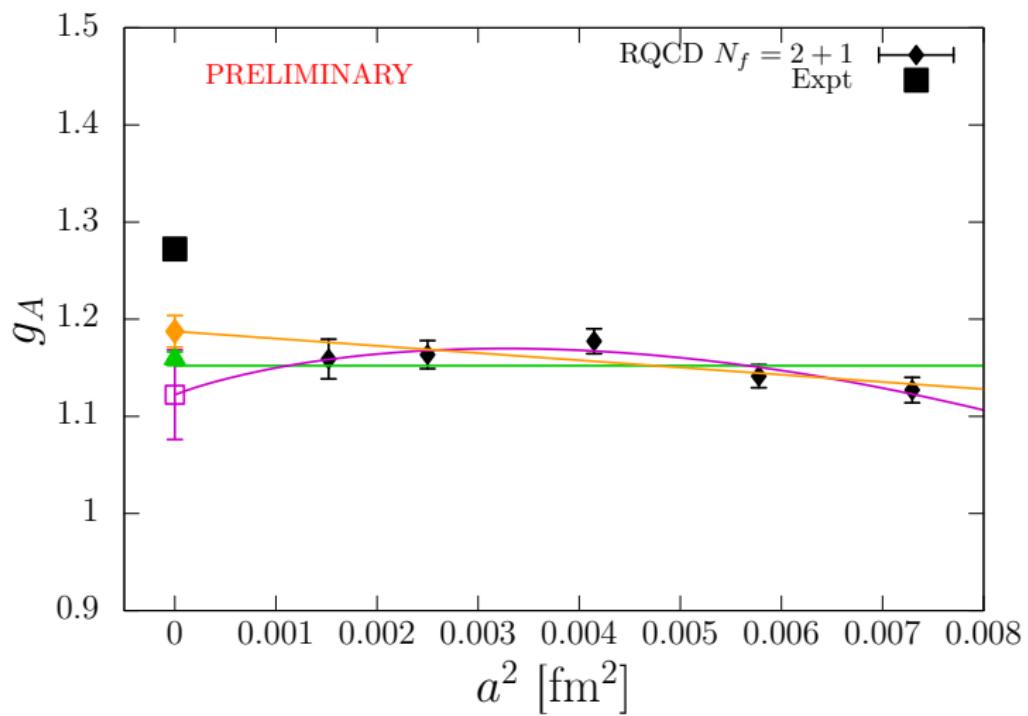


## Continuum limit of $g_A$ at $M_\pi \approx 415$ MeV



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  $a \rightarrow 0$
- long term effort within CLS

$\bar{m} = m_{\text{symm}}$  trajectory: Meson/Baryon Spectrum

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

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

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

Strategy allows us

- to determine SU(2) as well as 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