Towards the continuum limit
– Results on the light hadron spectrum on CLS ensembles –

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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

Simulation Overview

Lattice Action

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

∃ three different quark mass plane trajectories

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

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

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

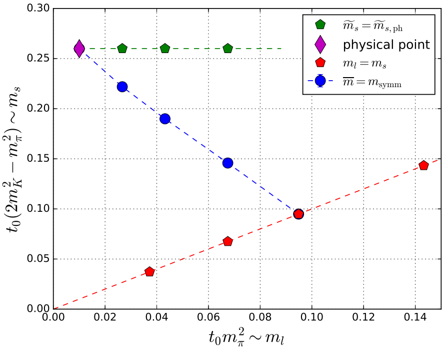
Strange AWI mass $\widetilde{m}_s = \text{const.} \rightarrow$ renormalized $\widehat{m}_s = \widehat{m}_{s,\mathrm{ph}}$, up to tiny $\mathcal{O}(a)$ effects.

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

For joint non-perturbative renormalization program

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

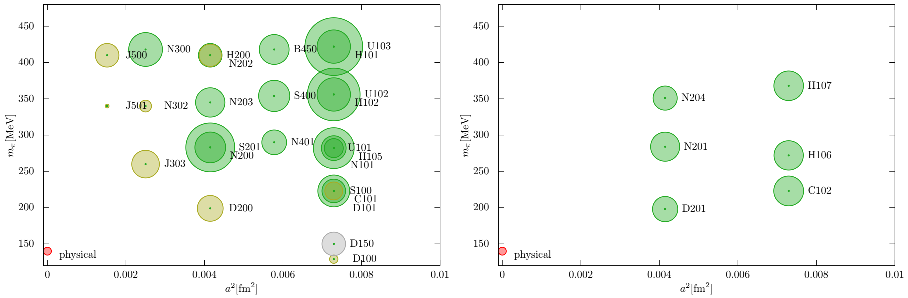
Overview of the simulation strategy → [hep-lat 1606.09039]



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.

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

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



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

Octet Baryons: Chiral + Continuum Extrapolation

Octet Baryon Masses m_B ($B = N, \Lambda, \Sigma, \Xi$)

Fitting Formula:

$$\sqrt{8t_0}m_B(\sqrt{8t_0}m_\pi, \sqrt{8t_0}m_K, a) = \sqrt{8t_0}m_B(\sqrt{8t_0}m_\pi, \sqrt{8t_0}m_K, 0)\left(1 + c\,a^2 + \bar{c}\,a^2\,t_0\overline{M}^2 + \delta c^B\,a^2\,t_0\delta M^2\right)$$

with

$$t_0\overline{M}^2 = \frac{1}{3}t_0(2m_K^2 + m_\pi^2) \sim 2B_0\overline{m} = 2B_0\frac{1}{3}(2m_l + m_s)$$

$$t_0\delta M^2 = 2t_0(m_K^2 - m_\pi^2) \sim 2B_0\delta m = 2B_0(m_s - m_l)$$

Details

- continuum chiral behavior given by: $\sqrt{8t_0}m_B(\sqrt{8t_0}m_\pi, \sqrt{8t_0}m_K, 0)$
- lattice spacing dependence parametrized by 6 parameters: c, $\bar{c}$, δc^N, δc^Λ, δc^Σ, δc^Ξ
- lattice spacing (intermediately) set by $t_0^\star/a^2$
  ($t_0^\star = t_0$ at the symmetric point at fixed $\phi_4 = 8t_0(m_\pi^2/2 + m_K^2) = \phi_4^{phys.} = 1.11$ → [hep-lat 1608.08900]

Octet Baryon Masses: Continuum Chiral Behavior

Chiral behavior of the masses in the continuum limit $m_B(m_\pi, m_K, 0)$

Parametrizations:

- linear fit (with enforced SU(3) constraints $\hat{=}$ NLO tree-level ChPT)
- NLO ChPT
- (NNLO ChPT)

Linear Fit Formula

$$\sqrt{8t_0}m_B(\sqrt{8t_0}m_\pi, \sqrt{8t_0}m_K, 0) = \sqrt{8t_0}m_0 + \bar{b}\,\sqrt{8t_0}\overline{M}^2 + \delta b^B\,\sqrt{8t_0}\delta M^2$$

Note:

$\Rightarrow$ $\bar{b} \equiv \bar{b}(b_0, b_D)$ and $\delta b^B \equiv \delta b^B(b_D, b_F)$

$\Rightarrow$ in total 4 fit parameters for chiral part: m_0, b_0, b_D and b_F

Octet Baryon Masses: Continuum Chiral Behavior

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- NLO ChPT
- (NNLO ChPT)

NLO Fit Formula

$$\sqrt{8t_0}m_B(\sqrt{8t_0}m_\pi, \sqrt{8t_0}m_K, 0) =$$
$$\sqrt{8t_0}m_0 + \bar{b}\,\sqrt{8t_0}\overline{M}^2 + \delta b^B\,\sqrt{8t_0}\delta M^2 + 3g_{B,\pi}f(m_\pi) + 4g_{B,K}f(m_K) + 4g_{B,\eta}f(m_\eta)$$

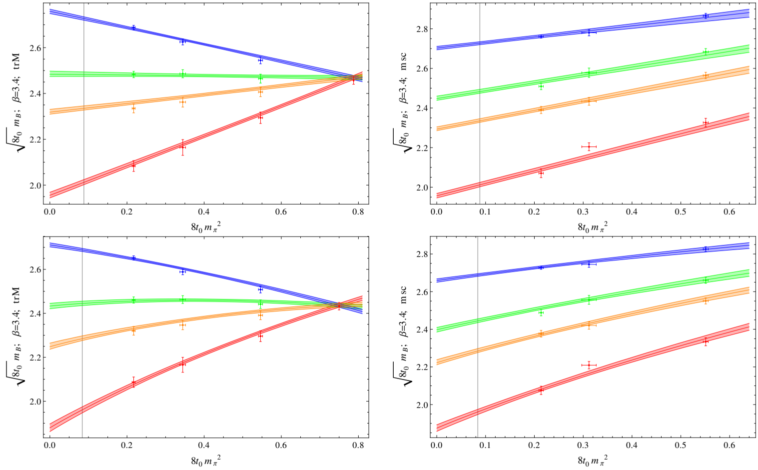
Note:

- $f(m)$ contains logs ($\sim \ln \frac{m^2}{\mu^2}$) (set $\mu \approx 1GeV$)

$\Rightarrow$ parameters $g_i \equiv g_i(F, D)$

$\Rightarrow$ in total 6 fit parameters for chiral part: m_0, b_0, b_D and b_F plus D, F

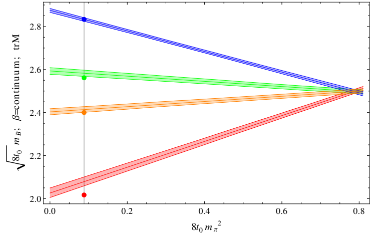
Linear+NLO Chiral Fits: $\overline{m} = m_{\mathrm{symm}}$ vs. $\widetilde{m}_s = \widetilde{m}_{s,\mathrm{ph}}$



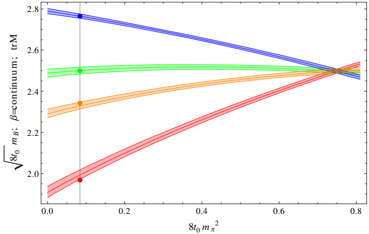
$\overline{m} = m_{\mathrm{symm}}$ $\widetilde{m}_s = \widetilde{m}_{s,\mathrm{ph}}$

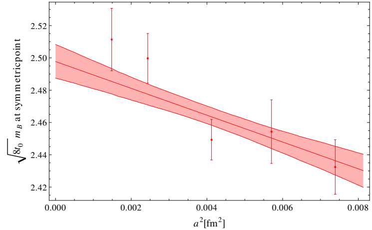
Chiral Fits in the Continuum limit

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



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





$m_s = m_\ell$

Preliminary Results and Outlook

Preliminary Results

- NLO fit describes data very well
- data compatible with lattice spacing effects of order a^2
- t_0 in agreement with BMW (and Zeuthen) determination with similar (eventually smaller) error
- sigma term $\sigma_{\pi N} \approx 40 MeV$
  (via Feynman-Hellmann; at phys. point + cont. limit from NLO fit)

Outlook

- check for systematics
- determine low energy constants
- compare different ways of scale settings

AWI masses and $\mathrm{O}(a)$-Improvement [hep-lat 1606.09039]

AWI masses

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

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

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

Problem: Different renormalization of flavour-singlet and non-singlet

quark mass combinations (without order a improvement):

$$\frac{Z}{2}\,\delta m = \frac{Z}{2}(m_s - m_\ell) = \frac{Z}{4a}\left(\frac{1}{\kappa_s} - \frac{1}{\kappa_\ell}\right) = \frac{Z_P}{2Z_A}(\widehat{m}_s - \widehat{m}_\ell) = (\widetilde{m}_{13} - \widetilde{m}_{12}) = \delta\widetilde{m}$$

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

$\rightarrow Z = Z_m Z_P / Z_A$, renormalized quark masses: $\widehat{m}_\ell, \widehat{m}_s$

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

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

Full order *a* improvement

$$\delta\widetilde{m} = \frac{Z}{2}\delta m\left[1 - \frac{\mathcal{A}}{12}(a\,\delta m) - \mathcal{B}_0 a\overline{m}\right], \qquad \widetilde{\overline{m}} = Zr_m\overline{m}\left[1 - \frac{\mathcal{C}_0}{36}\frac{(a\,\delta m)^2}{a\overline{m}} - \frac{\mathcal{D}_0}{2}(a\overline{m})^2\right]$$

- four combinations of improvement coefficients appear $\rightarrow \mathcal{A}, \mathcal{B}_0, \mathcal{C}_0$ and $\mathcal{D}_0$.
- $\mathcal{A}, ..., \mathcal{D}_0$ are combinations of $r_m, b_P, b_A, b_m, d_m, \tilde{b}_P, \tilde{b}_A, \tilde{b}_m, \tilde{d}_m$

Fitting

- simultaneous fit of light and strange AWI masses $\widetilde{m}_{(\ell,s)}(\kappa_\ell, \kappa_s)$
- use $\mathcal{A}$ from Ref. [Korcyl and Bali, arXiv:1607.07090] as input
- sensitive parameters: $Z \equiv \frac{Z_P Z_m}{Z_A}$, Zr_m, κ_{crit}, $\mathcal{C}_0$
- less sensitive parameters: $\mathcal{B}_0$, $\mathcal{D}_0$, ($\mathcal{A}$)

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

Full order a improvement

$$\delta\widetilde{m} = \frac{Z}{2}\delta m\left[1 - \frac{\mathcal{A}}{12}(a\,\delta m) - \mathcal{B}_0 a\overline{m}\right], \qquad \widetilde{\overline{m}} = Zr_m\overline{m}\left[1 - \frac{\mathcal{C}_0}{36}\frac{(a\,\delta m)^2}{a\overline{m}} - \frac{\mathcal{D}_0}{2}(a\overline{m})^2\right]$$

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Results

β	Z	r_m	$\kappa_{\rm crit}$	$\mathcal{A}$ (input)	$\mathcal{B}_0$	$\mathcal{C}_0$	$\mathcal{D}_0$
3.4	0.8710(30)(10)	2.635(94)(5)	0.1369115(27)(1)	2.91(33)	$-1.55(76)(1)$	3.43(30)	10.0(9.1)(0.3)
3.46	0.923(1)	1.98(5)	0.137057(3)	2.58(18)	-1.0 (fixed)	1.3(8)	4(3)
3.55	0.9841(25)(3)	1.530(14)(1)	0.1371718(10)	2.27(14)	$-0.81(45)(1)$	1.89(25)(1)	1.2(1.2)
3.7	≈ 1.05	≈ 1.27	–	1.96(14)	–	($\approx 1.7(7)$)	–

Simulations at the Physical Point

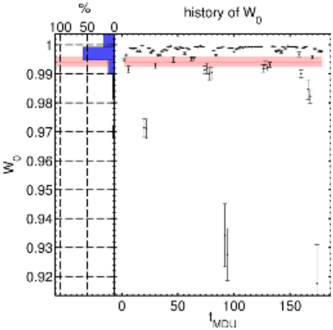
Simulations with open boundary conditions in time

- Ensemble D100 at $a \approx 0.086 fm$ ($m_\pi \approx 130 MeV$, low statistics)

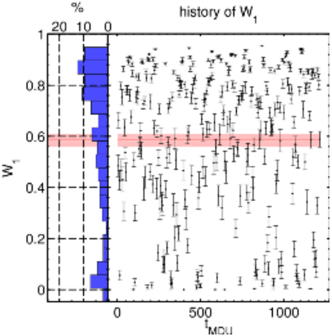
Simulations with anti-periodic boundary conditions in time

- Ensemble D150 at $a \approx 0.086 fm$ ($m_\pi \approx 150 MeV$, generation in progress)
- Ensemble E250 at $a \approx 0.064 fm$ (thermalized/low statistics $\rightarrow$ planned) $\rightarrow$ talk by Daniel MOHLER on Tue

Simulations at the Physical Point: Reweighting



D100 (small twisted mass parameter)

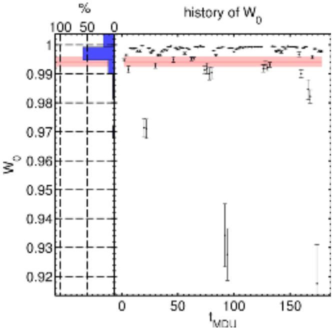


D150 (large twisted mass parameter)

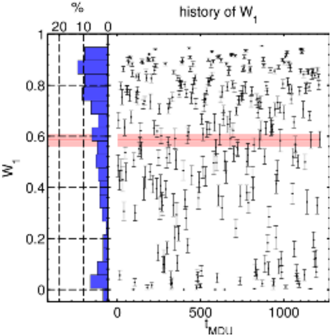
Simulations and reweighting

- ⇒ twisted mass reweighting
  → add a twisted mass term to light quark action in the simulations to stabilize HMC runs
- ⇒ $\langle O \rangle = \frac{\langle RO \rangle}{\langle R \rangle}$ with observable O and rwt. factor R
- ⇒ cancellations of fluctuations between observable and reweighting factor?

Simulations at the Physical Point: Reweighting



D100 (small twisted mass parameter)



D150 (large twisted mass parameter)

Simulations and reweighting

⇒ error on kaon mass (stats=500MDU):
D100: $m_K a = 0.20880(44)$
D150: $m_K a = 0.20928(40)$

⇒ error on t_0:
D100: $t_0/a^2 = 2.9538(15)$ (stats=500MDU)
D150: $t_0/a^2 = 2.9397(09)$ (stats=1200MDU)

⇒ beneficial cancellations of fluctuations between observable and reweighting factor!

Disclaimer

The work presented was carried out in collaboration with

Gunnar Bali, Sara Collins, Meinulf Göckeler, Fabian Hutzler,

Rudolf Rödl, Andreas Schäfer, Enno Scholz, Jakob Simeth,

André Sternbeck, Philipp Wein ($\rightarrow$ chiral fits) 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

AWI mass and order *a* improvement

- extended study of order *a* improvement

Physical Point

- reweighting works well, even for rather large twisted mass parameter
- simulations at the physical point planned/in progress

Octet Baryon Spectrum

- fitting to linear and NLO SU(3) ChiPT in progress
- good agreement at the physical point of NLO SU(3) ChiPT

Outlook

- check for systematics
- nucleon structure and other additional observables