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

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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 $a \gtrsim 0.05$ fm

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

$[\text{Lüscher and Schaefer 2011}]$

$\rightarrow$ 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 Details

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. \( \bar{m} = m_{\text{symm}} \)

\(3\bar{m} = 2m_{(\ell)\text{ght}} + m_{(s)} = \text{const.} \iff \frac{2}{\kappa_{\ell}} + \frac{1}{\kappa_{s}} = \text{const.} \rightarrow \text{renormalized } 2\hat{m}_{\ell} + \hat{m}_{s} = \text{const.} + O(a).\)

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

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

3. \( m_{s} = m_{\ell} \) (Mainz/Regensburg)

For joint non-perturbative renormalization program

→ simulations with anti-periodic boundary conditions (for \( a > 0.05 \text{ fm} \))
Overview of the simulation strategy → 1606.09039

1. generate the $\bar{m} = m_{\text{symm}}$ 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 $\bar{m} = m_{\text{symm}}$ line, imposing $\bar{m}_S/\bar{m}_\ell = 27.46(44)$ [FLAG 2] → $\bar{m}_{S,\text{ph}}$

5. predict $\kappa_\ell, \kappa_S$ pairs for which $\bar{m}_S = \bar{m}_{S,\text{ph}}$ from the parametrization in order to add $\bar{m}_S = \bar{m}_{S,\text{ph}}$ simulation points.
How to predict $\kappa_S$ as a function of $\kappa_\ell$ for $\tilde{m}_s$ fixed

Average AWI masses:
\[
\frac{\tilde{m}_j + \tilde{m}_k}{2} = \tilde{m}_{jk} = \frac{\partial_4 \langle 0 | A_{4j}^{jk} | \pi^{jk} \rangle}{2 \langle 0 | P_{jk} | \pi^{jk} \rangle}
\]

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

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

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

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

where $Z = Z_mZ_P/Z_A$. Setting $\tilde{m}_s = \tilde{m}_s,\text{ph}$ gives

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

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

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

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

$$\frac{1}{\kappa_\ell} = \frac{1}{\kappa_{\ell,\text{ph}}} + \frac{2a(2 + r_\text{m})}{3Zr_\text{m}}(\tilde{m}_\ell - \tilde{m}_{\ell,\text{ph}}).$$
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 $\overline{m} = \text{const.}$ 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 $m = \overline{m} = m_s = m_\ell$ line.
- We carry out full order $a$ improvement. In this case four combinations of improvement coefficients ($A, B_0, C_0$ and $D_0$) appear.

Does the $\kappa_s$ prediction strategy work?

To be addressed later: Scale setting/tuning; we assumed that the physical point is on the $\overline{m} = m_{\text{symm}}$ 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:

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

\[ \bar{m} = m_{\text{symm}} \]

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

\[ m_\pi \text{[MeV]} \]

\[ a^2 \text{[fm}^2\text{]} \]

Physical

- 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: $192 \times 64^3$

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RQCD results on CLS open BC ensembles

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Tuning details and results for the $\bar{m} = m_{\text{symm}}$ trajectory
Tuning strategy: $\bar{m} = m_{\text{symm}}$

- $\phi_2 = t_0 m_\pi^2 \sim m_l, \quad \phi_4 = 8 t_0 (m_K^2 + m_\pi^2 / 2) \sim \bar{m}$
- 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: $\bar{m} = m_{\text{symm}}$ → hep-lat 1606.09039

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

$\beta = 3.4 \, a \approx 0.085 \text{ fm}$

$\beta = 3.55 \, a \approx 0.064 \text{ fm}$
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

$\beta = 3.4$

$\beta = 3.55$

Relevant parameters: $Z \equiv \frac{Z_P Z_m}{Z_A}$, $A$, $B_0$ ($\rightarrow$ slope is due to $Z$)

- use $A$ from Ref. [Korcyl and Bali, arXiv:1607.07090] as input
- Sums of quark masses are sensitive to $Z r_m, \kappa_{\text{crit}}, C_0, (D_0)$
- $A, \ldots, D_0$ 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]

\[ m_s = m_{s,\text{ph}} \text{ line} \]

For \( \beta = 3.4 \)

\[ \tilde{m}_s / \tilde{m}_\ell \text{ along } \bar{m} = m_{\text{symm}} \text{ determined from the global fit.} \]

\[ \text{physical value} = 27.46(44) \text{ from [FLAG 2] used to define the physical point.} \]
Is the FLAG value consistent with our results?

\[ m_s = m_{s,\text{ph}} \]

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.
Fitting Details

Nucleon: Effective mass

Ensemble = N300, Run = run4

- fit range = [2, 35]
- fit range = [2, 30]
- fit range = [2, 35]

N300 Ensemble

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

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

→ binning analysis, extrapolate error to infinite bin size
Pion: Effective mass

Ensemble = N300, Run = run4

Fit range = [4, 66]

fit range = [4, 34]

fit range = [4, 52]

N300 Ensemble

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

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

→ 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 ChiPT $\propto \bar{m}$ and $\propto (m_s - m_\ell)^2$. 

$m_s = m_{s,\text{ph}}$ line
Comparing extrapolations along the two mass trajectories

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

Preliminary

$M = K$

$M = \pi$

physical point

$\beta = 3.4, \bar{m} = m_{\text{symm}}$

$\beta = 3.55, \bar{m} = m_{\text{symm}}$

$X^2/\pi^2_{\text{symm}}$

$X^2/\pi^2_{\text{symm}}$

$\tilde{m}/\tilde{m}_{\text{ph}}$

$\tilde{m}/\tilde{m}_{\text{ph}}$

$\tilde{m}/\tilde{m}_{\text{ph}}$

$\tilde{m}/\tilde{m}_{\text{ph}}$

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RQCD results on CLS open BC ensembles

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Comparing extrapolations along the two mass trajectories

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

preliminary
Comparing extrapolations along the two mass trajectories

Octet baryons $\vec{m} = m_{symm}$

Preliminary

$m_B/X_{N,symm}$

$m_{\pi}/m_{\pi,ph}$

Physical point $\beta = 3.4$, $\vec{m} = m_{symm}$

Physical point $\beta = 3.55$, $\vec{m} = m_{symm}$
Comparing extrapolations along the two mass trajectories

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

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

preliminary

![Graphs showing extrapolations for different mass trajectories](image)

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Comparing extrapolations along the two mass trajectories

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

preliminary
Comparing extrapolations along the two mass trajectories

\[ \hat{X}_N, \hat{X}_\Delta \]

\[ \hat{X}_N, \hat{X}_\Delta \]

\[ \hat{X}_N, \hat{X}_\Delta \]

\[ \hat{X}_N, \hat{X}_\Delta \]

\[ \beta = 3.4, \bar{m}_s = \bar{m}_{s, ph} \]

\[ \beta = 3.4, \bar{m} = \bar{m}_{symm} \]

\[ \beta = 3.55, \bar{m}_s = \bar{m}_{s, ph} \]

\[ \beta = 3.55, \bar{m} = \bar{m}_{symm} \]

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\[ \beta = 3.4 \text{ RQCD(CLS) data} \]

\[ \beta = 3.55 \text{ RQCD(CLS) data} \]

Compare scale setting

- relative error on \( a \) from \( m_\Xi \approx 0.4\%, m_\Xi^* \approx 0.9\%, m_\Omega \approx 0.7\%, X_N \approx 0.6\% \) \( \rightarrow \) from BMW \( t_0 \approx 1.7\% \)
- \( a \) for \( \beta = 3.40 \): \( a_{X_N} \approx 0.0833(4) \text{ fm} \) \( \rightarrow \) from BMW \( a_{t_0} = 0.0854(15) \text{ fm} \)
- \( a \) for \( \beta = 3.55 \): \( a_{X_N} \approx 0.0632(5) \text{ fm} \) \( \rightarrow \) from BMW \( a_{t_0} = 0.0644(11) \text{ fm} \)
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)
weak dependence on $\overline{m}$ allows for a continuum extrapolation
Continuum limit of $g_A$ at $M_\pi \approx 415$ MeV

Preliminary result for $RQCD$ with $N_f = 2 + 1$ quark flavors:

- $g_A$ as a function of $a^2$ [fm$^2$]
- The plot shows the trend of $g_A$ with $a^2$ and includes experimental data.

RQCD results on CLS open BC ensembles

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

Continuum Extrapolation

$g_A$ vs. $a^2$ [fm$^2$]

RQCD $N_f = 2 + 1$

Expt

PRELIMINARY
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.

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Summary

Lattice Simulations with Open Boundaries

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

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