Benchmark Continuum Limit Results for Spectroscopy with Stabilized Wilson Fermions

Giovanni Pederiva

On behalf of the OPEN LATtice Initiative:

F. Cuteri, A. Francis, P. Fritzsch, A. Rago,
A. Shindler, A. Walker-Loud, S. Zafeiropoulos

OPEN
LATtice
initiative

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on Lattice Field Theory

OpenLat Initiative

Bringing together researchers from different institutes. Our aim is to generate state-of-the-art QCD gauge en- sembles for physics applications and to share them with the community to strengthen open science.

- define and uphold quality standards
- share and maintain repository
- community boosting
- grant and enable access

Stabilized Wilson Fermions Generation

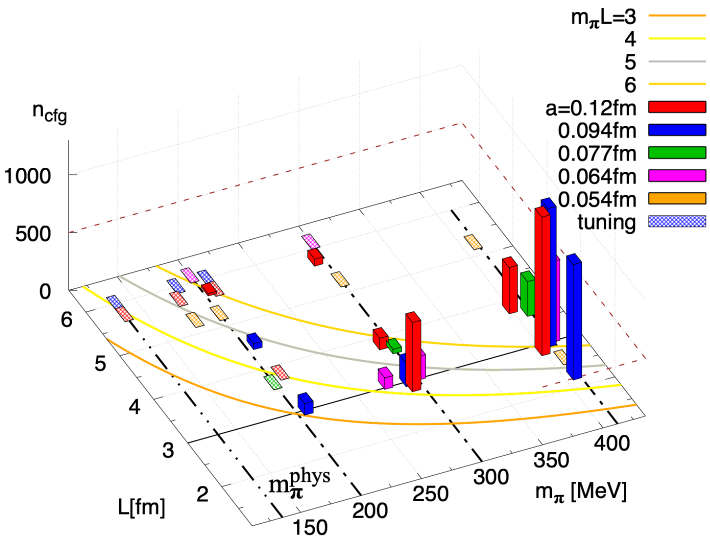
We use the SWF package, a set of algorithmic improvements:

- SMD (stochastic molecular dynamics)
- increase precision of internal numbers to quad
- use supremum-norm to ensure minimum solve quality
- exponentiated Clover action

On top of more commonly used practices:

- twisted mass reweighting for light quarks
- mass preconditioning through Hasenbusch chains
- using improved solvers (deflated SAP)
- high accuracy approximations for the strange quark RHMC

Ensembles at the SU(3) flavor Symmetric Point m_π 410 MeV



Ensembles at the SU(3) flavor Symmetric Point m_π 410 MeV

β	Size	a[fm]	m_π	L [fm]	$m_\pi L$	N_{cfg}
3.685	$24^3 \times 96$	0.12	411.54(46)	2.9	6.0	1200
3.8	$24^3 \times 96$	0.094	410.58(84)	2.3	4.5	1200
	$32^3 \times 96$	0.094	409.57(46)	3.0	6.0	1300
3.9	$48^3 \times 96$	0.077	410.39(22)	3.6	7.5	300
4.0	$48^3 \times 96$	0.064	408.93(25)	3.0	6.4	600

Software Stack

Gauge generation and basic flowed observables are obtained using `openQCD 2.0`and `openQCD 2.4` [1]

To perform the spectroscopy analysis we used these tools:

- The `CHROMA` stack[2], including `QUDA`[3] and `QPHIX`
- `LALIBE`[4], a code built on top of `CHROMA` with many useful tools for spectroscopy
- `gvar` and `lsqfit`[5] for bayesian fitting

[1] `https://luscher.web.cern.ch/luscher/openQCD/`

[2] R. G. Edwards, B. Joó, *The Chroma Software System for Lattice QCD*, 2005, POS Lattice2004

[3] M. A. Clark, R. Babich, K. Barros, R. Brower, and C. Rebbi, *Solving Lattice QCD systems of equations using mixed precision solvers on GPUs*, Comput. Phys. Commun. 181, 1517 (2010) [arXiv:0911.3191 [hep-lat]].

[4] `https://github.com/callat-qcd/lalibe`

[5] Created by G. Peter Lepage (Cornell University) 2008, copyright (c) 2008-2020 G. Peter Lepage

Gauge Observables

Estimation of t_0

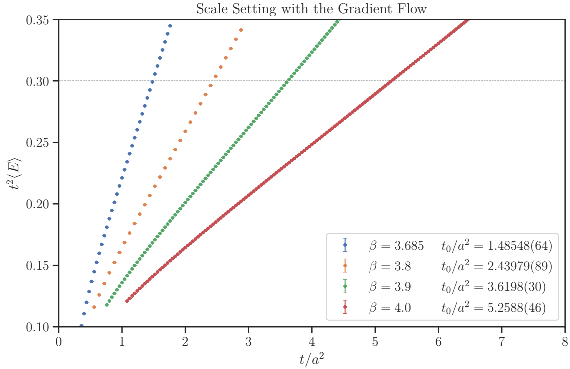
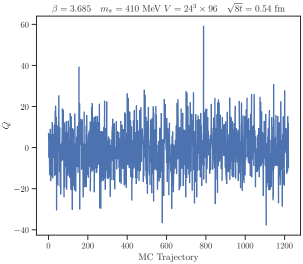


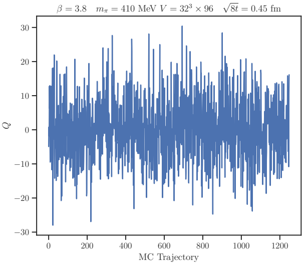
Figure 1: Setting the scale with the Gradient Flow and the condition $t^2\langle E\rangle = 0.3$.

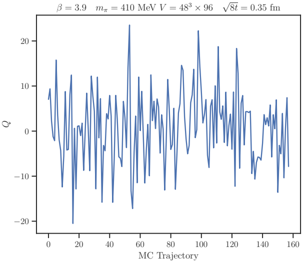
We use $\sqrt{t_0} = 0.1464(18)$ fm to fix the scale in physical units[6]

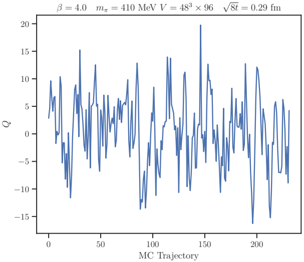
[6] M. Bruno, T. Korzec and S. Schaefer *Setting the scale for the CLS 2 + 1 flavor ensembles*

Topological Charge Distribution

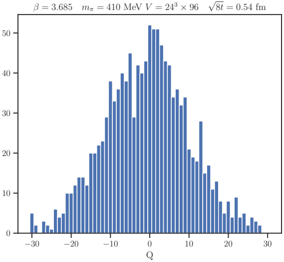


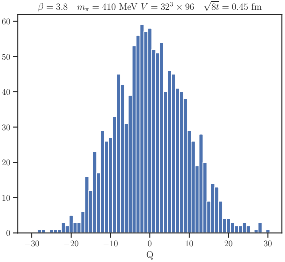


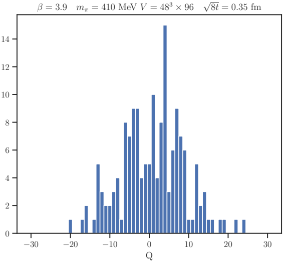


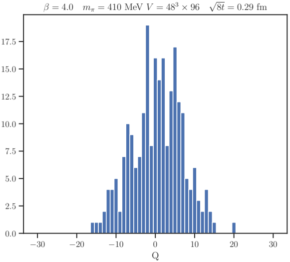


Topological Charge Distribution









Hadron Spectroscopy

Ensembles' Properties

Ensemble	t_0/a^2	a [fm]	N_{cfg}	N_{srcs}
a12m400mL6.0	1.48548(64)	0.12	600	100
a094m400mL4.5	2.44202(98)	0.094	500	100
a064m400mL6.0	2.43979(89)	0.094	1200	100
a077m400mL6.0	3.6198(30)	0.077	900	100
a064m400mL6.4	5.2588(46)	0.064	1000	100

Using Gaussian smearing, we compute both smeared-point (PS) and smeared-smeared (SS) correlators.

Bayesian Fitting of Correlation Function

For the analysis we used a Bayesian framework with constraints[7]. The n-state function used as ansatz reads:

$$C(t, Z_{P,n}, Z_{S,n}, E_n) = \sum_{n=0}^{n=N} Z_{S,n} Z_{S/P,n} e^{-E_n t}$$

Where $Z_{P,n}$ and $Z_{S,n}$ are the amplitudes for the point and smeared sources/sinks. We fit both the PS and SS correlators at once.

[7] G.P. Lepage, B. Clark, C.T.H. Davies, K. Hornbostel, P.B. Mackenzie, C. Morningstar, and H. Trottier, *Con- strained curve fitting*, Nucl. Phys. B Proc. Suppl. 106, 12–20 (2002

Bayesian Fitting of Correlation Function

To constrain the fit we used a set of priors for the energies and the amplitudes. These enter the fit through an addition to the χ^2 function to be minimized:

$$\chi^2_{prior} = \sum_{n=0}^{N} \frac{(Z_{P,n} - \tilde{Z}_{P,n})^2}{\tilde{\sigma^2}_{Z_{P,n}}} + \sum_{n=0}^{N} \frac{(Z_{S,n} - \tilde{Z}_{S,n})^2}{\tilde{\sigma^2}_{Z_{S,n}}} + \sum_{n=0}^{N} \frac{(E_n - \tilde{E}_n)^2}{\tilde{\sigma^2}_{E_n}}$$

The priors for $E_0, Z_{P,n}, Z_{S,n}$ are chosen as normally distributed, while the excited-state energy priors are set to be log-normal. The excited-state energy splittings are set to the value of $2m_\pi$ with a width allowing for fluctuations down to one pion mass within one standard deviation.

Fit Model Averaging

To determine an **unbiased** value for the mass of the hadrons, we use a bayesian model averaging procedure based on the Akaike Information Criterion (AIC)[8].

For each possible fit we compute:

$$pr(M|D) = \exp\left[-\frac{1}{2}(\chi^2_{aug} + 2k + 2N_{cut})\right]$$

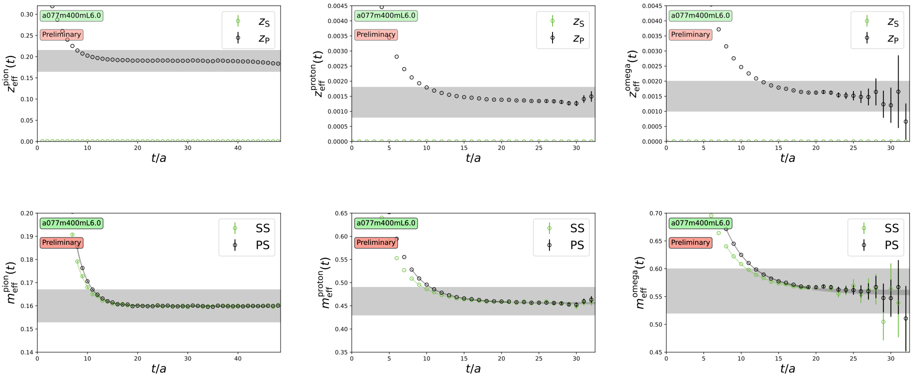
where k is the number of fit parameters and N_{cut} is the number of points removed from the fitting window.

$pr(M|D)$ is used as weights in the weighted mean that gives the final result. The uncertainty on a given fit parameter a is given by the bias corrected variance on the weighted mean:

$$\sigma_a = \sum_{i=1}^{N_M} \sigma_{a,i} pr(M|D) + \sum_{i=1}^{N_M} \langle a \rangle_i^2 pr(M|D) - \left(\sum_{i=1}^{N_M} \langle a \rangle_i pr(M|D)\right)^2$$

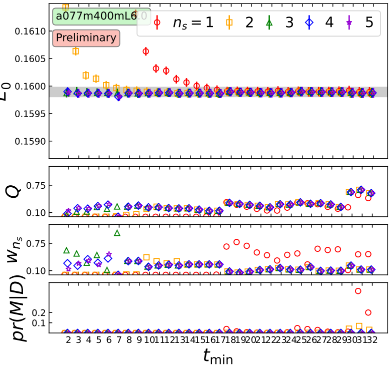
[8] W. I. Jay and E. T. Neil *Bayesian model averaging for analysis of lattice field theory results* Phys. Rev. D 103, 114502

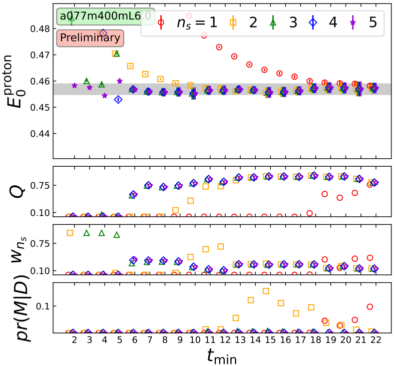
Example of Effective Mass Fit Results



The first step consists on fixing the priors on the values for the amplitudes and the masses (gray bands in the figures).

Fit Stability Considerations

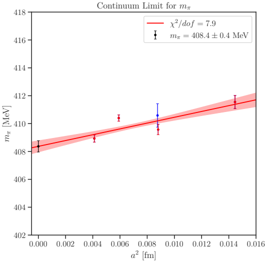


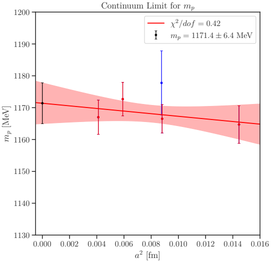


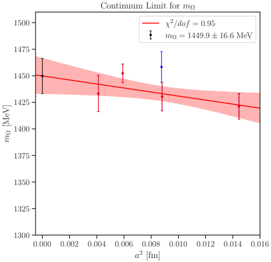
Stability for the ground state as the t_{min} of the fitting window is changed for fits with different number of states. Here Q is the probability that the augmented χ^2 from the fit could have been larger, by chance, assuming the best-fit model is correct and W_{n_s} is the relative weight one the fit over the others, at fixed t_{min}

$pr(M|D)$ is the a likelihood of the model given the data. This is what is used as a weight.

Continuum Limit Extrapolation







The blue point is the smaller volume at $\beta = 3.8$. Since we see some small finite volume effects, it is not included in the continuum extrapolation.

Autocorrelation Considerations

With the data we gathered, we estimated these integrated autocorrelation times:

Ensemble	τ_Q	τ_π	τ_N	τ_Ω
a12m400mL6.0	0.53(4)	1.56(26)	0.53(4)	0.50(4)
a094m400mL4.5	0.54(10)	0.51(6)	0.54(6)	0.51(6)
a064m400mL6.0	0.64(6)	0.55(6)	0.51(4)	0.44(6)
a077m400mL6.0	0.54(10)	0.63(8)	0.72(10)	0.75(13)
a064m400mL6.4	1.52(42)	0.50(6)	0.57(11)	0.66(11)

τ_{int} is estimated using the Madras-Sokal windowing procedure and shown in units of MC saves

Moving Forward

Summary:

- Stage 1 of gauge generation of SWF ensembles almost completed
- First results of continuum extrapolation at the $SU(3)$ flavor symmetric point give encouraging results
- Bayesian method applied to determine ground-state masses gives unbiased and reliable estimates

Going Forward:

- Further refine the analysis for all the benchmark observables
- Repeat analysis once new ensembles enter production stage
- Refine the analysis and perform infinite volume and chiral extrapolations when possible
- Establish robust results as future benchmarks for the openLAT initiative

Thank You

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https://openlat1.gitlab.io/

Standard Wilson-Dirac Clover Action for LQCD

The standard $O(a)$-improved Wilson-Dirac operator can be split as:

$$D = D_W + C + m_0 = D'_W + C + 4 + m_0$$

Here D_W is the regular Wilson-Dirac operator, while D'_W is the off-diagonal part only. C is the clover term:

$$C = c_{SW} \frac{i}{4} \sigma_{\mu\nu} F_{\mu\nu}$$

This term is diagonal in spacetime.

A New Clover Action

An exponential variant has recently been proposed [9]

$$(4+m_0)+C \Rightarrow (4+m_0)\exp\left\{\frac{C}{(4+m_0)}\right\} = (4+m_0)\exp\left\{\frac{i}{4}\frac{c_{SW}}{(4+m_0)}\sigma_{\mu\nu}F_{\mu\nu}\right\}$$

The regular clover term can be understood as the first part of an expansion. For more details refer to the previous talk by A. Francis *Properties and ensembles of Stabilised Wilson Fermions*

[9] A. Francis, P. Fritzsch, M. Luscher, A. Rago, *Master-field simulations of O(a)-improved lattice QCD: Algorithms, stability and exactness*, Comput.Phys.Commun. 255 (2020) 107355

Numerical Implementation in CHROMA

- The exponential clover term has been implemented in CHROMA[10], on top of the regular QDP Clover term, to allow computation of more advanced observables.
- Publicly available for the LQCD community
- Tested against the existing openQCD implementation.

The key part of the implementation of the action is calculating $\exp[\sigma_{\mu\nu} F_{\mu\nu}]$, which is a 12×12 matrix, block diagonal (6×6). The exponential needs to be calculated as precisely as possible. This is only computed once before calling the solver, while creating the linear operator.
Using the Cayley-Hamilton theorem we can show that:

$$A^m = \sum_{i=0}^{n} c_i(m, A) A^i \;\; \rightarrow \;\; \exp(A) = \sum_{m=0}^{\infty} \frac{1}{m!} \sum_{i=0}^{n} c_i(m, A) A^i = \sum_{i=0}^{n} b_i(N, A) A^i$$

The coefficients $b_i(N, A)$ are found iteratively using Horner's scheme and the coefficients of the characteristic polynomial of A

[10] R. G. Edwards, B. Joó, *The Chroma Software System for Lattice QCD*, 2005, POS Lattice2004

Smearing Parameters

We performed a scan for the Gaussian smearing [11] [12] parameters to use, we selected $N_s = 32$ iteration and $\sigma = 3.86$ for the smearing width.

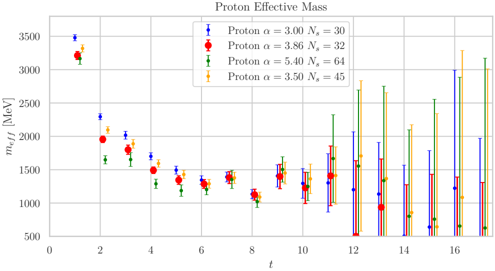

Figure 10: Nucleon mass on the a094m200mL3.3trMc ensemble with different Gaussian smearing parameters.

[11] T. A. DeGrand and R. D. Loft, Comput. Phys. Commun. 65, 84 (1991)

[12] Stephan Güsken, *A study of smearing techniques for hadron correlation functions*, Nuclear Physics B, (1990)