Progress in generating gauge ensembles with Stabilized Wilson Fermions

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For OpenLat:
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OPEN LATtice initiative

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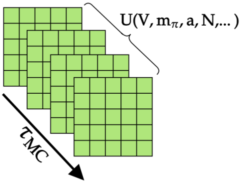
Lattice QCD as an engine to progress

Lattice provides key inputs for ...	... and impacts (small selection)
- HVP and HLBL, - Resonances, - Decay Constants, - Form Factors, - CKM Matrix, - QCD Spectrum, - 2-,3-Scattering, - Exotic Hadrons, - Matrix elements, - BSM / DM, ...	

Successes have been possible due to:

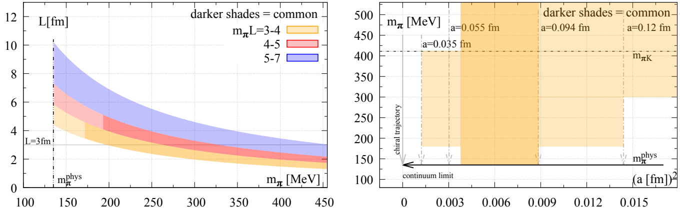
- Improved theoretical tools and understanding.
- Gauge configurations that enable controlled extrapolations for:
  - chiral / quark mass effects
  - finite size / volume effects
  - discretisation effects and continuum limit



- Configurations generated via Markov Chain Monte Carlo:
  - Many samples to reduce *statistical uncertainties*
  - Long trajectories to control *auto-correlations*
- *"New physics"*: With a good set of configurations more research areas open up.
- Not having ensembles is often the road-block. Need infrastructure (e.g. MILC, JLDG, ILDG revitalised)

The **quantity and quality of the set of configurations drives** the accessible precision.

Simulation bounds - accessible parameter window



With a good set of configurations precision becomes accessible. **But:**

(1.) Discretisation / Volume effects: Continuum extrapolation not always clear.

- Cost bound on finest $[a]$ due to lower bound V constraints. (L=3 fm and $m_\pi L \sim 4$ hard to fulfil)
- Cost bound on largest V. ($m_\pi L \geq 6$ hard to reach)

(2.) Stability issues: $m_\pi \to m_\pi^{\text{phys}}$ increases numerical problems associated with generation as fluctuations go with $\mathcal{O}(1/m_\pi, a)$.

- Algorithmic bound on m_π at given $[a]$. (Coarse $[a]$ = hard to go light)
- Smearing? Not a silver bullet.

(3.) Critical slowing down: As $[a] \downarrow$ the topology tunneling probability drops.

- Topology bound on $[a]$. (Topology freezes → autocorrelation explodes)
- Frozen topology induces $\propto Q/V$ contamination of observables.

⇝ some dependence on action for these statements.

Open lattice initiative - Est. 2019

Motivation:

- Quantity and quality of ensembles drives precision.

OpenLat: Generate and share configurations with community.

⇒ Choose new, complementary, actions and algorithms.
⇒ Aim to benefit from (and be ready for) new developments.
⇒ First focus on providing auxiliaries (rwf, m_π, f_π, Z_A, ...) for broad use.

OpenLat's setup: Stabilized Wilson fermions (SWF)

- Algorithmic improvements: SMD = stochastic molecular dynamics
  - SMD decreases fluctuations and makes for a generally more stable run
  - Supremum-norm to ensure best, volume independent, solve quality
- Fermion discretisation: Wilson - exponentiated Clover

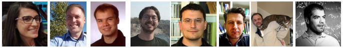
$$D = \frac{1}{2}\Big[\underbrace{\gamma_\mu\Big(\nabla^*_\mu + \nabla_\mu - a\nabla^*_\mu\nabla_\mu\Big)}_{\text{Wilson term}}\Big] + \underbrace{m_0 \exp\Big[\frac{c_{SW}}{m_0}\frac{i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}\Big]}_{\text{exponentiated Clover term}}$$

AF, Fritzsch, Lüscher, Rago; Comput.Phys.Commun. 255 (2020) 107355, [2106.09080]

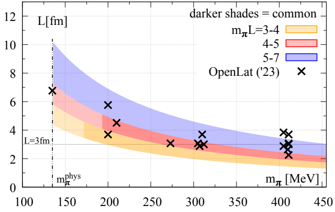
SWF toolkit implemented from `openQCD-2.0` onwards

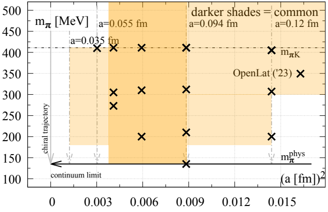
Open lattice initiative - Est. 2019



Lattice '21 and '22: [2212.11048], [2212.10138], [2212.07314], [2201.03874]

Cover a broad region in common area and expand:





⇝ Coarse $a = 0.12$ fm line outside of common WCF area.

⇝ New results at $a = 0.94$ fm at physical point.

⇝ First determination of f_π at $SU(3)_F$.

SWF in action:

(1.) Discretisation / Volume effects:

- Stabilized Wilson Fermions exhibit flatter continuum extrapolations

⇝ J. Green and A. Nicholson for BaSc, and G. Pederia for OpenLat, all Lattice'22

(2.) Stability issues:

- Observed smoother behavior, coarser $[a]$ and lighter m_π accessible

(3.) Critical slowing down: ⇝ No direct benefit expected.

- SWF are large volume safe. ⇝ no limitation on master-field type sims, not our focus.

Criteria that have to be fulfilled by a chain of configurations:

- $\phi_4 = 8t_0(m_K^2 + m_\pi^2/2) = 1.115$ within 0.5%, with an error of max. 1σ.
- Total reweighting factor fluctuations are mild, and ideally below 5%.
- SMD step distance $\delta\tau$ maximises the backtracking period.
- Distribution of δH matches the one set by the acceptance rate.
- Distribution of the lowest $\sqrt{D^\dagger D}$ eigenvalue is well-behaved & gapped.
- Distribution of the bounds of the strange quark spectral gap are within the input ranges, and the degree of the Zolotarev is sufficiently high, $12(V/2)\delta^2 < 10^{-4}$.
- There is no significant loss of precision caused by unbalanced contributions to the total action that might drive instabilities in the evolution.
- Distribution of the topological charge is symmetric around zero with no metastability.

Current resources and repository

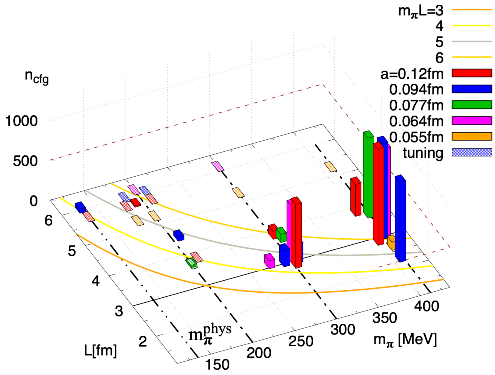
- Running allocation of **260 Mch** computing time*
- **22k configurations** generated, **40k** by end of 2023
- Total of **500 TB data** projected by end of 2023

*combined on several machines.

Configuration access

- No embargo time after publication.
- User access for unpublished configurations (case-by-case)
- Working on public hosting (JLDG? ILDG? NERSC?)

Gauge generation status



Main updates:

Ensemble	N_{conf}
a12m412	1200
a12m300	→ 700
a12m200*	→ 20*
a094m412	1500
a094m300**	→ 250**
a094m200	50
a094m135	→ 40
a077m412	→ 1000
a077m300	→ 100
a077m200	→ 50
a064m412	→ 1100
a064m300	→ 700
a055m412	→ 100

*not yet finalised in tuning.

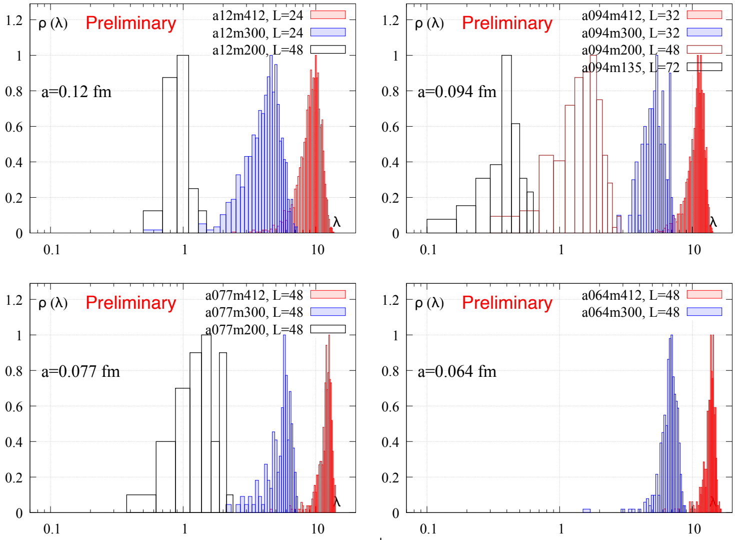
**a094m300: $m_\pi = 293 \rightarrow 307$ MeV

for better match on [a]-line.

Production plan overview:

Stage 1.: $SU(3)_F$ $(M_\pi = M_K = 412\text{MeV})$.
$\rightsquigarrow$ *Complete. Publication soon.*
Stage 2.: $M_\pi = 300\text{MeV}$ and 200MeV.
Stage 3.: $M_\pi = 135\text{MeV}$.

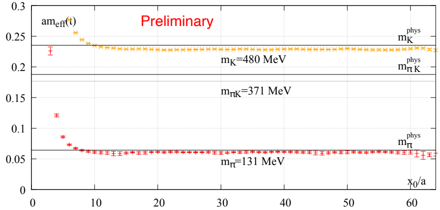
Gauge generation status - Lowest Dirac eigenvalue distributions

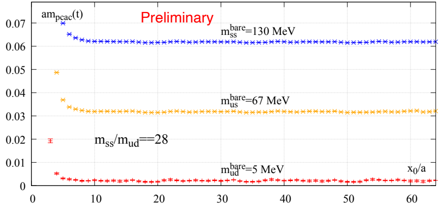


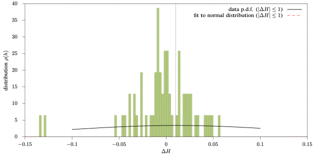
- Distribution of lowest Dirac EV $\rho(\lambda)$
- Dirac EV: $\lambda = \sqrt{D^\dagger D}$
- $\sqrt{8t_0} = 0.414(5)\ fm$ [1608.08900]

- Production = shaded (red, blue)
- Tuning / New = open (black, brown)
- Normalised to peak maximum

Updates I: Light and physical quark masses at $a = 0.094$ fm







New push towards $m_\pi = 135$ MeV:

- Deployed gathered experience from previous runs
- New thermalisation chain
- New volume: $L = 72$, $m_\pi L \simeq 4.6$
- $\rho(\lambda)$ gapped (previous slide)
- Reached:
  $\rightarrow m_{ss}/m_{ud} \simeq 28$
  $\rightarrow m_\pi \simeq 131$ MeV

More work ongoing

- MC chain very short
- More auxiliary measurements
- Sign of RWF particularly important

If all tests pass:
$\rightarrow$ Budgeted to gather 100 cfgs

Updates II: Renormalised f_π on $SU(3)_F$ line

Aside of introducing the SWF, in [2106.09080] we also demonstrated a different way to determine the **renormalized decay constant** f_π in

$$C_{PP} = \frac{GG_t}{m_\pi} e^{-m_\pi x_0} + \ldots \quad \text{and} \quad C_{AP} = \frac{f_\pi G_t}{m_\pi} e^{-m_\pi x_0} + \ldots$$

Idea: Determine the renormalization factors by probing chiral symmetry at positive flow time.

$\rightsquigarrow$ `Builds heavily on [1302.5246] and extended by Martin Lüscher.`

Observations:

- Renormalized decay constants are insensitive to improvement coefficient c_A
- Statistical errors for f_π small. (Z_{ren} sims = bare parameter sims)
- Decay constants seen to depend only mildly on $[a]$

Insensitivity to c_A:

- The PCAC relation forms the basis to compute f_π.
- At positive flow time t one needs to consider correlators, e.g. $\mathcal{O} = P$ in ud-case:

$$\mathcal{C}_P(t,d) = \sum_{x_0=y_0-d}^{y_0+d} \sum_{\vec{x}} \langle P(x) P_t(y) \rangle$$

where the dependence on d becomes negligible once excited states are suppressed.

Updates II: Renormalised f_π on $SU(3)_F$ line

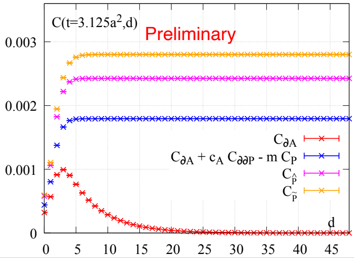
Insensitivity to c_A cont'd: PCAC relation in terms of flowed correlators is:

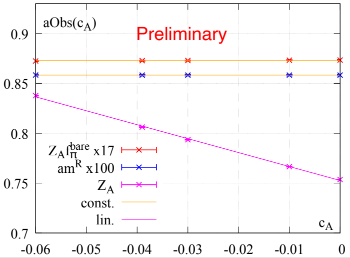
$$Z_A[\mathcal{C}_{\partial A} + c_A\, \mathcal{C}_{\partial\partial P} - m\, \mathcal{C}_P] - 2c_{fl}\mathcal{C}_{\hat{P}} = -(1 - Z_A \tilde{c}_P m)\mathcal{C}_{\tilde{P}}$$

- Comparing two flow times: $\frac{Z_A}{1-Z_A\tilde{c}_P m}$ and $\frac{c_{fl}}{1-Z_A\tilde{c}_P m}$ where $1 - Z_A\tilde{c}_P m \sim 1$.
- Key insight: The correlators are evaluated at large d. In particular in the limit $d \to \infty$ they are constant and $\mathcal{C}_{\partial A}$ and $\mathcal{C}_{\partial\partial P}$ are zero. $\Rightarrow$ **Explicit c_A vanishes.**
- There are still implicit dependences but in $f_\pi = Z_A f_\pi^{bare}$ these are $a^3 c_A m_\pi^2 G$ =small and in $m^R = Z_A m^{bare}$ they are removed.

  $\Rightarrow$ **f_π and m^R do not need a determination of c_A, but Z_A does.**

Examples on a094m412 (new statistics):

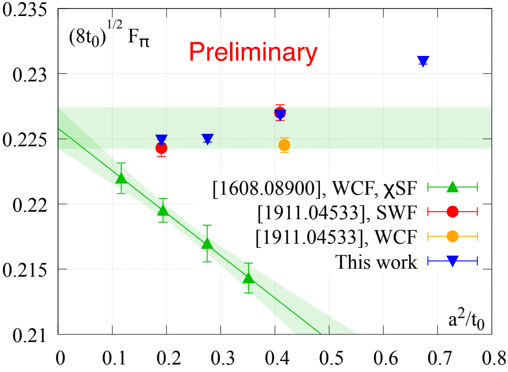




Updates II: Renormalised f_π on $SU(3)_F$ line

Updates for all $SU(3)_F$ ensembles:

- New addition of points at $a = 0.12$ and 0.077 fm.
- New statistics for $a = 0.094$ and 0.064 fm, $N \sim \mathcal{O}(10\, N_{old})$.
- Continuum limit: We follow a recipe where the flow times are fixed in physical units for all lattice spacings ($t_f \sim 0.38, 0.47$ and 0.56 fm).



- Compared to results from χSF by Bruno et al. (green)
- χSF continuum result (vertical green band)
- Previous SWF results (red), and WCF comparison (orange)
- New results (blue)

Coming soon:

- Continuum limit of f_π and m^R
- Z_A (needs c_A, either from SF or LANL method)

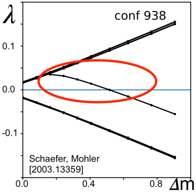
Updates III: RWF signs


Chiral symmetry breaking in Wilson fermions: Negative $\lambda(\hat{D})$ of the Dirac operator.

- $\Rightarrow$ RHMC: Assume the mass is large enough to avoid them.
- $\Rightarrow$ But: **negative** RWF sign observed in WCF configurations [2003.13359].

Diagnostic test:

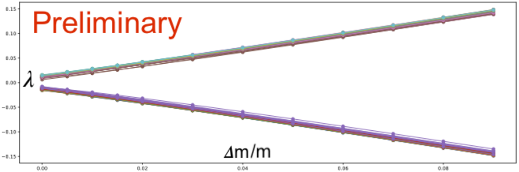
- Direct evaluation via $\lambda(\hat{D})$ not practical.
- Hermitian: $\hat{Q} = \gamma_5 \hat{D}$



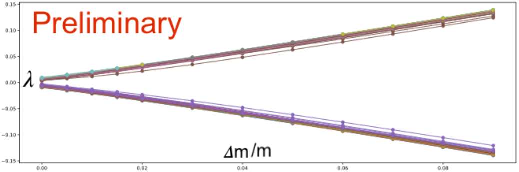
Recipe:

- $\Rightarrow$ pairs $\pm\lambda(\hat{Q})$ for $m =$large
- $\Rightarrow$ mismatch implies $-\lambda(\hat{D})$
- $\Rightarrow$ track $\lambda(\hat{Q})$ with $m_{valence}$, then 0-crossing implies negative real $\lambda(\hat{D}(m))$

Status in OpenLat ensembles



$a = 0.094$ fm, $m_\pi = m_K = 412$ MeV, $SU(3)_F$ point



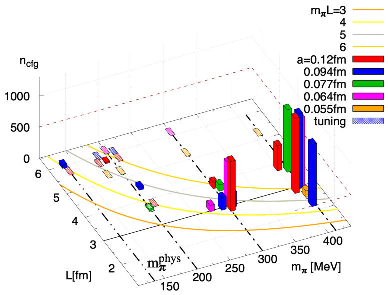
$a = 0.094$ fm, $m_\pi = 293, m_K = 454$ MeV

Summary - SWF in Action

SWF and OpenLat

- Benefits of SWF continue in production.
  - → Coarse and light parameter extension
  - → Stable generation after tuning
  - → Discretisation effects seem reduced
- Further research on the action ongoing.
  - → RWF signs
  - → Optimised run parameters
  - → Valence software (`Chroma`, `openQCD`)
- OpenLat as initiative to generate and provide ensembles for the community.
  - → Working on hosting and integration
  - → Publication of stage 1 very soon

Production update



Observables update

- First results at physical pion mass in $m_\pi L = 4.6$ volume. → Stable so far.
- Determination of f_π via gradient flow. → Advocate broader use of this method.
- Preliminary look at RWF signs. → No negative signs seen so far.

Thank you for your attention.