Details on Gauge Generation with Stabilized Wilson Fermions

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With OpenLat:
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OPEN LATtice initiative

Field Theory Research Team Seminar,
R-CCS, Kobe, 22.Jan.2024

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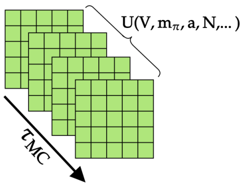
Lattice QCD as an engine to progress

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

Successes have been possible due to:

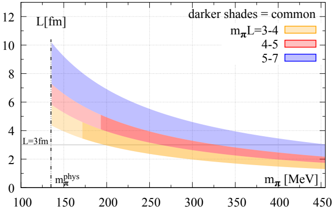
- Improved theoretical tools and understanding.
- Gauge configurations that enable controlled extrapolations for:
  - chiral / quark mass effects
  - finite size / volume effects
  - discretisation effects and continuum limit

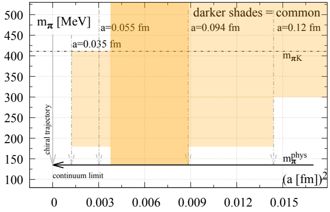


- Configurations generated via Markov Chain Monte Carlo:
  - Many samples to reduce *statistical uncertainties*
  - Long trajectories to control *auto-correlations*
- "*New physics*": With a good set of configurations more research areas open up.
- Not having ensembles is often the road-block. Need infrastructure (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 $\to$ autocorrelation explodes)
- Frozen topology induces $\propto Q/V$ contamination of observables.

$\rightsquigarrow$ 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.

$\Rightarrow$ Choose new, complementary, actions and algorithms.
$\Rightarrow$ Aim to benefit from (and be ready for) new developments.
$\Rightarrow$ 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

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

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

SWF toolkit implemented from `openQCD-2.0` onwards

A brief excursion into the details of stabilized Wilson fermions

SWF action and algorithms

A toolkit for more stability

SMD = stochastic molecular dynamics $\rightsquigarrow$ (algorithm between HMC and Langevin)

- Algorithmic improvements:
  - SMD decreases fluctuations and makes for a generally more stable run
  - SMD algorithm shows net gain in reduced autocorrelations at same cost
  - increase precision of internal numbers to quad
  - use supremum-norm to ensure minimum solve quality
- Fermion discretisation:
  - exponentiated Clover action
  - bound from below and guaranteed invertibility for Clover term
  - indication of scaling benefits (see further below)

These go on top of the measures already deployed:

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

$\rightsquigarrow$ Combine all for the best, i.e. most stable in our experience, results.

Note, that the eClover action preserves the PT-expansion, particularly important for renormalisation, and the change to the action is local only.

Three ingredients to improve stability of MD evolution:

1. Use the SMD

In usual HMC:

- ∘ possible jumps in phase space trajectory, e.g. from accumulated integration errors.
- ∘ re-thermalisation necessary, can lead to extended autocorrelation times.

Alternative approach: **stochastic molecular dynamics (SMD)**

*Horowitz et al. ('85, '86, '91), Jansen et al. ('95)

1.	Refresh $\pi(x,\mu)$ and $\phi(x)$ by a random field rotation:	$\pi \to c_1\pi + c_2 v$ $\phi \to c_1\phi + c_2 D^\dagger \eta$ (v and η normal distributed)
	$c_1^2 + c_2^2 = 1$, $c_1 = e^{-\epsilon\gamma}$, $\epsilon =$ MD integration time,	$\gamma =$ friction parameter
2.	short MD evolution	
3.	Accept/Reject-step	(algorithm exact)
4.	Repeat ↻	

- ∘ exact algorithm, coincides with HMC (for $\epsilon =$ fixed, $\gamma =$ large)
- ∘ shown to be ergodic for small ϵ
- ∘ effective reduction of unbounded energy violations $|\delta H| \gg 1$
- ∘ shorter autocorrelation times compensate longer time per MDU

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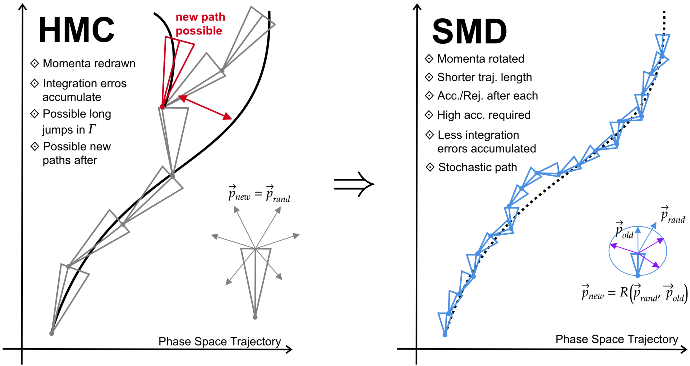


Three ingredients to improve stability of MD evolution:

2. Use a volume-independent norm for solver stopping criterion

$\|\eta - D\tilde{\psi}\|_2 \leq w\|\eta\|_2,$	$\|\eta\|_2 = \left(\sum_x (\eta(x), \eta(x))\right)^{1/2} \propto \sqrt{V}$
uniform norm:	$\|\eta\|_\infty = \sup_x \|\eta\|_2$, V-independent

- norm guarantees the quality of a given solve
- gives insurance against precision losses from local effects in large but also traditional volumes

3. Use quadruple precision in global sums

For the global accept/reject step $\delta H \propto \epsilon^P \sqrt{V}$. This can lead to accumulation errors for global sums. Quadruple precision remedies this

SWF action and algorithms - the eClover

Improve aspects of the fermion discretisation:
$\rightarrow$ This marks a departure from the standard WCF setup and defines a new action.

The Wilson-Clover action reads:

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

$\rightsquigarrow$ unbounded below $\qquad$ $\rightsquigarrow$ unbounded below

Typically one next classifies the lattice points as even/odd and writes the preconditioned form, $\hat{D} = D_{ee} - D_{eo}(D_{oo})^{-1}D_{oe}$ with diagonal part ($M_0 = 4 + m_0$):

$$D_{ee} + D_{oo} = M_0 + c_{SW}\frac{i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu} \quad .$$

Clover term can saturate $\|\frac{i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}\|_2 \leq 3$ while $c_{sw} \geq 1$ and rising with g_0^2.
$\rightarrow$ Dirac operator is not protected from arbitrarily small eigenvalues

Solution: Define a bounded-from-below Clover term

$$D_{ee} + D_{oo} = M_0 + c_{SW}\frac{i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu} \;\rightarrow\; M_0 \exp\Big[\frac{c_{SW}}{M_0}\frac{i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}\Big] \quad .$$

- local change of action
- valid in terms of Symanzik improvement
- guarantees invertibility of the Clover

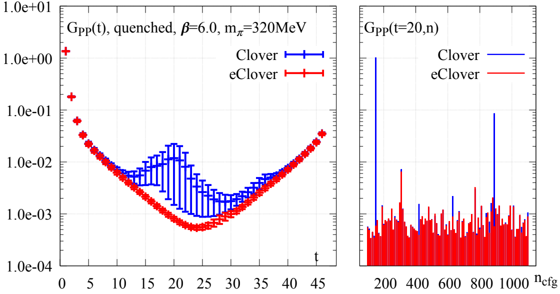
The eClover offers a new perspective on an old problem:

- In quenched QCD the absence of dynamical flavors increases the probability of an "exceptional" configuration
  - almost-zero mode in the (valence) Dirac operator encountered
  - leadas to extreme outliers affecting observables
  - highly anomalous behaviour in the correlation function observed

Around the beginning of the use of the WCF action it was observed that

- the introduction of the Clover term further increased this probability.
- it was never really understood why this is the case.

How is it now with the eClover?



Quenched demo:

- npt c_{SW} via tuning in SF
- cfg's: $\beta = 6.0$, $L = 48^4$
- $G_{PP}(t)$ tuned to $m_\pi = 320$MeV

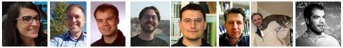
Measurement on identical cfg's using the same solver**.

**Only a selection of results here, it looks the same on smaller lattices and quark masses

In the **SWF action** we do not see the near-zero modes.

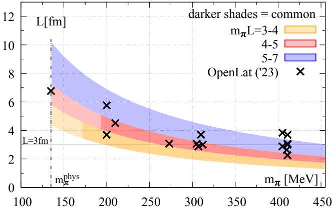
Back to the main topic

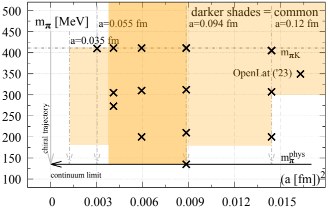
Open lattice initiative - Est. 2019



Lattice '21 - '23: [2312.11298], [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.`

SWF in action:

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

(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, see extra material.`

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

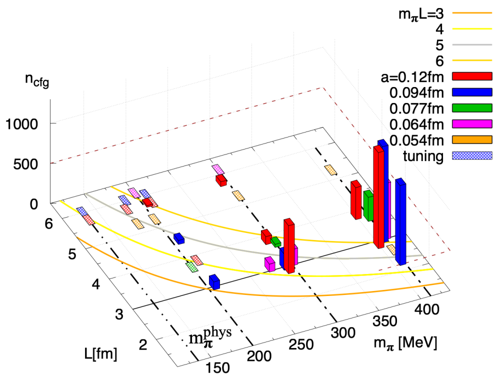
- Running allocation of **260 Mch** computing time*
- **22k configurations** generated, **40k** by end of 2024
- Total of **500 TB data** projected by end of 2024

*combined on several machines.

Configuration access

- No embargo time after publication. (500 cfgs min. goal)
- User access for unpublished configurations (case-by-case)
- Working on public hosting (JLDG? ILDG? NERSC?)

Gauge generation status - 2022



Main updates:

Ensemble	N_{conf}
a12m412	1200
a12m300	600
a12m200*	20*
a094m412	1500
a094m300**	300
a094m200	0
a094m135	20
a077m412	300
a077m300	100
a077m200	0
a064m412	600
a064m300	200
a055m412	100

*not yet finalised in tuning.

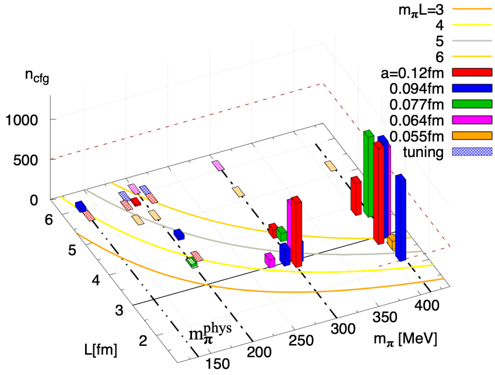
**a094m300: m_π = 293 $\rightarrow$ 307 MeV

for better match on [a]-line.

Production plan overview:

Stage 1.: $SU(3)_F$ ($M_\pi = M_K = 412$MeV).
Stage 2.: $M_\pi = 300$MeV and 200MeV.
Stage 3.: $M_\pi = 135$MeV.

Gauge generation status - 2023



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a094m300**	$\rightarrow$ 500
a094m200	$\rightarrow$ 100
a094m135	$\rightarrow$ 40
a077m412	$\rightarrow$ 1000
a077m300	$\rightarrow$ 500
a077m200	$\rightarrow$ 50
a064m412	$\rightarrow$ 1100
a064m300	$\rightarrow$ 700
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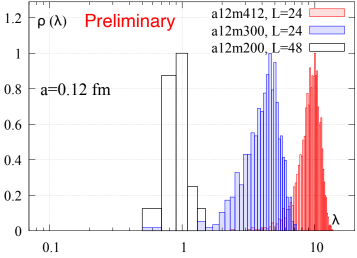
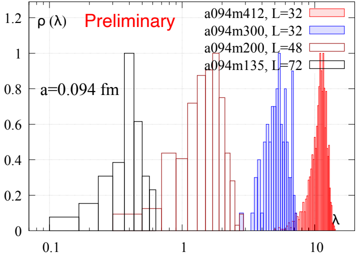
Production plan overview:

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

Publication of $SU(3)_F$ and $M_\pi = 300$MeV soon.

Gauge generation status - Lowest Dirac eigenvalue distributions I

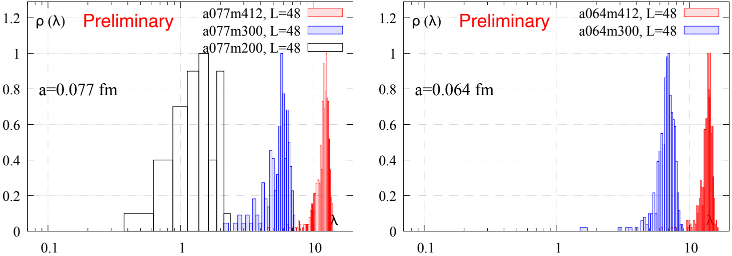




- Distribution of lowest Dirac EV $\rho(\lambda)$
- Dirac EV: $\lambda = \sqrt{D^\dagger D}$
- $\sqrt{8t_0} = 0.414(5)$ *fm* [1608.08900]

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

Gauge generation status - Lowest Dirac eigenvalue distributions II



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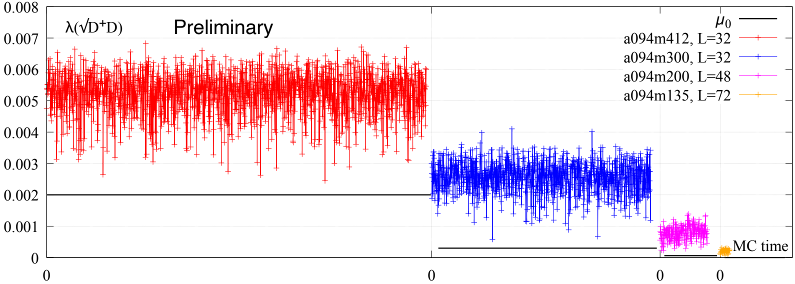
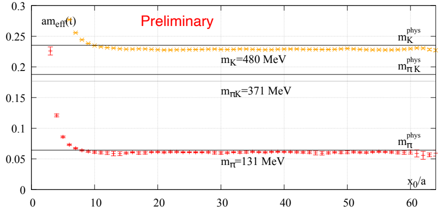
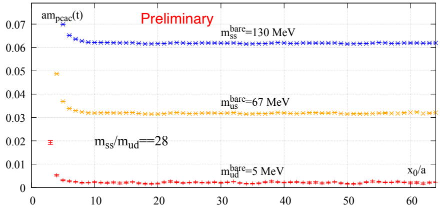


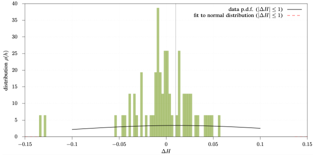
In the case of twisted mass reweighting:
An interesting auxiliary test is to compare the fluctuations of the lowest Dirac EV ($\lambda = \sqrt{D^\dagger D}$) with the lowest Hasenbush mass parameter μ_0.

- We observe best stability, if the fluctuations of λ stay above μ_0
- Otherwise: strong fluctuations in the reweighting factor observed.
- In certain cases it can make sense to set $\mu_0 = 0$ and to remove the twisted mass reweighting (esp. if μ_0 becomes much smaller than physically reasonable values).

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

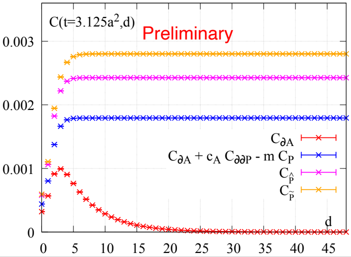
Insensitivity to c_A cont'd: PCAC relation in terms of flowed correlators is:

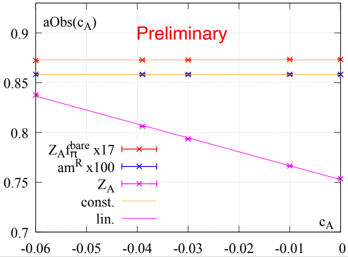
$$Z_A[\mathcal{C}_{\partial A} + c_A\,\mathcal{C}_{\partial\partial P} - m\,\mathcal{C}_P] - 2c_{fl}\mathcal{C}_{\hat{P}} = -(1 - Z_A\tilde{c}_P m)\mathcal{C}_{\tilde{P}}$$

- 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):

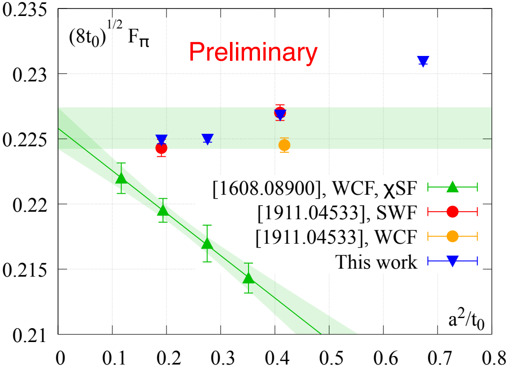




Updates II: Renormalised f_π on $SU(3)_F$ line

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)

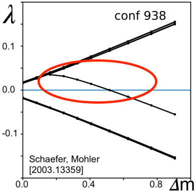
Updates III: RWF signs  

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:

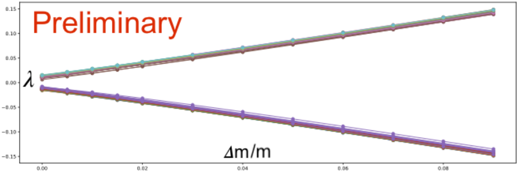
- Direct evaluation via $\lambda(\hat{D})$ not practical.
- Hermitian: $\hat{Q} = \gamma_5 \hat{D}$



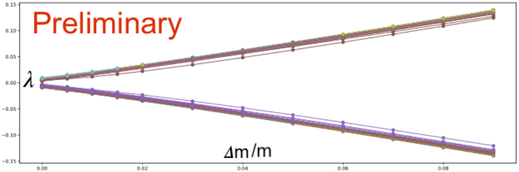
Recipe:

- $\Rightarrow$ 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



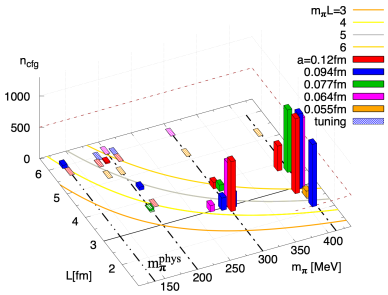
$a = 0.094$ fm, $m_\pi = 293, m_K = 454$ MeV

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.

Extra topic (outside of OpenLat):

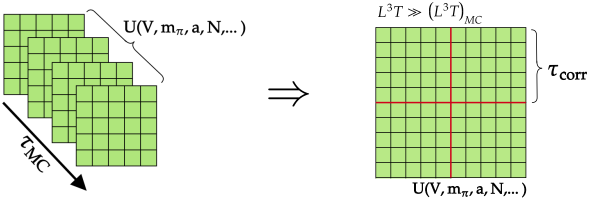
Circumventing topological contamination through stochastic locality

A special thanks to my long-term collaborators:
John Bulava, Mattia Bruno, Marco Cè, Patrick Fritzsch, Jeremy Green, Max Hansen, Martin Lüscher and Antonio Rago

A different way of looking at sampling

The SWF framework by definition does not help with the topological freezing problem.

But there is one path towards addressing this problem that has led to a new look at sampling:



Change our perspective of building $\langle ... \rangle$ via averages over MC time histories into one in which we understand the same process as a translational averaging over locally de-correlated regions $\langle\!\langle ... \rangle\!\rangle$: *arxiv[1707.09758]

$$\langle\!\langle O(x) \rangle\!\rangle = \frac{1}{V}\sum_z O(x+z), \quad \langle O(x) \rangle = \langle\!\langle O(x) \rangle\!\rangle + \mathcal{O}(V^{-1/2})$$

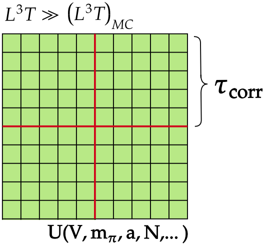
- *Extreme (N=1):* $\langle ... \rangle$ = averaging the local fluctuations in this one **master-field**.
- With large V the single value of Q becomes irrelevant as corrections are $\sim 1/V$ suppressed, while statistical uncertainties are $\sim 1/\sqrt{V}$.

⇝ arxiv[hep-lat/0302005], arxiv[0707.0396]

Stochastic locality

Translational averaging is possible due to stochastic locality.

⇝ M. Lüscher, EPJ Web Conf. 175 (2018) 01002 [1707.09758]



- QCD gauge-invariant local fields at large physical separations are stochastically independent.
- field distributions are the same everywhere (PBCs).
- due to the short-range interaction and mass gap.
- localisation range ∼ pion length scale $\mathcal{O}(m_\pi^{-1})$.

Towards generating master-fields

*P. Fritzsch, Lattice'22.

- $N_f = 2 + 1$ with $m_\pi = 270\text{MeV}$ and $m_K = 460\text{MeV}$

$\beta/a[\text{fm}]/\phi_4$	L	T	N_{cfg}	$m_\pi L$	$L[\text{fm}]$	cost (thermal.)(cfg.)
3.8/0.094/1.115	96	96	5	12.3	9.0	(3 + 0.2) Mch
	192	192	2	24.7	18.0	(45 + 9) Mch
4.0/0.064/1.117	144	144	-	12.6	9.2	(20 + 13) Mch

⇝ Generated using PRACE resources.

Hadronic observables - master-field errors and correlators

Translation average replaces the MC average and the variance becomes:

$$\sigma^2_{\langle\langle \bar{O}\rangle\rangle}(x) = \frac{1}{N}\sigma^2_{\langle\langle O\rangle\rangle}(x) = \frac{1}{V}\Big[\sum_{|y|\leq R}\langle\langle \bar{O}(y)\bar{O}(0)\rangle\rangle_c + \mathcal{O}(e^{-mR}) + \mathcal{O}(V^{-1/2})\Big]$$

In a hadron correlator, e.g. $G_{\Gamma_1\Gamma_2}(x,0) = [\bar{u}\Gamma_1 d](x)[\bar{d}\Gamma_2 u](0)$, the master-field error is given by the connected **four-point function**:

$$\Big\langle [\langle\langle G(x,0)\rangle\rangle \langle G(x,0)\rangle]^2 \Big\rangle \;=\; \frac{1}{V}\Big[\sum_{|y|\leq R}\langle\langle C(x{+}y,y)\, C(x,0)\rangle\rangle_c {+}\mathcal{O}(e^{-mR}){+}\mathcal{O}(V^{-1/2})\Big]$$

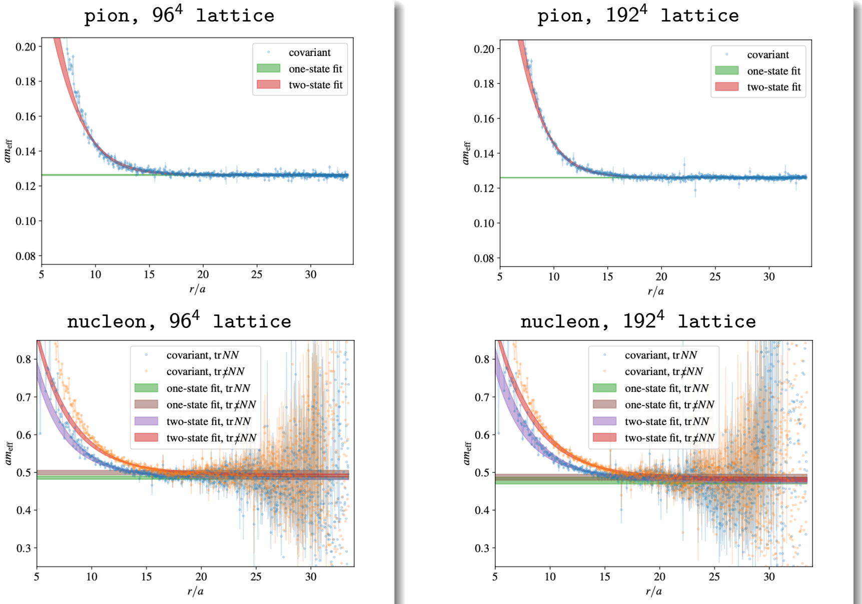
$\rightsquigarrow$ `y can be sampled and no all-to-all needed`

- Also works in TMR as $\tilde{C}(x_0,\vec{p}) = \sum_{\vec{x}} e^{-i\vec{p}\vec{x}} C(x,0)$. But: large footprint in space.
- Extract hadronic observables from *position-space correlators*?
- Would be more "in-line" with large volume, localisation idea too...
- Asymptotically:

$$C_{PP}(x) \to \frac{|c_P|^2}{4\pi^2}\frac{m_P^2}{|x|}\,K_1(m_P|x|)\;,\quad C_{NN}(x) \to \frac{|c_N|^2}{4\pi^2}\frac{m_N^2}{|x|}\,\Big[K_1(m_N|x|) + \frac{\cancel{x}}{|x|}K_2(m_N|x|)\Big]$$

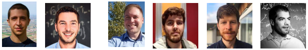
$\rightsquigarrow$ `Note: axis/off-axis directions have different cut-off effects`

- For many more details see: *JHEP 11 (2023) 167, [2307.15674]*

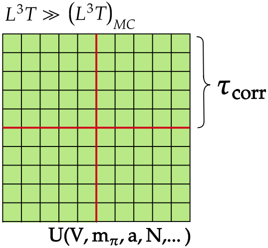


PoS LATTICE2022 (2023) 052, [2301.05156] , PoS LATTICE2021 (2022) 465, [2111.11544] , PoS LATTICE2021 (2022) 383, [2110.15375]

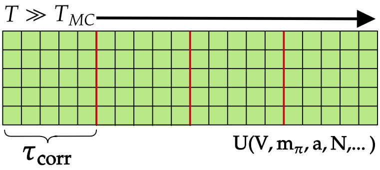
The long-T approach



PoS LATTICE2022 (2023) 368, [2212.09533]



$\Rightarrow$



A variation of the idea: The MF regime is reached through scaling the volume, this is true in particular also via

$$L = L_{trad}\,,\; T \gg T_{trad} \rightarrow \text{long-T approach}$$

Motivations:

- In MF position space very attractive - but not optimal for all observables.
- For example in spectroscopy, we commonly exploit and use as tools:
  - sparseness of the spectrum, finite volume formalism where ideally $m_\pi L \in [4:6]$
  - translation invariance for boosting statistics, small volumes for EV evaluation

$\rightarrow$ `especially important for distillation`

MF regime is reached through scaling the volume, this is true in particular also via

$$L = L_{trad},\, T \gg T_{trad} \to \text{long-T approach}$$

Can it be reached also in practice? Can it be used to study topology freezing effects?

Generating long-T configurations

*on Irene Jolliot Curie of TPCC

β/a[fm]/ϕ_4	L	T	N_{cfg}	BC's	$\bar{Q}$	$V_{rel} = \frac{V}{V_{96}}$
4.1/0.055/1.17	48	96	488	P	1.3(2)	1
		384	101	P	3.0(5)	4
		1152	94	P	-8(1)	12
		2304	38	P	-50(1)	24
		2304	36	P	-12(2)	24
$\to$		96	495	O	-1.0(3)*	1

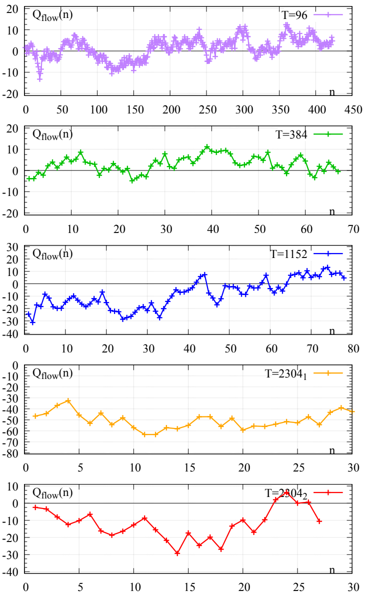
$\rightsquigarrow$ definition of $\bar{Q}$ with OBC's not clean

- SU(3) flavor symmetric point, $m_\pi = m_K = 418\,\text{MeV}$ (a bit off 412 MeV target)
- Lattice spacing $a = 0.055$fm exhibited significant slowing down of topological tunnelling in tuning runs

*unpublished, part of arxiv[1911.04533]

- To reach long T's we use an upfolding strategy with aperiodic extensions.
- $T = 2304$: 2 strings with different $\bar{Q}$ through different seed configuration upfolding.

Observations during generation - topological charge



- One key observable during generation is the topological charge:

$$Q = \sum_V q(x)$$

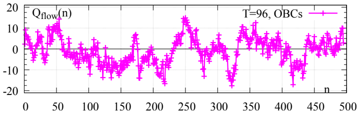
$$q(x) = -\frac{1}{32\pi^2}\epsilon_{\mu\nu\rho\sigma}\mathrm{Tr}[F_{\mu\nu}(x)F_{\rho\sigma}(x)]$$

$\rightarrow$ evaluated at pos. flow time $t_{flow} = 1.3t_0$

*arxiv[1006.4518]

- We see:
  - Slow evolution over MC time*
  - Still, not completely frozen
  - Thermalization effects?

*local decorrelation visually observed (see appendix)

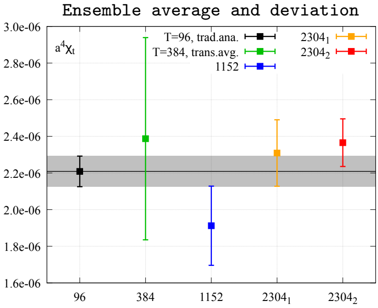


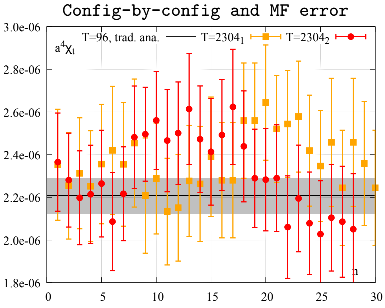
*definition of Q with OBC's not clean, shown for completeness

Effective translational averages - topological susceptibility

*following arxiv[1707.09758]

$$\chi_t := \frac{\langle Q^2 \rangle}{V} = \sum_y \langle q(y)q(0)\rangle = \sum_{|y|\leq R} \langle\langle q(y)q(0)\rangle\rangle + \sum_{|y|>R} \langle q(y)q(0)\rangle + \mathcal{O}(V^{-1/2})$$





⇝ $T = 96$: Traditional analysis (not using TMR method)
⇝ $T > 96$: Translation averages and errors following MF prescription

At T=2304 we see indications that:

- each configuration gives the same topological susceptibility (MF errors)
- the result is the same irrespective of global topological charge (MF defrosting)
- T is long enough to suppress topo. contamination below the level of the error.

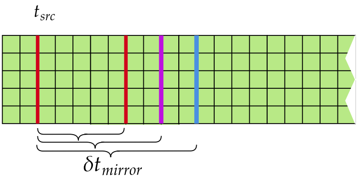
Long-T hadrons - meson correlation functions

- Calculation of hadron correlators, e.g. mesons

$$G_{\mathcal{O}_1\mathcal{O}_2}(t = t' - t_{\rm src}) = \sum_x \langle \mathcal{O}_2(x, t')\mathcal{O}_1(x_{\rm src}, t_{\rm src})\rangle \ ,$$

where: $\mathcal{O}_i = \bar{\psi}\Gamma_i\psi$ and $\Gamma = \gamma_5, \mathbf{1}$. Only connected channels. Shorthand: $\mathcal{O}_1 - \mathcal{O}_2 \hat{=} G_{\mathcal{O}_1\mathcal{O}_2}(t)$.

  - $U(1)$ noise wall sources
  - $N_{mirror} = T/\delta t_{mirror}$ sources per cfg per solve
  - sources spread with δt_{mirror} starting from t_{src}
  - δt_{mirror} varied but only $\delta t_{mirror} = 96$ shown
  - t_{src} =randomly varied to suppress correlations



- In OBC, two setups:
  - sources close to boundary, $t_{src} = 1, T - 1$
  - sources in the central region, $t_{src} = T/4, T3/4$

Source	$m_\pi = m_K$	T	$N_{src} * N_{noise}$	δt_{mirror}
$U(1)$ wall	418 MeV	96	$48_{t=rnd}$	-
	$\kappa = 0.137945$	384	$48_{t=rnd}$	96
	$a = 0.055$fm	1152	$48_{t=rnd}$	64/96/128
		2304_1	$48_{t=rnd}$	96
		2304_2	$48_{t=rnd}$	64/96/128/192
		$96^{boundary}_{obc}$	$12_{t=1,95}$	-
		$96^{central}_{obc}$	$12_{t=24,72}$	-

$\rightsquigarrow$ here only $\delta t_{mirror} = 96$ results will be shown.

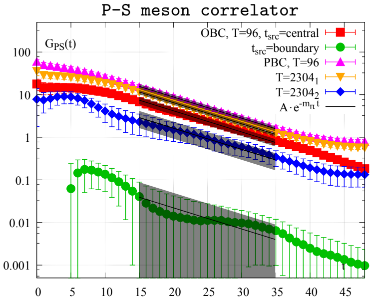
Defrosting - isovector mesons as sensitive probe

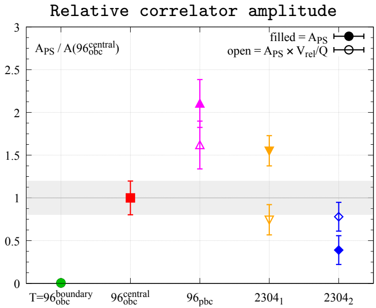
*arxiv[0707.0396] and arxiv[1406.5449]

- **In QCD:** The parity-odd $P - S$ correlator is zero (stochastically)
- **Also:** The parity-even $S - S$ correlator at long distance creates/annihilates a pion at LO (inserting Q^2) $\rightsquigarrow$ like in the η'

$\Rightarrow$ In case of topological contamination the $P - S$ correlator obtains *non-zero signal*:

$$G_{PS}(t) \sim A_{PS} \cdot \exp[-m_\pi t] \quad \rightarrow \quad \text{the amplitude scales as } A_{PS} \sim Q/V$$





- ○ $P - S$ correlator visibly affected by topological freezing effects. Even with OBC.
- ○ Long-T results show suppression, competitive with central OBC results.

Summary - SWF in Action

SWF and OpenLat

- First production level SWF studies continue to show benefits.
- Further research to study the action ongoing.
- OpenLat as initiative to generate and provide ensembles for research.
- Indications that the parameter window can be extended to coarser+lighter regime with acceptable discretisation effects and stable generation.

Master-field simulations

- A different way to look at sampling. Potentially circumvents topology freezing.
- First dedicated studies ongoing. Methods being worked out.
- Requires a careful re-evaluation of what it means to determine an uncertainty.

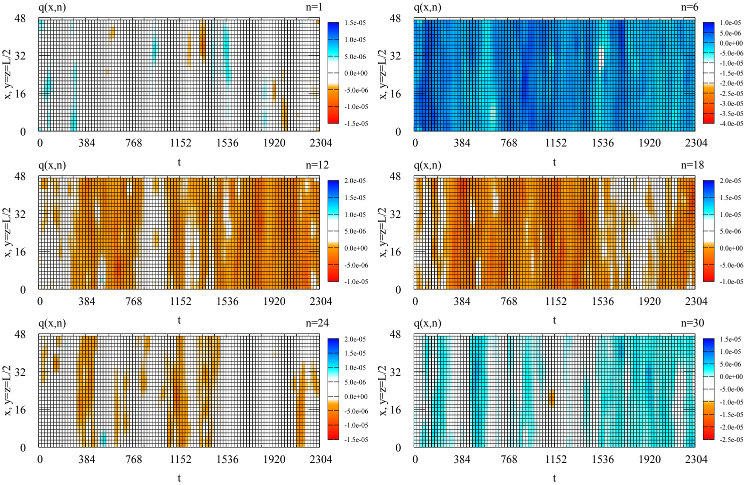
Long-T simulations

- A master-field variation. Want to understand topology freezing for a potential way to "defrost" observables.
- First results indicate translational averaging can be made effective.
- Can be made competitive with other methods to handle topology freezing.

Thank you for your attention.

Further material

Visualisation of thermalisation through topological charge density



- Locally topological charge is evolving
- Correlations in SMD time in line with autocorrelation analysis

Extra highlight: Spectral reconstruction and inverse problems

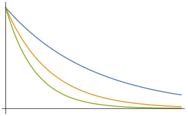
Extractable from an **Euclidean expectation value** by solving an **inverse problem**

⇝ see plenaries by John Bulava, Kadir Utku Can, Francesca Cuteri, Takashi Kaneko, Joe Karpie at Lattice'22

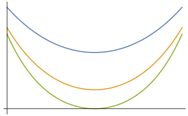
- $N \to N'$ hadronic scattering amplitude at any $s = E_{\text{cm}}^2$
  $(\pi\pi \to \pi\pi, \;\; N\pi \to N\pi\pi, \;\; \pi\pi \to \pi\pi\pi\pi)$
- $N + j \to N'$ transitions at any s
  $(K \to \pi\pi, \quad D \to \pi\pi, K\overline{K}, \quad \gamma \to \pi\pi, \quad B \to K^* \to K\pi)$
- Non-local matrix elements
  (R-ratio, hadronic tensor, **inclusive decay rates**, $D\overline{D}$ mixing)
- Distribution functions
  (PDFs, distribution amplitudes, TMDs)
- Finite-temperature observables
  (transport coefficients, viscosity, thermal broadening effects)

$$\boxed{G_{\mathrm{E}}(\tau) = \int_0^\infty d\omega \, \rho(\omega) \, K(\omega, \tau)}$$

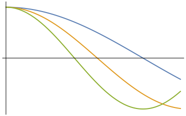
The specific set-up will modify the kernel entering the inverse problem



Zero-temperature quantities:
$K(\omega, \tau) = e^{-\omega\tau}$



Nonzero-temperature:
$K(\omega, \tau) = \frac{\cosh(\omega(\beta/2 - \tau))}{\sinh(\omega\beta/2)}$



qPDFs:
$K(\nu, x) = \cos(\nu x)\, \Theta(1 - x)$

Setting expectations - an ill-posed problem

Three conditions for a well-posed problem:

- Existence
- Uniqueness
- Stability (solution behavior changes continuosly with the initial conditions)

$\rightsquigarrow$ J. Hadamard

The problems we consider fail in the sense of 3 and are thus **ill-posed**.

This is a problem due to **discrete sampling + finite precision**.

Many methods attempt the task

- Frequentist: Model fits
- Bayesian: MEM, BR, SAI, ...
- Linear: BGM, Chebychev, HLT, ...
- Non-linear: Machine Learning

Limitation: Lack of precision, data points, systematic control, ...
$\rightsquigarrow$ In general: constraints and information

No method objectively better!

A bird's eye view

All methods can be understood as a master function

$$\mathcal{F}[\mathbf{G}, \mathbf{C}_G] = \left(\boldsymbol{\rho}, \mathbf{C}_\rho \right)$$

where

- $\mathbf{G}$ = discrete samples of $G(\tau)$
- $\mathbf{C}_G$ = covariance of $\mathbf{G}$
- $\boldsymbol{\rho}$ = discrete estimator of $\rho(\omega)$
- $\mathbf{C}_\rho$ = covariance of $\boldsymbol{\rho}$

Challenges

- For $\boldsymbol{\rho}_i = \rho(\omega_i)$

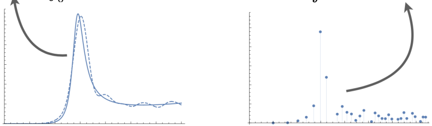
$$\left| \mathcal{F}[\mathbf{G} + \delta\mathbf{G}, \mathbf{C}_G + \delta\mathbf{C}_G] - \mathcal{F}[\mathbf{G}, \mathbf{C}_G] \right|$$

  and thus $\left|\mathbf{C}_\rho\right|$ explode.
- For cases where $|\mathbf{C}_\rho|$ is under control, relation between $\rho(\omega) \Leftrightarrow \boldsymbol{\rho}$ may be obscured.

Spectral estimators - embracing the smearing

Role of the discrete spatial volume

$$\widehat{\rho}_L(\bar{\omega}) \equiv \int_0^\infty d\omega\, \widehat{\delta}_\Delta(\bar{\omega},\omega)\, \rho_L(\omega) \qquad G_L(\tau) = \int d\omega\, e^{-\omega\tau}\, \rho_L(\omega)$$



Do not want $\rho_L(\omega)$ but rather the **smeared estimator** $\widehat{\rho}_L(\bar{\omega})$ with $1/L \ll \Delta \ll \mu_{\text{physical}}$.

At the same time: Resolution $\widehat{\delta}_\Delta$ will satisfy $1/L \ll \Delta$, provided $\delta G(\tau)_{L-\text{effects}} \ll \delta G(\tau)_{\text{statistical}}$

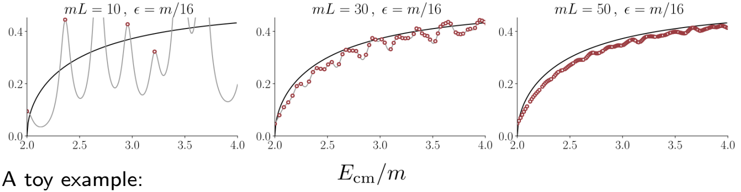
With a smeared estimator $\widehat{\rho}_L(\bar{\omega})$

- $L \to \infty$ limit of $\widehat{\rho}(\bar{\omega}, \Delta, L)$ is well defined.
- Of $\rho(\omega, L)$ it is not!
- One can retrieve the infinite volume spf through the double limit:

$$\rho(\bar{\omega}) = \lim_{\Delta \to 0} \lim_{L \to \infty} \widehat{\rho}(\bar{\omega}, \Delta, L)$$

⇝ [Hansen, Meyer, Robaina ('17)]

⇝ see plenary by John Bulava, Lattice '22

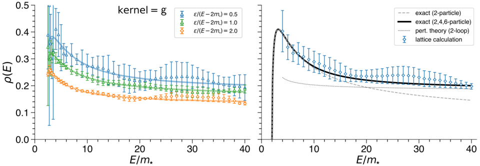


A toy example:

- Free/continuous spectral function
- Large volume/control over L-effects crucial

Towards the R-ratio - a new frontier

Another toy example: $2d$ $O(3)$-linear sigma model

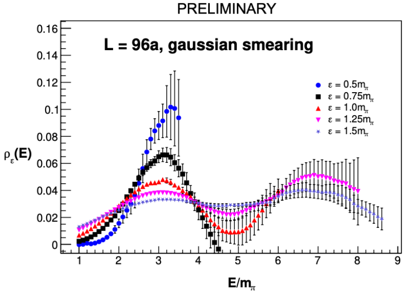


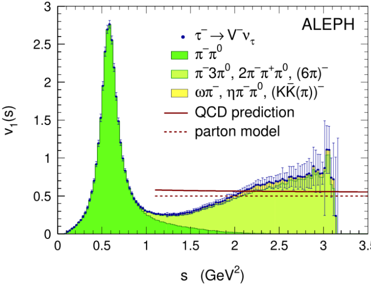
$\Rightarrow$ Accurate spectral reconstruction seems possible!

Becoming realistic: The R-ratio

- R-ratio is a key experimental quantity
- Large volume/control over L-effects crucial
- Our attempt: Use Masterfield QCD ensembles

$\rightsquigarrow$ see plenaries by John Bulava, Patrick Fritzsch and parallel by Marco Cè (all coll. AF), Lattice '22





$\Rightarrow$ First results look promising!