Stabilised Wilson Fermions in Action

- An overview of recent developments

Anthony Francis

Challenges and opportunities in
Lattice QCD simulations and related fields
RIKEN R-CCS workshop

Kobe, Japan, 17.02.2023

陽明交大物理研究所
NYCU Institute of Physics

OPEN LATtice initiative

Lattice QCD for HEP - non-perturbative precision inputs

(Next-gen) experiments continue to probe nature with higher and higher precision

- Tensions with SM at few-σ level
- Understanding QCD uncertainties is key
- Lattice provides tool towards QCD without approximations

Lattice community is ...

- entering a new precision era for simple systems and "standard" observales (e.g. α_s and **decay constants**).
- tackling more complicated systems with heightened confidence (e.g. **resonances** and **exotic hadrons**)
- expanding towards reliable results for **(inclusive) decay rates** and **nuclear matrix elements**.

Lattice QCD can provide input for

Input	Program
HVP and HLBL, Resonances	
Decay Constants, Form Factors, CKM Parameters, Exotic Hadrons	
Parton Distribution Functions	
Nucleon Matrix Elements, TMDs, Multi-Nucleons	
Neutrino-Nucleus Int., DM-nucleus/-on Int. and more ...	...

In the following:

- Focus on technical work for the next level of precision
- Status updates up to Lattice'22

Disclaimer: Will not talk about physics results per se.

Lattice QCD - ab initio approach using supercomputers

Discretise QCD on space-time grid

- Lagrangian approach
- Consistent at all energies
- Euclidean signature ($t \to it$)
- Efficient parallelisation

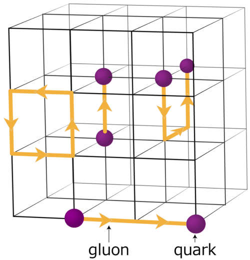


figure from: P. Shanahan, '18

Spectrum from Euclidean correlation functions

$$G_{\mathcal{O}_1\mathcal{O}_2}(t) = \langle \mathcal{O}_1 \mathcal{O}_2^\dagger \rangle \overset{e.g.}{=} \langle 0 | \bar{q}\Gamma q' \; (\bar{q}\Gamma q')^\dagger | 0 \rangle$$
$$\text{or} \quad \langle \pi | \bar{q}\Gamma q \; \bar{q}'\Gamma q' | \pi \rangle$$

$$\textbf{(1.)} \rightsquigarrow \sum_i \frac{\langle 0|\mathcal{O}_1|n\rangle\langle n|\mathcal{O}_2|0\rangle}{2m_i} e^{-m_i t}$$

- $t \gg$: $m_i = m_0$, $f_i \simeq \langle 0|\mathcal{O}_i|n\rangle$
- interpolating operator GEVP for multiple m_i
- F.Vol. quantisation for scattering phase shifts

$$\textbf{(2.)} \rightsquigarrow \int d\omega \rho(\omega) K(\omega, t) \;, \rho(\omega) \overset{e.g.}{=} \textit{R-ratio}$$

- *inverse transform:* (numerically) ill-posed

Connection to physics

- renormalisation Z_{NP}
- chiral/phys.point limit $m_\pi \to m_{\text{phys}}$
- volume limit $L \to \infty$
- continuum limit $a \to 0$

$\Longrightarrow$

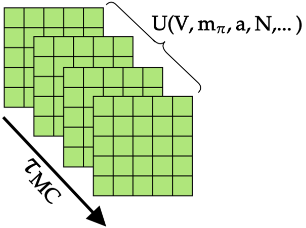
Systematic effects to control

- cut-off $\mathcal{O}(a, a^2)$
- heavy quarks $\mathcal{O}(aM_Q)$
- finite volume effects $\mathcal{O}(m_\pi L)$

Gauge field configurations - the engine to progress

Successes have been possible due to:

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



- Generating configurations is done via Markov-Chain Monte Carlo:
  - *Samples are checkpoints* in the MC time history of the Markov-Chain
  - Number of samples affects the *uncertainty* of observables (statistics error)
  - Observables are correlated and **autocorrelations** have to be controlled

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

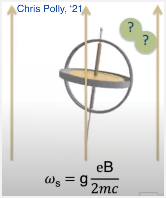
Ensembles dictate research we can and cannot do

- "New physics": With a good set of configurations more research areas open up.
- Indeed: Often not having the required ensembles is the main road-block.

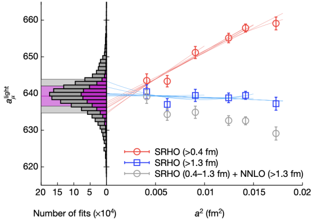
An impactful example - the anomalous magnetic moment of the muon

The g-factor: muon spin precesses around an external $\vec{B}$ field. The strength of this magnetic moment is $\vec{\mu} = g\frac{e}{2m}\vec{S}$ (class.mech.: $g = 1$, quant.mech.: $g = 2$ [Dirac])

- $a_\mu = \frac{g-2}{2}$ is sensitive to all particle interactions
- Precision measurements make further particle interactions visible. **SM test and probe for new physics!**
- **Today:** 4.2σ discrepancy between a_μ exp. vs. pheno.



- In `Nature 593 (2021)` the BMW collaboration published a lattice result for the hadronic (=most uncertain) contribution a_μ^{HLO} whose accuracy rivals that of current phenomenological estimates.



Success has been possible due to:

- Improved theoretical tools, notably the TMR and bounding methods `[Bernecker, Meyer ('11); AF et al. ('13); Feng et al. ('13)], [Lehner ('16); Borsyani et al. ('17)]`
- BMW has gathered a large set of *(staggered)* configurations at physical quark masses, with large volumes and many lattice spacings.

With a good set of configurations precision becomes accessible.

- **g-2:** Example where continuum limit is (now) the main difficulty
- **Spacing window:** Commonly $0.05 \lesssim a \lesssim 0.15$fm (some exceptions, but not many)
- **Solution:** Generate and make available more ensembles at finer lattice spacings and at physical quark masses. $\rightsquigarrow$ Revitalisation of the ILDG, see plenary by Frithjof Karsch, Lattice'22

But:

(1.) Discretisation effects:

Continuum extrapolation of actions not always clear. Higher order terms important! $\rightsquigarrow$ see plenary by Nikolai Husung, Lattice'22

(2.) Stability issues:

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

- Often addressed by smearing in the action. However: Not a silver bullet.

$\rightsquigarrow$ see parallel by Andreas Rish, Lattice'22

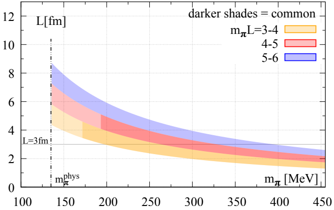
- Possible extra discretisation effects from dominating length scale of observable.

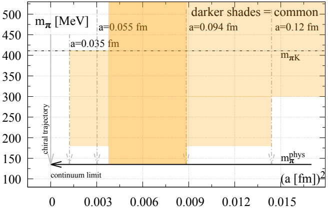
(3.) Critical slowing down:

$\tau_Q \uparrow$ increases such that updating becomes unrealistic.

- As $[a] \downarrow$ the tunneling probability to a new topological sector drops. The topology freezes and induces $\sim Q/V$ contamination of observables!

Simulation bounds - accessible parameter window





- 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)
- Algorithmic bound on lightest m_π at given [a]. (Coarse [a] = hard to go light)
- "Topology" bound on finest [a].
  (Topology freezes $\to$ autocorrelation explodes, esp. important for cont.lim)

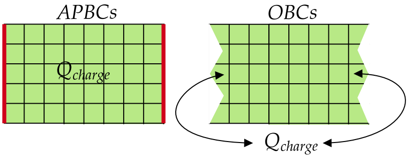
$\rightsquigarrow$ some dependence on action for these statements.

Conceptual research in algorithms intensified - especially for topological freezing

- ML for gauge generation? Trivialising map? $\rightsquigarrow$ see this Workshop, esp. Nobuyuki Matsumoto
- Metadynamics? Modify detailed balance? $\rightsquigarrow$ see e.g. Joao Pinto Barros, Lattice'22
- Master-field simulations? Defrosting through ultra-cold, long-T lattices?

Topology freezing - simulations with open boundary conditions

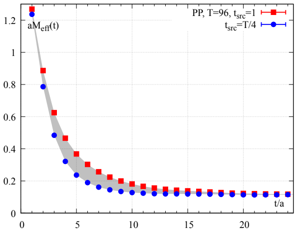
Open boundary conditions in time are one way to approach topology freezing:



1. Replace anti-periodic boundary conditions in time
2. Topology can now flow in/out in the T-direction
3. But: Boundary effects affect measurements

Price: loss of **time translation invariance** (and $T > 0$ sims plus clear definition of Q)

Example: Boundary effects in the pion



- In principle, OBC's solve the freezing problem.
- In practice, measurements only in the central region.
- There topology evolves more slowly and some observables can still be affected. (will see one later on)

At the same time:

- Calculations in hadron spectroscopy rely (heavily) on translational invariance to increase statistical precision.
- Losing translational invariance can seem a high price.

(especially on the analysis side for some obs.)

One continued motivation: Find solutions without losing time translation invariance.

Stabilised Wilson Fermions

Anthony

Francis

Patrick

Fritzsch

Martin

Lüscher

Antonio

Rago

Comput.Phys.Commun. 255 (2020) 107355, [2106.09080]

Wilson-Clover fermions - an attractive setup with its drawbacks

- Wilson-Clover fermions are popular in the community
  $\rightsquigarrow$ @Lattice'21: $\mathcal{O}(120)$ WCF, $\mathcal{O}(70)$ STG, $\mathcal{O}(40)$ DWF, $\mathcal{O}(20)$ TMW - [dynamical]

- They are conceptually clear, with many advanced methods available, relatively cheap, and pose little restrictions on what observables can be computed.
- Together with a rigorous improvement program they can also be made $O(a^2)$.

There are also some drawbacks:

- without automatic $O(a)$ improvement observables often
  - require finer a or extra investment to implement improvement
  - have to deal with autocorrelations in gauge generation (as others).
    $\rightsquigarrow$ topology freezing problems
- without chiral symmetry the lowest DEV is not protected
  - exceptionally low values possible
  - problem especially when a=coarse or m_π=light or L_V=small

- in general for all actions errors can accumulate during gauge generation
  - large fluctuations have the potential to increase autocorrelation times
  - precision losses possible through global volume sums and integration errors

Action and algorithms - a toolkit for more stability

Stabilised Wilson fermions (SWF)

AF, Fritzsch, Lüscher, Rago ('19)

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)

SWF toolkit implemented from `openQCD-2.0` onwards

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 SWF preserve the PT-expansion, particularly important for renormalisation, and the change to the action is local only.

Actions and algorithms - algorithmic ingredients of SWF

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

Actions and algorithms - algorithmic ingredients of SWF

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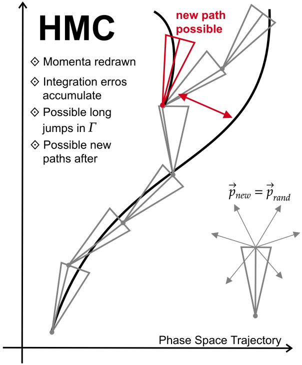
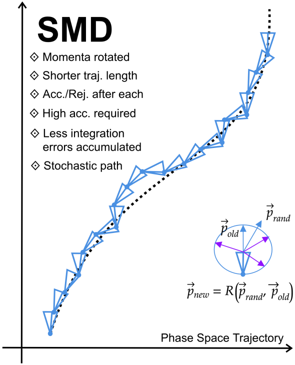


$\Longrightarrow$



Actions and algorithms - algorithmic ingredients of SWF

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

Actions and algorithms - action ingredient of SWF

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:

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

$\rightsquigarrow$ unbounded below $\quad\quad$ $\rightsquigarrow$ 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

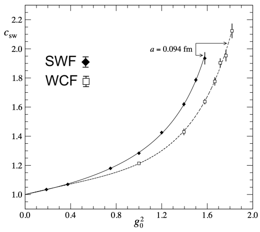
Solution: Define a bounded-from-below Clover term

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

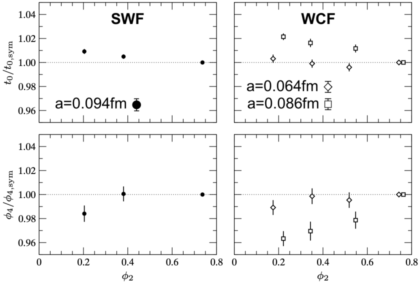
- local change of action
- valid in terms of Symanzik improvement
- guarantees invertibility of the Clover

SWF simulations - the initial, dynamical results

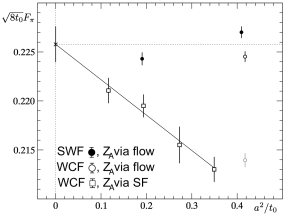
NP tuned c_{SW} (in SF)



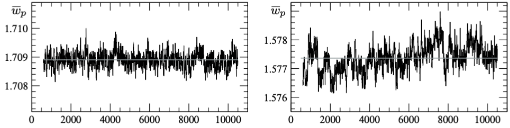
Chiral scaling at fixed a



f_π scaling in a



plaquette (energy density) with SMD: $a = 0.095\,\mathrm{fm}$



exp. clover (A_1) std. clover (X_1)

Observed smoother fluctuations and smaller discretisation effects

SWF and OpenLat

Francesca Cuteri

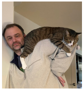
Anthony Francis

Patrick Fritzsch

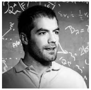
Giovanni Pederiva

Antonio Rago

Andrea Shindler



André Walker-Loud



Savvas Zafeiropoulos

PoS LATTICE2022 (2023) 074, [2212.11048]

PoS LATTICE2022 (2023) 203, [2212.10138]

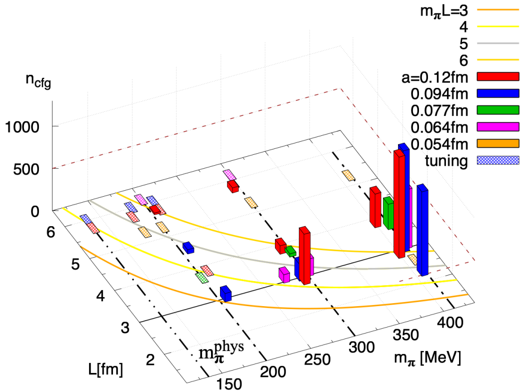
PoS LATTICE2022 (2023) 426, [2212.07314]

PoS LATTICE2021 (2022) 118, [2201.03874]

Initial successes - prompted us to do more ...

OPEN LATtice initiative

Our aim is to generate state-of-the-art QCD gauge ensembles for physics applications and to share them with the community to strengthen open science.
Policies and info: `https://openlat1.gitlab.io`



- ⇝ Phase 1: 500+ configurations at $SU(3)_F$ points. Status: complete.
- ⇝ Phase 2: add $m_\pi = 300,\ 200$ MeV. Status: production.
- ⇝ Phase 3: add $m_\pi = 145$ MeV. Status: tuning.

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.
- The total reweighting factor fluctuations are mild, and ideally below 5%.
- The SMD step distance $\delta\tau$ maximises the backtracking period.
- The distribution of δH matches the one set by the acceptance rate.
- The distribution of the lowest $\sqrt{D^\dagger D}$ eigenvalue is well-behaved & gapped.
- The distribution of the lower and upper bounds of the spectral gap for the strange quark 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.
- The distribution of the flowed topological charge is symmetric around zero with no signs of metastability.

Current resources and repository

- Running allocation of **300 Mch** computing time*
- **22k configurations** generated, **40k** by end of 2023
- Total of **500 TB data** projected by end of 2023

*on Tier-0 machines in US and EU.

SWF related talks at Lattice'22

*AF; *John Bulava; *Giovanni Pederiva, *Rocco Francesco Basta, *Justus Kuhlmann, *Marco Cè, *Jeremy Green, *Fabian Joswig, *Patrick Fritzsch

Encouraging results - OpenLat and user projects

Publication plan:

1. Each completed phase is accompanied by a reference publication.
2. All configurations and metadata are made openly available. (OpenLat and ILDG)
3. No further embargo time.

- Users may obtain access to the configurations of ongoing stages.
- User-access is granted on a case-by-case basis.

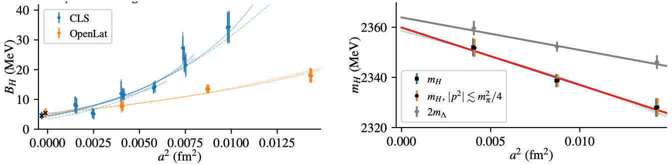
Current user projects: multi-nucleons (BaSc), nEDM, $T > 0$, hadronic decays (EDI)

$\rightarrow$ Simple and complex observable results becoming available at the same time.

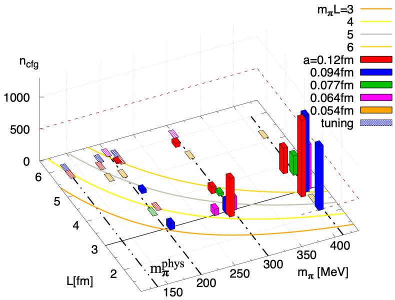
Example: Ab initio nuclear physics ⇝ J. Green and A. Nicholson (for BaSc, coll. AF), Lattice'22

- *H*-**dibaryon** at $SU(3)_F$ point continuum limits with two actions - CLS and OpenLat
- Paving the way for ab initio nuclear physics inputs. ⇝ btw: no indication of deeply bound *uuddss*.

⇝ also: not all projects need physical pions to have an impact.



$\rightarrow$ SWF continue to show benefits!



Status overview

- SWF show signs of better behaved discretisation effects.
- SWF designed with more stable/safe generation in mind:
  $\rightarrow$ remedy large-volume pathologies
  $\rightarrow$ choose algorithm that better controls "spikes"
- Expanded parameter window:
  $\rightarrow$ up to $a = 0.1$ fm with $m_\pi = 300$ MeV for WCF(!) (also: first hints at 200 MeV)
- User projects:
  $\rightarrow$ Simple and complicated observable results being presented already

But what about going to finer [a] and topology freezing?

Stochastic locality and master-field simulations

John Bulava

Mattia Bruno

Marco Cé

Anthony Francis

Patrick Fritzsch

Jeremy Green

Max Hansen

Martin Lüscher

Antonio Rago

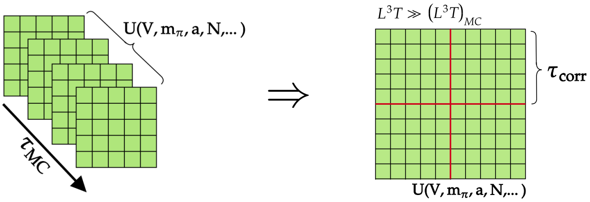
PoS LATTICE2022 (2023) 052, [2301.05156]

PoS LATTICE2021 (2022) 465, [2111.11544]

PoS LATTICE2021 (2022) 383, [2110.15375]

Master-field simulations - a different way of looking at sampling

Among other ideas to address the topological freezing problem, one path has led to a new look at sampling:



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

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

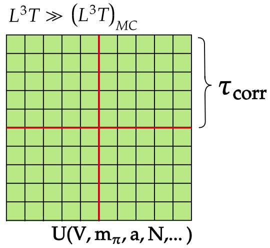
- *Extreme (N=1):* $\langle \ldots \rangle$ = averaging the local fluctuations in this one **master-field**.
- With large V the single value of Q becomes irrelevant as corrections are $\sim 1/V$ suppressed, while statistical uncertainties are $\sim 1/\sqrt{V}$.

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

Stochastic locality - a feature of QCD

Translational averaging is possible due to stochastic locality.

⤳ M. Luscher, 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 $\sim$ pion length scale $\mathcal{O}(m_\pi^{-1})$.

Towards generating master-fields

*P. Fritzsch, Lattice'22.

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

β/a[fm]/ϕ_4	L	T	N_{cfg}	$m_\pi L$	L[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**:

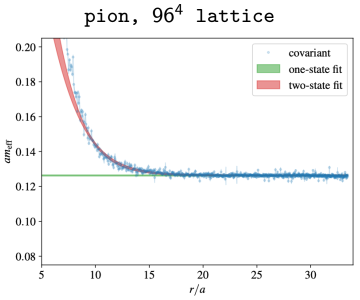
$$\Big\langle[\langle\langle G(x,0)\rangle\rangle\langle G(x,0)\rangle]^2\Big\rangle \; = \; \frac{1}{V}\Big[\sum_{|y|\leq R}\langle\langle C(x+y,y)\,C(x,0)\rangle\rangle_c+\mathcal{O}(e^{-mR})+\mathcal{O}(V^{-1/2})\Big]$$

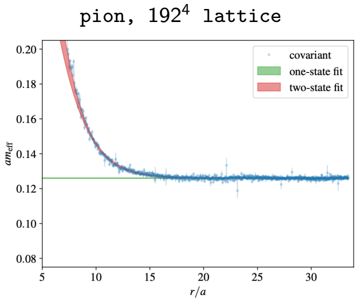
$\rightsquigarrow$ y can be sampled and no all-to-all needed

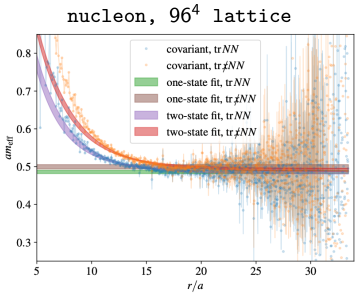
- Also works in TMR as $\tilde{C}(x_0,\vec{p}) = \sum_{\vec{x}} e^{-i\vec{p}\vec{x}}C(x,0)$. But: large footprint in space.
- Extract hadronic observables from *position-space correlators*?
- Would be more "in-line" with large volume, localisation idea too...
- Asymptotically:

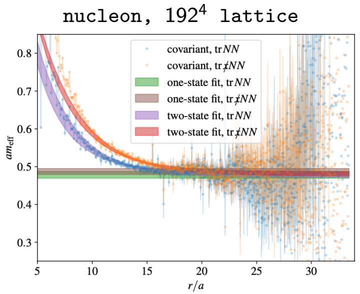
$$C_{PP}(x) \to \frac{|c_P|^2}{4\pi^2}\frac{m_P^2}{|x|}K_1(m_P|x|)\,, \quad C_{NN}(x) \to \frac{|c_N|^2}{4\pi^2}\frac{m_N^2}{|x|}\Big[K_1(m_N|x|) + \frac{\cancel{x}}{|x|}K_2(m_N|x|)\Big]$$

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


pion, 96^4 lattice
covariant
one-state fit
two-state fit
am_{eff}
r/a


pion, 192^4 lattice
covariant
one-state fit
two-state fit
am_{eff}
r/a


nucleon, 96^4 lattice
covariant, tr NN
covariant, tr $\not{t}NN$
one-state fit, tr NN
one-state fit, tr $\not{t}NN$
two-state fit, tr NN
two-state fit, tr $\not{t}NN$
am_{eff}
r/a


nucleon, 192^4 lattice
covariant, tr NN
covariant, tr $\not{t}NN$
one-state fit, tr NN
one-state fit, tr $\not{t}NN$
two-state fit, tr NN
two-state fit, tr $\not{t}NN$
am_{eff}
r/a

Stochastic locality and the long-T approach

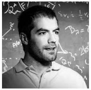
Mattia Bruno

Marco Cé

Anthony Francis

Jeremy Green

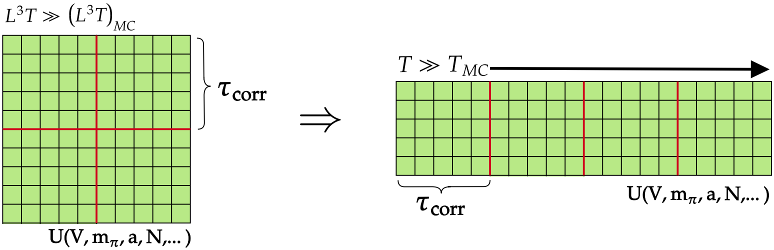
Max Hansen



Savvas Zafeiropoulos

PoS LATTICE2022 (2023) 368, [2212.09533]

The long-T approach - a master-field variation



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`

long-T approach: aims to get the best of both worlds and to open a way towards finer a[fm] without giving up on current, advanced, spectroscopy methods.

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

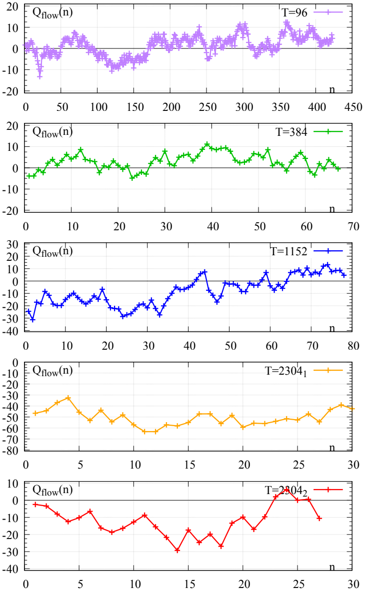
*on Irene Jolliot Curie of TPCC

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:

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

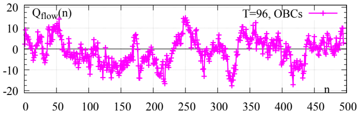
$$q(x) = -\frac{1}{32\pi^2}\epsilon_{\mu\nu\rho\sigma}\mathrm{Tr}[F_{\mu\nu}(x)F_{\rho\sigma}(x)]$$

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

*arxiv[1006.4518]

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

*local decorrelation visually observed (see appendix)

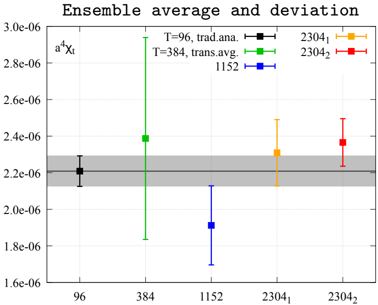


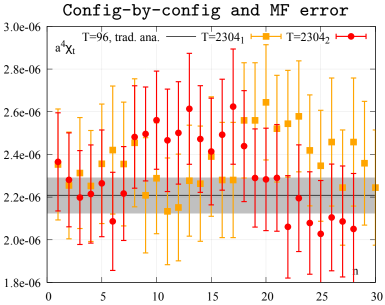
*definition of Q with OBC's not clean, shown for completeness

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.

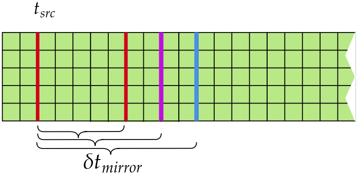
Long-T hadrons - meson correlation functions

- Calculation of hadron correlators, e.g. mesons

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

where: $\mathcal{O}_i = \bar{\psi}\Gamma_i\psi$ and $\Gamma = \gamma_5, 1$. 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.

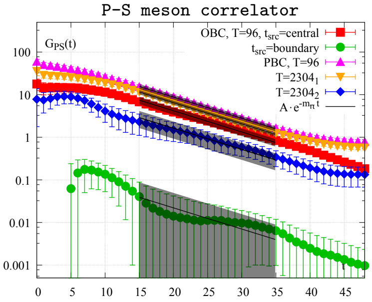
Defrosting - isovector mesons as sensitive probe

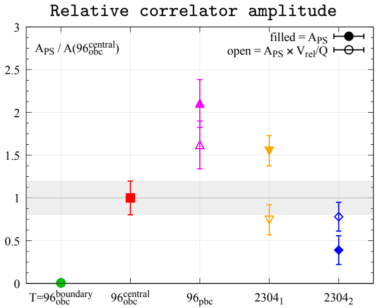
*arxiv[0707.0396] and arxiv[1406.5449]

- **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.

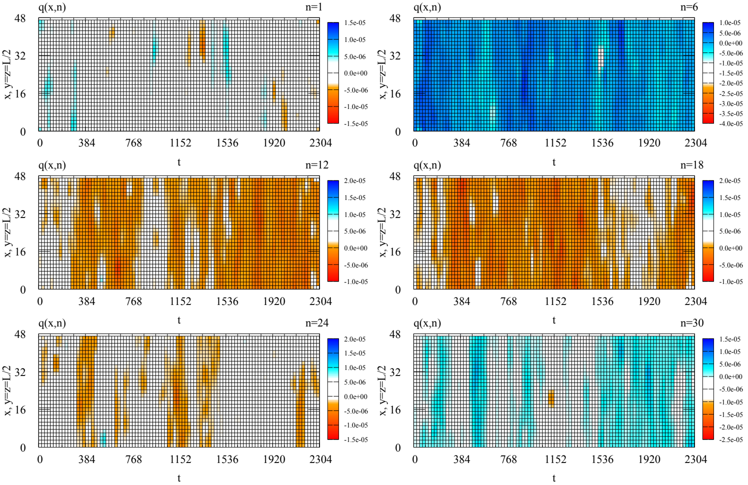
Long-T simulations

- 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

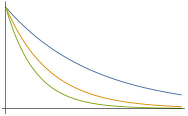
Extractable from an **Euclidean expectation value** by solving an **inverse problem**

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

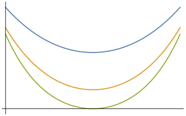
- $N \to N'$ hadronic scattering amplitude at any $s = E_{\rm cm}^2$
  ($\pi\pi \to \pi\pi$, $N\pi \to N\pi\pi$, $\pi\pi \to \pi\pi\pi\pi$)
- $N + j \to N'$ transitions at any s
  ($K \to \pi\pi$, $D \to \pi\pi, K\overline{K}$, $\gamma \to \pi\pi$, $B \to K^* \to K\pi$)
- Non-local matrix elements
  (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)

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

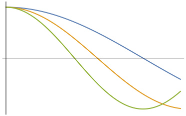
The specific set-up will modify the kernel entering the inverse problem



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

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

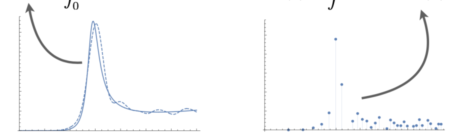
  and thus $\left|\mathbf{C}_\rho\right|$ explode.

- 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 $\delta G(\tau)_{L-\text{effects}} \ll \delta G(\tau)_{\text{statistical}}$

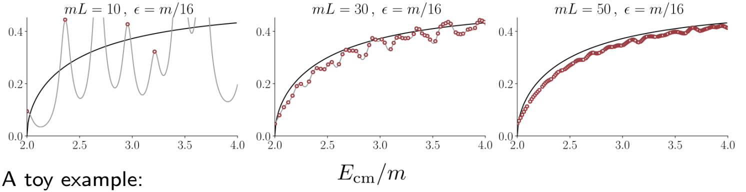
With a smeared estimator $\widehat{\rho}_L(\bar{\omega})$

- $L \to \infty$ 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

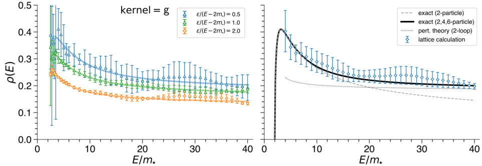


A toy example:

- 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

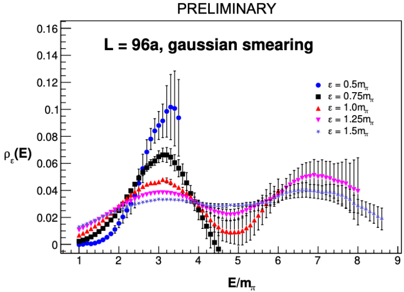


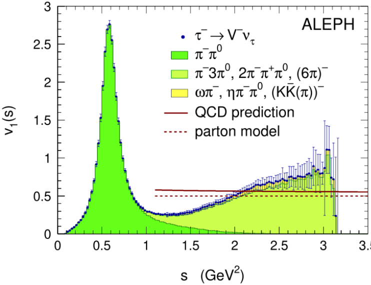
$\Rightarrow$ Accurate spectral reconstruction seems possible!

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!