Translating topological benefits in very cold master-field simulations

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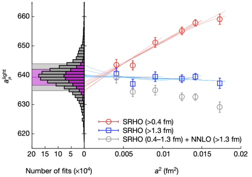
Preliminary

Precision lattice simulations

- Lattice QCD is entering a new precision era. And, the results are impacting in some of the most interesting areas of particle physics.
- One example among many: the BMW result on a_μ^{HLO} with an accuracy that rivals current phenomenological estimates.

Nature 593 (2021)



Successes like this have been possible due to:

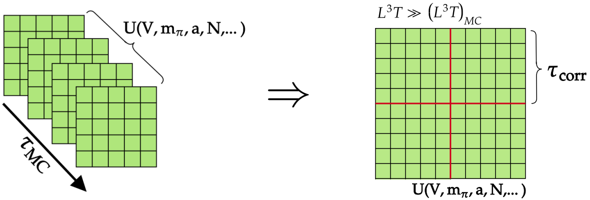
- Improved theoretical tools. TMR+bounding,arxiv[1107.4388, 1306.2532, 1305.5878, 1512.09054, 1612.02364]
- Gauge configurations that enable controlled extrapolations and error estimates for:
  - chiral / quark mass effects
  - finite size / volume effects
  - discretisation effects and continuum limit

With a good set of configurations precision becomes accessible.

- **g-2:** Example where continuum limit is (now) the main difficulty
- **Spacing window:** Commonly $0.06 \lesssim a \lesssim 0.15$fm (some exceptions, but not many)
- **Solution:** Generate more ensembles especially at finer lattice spacings
- **But:** As $\downarrow a$ the tunneling probability to a new topological sector drops.
  $\Rightarrow$ topology freezes, inducing $\sim Q/V$ contamination of observables.
- **Critical slowing down:** $\uparrow \tau_Q$ increases to a level that generating an update becomes unrealistic. (In addition to larger V for $L \gtrsim 3$fm and $m_\pi L \geq 4$)

A new way of looking at sampling: Master-field simulations

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]

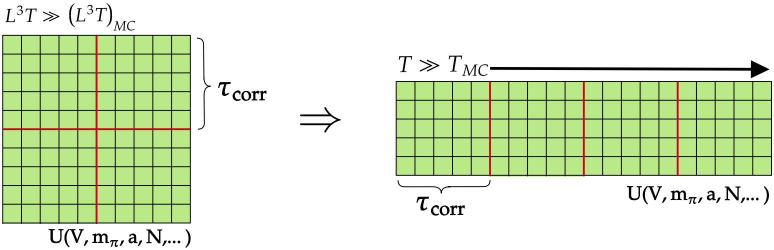
$$\langle\!\langle O(x) \rangle\!\rangle = \frac{1}{V}\sum_z O(x+z), \quad \langle O(x) \rangle = \langle\!\langle O(x) \rangle\!\rangle + \mathcal{O}(V^{-1/2})$$

- **Extreme (N=1):** $\langle \ldots \rangle$ = averaging the local fluctuations in this one master-field.
- The single value of Q becomes irrelevant as corrections are $\sim 1/V$ suppressed - provided the volume is large enough.
- Uses the result that corrections due to topology typically go as

$$\sim \frac{Q}{L^3 T}$$

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

A master-field variation: the long-T approach



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 always optimal for some obs.

*Marco Cè, Thu. 11.08., 11:50; *John Bulava, Tue. 9.08., 9:20

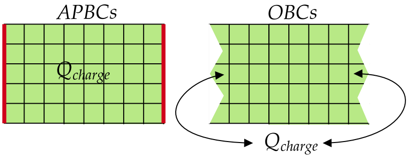
- For spectroscopy, we commonly exploit and use as tools:
  - sparseness of the spectrum, finite volume formalism where ideally $m_\pi L \in [4:6]$
  - translation invariance for boosting statistics, small volumes for EV evaluation

$\rightarrow$ 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.

Excursion: Simulations with open boundary conditions

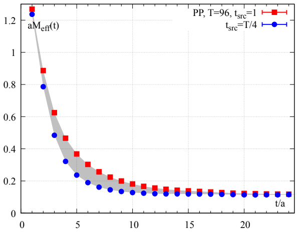
Open boundary conditions in time elegantly solve the topology freezing problem.



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)

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 more motivation: Find paths without losing time translation invariance.

Towards the first long-T master-fields

- Configurations are generated using Stabilized Wilson Fermions *arxiv[1911.04533]
  $\rightarrow$ SMD update algorithm, supremum norm, quad precision arithmetic, ...
  $\rightarrow$ exponentiated Clover action
- SWF make simulations safe for very large volumes. *Patrick Fritzsch, Sat. 13.08., 9:20
  $\rightarrow$ non-invertibility of Clover term is avoided (pathology in WCF)
- To reach long T's we use an upfolding strategy with aperiodic extensions.

Generated configurations

*generated 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
$\rightarrow$		96	495	O	-1.0(3)*	1

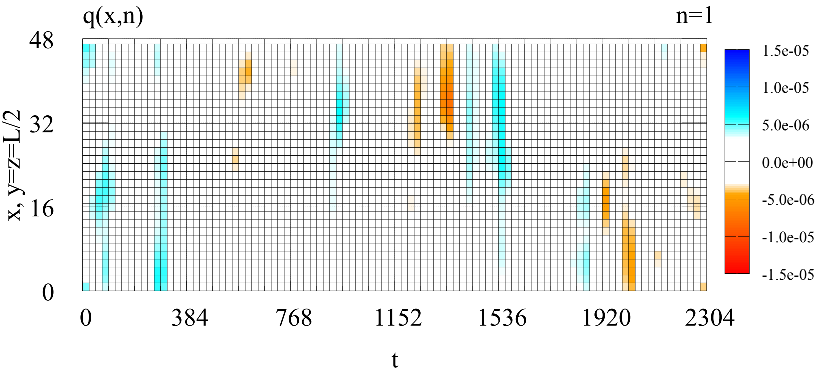
$\rightsquigarrow$ definition of $\bar{Q}$ with OBC's not clean

- SU(3) flavor symmetric point, $\phi_4 = 1.115 \rightsquigarrow m_\pi = m_K = 412$MeV
- Lattice spacing $a = 0.055$fm exhibited significant slowing down of topological tunneling in tuning runs *unpublished, part of arxiv[1911.04533]
- $T = 2304$: 2 strings with different $\bar{Q}$ through different seed configuration upfolding.

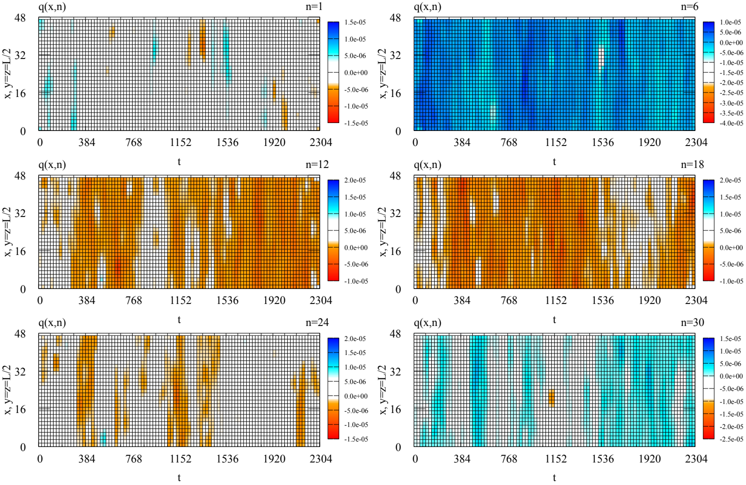
Visualisation of thermalisation through topological charge density

⇝ animation, might have to skip to next slide

- Effective thermalisation is a key question in MF type simulations.
  → First, we check the evolution of the (local) topological charge density $q(x)$
  → Here just a rough look, a quantitative study is left for the future

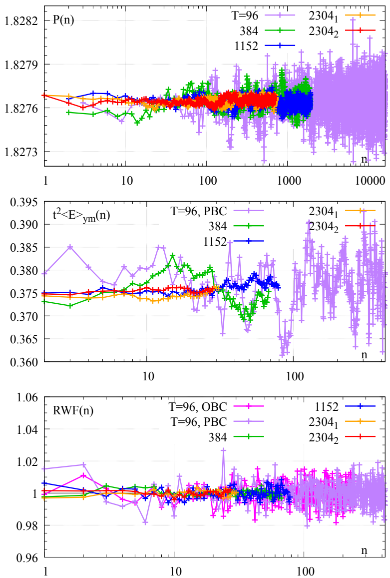


Visualisation of thermalisation through topological charge density



- No obvious thermalisation effects
- Locally topological charge is evolving
- Correlations in SMD time in line with autocorrelation analysis (⇝ next slide)

Plaquette, action and RWF histories



⇝ $log(x)$ axis for legibility, opening spread is optical effect

Further run tests and info:

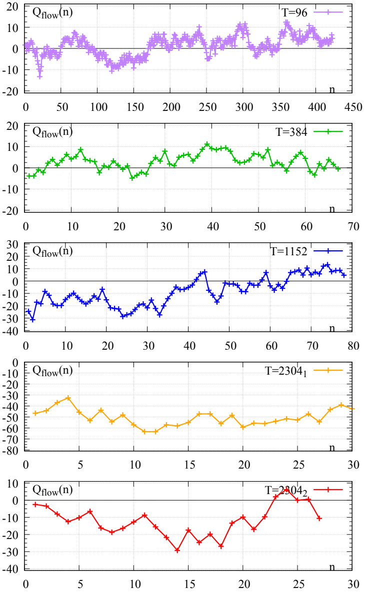
- Reweighting well behaved within 3%
- Expected distribution in δH, no outliers
- Zolotarev spectral ranges well respected
- Pole number gives high quality approx
- (So far) generation was unremarkable

Observed autocorrelation times

T	τ_Q	τ_E
96	11.1(4.1)	4.7(1.7)
384	2.7(1.3)	3.7(1.8)
1152	3.6(1.6)	3.0(1.4)
2304_1	1.6(1.0)	2.0(1.3)
2304_2	1.5(1.0)	2.5(1.0)
96_{obc}	7.1(2.6)*	3.3(1.2)*

⇝ Caveat: MC strings not long

Topological charge



- One key observable during generation is the topological charge:

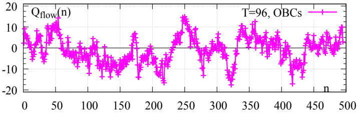
$$Q = \sum_V q(x)$$

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

$\rightarrow$ 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
  - Fixed topology simulations in future?



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

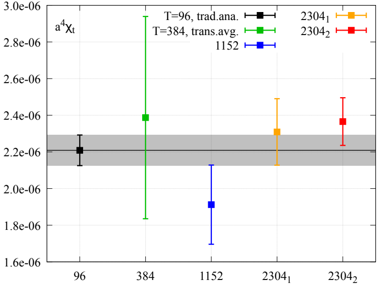
Topological susceptibility

*we follow arxiv[1707.09758]

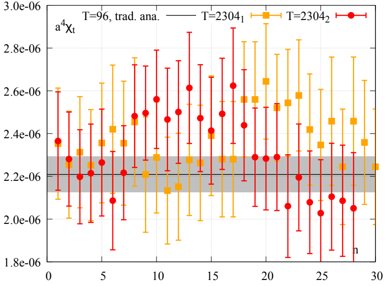
$$\chi_t = \sum_{|y| \leq R} \langle q(y) q(0) \rangle + \delta(R) = \sum_{|y| \leq R} \langle\!\langle q(y) q(0) \rangle\!\rangle + \sum_{|y| > R} \langle q(y) q(0) \rangle + \mathcal{O}(V^{-1/2})$$

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

Ensemble average and deviation



Config-by-config and MF error



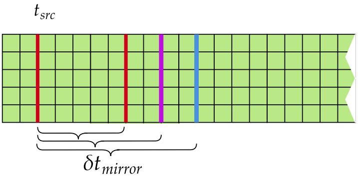
At T=2304 we see indications that:

- ◦ each configuration gives the same topological susceptibility (MF errors)
- ◦ the result is the same irrespective of global topological charge (MF defrosting)

→ Other lattices unclear, more work ongoing

Defrosting meson correlation functions

- Calculation of hadron correlators:
  - $U(1)$ 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.

Isovector meson correlators as sensitive probe

*arxiv[0707.0396] and arxiv[1406.5449]

- **Note:** The $P-S$ correlator should be zero (stochastically)
- **But:** At leading order the insertion of Q^2 into the $S-S$ correlator at long distance creates/annihilates a pion $\rightsquigarrow$ like in the η'

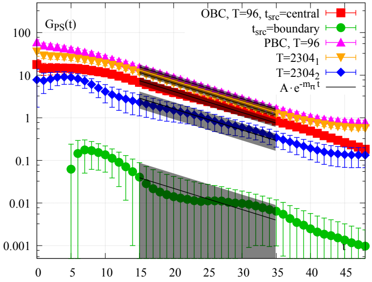
$\Rightarrow$ In case of contamination the P-S correlator obtains *non-zero signal* that behaves as:

$$G_{PS}(t) \sim A_{PS} \cdot \exp[-m_\pi t]$$

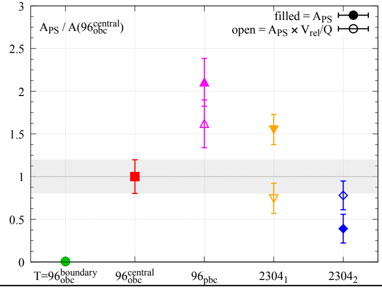
$\rightarrow$ the amplitude scales as $A_{PS} \sim Q/V$

- ○ Can be checked by comparing A_{PS} in traditional and long-T simulations
- ○ Naively, factor relative to reference lattice can be cancelled out $A_{PS} \cdot V_{rel}/\bar{Q}$

P-S meson correlator

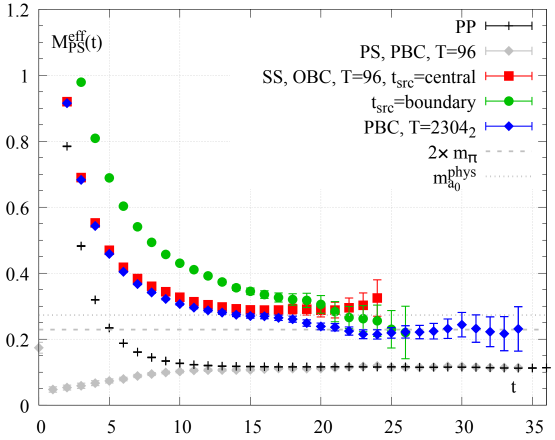


Relative correlator amplitude



Isovector meson correlators as sensitive probe

Effective masses



A variation of the master-field approach

- Continuum limit (and thus topological freezing) is becoming a main systematic.
- MF approach gives new ways of looking at both.
- Combinations of translational and MC time averages can be a powerful tool.
- Long-T variation could be a way towards finer a[fm] without losing time trans.inv.

Generating long-T, "defrosted", ensembles

- Upfolding strategy followed, no obvious signs of thermalisation contamination.
- Indications of MF behaviour in χ_t for $T = 2304$, i.e. $V/V_{trad} = 24$.

Topologically sensitive observables

- Isovector meson correlators are particularly sensitive to topological effects.
- P-S contamination visible, also in OBC study with sources in central region.
- Indication of effective A_{PS} topo suppression in $T = 2304$.

Outlook

- Work has only just begun, many open questions to tackle. Some next steps:
  - Study thermalisation (combine with multiscale equilibration).
  - Combine hadronic measurements with fermion factorisation algorithm?
  - Work out formal aspects. Length scales criterion for "runners" to decide T?
  - Simulations at lower a[fm] (or at fixed topology) for further investigations?

Thank you for your attention.