Hadronic observables from master-field simulations

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master-fields: motivation

with state-of-the-art supercomputers and algorithms, we can generate gauge field configurations with

[Lüscher Lattice 2017, Francis, Fritzsch, Lüscher, Rago 2020; plenary talk by P. Fritzsch on Saturday]

- 192^4 lattice points • up to $\approx 18\,\mathrm{fm}$ length • $m_\pi L = 25$
- stochastic locality ⇒ expectation values from volume average, on a single gauge field configuration
- also errors estimated using volume average

standard MC errors

for an observable $O(x)$ localized to a region around x,
the estimator of its field-theoretical expectation value $\langle O(x)\rangle$ is, traditionally, the Monte Carlo average

$$\bar{O}(x) = \frac{1}{n}\sum_{i=1}^{n} O\Big|_{U_i}, \qquad \sigma_{\bar{O}}(x) = \frac{1}{n^{1/2}}\sigma_O(x)$$

where the field-theoretical distribution variance is $\sigma_O^2(x) = \langle [O(x) - \langle O(x)\rangle]^2\rangle$

master-field errors

in the master-field approach, the Monte Carlo average is replaced with the translation average [Lüscher Lattice 2017]

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

whose distribution has variance

$$\begin{aligned}
\sigma^2_{\langle\!\langle O \rangle\!\rangle}(x) = \Big\langle [\langle\!\langle O(x) \rangle\!\rangle - \langle O(x) \rangle]^2 \Big\rangle &= \frac{1}{V} \sum_y \langle O(y) O(0) \rangle_c \\
&= \frac{1}{V} \Bigg[\sum_{|y| \leq R} \langle O(y) O(0) \rangle_c + \mathcal{O}\big(\mathrm{e}^{-mR}\big) \Bigg] \\
&= \frac{1}{V} \Bigg[\sum_{|y| \leq R} \langle\!\langle O(y) O(0) \rangle\!\rangle_c + \mathcal{O}\big(\mathrm{e}^{-mR}\big) + \mathcal{O}\big(V^{-1/2}\big) \Bigg]
\end{aligned}$$

and for n master-fields

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

hadronic observables

hadron propagator, *e.g.* Wick-connected meson contraction for source $y = 0$ to sink x

$$C_{\Gamma\Gamma'}(x,0) = [\bar{u}\Gamma d](x)[\bar{d}\Gamma' u](0) = \mathrm{tr}\left\{\Gamma\gamma_5 D^{-1}(x,0)\gamma_5\Gamma' D^{-1}(x,0)\right\}$$

- $\|D^{-1}(x,0)\| \propto \mathrm{e}^{-m_\pi|x|/2}$: non-*ultralocal* but still localized $\sim m_\pi^{-1}$
- the master-field error is given by the four-point function

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

  - large footprint
  - y can be sampled $\Rightarrow$ no all-to-all needed

everything works also replacing $C(x,0)$ with time-momentum correlators

$$\tilde{C}(x_0,\vec{p}) = \sum_{\vec{x}} \mathrm{e}^{-\mathrm{i}\vec{p}\cdot\vec{x}} C(x,0)$$

but these have a large footprint in space $\Rightarrow$ extract hadronic observables from position-space correlators?

e.g. • basic spectroscopy: m_π, m_N, • decay constants: f_π, • vector correlator physics: a_μ^{HVP}

alternative: inexact momentum projection, localized in space

position-space correlators

$$C_{PP}(x) \to \frac{c_P^2}{4\pi^2}\frac{m_\pi}{|x|}K_1(m_\pi|x|), \qquad C_{AP,\mu}(x) \to \frac{c_A c_P}{4\pi^2}\frac{x_\mu}{|x|}\frac{m_\pi}{|x|}K_2(m_\pi|x|),$$

$$C_{AA,\mu\nu}(x) \to \frac{c_A^2}{4\pi^2}\left[-\delta_{\mu\nu}\frac{1}{x^2}K_2(m_\pi|x|) + \frac{x_\mu x_\nu}{x^2}\left(\frac{m_\pi}{|x|}K_1(m_\pi|x|) + \frac{4}{x^2}K_2(m_\pi|x|)\right)\right],$$

$$C_{NN}(x) \to \frac{c_N^2}{4\pi^2}\frac{m_N^2}{|x|}\left[K_1(m_N|x|) + \frac{\not{x}}{|x|}K_2(m_N|x|)\right]$$

assuming the (Euclidean) Lorentz symmetry of the theory in the continuum, we can work with correlators that transform as scalars:

- $\mathring{C}_{PP}(r) \equiv C_{PP}(x)$, $\mathring{C}_{AP}(r) \equiv x_\mu C_{AP,\mu}(x) \to \frac{c_A c_P}{4\pi^2} m_\pi K_2(m_\pi r)$
- two ways to contract the μ, ν indices of the axial correlator

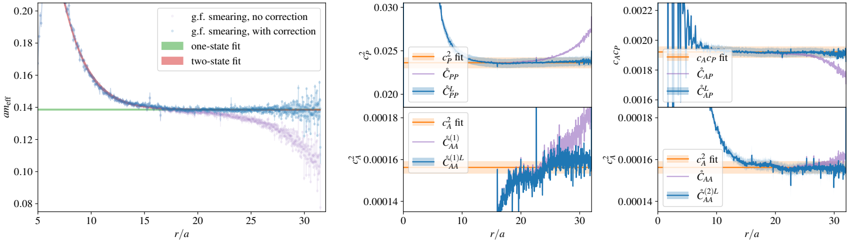
$$\mathring{C}^{(1)}_{AA}(r) \equiv \delta_{\mu\nu}C_{AA,\mu\nu}(x), \qquad \mathring{C}^{(2)}_{AA}(r) \equiv x_\mu x_\nu C_{AA,\mu\nu}(x)$$

- two structures for the nucleon correlator

$$\mathring{C}^{(1)}_{NN}(r) \equiv \mathrm{tr}\, C_{NN}(x), \qquad \mathring{C}^{(2)}_{NN}(r) \equiv \mathrm{tr}\, \not{x} C_{NN}(x)$$

position-space correlators – radial direction

- asymptotic behaviour known for $a \to 0$, at $a \neq 0$, each direction has different cut-off effects
- we work with the radial correlator, averaged over $4d$ spheres $\mathring{C}(r) = (1/\mathrm{r}_4(r^2)) \sum_{|x|=r} C(x)$
  $\Rightarrow$ different cut-off effects are averaged together
- different rôle of finite-L, T effects, more complex treatment in general
  on a "small" $L = 64a$ lattice, we correct for this on pseudoscalar [MC *et al.* Lattice 2021] and axial correlators



$\Rightarrow$ not an issue in the large-volume regime $L, T \gg 1/\Lambda, 1/m_\pi$ (see next slides)

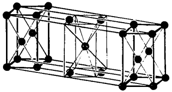
grid of point sources estimator

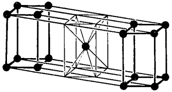
$L = T = 96a \approx 9\,\mathrm{fm}$ and $L = T = 192a \approx 18\,\mathrm{fm}$ boxes

$\Rightarrow$ we need a more efficient way to compute correlators

point sources on a regular grid with spacing $b = 48a \Rightarrow$ statistics scales with $(L/d)^4$, radial distances up to $b/2$

- we do not put Dirichlet boundary conditions on the b^4 blocks, differently that suggested in [Lüscher Lattice 2017], avoiding large boundary effects from the block boundary
- instead, for meson contractions, stochastic cancellation of unwanted contributions assigning a different $\mathrm{U}(1)$ phase to each point;
  at least $n_{\mathrm{src}} = 2$ sources are needed to cancel the bias, introducing a overhead cost factor of n_{src}
- no overhead for nucleon contractions!





- optimization: one can use only even (or odd) points $\Rightarrow$ cost factor of 2, radial distances up to $\sqrt{2}b/2$
- or a body-centred cell: in $4d$, same spacing along diagonal and non-diagonal directions

position-space correlators – two master-field volumes

on the $96^4 \approx (9\,\mathrm{fm})^4$ lattice

- grid of points with $b = 48a$, even points only $\Rightarrow r \leq 33.94a$
- $n_\mathrm{src} = 2$ $\mathrm{U}(1)$ noise sources for mesons
- 512 grids with offsets of $12a$
  $\Rightarrow$ 4096 point sources in a regular grid with spacing $12a$, times 5 gauge field configurations

on the $192^4 \approx (18\,\mathrm{fm})^4$ lattice

- grid of points with $b = 48a$, even points only $\Rightarrow r \leq 33.94a$
- $n_\mathrm{src} = 2$ (or 6) $\mathrm{U}(1)$ noise sources for mesons
- 32 grids with offsets of $24a$
  $\Rightarrow$ 4096 point sources in a regular grid with spacing $24a$, times 2 gauge field configurations

same (per configuration) statistics and computational effort on the two master-fields

position-space correlators – master-field errors

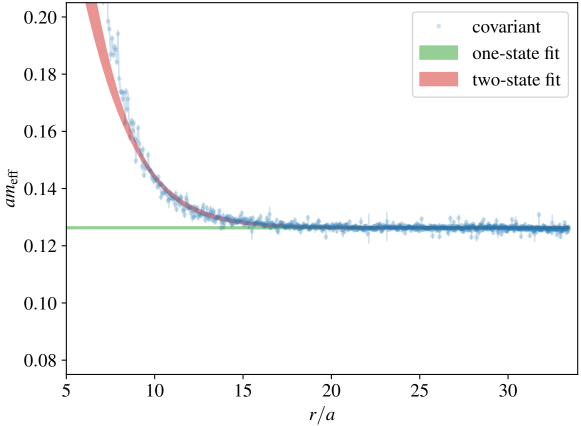
using averages and correlations over the sublattice of point sources location on y a grid

$$\left\langle [\langle\!\langle \mathring{C}(r) \rangle\!\rangle - \langle \mathring{C}(r) \rangle]^2 \right\rangle = \frac{1}{V}\left[\sum_{|y|\leq R} \langle\!\langle \mathring{C}(r;y)\mathring{C}(r;0) \rangle\!\rangle_c + \mathcal{O}\left(\mathrm{e}^{-mR}\right) + \mathcal{O}\left(V^{-1/2}\right) \right]$$

- "Γ-method-like" [Wolff 2003] to find the optimal R, applied to the space-time dimensions
  $\Rightarrow$ Madras-Sokal formula for the statistical error of the error [Madras, Sokal 1988]

- simpler alternative: blocks binning (blocking) and bootstrap
  we use blocks/bins of size $(24a)^4$ or $(48a)^4$ $\Rightarrow$ stable error estimate
  results shown for the more conservative case, $(48a)^4$

preliminary results – pion mass

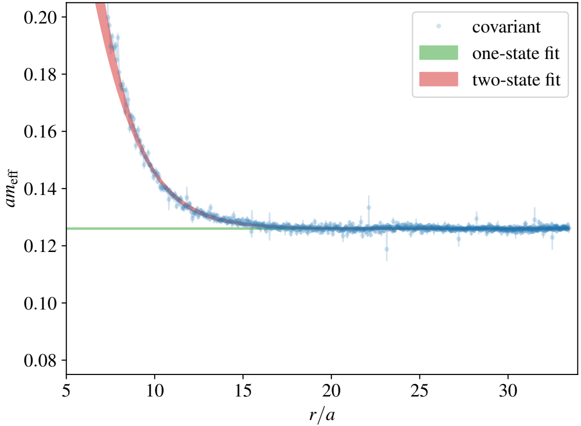


on the 96^4 ensemble, 5 configurations

$$m_\pi = 0.126\,28(33)/a \approx 265\,\mathrm{MeV}$$

and no boundary effect observed

preliminary results – pion mass

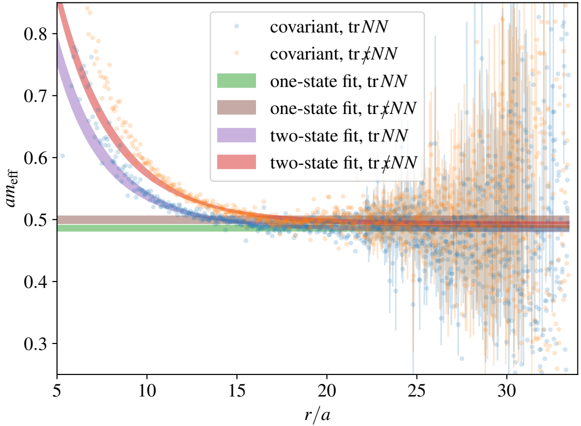


on the 192^4 ensemble, 2 configurations

$$m_\pi = 0.126\,01(19)/a \approx 265\,\text{MeV}$$

and no boundary effect observed

preliminary results – nucleon mass

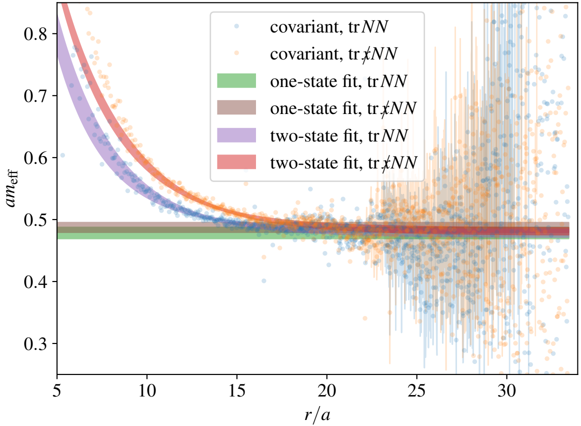


on the 96^4 ensemble, 5 configurations

$$m_N = 0.500(6)/a \approx 1049\,\mathrm{MeV}$$

and no boundary effect observed

preliminary results – nucleon mass

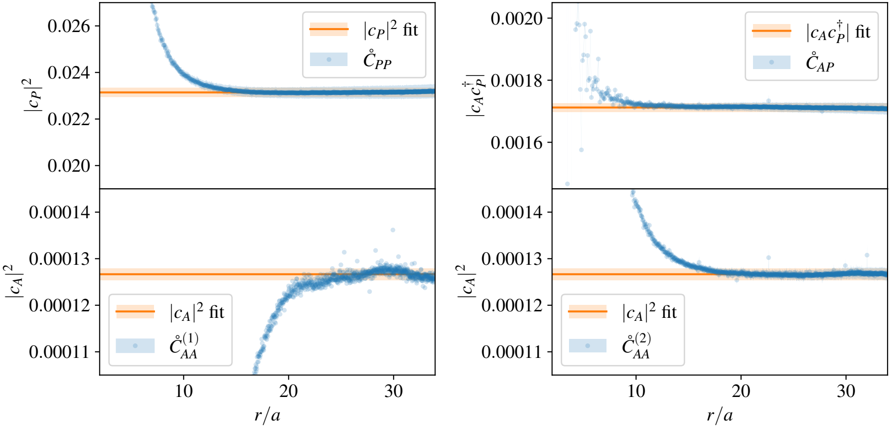


on the 192^4 ensemble, 2 configurations

$$m_N = 0.487(8)/a \approx 1023\,\mathrm{MeV}$$

and no boundary effect observed

preliminary results – pion decay constant

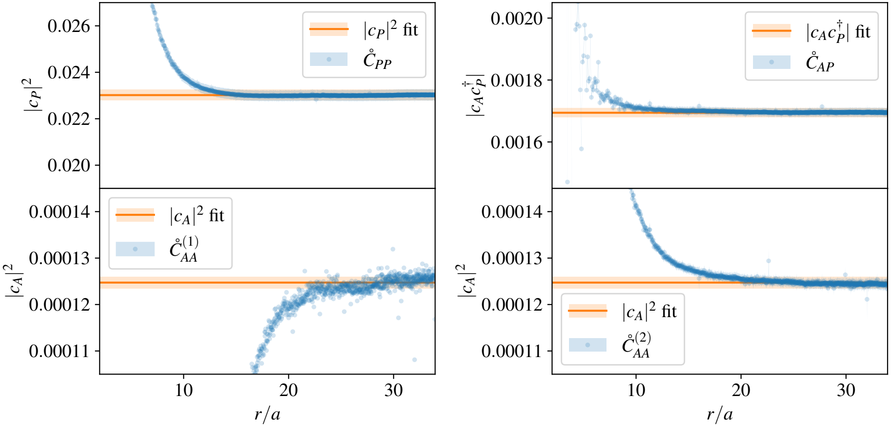


on the 96^4 ensemble, 5 configurations

$$f_\pi^{\mathrm{bare}} = 0.0890(3)/a \approx 187\,\mathrm{MeV}$$

and no boundary effect observed

preliminary results – pion decay constant



on the 192^4 ensemble, 2 configurations

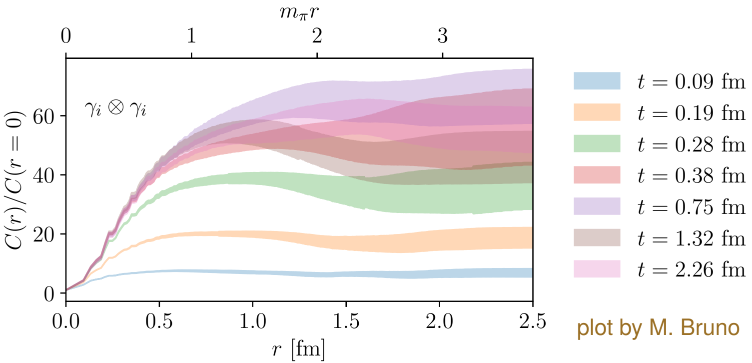
$$f_\pi^{\mathrm{bare}} = 0.0885(4)/a \approx 186\,\mathrm{MeV}$$

and no boundary effect observed, small shift but compatible with errors

momentum-projected correlators

using stochastic $3d$ volume sources, at $\vec{p} = 0$,
the master-field error is estimated with translation averages in space
(and time, with sources on two timeslices on the $T = 192a$)

tests on a "small" volume ($L = 64a$)



plot by M. Bruno

here, r is the radial direction in space, t is the source-sink separation in Euclidean time
$C(r)$ is the covariance between correlators separated by $r \Rightarrow$ integral is analogous to τ_{int}
$\Rightarrow$ large separation correlators have a larger footprint in space, but plateau due to limited statistics

conclusions

- position-space correlators can be used to extract hadron masses and decay constants
- short-distance and cut-off effects are under control
- with the statistical error estimated *à la* master-field
- and efficient volume scaling of the computational effort
- master-field error estimation also with momentum-projected correlators

more on this topic

[plenary talk by P. Fritzsch on Saturday @ Lattice 2022]

- on “small” volumes, corrections for boundary effects [MC *et al.*, in preparation]
- …and gluonic observables, *e.g.* topological susceptibility
  ⇒ “cold” (large T) master-field simulations [talk by A. Francis on Monday @ Lattice 2022]
- spectral reconstruction applications [plenary talk by J. Bulava on Tuesday @ Lattice 2022]
- position-space methods for HVP ($(g-2)_\mu$, $\Delta\alpha_{\text{had}}$) [Meyer 2017; MC, Gérardin, Ottnad, Meyer Lattice 2018]
  and the $(g-2)_\mu$ HVP windows [talk by J. Parrino on Tuesday @ Lattice 2022]

outlook

- go beyond the sphere-averaged radial correlator, understanding better cut-off effects on the $a \neq 0$ correlator
- $(4d)$ domain decomposition of the quark propagator?
- more complex hadronic observables …

thanks

for your attention!

questions?

backup slides

momentum-projected Euclidean-time correlators

or time-momentum correlators

$$\tilde{C}_{PP}(t,\vec{p}) \to \frac{\left|c_P(\vec{p})\right|^2}{2E_\pi(\vec{p})}\mathrm{e}^{-E_\pi(\vec{p})t},$$

$$\tilde{C}_{NN}(t,\vec{p}) \to \frac{\left|c_N(\vec{p})\right|^2}{2E_N(\vec{p})}(-i\not{p} + m_N)\mathrm{e}^{-E_N(\vec{p})t},$$

standard approach to lattice spectroscopy

- discrete spectrum in a L^3 box $\Rightarrow \tilde{C}(t,\vec{p})$ is a sum of exponentials, also at $a \neq 0$
- leading finite-T effects (back-propagating states) are easy to take into account

we considered point sources (that also work for position-space) and

- no smearing
- $3d$-fermion smearing with $\kappa_{3d} = 0.180, 0.190, 0.200$ [Papinutto, Scardino, Schaefer 2018]
- gradient-flow smearing ($4d$ smearing, modifies the transfer matrix but ok if $\sqrt{8t_{\mathrm{flow}}} \ll t$) [Lüscher 2013]