Error analysis from stochastic locality and master fields

Mattia Bruno

in collaboration with:
John Bulava, Marco Cé, Anthony Francis, Patrick Fritzsch,
Jeremy R. Green, Maxwell T. Hansen, Martin Lüscher, Antonio Rago

Domain-Wall Fermions at 25, BNL (Virtual)
December 13$^{\mathrm{th}}$, 2021

Stochastic locality

[Lüscher '17]

Observable $\mathcal{O}(s,x)$ at Monte Carlo time s at position x_μ

define true expectation value $\langle\mathcal{O}\rangle$

define $\langle\langle\overline{\mathcal{O}}\rangle\rangle = \frac{1}{VN}\sum_{s,x}\mathcal{O}(s,x)$

Stochastic locality implies $\lim_{V\to\infty}\langle\langle\overline{\mathcal{O}}\rangle\rangle = \langle\mathcal{O}\rangle$ at fixed N

parallelism to infinite statistics, $N\to\infty$

$\langle\langle\overline{\mathcal{O}}\rangle\rangle$ is our best estimator for $\langle\mathcal{O}\rangle$

its error from $\langle\big[\langle\langle\overline{\mathcal{O}}\rangle\rangle - \langle\mathcal{O}\rangle\big]^2\rangle = \frac{1}{VN}\sum_{s,x}\Gamma(s,x)$

$$\Gamma(s,x) = \langle\big[\mathcal{O}(s,x)-\langle\mathcal{O}\rangle\big]\big[\mathcal{O}(0)-\langle\mathcal{O}\rangle\big]\rangle$$

Master Fields

Translation invariance for error estimates

$\rightarrow$ unlocks the possibility to simulate very large lattices $m_\pi L \geq 12$

very expensive, likely small number of configs/fields

Master-field physics program

at fine lattice spacing suppression of topology freezing effects

at intermediate lattice spacing physics suffering from volume effects

i. magnetic background fields, fine momentum resolution

ii. intermediate windows HVP, finite vol. QED effects

iii. spectral reconstructions [talk by Hansen]

solutions to inverse laplace overcome 4-particle limit

possible w/ smeared kernel, e.g. $\frac{\epsilon}{\omega^2+\epsilon^2}$

ordered double limit $V \rightarrow \infty, \epsilon \rightarrow 0$

iv. ...

UNIVERSITA' DEGLI STUDI DI MILANO BICOCCA

Master-field errors - I

In practice our best estimator for Γ is given by

$\overline{\Gamma}(s,x) = \frac{1}{V}\frac{1}{N-s}\sum_{s',x'} \delta\mathcal{O}(s+s',x+x')\delta\mathcal{O}(s',x')$

w/ $\delta\mathcal{O}(s,x) = \mathcal{O}(s,x) - \langle\langle\overline{\mathcal{O}}\rangle\rangle$

For large volumes, likely few fields, i.e. N small [Lüscher '17]

pre-average all fields, $\overline{\mathcal{O}}(x) = \frac{1}{N}\sum_s \mathcal{O}(s,x)$

equivalent to $\overline{\Gamma}(x) = \frac{1}{N}\sum_s \overline{\Gamma}(s,x)$

truncated sum over space-time approximates the error

$$\sigma^2 = \frac{1}{V}\left[\sum_{|x|\leq r} \overline{\Gamma}(x) + O(e^{-mr}) + O(V^{-1/2})\right]$$

define $\overline{C}(r) = \sum_{|x|\leq r} \overline{\Gamma}(x)$

Master-field errors - II

In traditional simulations normally we perform volume average

take $\langle\langle O(s)\rangle\rangle = \frac{1}{V}\sum_x \mathcal{O}(s,x)$

its error given by $\Gamma(s) = \frac{1}{V}\sum_x \Gamma(s,x)$ [Madras, Sokal '88]

truncate sum over s to maximal window W [Wolff '03]

and the error of error is $O(\sqrt{W/N})$

Extend Γ-method for derived observables [e.g. Hernandez et al. '21]

linear error propagation $(\delta F)^2 = \sum_{\alpha\beta} \frac{\partial f}{\partial \mathcal{O}_\alpha} \Gamma_{\alpha\beta} \frac{\partial f}{\partial \mathcal{O}_\beta}$

We extended Wolff's derivation to the case of master fields

1. define an automatic summation radius R
2. quantitative grasp over error of error $O(\sqrt{R^D/V})$

Note that $\int d^D x \to \int d\Omega_D d|x||x|^{D-1}$

volumetric factor $|x|^{D-1}$ pushes optimal radius to large distance

UNIVERSITA' DEGLI STUDI DI MILANO BICOCCA

Our laboratory

A pre-master-field setup to test methods and ideas

Lattices w/ $N_f = 2 + 1$

$m_\pi = 293$ MeV, $a \approx 0.094$ fm
$L/a = 32, 48, 64 \quad \rightarrow \quad m_\pi L = 4.5, 6.7, 9$
approx. 100 configs for each ensemble

Observables:

1. energy density at positive flow time E_t
   1 point function: cheap, precise, known for all points
2. fermionic two-point correlators $\langle \mathrm{Tr}\left[\Gamma D^{-1}(x,y)\Gamma D^{-1}(y,x)\right]\rangle$
   $\Gamma = \gamma_5, \gamma_x, \gamma_y, \gamma_z$
   zero momentum, depends on source-sink sep $|x_0 - y_0|$
   position space, depends on radius $r^2 = \sum_\mu (x_\mu - y_\mu)^2$

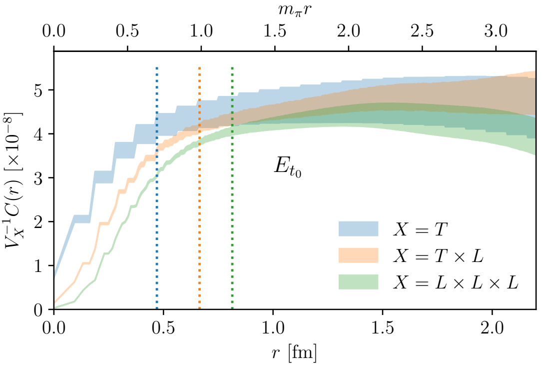
Master-field analysis

We study variance $C(r) = \sum_{|x|\leq r} \langle [\mathcal{O}(x) - \langle\mathcal{O}\rangle] [\mathcal{O}(0) - \langle\mathcal{O}\rangle] \rangle$

$\lim_{N\to\infty} \frac{1}{N} \sum_s \sum_{|x|<r} \overline{\Gamma}(s,x) = C(r)$

Monte-Carlo sampling of C $\to$ stat. error of C as error of error

master-field analysis along T, TL, L^3 (average other dimensions)

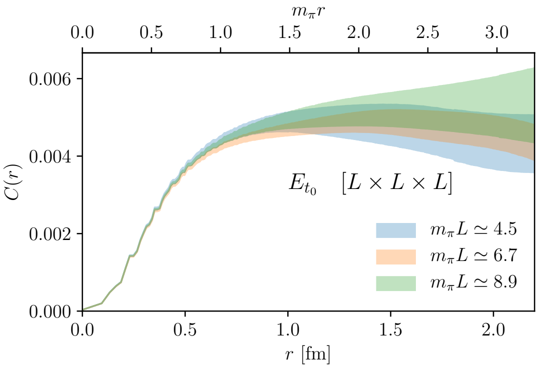


master-field error possible along any direction

$m_\pi L \simeq 6.7$

volumetric factor pushes saturation to right

Traditional MC: Markov chain long enough to estimate autocorrelations?
Master-field: is volume large enough to estimate spatial correlations?



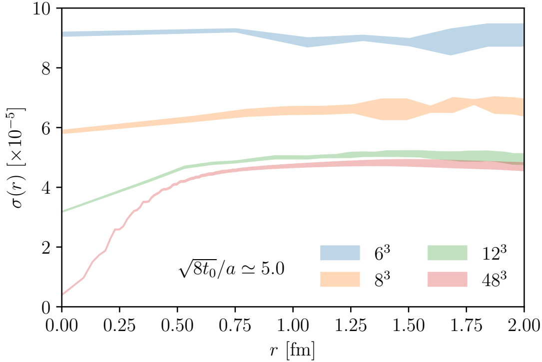
master-field error in space L^3

good agreement $m_\pi L = 4.5, 6.7, 9$ for E_{t_0}

Footprint ($=r$ such that error staturates) is observable dependent

Gauge Noise Limit

$\mathcal{O}$ known on subset of points (common for fermionic observables)
e.g. on a grid of points w/ equal distance



error of E_{t_0}

$m_\pi L \simeq 6.7$

less points smaller accuracy

master-field analysis in space L^3

checking saturation point useful to stop fermionic measurements
similar to check scaling with number random sources

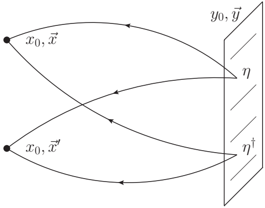
Fermionic correlators

Take zero mom. projection: how to study error a la master-field?

$G(x, |x_0 - y_0|) = \sum_{\boldsymbol{y}} \mathrm{Tr}\left[\Gamma D^{-1}(x,y)\Gamma D^{-1}(y,x)\right]$

use point-sources and perform master-field error over sampled points

use random-noise and perform master-field error



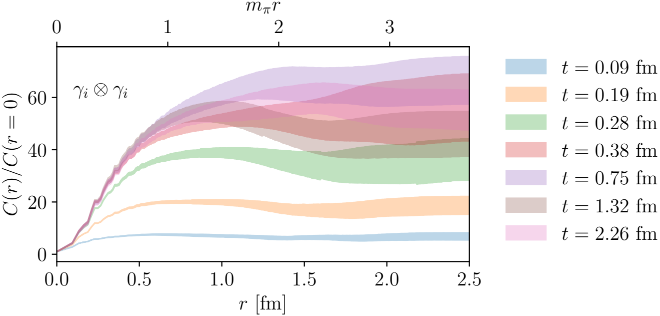
in time by changing position of wall source y_0

in 3D space at the sink $\boldsymbol{x}$, for fixed wall source

We take average over time (and hits), study MF error in 3D wall

Footprint

We study ud isovector two-point correlator (data from $m_\pi L \simeq 9$)
source-sink separation t related to footprint?



Footprint grows with source-sink sep, but then saturates
e.g. in master-field analysis fix summation radius to 1 fm
traditional Markov chain: "higher plateaus" $\leftrightarrow$ larger window W

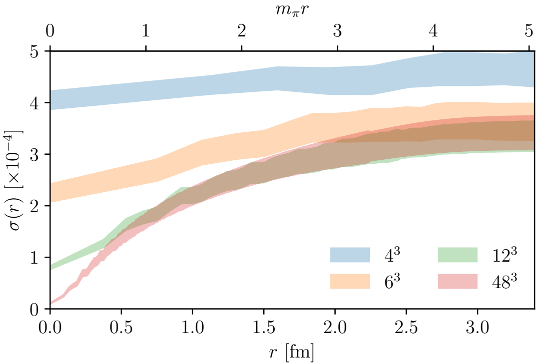
UNIVERSITÀ DEGLI STUDI DI MILANO BICOCCA

Pions

Pions play special role, due to absence of signal-to-noise problem

saturation at long distance → large volumes mandatory

→ several configurations



w/ few points reach gauge noise limit

master-field analysis less relevant in traditional simulations

$m_\pi L \simeq 6.7$

Footprint depends on observable

partially quenched theory to get asympt. behavior

Towards master fields - I

New challenges appear in several aspects of calculation

1. Stochastic locality naturally associated to coordinates
   correlators in position space more natural [e.g. x-space HVP by H. Meyer]
   truncated sum for mom. projections

2. Numerical methods for fermionic correlators w/ good volume scaling
   stochastic sampling of point sources [e.g. HLbL by RBC/UKQCD]
   (stoch.) grid of points [e.g. discon. HVP by RBC/UKQCD]
   factorization of observables [Cé et al.]

3. Production of master-fields [Friztsch Lattice '21]
   algorithmic considerations: SMD, infinite norm [Francis et al. '19]
   Wilson specific feature: exponentiated clover action [Francis et al. '19]
   → successful generation of L^4 fields w/ $L \simeq 9, 18$ fm
   $a \simeq 0.094$ fm, $m_\pi \simeq 270$ MeV, $m_\pi L = 12, 25$
   on-going efforts at $a \simeq 0.065$ fm

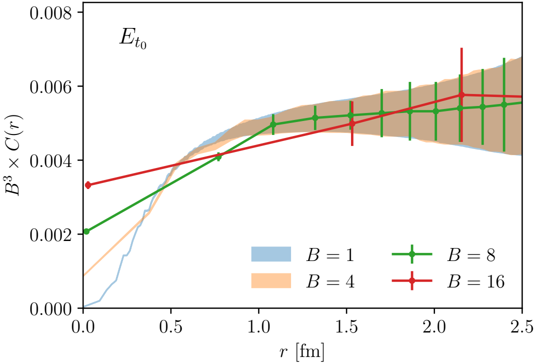
UNIVERSITA' DEGLI STUDI DI MILANO BICOCCA

Blocking

Analysis & storage costs grow w/ volume, e.g. E_t known on all points

perform blocking of points from averages of sub-volumes

similar to binning in traditional simulations



$m_\pi L \simeq 9$

master-field analysis in space L^3

blocking $L \to L/B$

If blocks large enough $\to$ jackknife, bootstrap

Towards master fields - II

[Cé Lattice 2021]

1. Position space $G_\pi(r) = \sum_{|x|=r} \langle \mathrm{Tr}\left[\gamma_5 D^{-1}(x,0)\gamma_5 D^{-1}(0,x)\right]\rangle$

   in the continuum asympt. behavior $G_\pi(r) \propto \frac{m_\pi}{r} K_1(m_\pi r)$

   not an exact representation, understand cutoff effects

   large finite volume contaminations

   for G_π mirror images $\rightarrow$ easy to correct

   like the $\cosh$ effect along temporal direction

   for nucleon $N\pi$ intermediate states

   average together points of same size

   $\rightarrow$ reduce noise w.r.t. zero momentum proj.

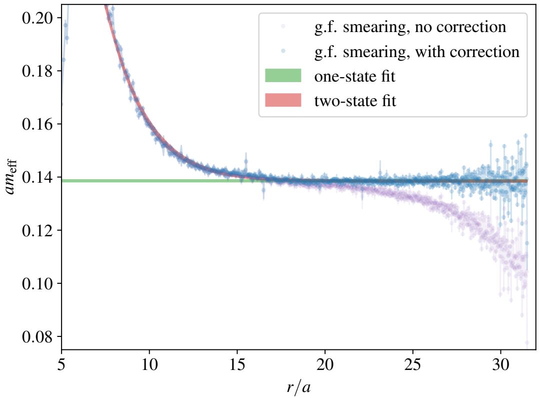
   encouraging results for mass extraction of nucleon

2. Grid of points w/ separation dictated by our study

   initial TMR study w/ wall sources relevant to get "saturation scales"

Towards master fields - III

Hadronic masses: one possibility given by position space correlators



$m_\pi L \simeq 9$

correction from mirror images working

excited states modeled w/ secondary K_1

discretization errors under investigation

Conclusions - I

Errors a la master-field

- may play interesting role w/ traditional simulations
  - e.g. DWF simulations expensive, fewer configurations
  - improved error estimators if consider $D+1$ theory?
- blocking, reduces analysis and storage costs
  - standard analysis techniques, like jackknife
- preliminary studies on intermediate volumes
  - identify relevant scales $\to$ planning of new simulation

Master-field observables: re-think definition and numerical methods

- first tests w/ position space correlators and common TMR
- sampling strategies (grids, point sources) under study
- investigations of spectral reconstructions under way

Conclusions - II

Master-field simulations

- exponentiated Clover formulation of Wilson fermions
  - important product, relevant beyond master-field program
- $m_\pi L = 12$ and 24 generated at coarse a for (eClover)-Wilson
  - $\to$ mesonic masses and decay const., spectral reconstruction
- interplay w/ domain decomposition will be crucial [talk by Boyle, Giusti]
  - $\to$ ratio network/computing power of new machines
- to really overcome topology freezing must go finer
  - thermalization challenge still open!
  - but many good ideas out there [e.g. talk by Matsumoto, Jung ...]

Thanks for your attention!!

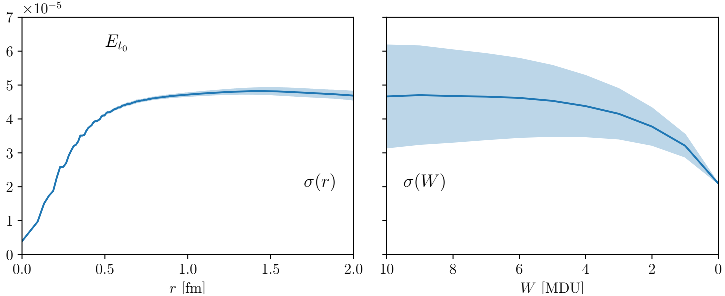
Improved error estimators

Master-field analysis

$V \simeq 48^3$ points

Traditional Monte-Carlo analysis

$N \simeq 10^2$ confs



Exactly same data both plots

If autocorrelations present [in prep.]

bin MC data w/ bin size τ_{int} before master-field analysis

or statistical analysis in full $D+1$ theory

UNIVERSITA' DEGLI STUDI DI MILANO BICOCCA