Performance of Low Mode Averaging on physical pion mass Twisted-Mass ensembles

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based on C. Alexandrou *et al.* – arXiv:2606.27072

University of Cyprus

Extended Twisted Mass Collaboration

43rd Lattice Conference

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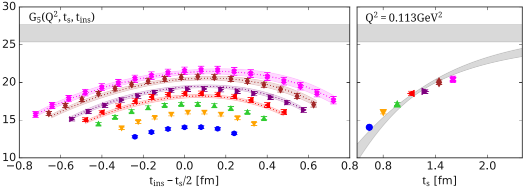
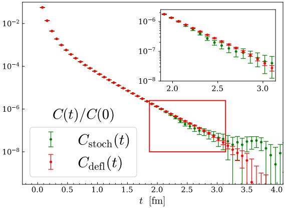
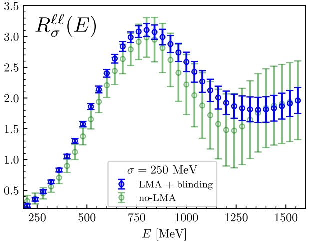
why low mode averaging?

in modern lattice QCD we need very precise correlators at large Euclidean distances!







- hadronic matrix elements
- hadron vacuum polarisation
- spectral densities reconstruction

to improve lattice correlators at long distances, deflation techniques played a central role!

the journey

- general feature of LMA
- results for mesonic and baryonic correlators
- a multigrid approach to LMA

improving the infrared part of correlators via propagator splitting

$$S \equiv D^{-1} = S^{\mathrm{IR}} + S^{\mathrm{UV}}$$

1. stochastic approach

$$S_\eta \equiv S H_\eta = S_\eta^{\mathrm{IR}} + S_\eta^{\mathrm{UV}}$$

2. low mode averaging approach

$$S_\eta^{\mathrm{LMA}} \equiv S^{\mathrm{IR}} + S_\eta^{\mathrm{UV}} = S_\eta + (S^{\mathrm{IR}} - S_\eta^{\mathrm{IR}})$$

mixed terms appear in *n*-propagator correlation functions

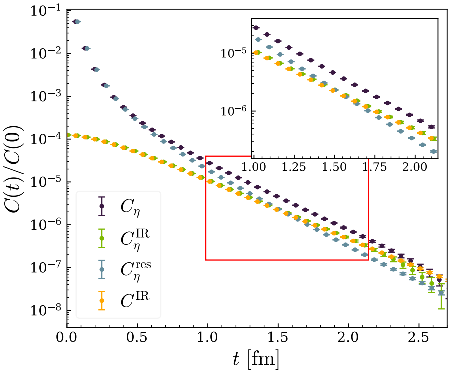
$$C_\eta^{\mathrm{LMA}} \equiv \mathcal{C}\Big[\underbrace{S_\eta^{\mathrm{LMA}}, \ldots}_{n \text{ times}}\Big] = \underbrace{\boxed{\mathcal{C}\Big[\underbrace{S^{\mathrm{IR}}, \ldots}_{n \text{ times}}\Big]}}_{C^{\mathrm{IR}}} + \underbrace{\boxed{\mathcal{C}\Big[\underbrace{S_\eta^{\mathrm{UV}}, \ldots}_{n \text{ times}}\Big]}}_{C_\eta^{\mathrm{UV}}} + \underbrace{\boxed{\mathcal{C}\Big[\underbrace{\left(S_\eta^{\mathrm{UV}}, S^{\mathrm{IR}}\right)}_{2^n-2 \text{ combinations}}\Big]}}_{C_{\eta,\mathrm{ex}}^{\mathrm{IR,UV}}}$$

$$C_\eta = C_\eta^{\mathrm{IR}} + C_\eta^{\mathrm{UV}} + \boxed{C_{\eta,\eta}^{\mathrm{IR,UV}}} \quad \longleftrightarrow \quad C_\eta^{\mathrm{LMA}} = C^{\mathrm{IR}} + C_\eta^{\mathrm{UV}} + \boxed{C_{\eta,\mathrm{ex}}^{\mathrm{IR,UV}}}$$

only the infrared part is improved

$$C_\eta^{\mathrm{LMA}}(t) = C_\eta(t) + C^{\mathrm{IR}}(t) - C_\eta^{\mathrm{IR}}(t)$$

for example for time-spin diluted or point spin-color diluted sources



1. C^{IR} can be *exactly* known on a given gauge configuration
2. C_η and C_η^{IR} to be computed on the same source H_η

   they share *exactly* the same fluctuations

   $C_\eta^{\mathrm{res}} \equiv C_\eta - C_\eta^{\mathrm{IR}}$ precisely up to very large t
3. $C^{IR} \Big/ C_\eta^{\mathrm{res}}$ crossover depend on the number of modes

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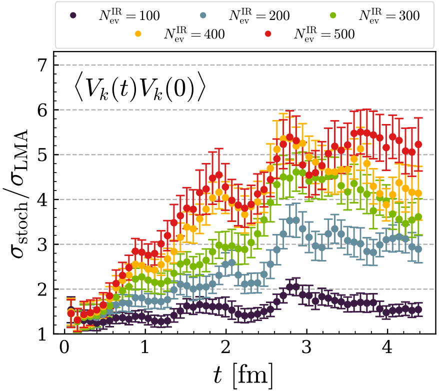

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$\longleftarrow$ saturation of S/N gain w.r.t. $N_{\mathrm{ev}}^{\mathrm{IR}}$

only the infrared part is improved

$$\boxed{C_\eta^{\mathrm{LMA}}(t) = C_\eta(t) + C^{\mathrm{IR}}(t) - C_\eta^{\mathrm{IR}}(t)}$$

for example for time-spin diluted or point spin-color diluted sources

computational convenience:

- contractions $\mathcal{C}$ number reduced $\longrightarrow$ **2^n to 3 for any correlator**
- separate runs for full and IR correlators $\longrightarrow$ **efficient scaling with the number of nodes**

  not possible in the standard approach where simultaneaus UV and IR projections are needed
- if sources of C_η are reproducible $\longrightarrow$ **improvement a posteriori is possible**

only the infrared part is improved

$$\boxed{C^{\mathrm{LMA}}_{\eta}(t) = C_{\eta}(t) + C^{\mathrm{IR}}(t) - C^{\mathrm{IR}}_{\eta}(t)}$$

for example for time-spin diluted or point spin-color diluted sources

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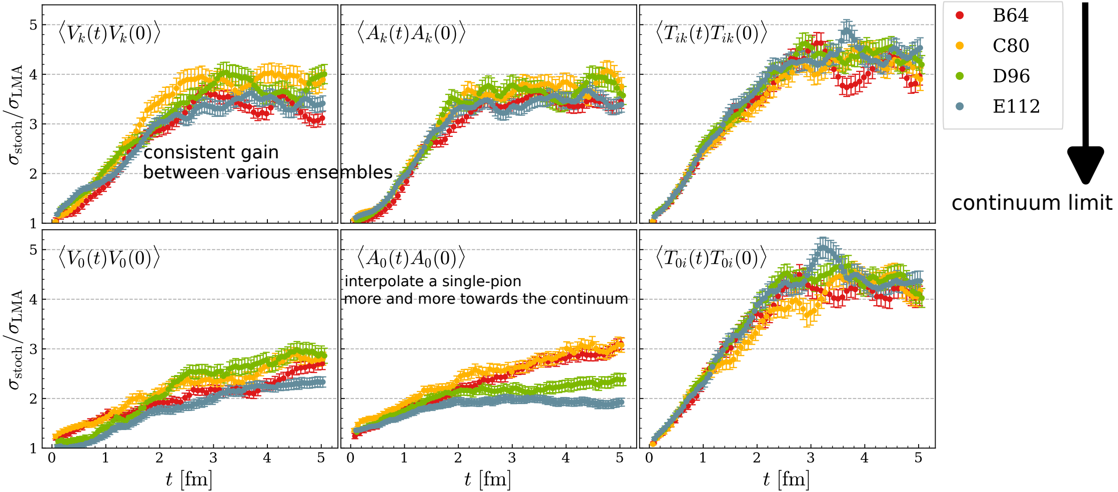
! if the relation does not hold exactly, it can still be used with some care !

improved mesonic correlators

1. **how many eigenvectors do we need?**
2. **does N_{ev}^{IR} depends on the Dirac structures considered?**



improved baryonic correlators

- $2+6$ mix. contractions $\longrightarrow$ 3 contractions

  using spin-colour diluted point sources

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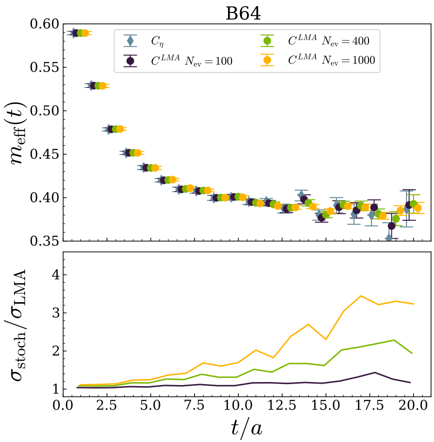
- **larger number of eigenvectors compared to mesons**
  unclear saturation on the gain with N_{ev}^{IR}



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  using spin-colour diluted point sources

- **larger number of eigenvectors compared to mesons**

  unclear saturation on the gain with N_{ev}^{IR}

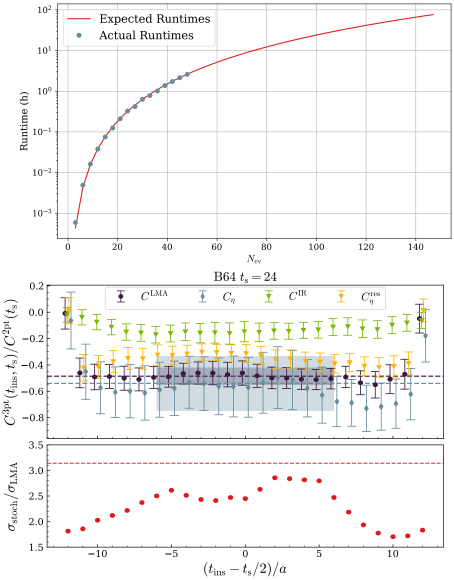
- contractions in C^{IR} scale $\propto \left(N_{ev}^{\mathrm{IR}}\right)^3$

  ~ 100 eigenvectors take more than a day

  ~ 1000 eigenvectors take more than a 3 years!!

$$C^{\mathrm{IR}}(t) \longrightarrow C^{\mathrm{IR}}_{\mathrm{impr.}} = \frac{1}{N^{\mathrm{IR}}_{x_s}} \sum_{x_s}^{N^{\mathrm{IR}}_{x_s}} C^{\mathrm{IR}}_{x_s}(t)$$

high-statistic realisation for two- and three-point functions



improved three-point functions

- Dirac structure dependence of the computational gain $\left(g_\Gamma \xleftarrow[a \ll t_{\text{ins}} \ll t_s]{} \frac{C_N^{3pt}(t_{\text{ins}}, t_s; \Gamma)}{C_N(t_s)} \right)$
- maximisation of the computational gain $G_{\mathcal{C}}\left(N_{x_s}, N_{x_s}^{\text{IR}}\right) = G_{\mathcal{E}}^2\left(N_{x_s}, N_{x_s}^{\text{IR}}\right) \cdot R_{\mathcal{C}}\left(N_{x_s}, N_{x_s}^{\text{IR}}\right)$

$$R_{\mathcal{C}} = \left[1 + \boxed{\frac{\mathcal{C}_{x_s}^{\text{IR}}}{\mathcal{C}_{x_s}}} \cdot \frac{N_{x_s}^{\text{IR}}}{N_{x_s}} \right]^{-1} \qquad G_{\mathcal{E}}^2(t) \simeq \left[1 - \boxed{\frac{\mathrm{Var}[C_{x_s}^{\text{IR}}(t)]}{\mathrm{Var}[C_{x_s}(t)]}} \cdot \frac{N_{x_s}^{\text{IR}} - N_{x_s}}{N_{x_s}^{\text{IR}}} \right]^{-1}$$

implementation dependent **observable dependent**

$\frac{\mathrm{Var}[C_{x_s}^{\text{IR}}(t_s)]}{\mathrm{Var}[C_{x_s}(t_s)]}$	g_A^{u-d}	g_A^{u+d}	g_S^{u-d}	g_S^{u+d}	g_T^{u-d}	g_T^{u+d}
$t_s/a = 16$	50.7%	42.3%	78.5%	82.7%	32.6%	23.4%
$t_s/a = 24$	87.6%	99.2%	99.0%	99.8%	55.5%	71.5%

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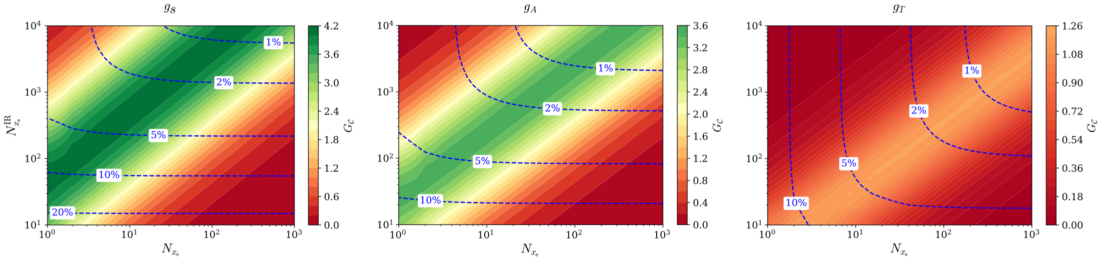

a multigrid approach to LMA

- MG as a preconditioner $\longrightarrow$ **dynamical adaptivity**

  K-cycle, lose precision, presence of a smoother

- MG for low mode averainging $\longrightarrow$ **static coarse operator**

  V-cycle, no-smoother (not tested)

  high-precision (particularly difficult for TM-fermions)

$$\boldsymbol{S} = \mathbb{P}_{\mathbf{MG}} \boldsymbol{S} + (\mathbb{1} - \mathbb{P}_{\mathbf{MG}})\, \boldsymbol{S}$$

$$\mathbb{P}_{\mathrm{MG}} \equiv P D_c^{-1} R D$$

$$\boldsymbol{S}^{\mathbf{MG}} = \mathbb{P}_{\mathbf{MG}} \boldsymbol{S} \;=\; P D_c^{-1} R$$

for TM-fermions computing exactly $\boldsymbol{S}^{\mathbf{MG}}$ is unfeasible

$$S^{\mathrm{MG}} \qquad \longrightarrow \qquad S^{\mathrm{MG,IR}} = P S_c^{\mathrm{IR}} P^{\dagger}$$

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$$\mathbb{P}_{\mathsf{MG}} \equiv PD_c^{-1}RD$$

$$\boldsymbol{S}^{\mathsf{MG}} = \mathbb{P}_{\mathsf{MG}}\boldsymbol{S} = PD_c^{-1}R$$

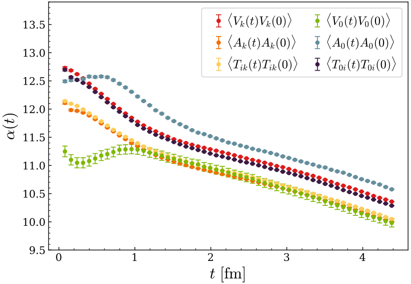
for TM-fermions computing exactly S^{MG} is unfeasible

$$S^{\mathsf{MG}} \longrightarrow S^{\mathsf{MG,IR}} = PS_c^{\mathsf{IR}}P^{\dagger}$$

! breaking of exact realisation of IR substitution !

$$C_\eta^{\mathsf{LMA,MG}}(t) \equiv C_\eta(t) + \alpha(t)\left(C_{\mathsf{impr.}}^{\mathsf{MG}}(t) - C_\eta^{\mathsf{MG}}(t)\right)$$

$$\alpha(t) = \frac{\mathrm{Cov}[C_\eta(t), C_\eta^{\mathsf{MG}}(t)]}{\mathrm{Var}[C_\eta^{\mathsf{MG}}(t)]}$$



why a multigrid approach is favourable on large volumes?

to keep the same performance level $N_{\mathrm{ev}}^{\mathrm{IR}}$ grows like V
the costs grows like V^2

$$\downarrow$$

on a $L \simeq 7.5$ fm ensemble ~ 4 times more eigenvectors compared to $L \simeq 5.5$ fm
a factor 16 in costs

$$\downarrow$$

in our experience exact LMA would require 950 GPUs (256 nodes on Leonardo)

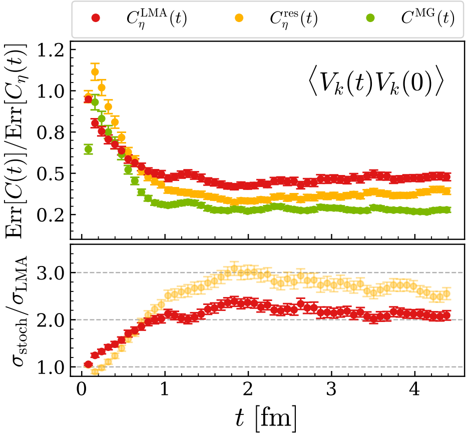
$$\Downarrow$$

via our multigrid approach, we have been able to reduce it to 54 nodes

our multigrid approach

- a high-statistic realisation requires less implementation effort and maintains generality

$$S^{\mathsf{MG,IR}} \quad \Longrightarrow \quad C^{\mathsf{MG}}_{\mathsf{impr.}}(t) = \frac{1}{N_\eta^{\mathsf{MG}}} \sum_\eta^{N_\eta^{\mathsf{MG}}} C_\eta^{\mathsf{MG}}(t),$$



$$C_\eta^{\mathsf{LMA,MG}}(t) \equiv C_\eta^{\mathrm{res},\mathsf{MG}}(t) + C^{\mathsf{MG}}(t)$$

$$C_\eta^{\mathrm{res},\mathsf{MG}}(t) \equiv C_\eta(t) - \alpha(t)\, C_\eta^{\mathsf{MG,IR}}(t)$$

$$C^{\mathsf{MG}}(t) \equiv \alpha(t)\, C^{\mathsf{MG,IR}}_{\mathsf{impr.}}(t)$$

- stochastic error of C^{MG} can be sent to 0

  implementation of $C^{\mathsf{MG,IR}}_{\mathsf{all-to-all}}$

- balance of errors is crucial for the costs

conclusions & outlooks

$$C_\eta^{\text{LMA}}(t) \equiv C_\eta(t) + \alpha(t)\Big(C_{\text{impr.}}^{\text{IR}}(t) - C_\eta^{\text{IR}}(t)\Big) \qquad \alpha(t) = \frac{\mathrm{Cov}[C_\eta(t), C_\eta^{\text{IR}}(t)]}{\mathrm{Var}[C_\eta^{\text{IR}}(t)]}$$

for particular choices of sources $\alpha = 1$ is possible

- LMA improve only the IR part of correlators
- $N_{\text{ev}}^{\text{IR}}$ needed to describe nucleons is higher than that for mesons
- at fixed target gain $N_{\text{ev}}^{\text{IR}} \propto \mu V$
- our implementation of mgLMA is quite effective on large volumes and can be improved

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Thank you for the attention!

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EXCELLENCE/0524/0459, EXCELLENCE/0524/0017

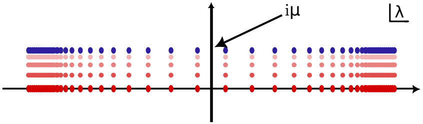
Backup

$$D(\mu) = D_W + i\gamma_5\,\mu \quad \longleftrightarrow \quad Q(\mu) \equiv D(\mu)\gamma_5 = Q_W + i\mu$$

since Q_W is hermitian his spectrum is real

$\downarrow$

the spectrum and eigenvectors are μ independent



$$D(\mu) = D_{\mathrm{W}} + i\gamma_5\,\mu \quad \longleftrightarrow \quad Q(\mu) \equiv D(\mu)\gamma_5 = Q_{\mathrm{W}} + i\mu$$

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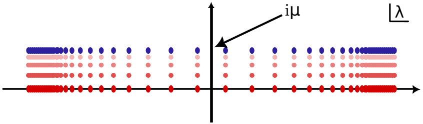

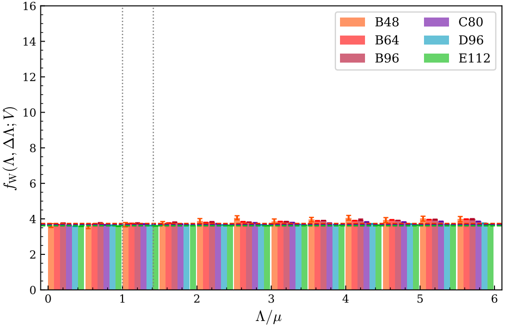

for large enough volumes the IR region is dense

1. physical space-time volume V scaling
2. density is constant in a fixed $\delta\Lambda$ interval

$$f_{\mathrm{W}} \equiv \frac{1}{V\,\delta\Lambda}\int_{\Lambda}^{\Lambda+\delta\Lambda} \rho_{\mathrm{W}}(\tilde{\Lambda}; V)\,\mathrm{d}\tilde{\Lambda} \;=\; \bar{\rho}_{\mathrm{W}} + df_{\mathrm{W}}$$

true for massless Wilson fermions

$$D(\mu) = D_{\mathrm{W}} + i\gamma_5\,\mu \quad \longleftrightarrow \quad Q(\mu) \equiv D(\mu)\gamma_5 = Q_{\mathrm{W}} + i\mu$$

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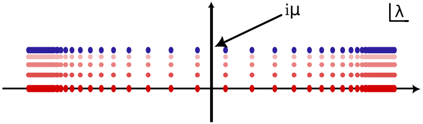

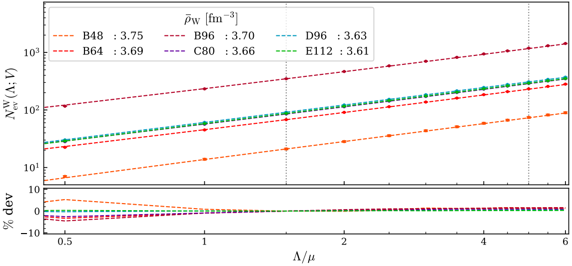

for large enough volumes the IR region is dense

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2. density is constant in a fixed $\delta\Lambda$ interval

$$N^{\mathrm{W}}_{\mathrm{ev}}(\Lambda; V) \equiv \int_0^{\Lambda} \rho_{\mathrm{W}}(\tilde{\Lambda}; V)\, \mathrm{d}\tilde{\Lambda} \simeq \bar{\rho}_{\mathrm{W}}\,\Lambda\, V$$

$\bar{\rho}_{\mathrm{W}}$ **related to the chiral condensate**

$$\Lambda \le \mu \quad \longrightarrow \quad \mu \le \left(|\lambda(\mu)| = \sqrt{\Lambda^2 + \mu^2} \right) \le \sqrt{2}\,\mu$$

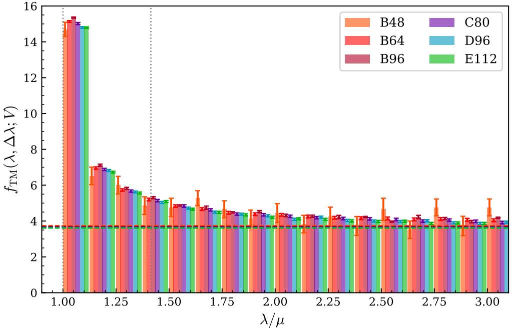
compression of eigenvalues

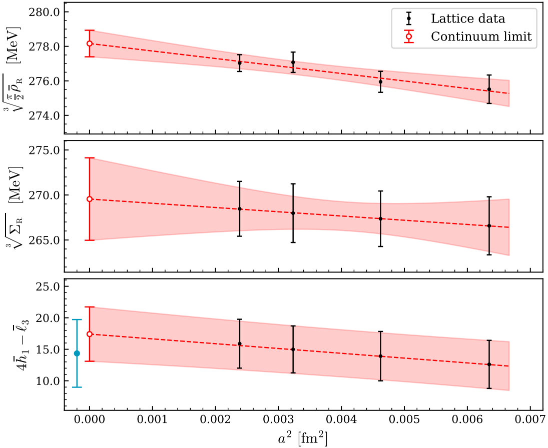
$$N_{\mathrm{ev}}^{\mathrm{TM}}(\sqrt{2}\mu; V) \equiv \int_{\mu}^{\sqrt{2}\mu} \rho_{\mathrm{TM}}(|\lambda|; V, \mu)\,\mathrm{d}|\lambda|$$

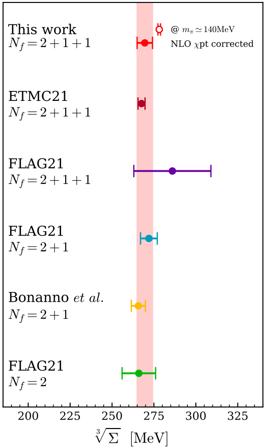
$$= \int_0^{\mu} \rho_{\mathrm{W}}(\Lambda; V)\,\mathrm{d}\Lambda \equiv N_{\mathrm{ev}}^{\mathrm{W}}(\mu; V)$$

	$N_{\mathrm{ev}}^{\mathrm{TM}}(\sqrt{2}\mu)$	$\bar{\rho}_{\mathrm{W}}\,\mu\,V$
B48	13	14
B64	44	45
B96 $V_{B48}\times 16$	232	229

- LMA production scale as $\propto \mu V \cdot \frac{V}{a^4}$
- at fixed $N_{\mathrm{ev}}^{\mathrm{IR}}$ LMA deteriorate with increasing μ
- in mixed correlators, the higher mass dominates the improvement



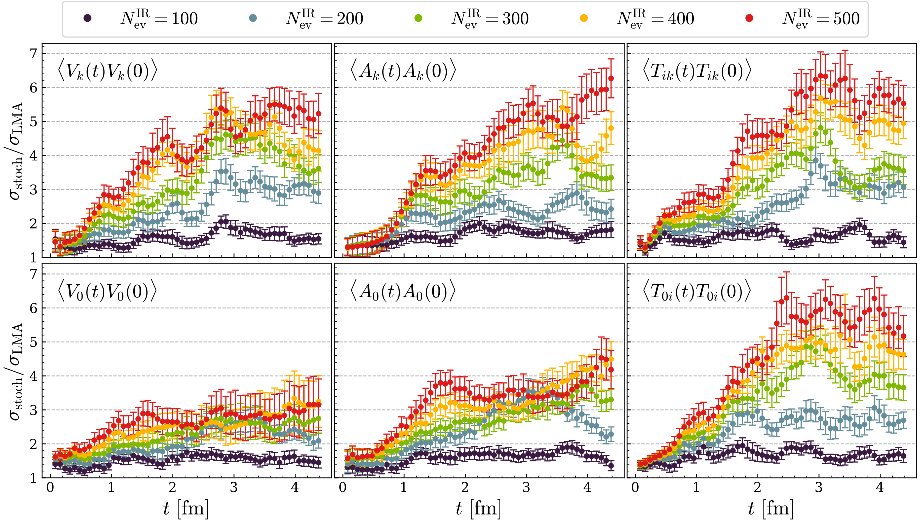




the Bank-Casher relation

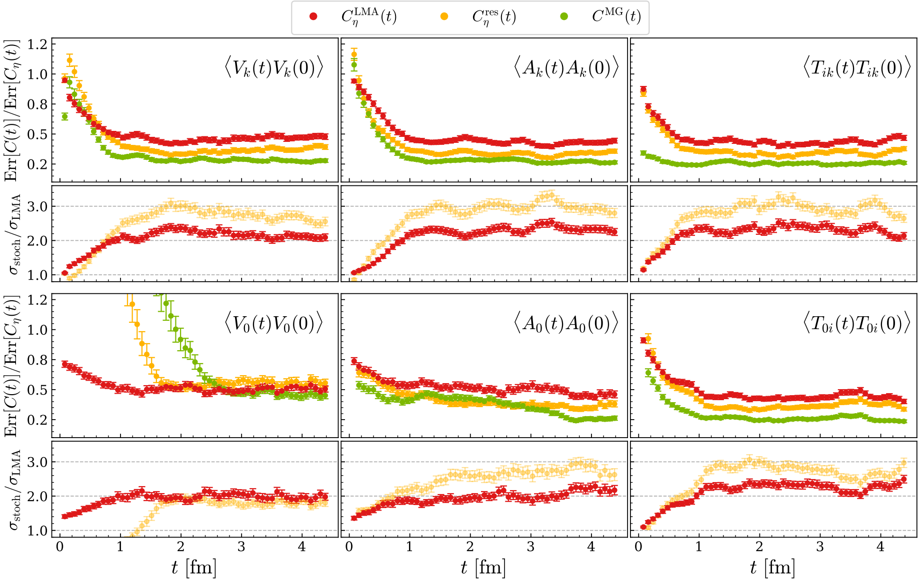
$$\Sigma_{\rm R} = -\frac{1}{2}\lim_{\mu\to 0}\left\langle\left(\bar{u}u + \bar{d}d\right)_{\rm R}\right\rangle(\mu) = \frac{\pi}{2} Z_P\,\bar{\rho}^{\,0}_{\rm W} \quad \text{with} \quad \bar{\rho}^{\,0}_{\rm W} = \lim_{\mu\to 0}\bar{\rho}_{\rm W}$$

$$Z_P\,\bar{\rho}_{\rm W}(\xi_\pi) = \frac{2\,\Sigma_{\rm R}}{\pi}\left(1 + \xi_\pi(4\bar{h}_1 - \bar{l}_3) + \mathcal{O}(\xi_\pi^2)\right) \quad \text{with} \quad \xi_\pi = \frac{m_\pi^2}{16\pi^2 f_\pi^2}$$



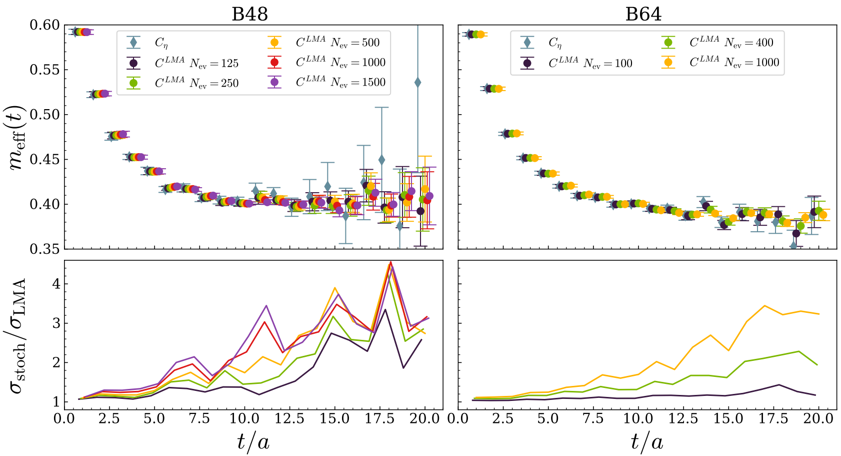
$N_{\rm ev}^{\rm IR} = 100$
$N_{\rm ev}^{\rm IR} = 200$
$N_{\rm ev}^{\rm IR} = 300$
$N_{\rm ev}^{\rm IR} = 400$
$N_{\rm ev}^{\rm IR} = 500$
$\langle V_k(t)V_k(0)\rangle$
$\langle A_k(t)A_k(0)\rangle$
$\langle T_{ik}(t)T_{ik}(0)\rangle$
$\langle V_0(t)V_0(0)\rangle$
$\langle A_0(t)A_0(0)\rangle$
$\langle T_{0i}(t)T_{0i}(0)\rangle$
$\sigma_{\rm stoch}/\sigma_{\rm LMA}$
t [fm]

exLMA gain



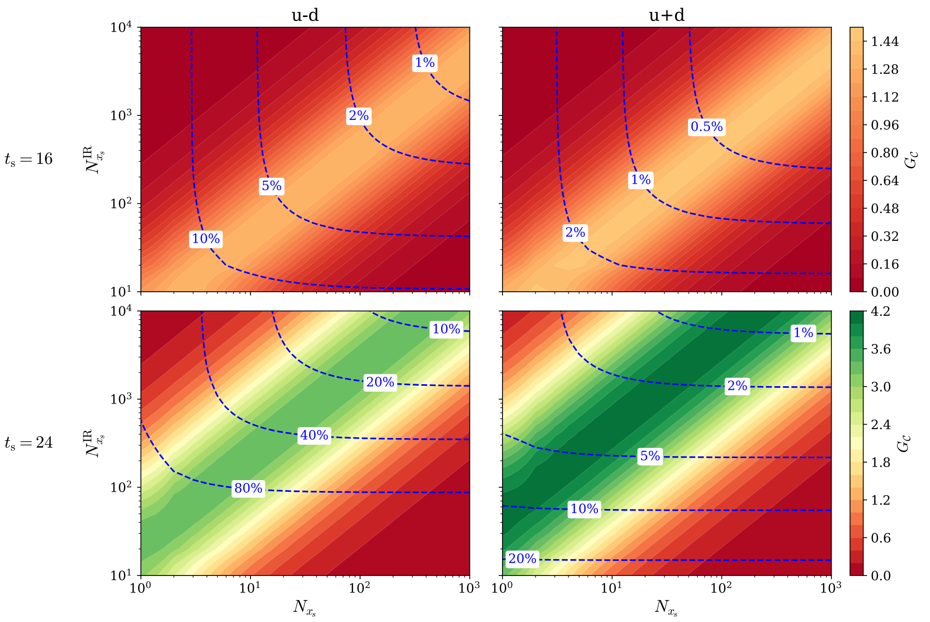
$C_\eta^{\mathrm{LMA}}(t)$
$C_\eta^{\mathrm{res}}(t)$
$C^{\mathrm{MG}}(t)$
$\langle V_k(t)V_k(0)\rangle$
$\langle A_k(t)A_k(0)\rangle$
$\langle T_{ik}(t)T_{ik}(0)\rangle$
$\langle V_0(t)V_0(0)\rangle$
$\langle A_0(t)A_0(0)\rangle$
$\langle T_{0i}(t)T_{0i}(0)\rangle$
$\mathrm{Err}[C(t)]/\mathrm{Err}[C_\eta(t)]$
$\sigma_{\mathrm{stoch}}/\sigma_{\mathrm{LMA}}$
t [fm]

mgLMA gain



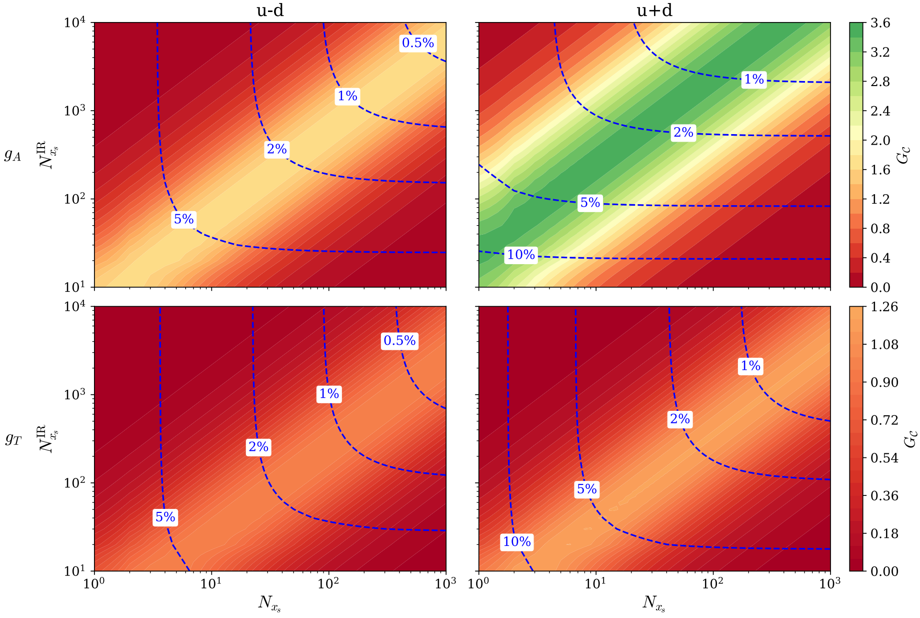
nucleon m_{eff}
factor 3 in volume
B48 vs B64

B64 saturation expected between 1000-1500



u-d
u+d
$t_s = 16$
$t_s = 24$
$N_{x_s}^{\mathrm{IR}}$
N_{x_s}
$G_{\mathcal{C}}$
1%
2%
5%
10%
0.5%
1%
2%
10%
20%
40%
80%
1%
2%
5%
10%
20%

gS cost gain



gA and gT cost gain

the multigrid approach

1. constructing a coarse operator through prolongation and restriction operators

$$\boldsymbol{D_c \equiv RDP}$$

- preserve the identity $\mathbb{1}_c \equiv R\mathbb{1}P$
- D_c retains a nearest-neighbour structure
- preserve γ_5-hermiticity $\longrightarrow$ $R = P^\dagger$
- for TM-fermios γ_5-compatibility

2. construct a projector acting on the fine space $\mathbb{P}_{\text{MG}} \equiv PD_c^{-1}RD$

$$\boldsymbol{S} = \mathbb{P}_{\mathbf{MG}}\boldsymbol{S} + (\mathbb{1} - \mathbb{P}_{\mathbf{MG}})\,\boldsymbol{S} \qquad \Longrightarrow \qquad \boldsymbol{S}^{\mathbf{MG}} = \mathbb{P}_{\mathbf{MG}}\boldsymbol{S} \;=\; PD_c^{-1}R$$

3. direct connection to exact deflation if P and R are constructed from eigenvectors of the Dirac operator

$$\boldsymbol{P}{=}\boldsymbol{V}^{\mathbf{IR}} \qquad \Longrightarrow \qquad \boldsymbol{D_c} = \left(\boldsymbol{V}^{\mathbf{IR}}\right)^\dagger \boldsymbol{D}\boldsymbol{V}^{\mathbf{IR}} = \Lambda^{\mathbf{IR}} \qquad \Longrightarrow \qquad \boldsymbol{S}^{\mathbf{MG}} = \boldsymbol{S}^{\mathbf{IR}}$$