Towards the proton mass decomposition from lattice QCD

University of Cyprus

Constantia Alexandrou

The Cyprus Institute

Extended Twisted Mass Collaboration

STIMULATE
European Joint Doctorates

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Extended Twisted Mass Collaboration (ETMC)

- **Gauge ensembles are generated by ETMC**
  We have now ensembles generated with 2+1+1 flavours at physical values of the light, strange and charm quark masses (physical point)

- **We perform an analysis of these ensembles for various observables**

Collaborators on the topic of this talk:

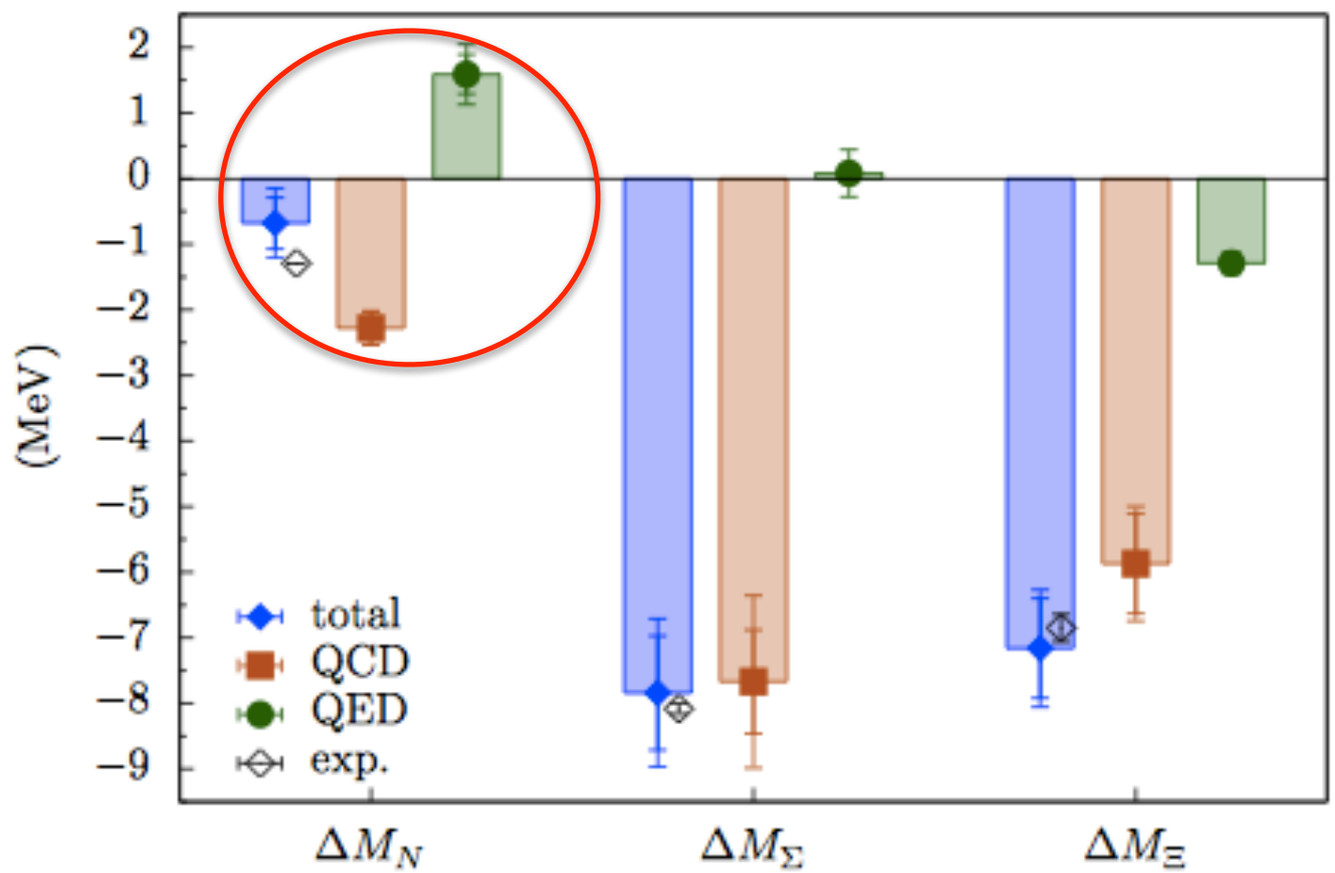
- *S. Bacchio, University of Cyprus & The Cyprus Institute*
- *M. Constantinou, Temple University*
- *M. Dalla Brida, University of Milano*
- *J. Finkenrath, The Cyprus Institute*
- *K. Hadjiyiannakou, The Cyprus Institute*
- *K. Jansen, DESY-Zeuthen*
- *G. Koutsou, The Cyprus Institute*
- *H. Panagopoulos, University of Cyprus*
- *G. Spanoudes, University of Cyprus*
- *S. Yamamoto, The Cyprus Institue*

Outline

- Decomposition of proton mass
- Lattice calculation of various components - what must be done to get results at ~1-2% accuracy as per X. Ji's wish
- Renormalisation
- Results
- Future prospectives

Insights on hadron mass splittings from lattice QCD

1+1+1+1 and QED



BMW Collaboration, Sz. Borsanyi et al., Science 347 (2015)

- **Mass splitting due to isospin and QED calculated in lattice QCD reproduces the neutron-proton mass splitting**

Energy and momentum tensor

Energy and momentum tensor taken to be symmetric

$$T^{\mu\nu} = \bar{T}^{\mu\nu} + \hat{T}^{\mu\nu}$$

X. Ji, PRD 52, 271,1995, hep-ph/9502213

Traceless and trace parts

❋Physical matrix elements of the traceless part can be written in terms of two gauge invariant terms

$$\bar{T}^{\mu\nu} = \bar{T}_q^{\mu\nu} + \bar{T}_g^{\mu\nu}$$

$$\bar{T}_q^{\mu\nu} = \bar{\psi} i \gamma^{\{\mu} \overleftrightarrow{D}^{\nu\}} \psi \,, \qquad \bar{T}_g^{\mu\nu} = F^{\{\mu\rho} F^{\nu\}}{}_{\rho}$$

Symmetrisation over indices and subtraction of trace

Scheme and scale dependent

quark and gluon momentum

Energy and momentum tensor

X. Ji, PRD 52, 271,1995, hep-ph/9502213

❋**Hadron matrix elements of the trace part can be written as**

$$\hat{T}^{\mu\nu} = \hat{T}^{\mu\nu}_m + \hat{T}^{\mu\nu}_a$$

quark mass and trace anomaly contributions

Renormalisation group invariants:

$$\hat{T}^{\mu\nu}_m = \frac{1}{4} g^{\mu\nu} m \bar{\psi}\psi \qquad \hat{T}^{\mu\nu}_a = \frac{1}{4} g^{\mu\nu} \left(\gamma_m m \bar{\psi}\psi + \frac{\beta(g)}{2g} F^{\rho\sigma} F_{\rho\sigma} \right)$$

❋**Decomposition into gluonic and quark contributions is scheme and scale dependent**

For other decompositions see e.g. talk by M. Constantinou

Nucleon mass decomposition in lattice QCD

❋ In Euclidean space and in the rest frame of the nucleon we have

$$M = -\langle T^{44} \rangle = \langle H_q \rangle(\mu) + \langle H_g \rangle(\mu) + \langle H_m \rangle + \frac{1}{4}\langle H_a \rangle$$

$$M = -\langle T^{\mu\mu} \rangle = \langle H_m \rangle + \langle H_a \rangle$$

$$H_m = \sum_q \int d^3x\, m_q \bar{\psi}_q \psi_q$$

$$H_q = \sum_q \int d^3x\, \bar{\psi} \vec{D}.\vec{\gamma} \psi$$

$$H_g = \frac{1}{2} \int d^3x \left(B^2 - E^2\right) \psi$$

$$H_a = \frac{-\beta}{g} \int d^3x \left(E^2 + B^2\right) + \gamma_m H_m$$

X. Ji, PRD 52, 271,(1995)

Yi-Bo Yang et al., PRL 121, 212001 (2018)

❋ Decompose mass into sum of four terms

Quark mass: $M_m = \langle H_m \rangle = \sum_q \sigma_q$ ← Nucleon σ-terms

Quark energy: $M_q = \langle H_q \rangle = \frac{3}{4}\left(M \sum_q \langle x \rangle_q - \langle H_m \rangle \right)$

Gluon energy: $M_g = \langle H_g \rangle = \frac{3}{4} M \langle x \rangle_g$

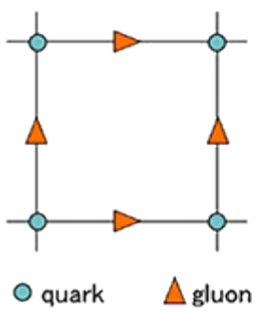
Renormalised momentum fraction

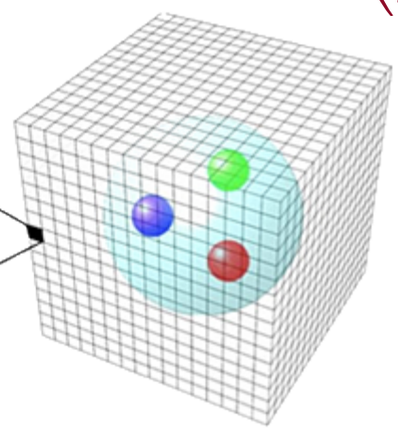
Trace anomaly term: $M_a = \frac{1}{4}\langle H_a \rangle = \frac{1}{4}\left(M - \sum_q \sigma_q \right)$

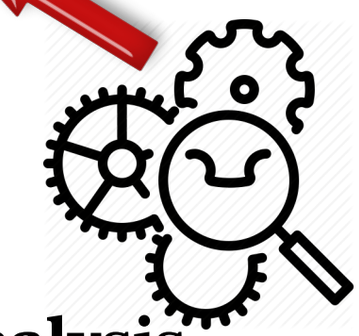
→ $\langle x \rangle_{q,g}$ and σ_q calculable within lattice QCD

Computation of hadron structure observables

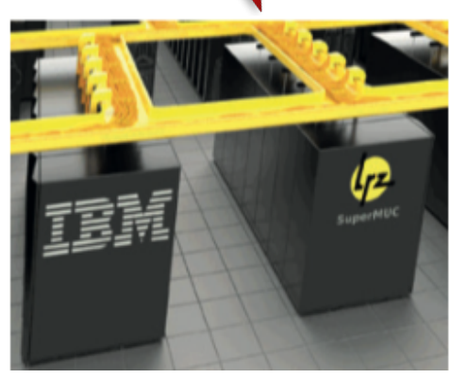
$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}[U] \mathcal{O}(D^{-1}[U], U) \left(\prod_{f=u,d,s,c} Det(D[U]) \right) e^{-S[U]}$$







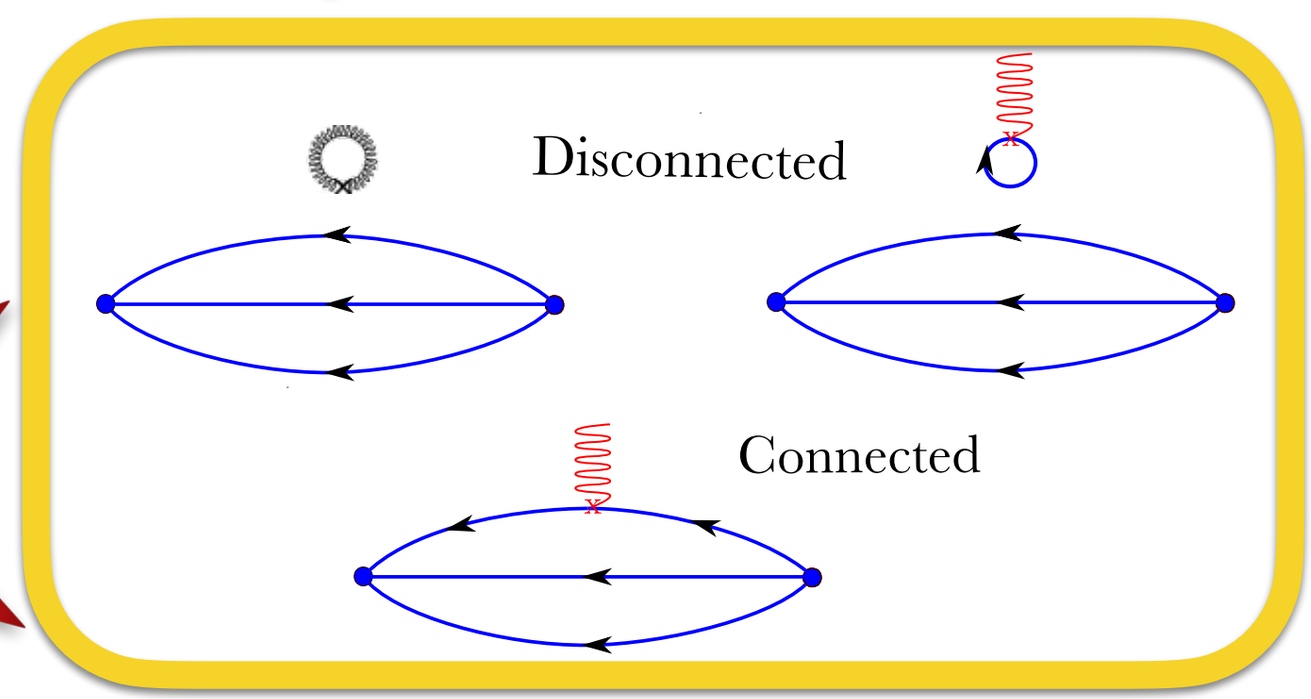
Simulation of gauge configurations U



Quark propagators

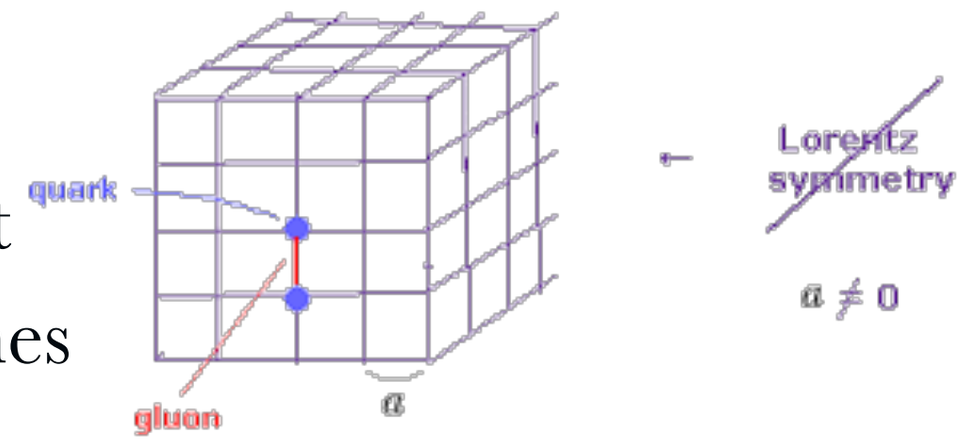
contractions

Data Analysis



Systematics & Challenges

- **Discretisation effect:** Continuum limit —> need simulations for at least 3 lattice spacings



- **Finite volume effects:** Infinite volume limit —> need simulations for at least 3 volumes
- **Simulations directly at the physical point**
  Systematic effects from chiral extrapolation are eliminated
- **Ground-state identification**
  Cross-check (one-, two- and three-state fits, summation)
- **Renormalisation**
  Non-perturbatively with improvements e.g using perturbative subtraction of lattice artefacts. Challenging for the trace anomaly

to obtain ~1-2% accuracy we need to have a good control of these systematics

Lattice ensemble at physical pion mass

N_f=2+1+1 twisted mass fermions with a clover term

- Lattice size 64^3 x 128
- a=0.08 fm
- m_π=139 MeV
- Lm_π=3.6

Mass of nucleon extracted from two-point function

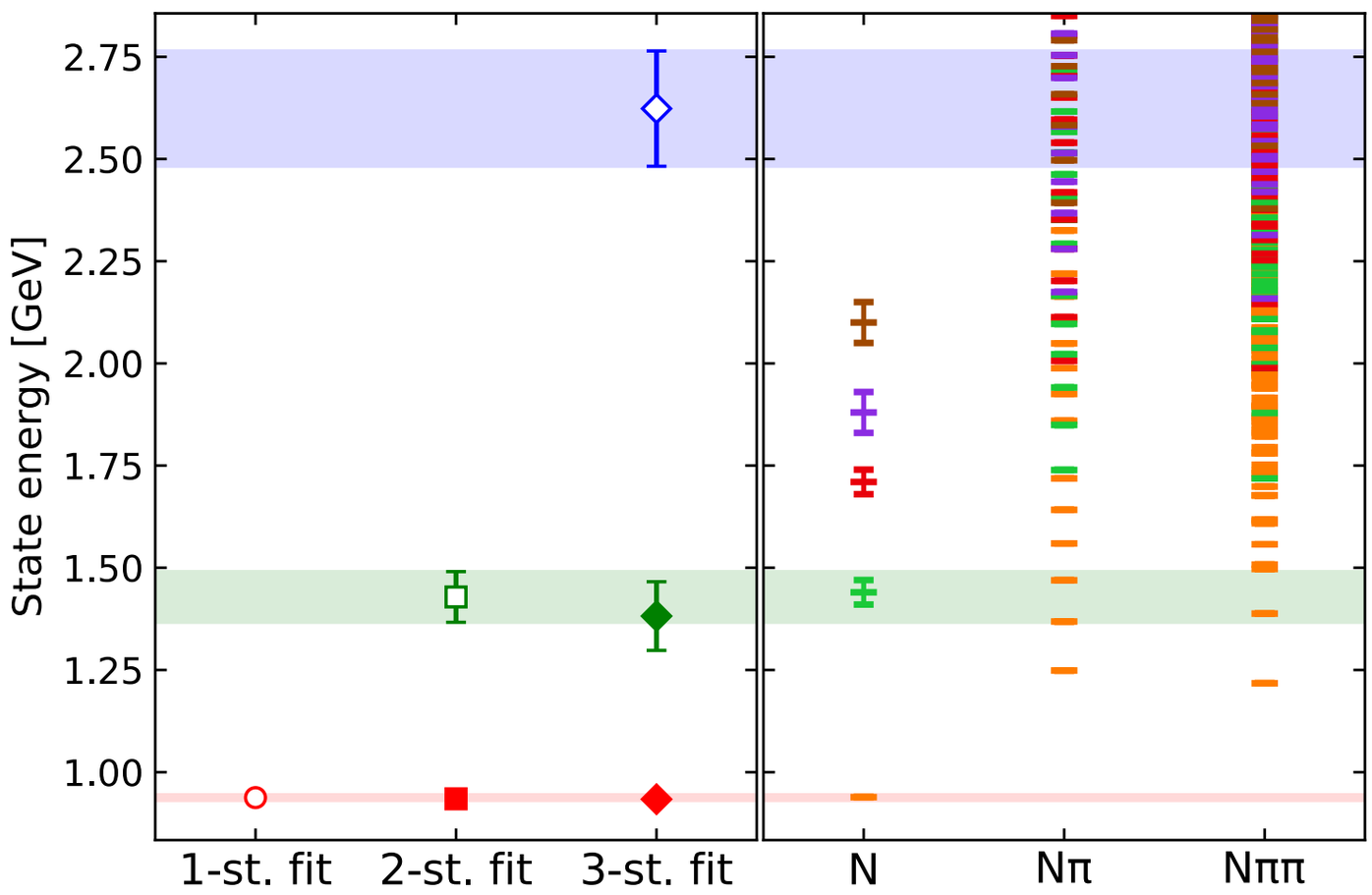
$$C_{2\mathrm{pt}}(\Gamma_0;\vec{p}=\vec{0},t_s)=\sum_{\vec{x}_s}\mathrm{Tr}\left[\langle\Gamma_0 J_N(t_s,\vec{x}_s)\bar{J}_N(t_0,\vec{x}_0)\rangle\right]$$

Nucleon mass

Mass of nucleon extracted from two-point function

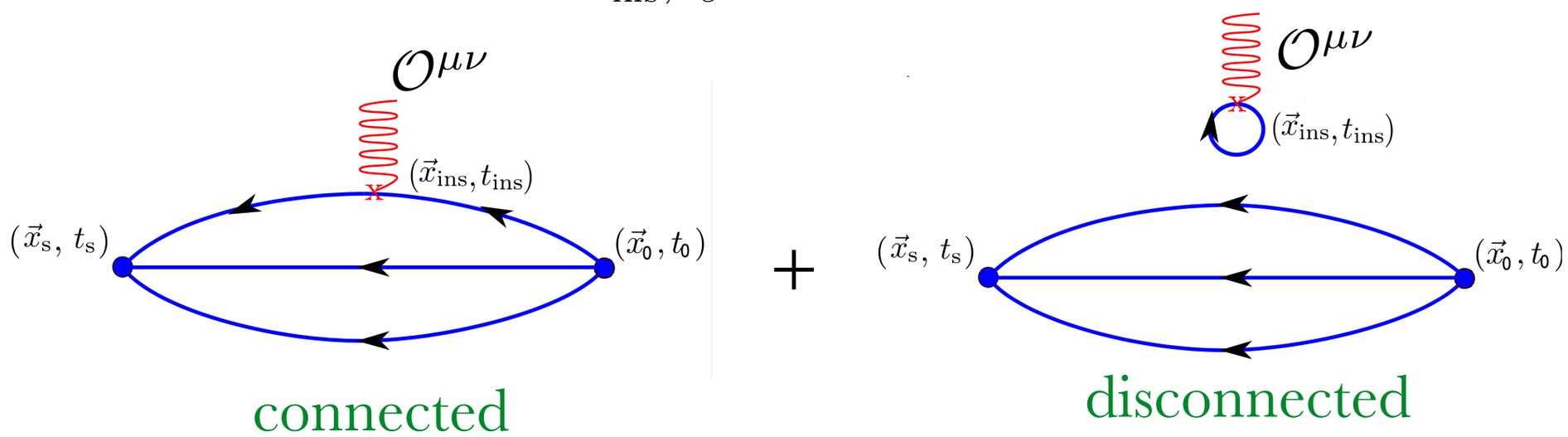
In a real computation t_s finite but large

$$C_{2\mathrm{pt}}(\Gamma_0;\vec{p}=\vec{0},t_s)=\sum_{\vec{x}_s}\mathrm{Tr}\left[\langle\Gamma_0 J_N(t_s,\vec{x}_s)\bar{J}_N(t_0,\vec{x}_0)\rangle\right]=\sum_j A_j e^{-M_j t_s}\overset{t_s\to\infty}{\longrightarrow} M$$



Nucleon matrix elements

$$C^{\mu\nu}_{3\mathrm{pt}}(\Gamma;\vec{q}=0,t_s,t_{\mathrm{ins}}) = \sum_{\vec{x}_{\mathrm{ins}},\vec{x}_s} \mathrm{Tr}\left[\langle \Gamma J_N(t_s,\vec{x}_s)\mathcal{O}^{\mu\nu}(t_{\mathrm{ins}},\vec{x}_{\mathrm{ins}})\bar{J}_N(t_0,\vec{x}_0)\rangle\right]$$



❋ Identification of nucleon matrix element *M* (t_0=0)

Plateau and two-state fit:

$$R^{\mu\nu}(\Gamma;\vec{q}=\vec{0},t_s,t_{\mathrm{ins}}) = \frac{C^{\mu\nu}_{3\mathrm{pt}}(t_s,t_{\mathrm{ins}})}{C_{2\mathrm{pt}}(\Gamma_0,t_s)} \longrightarrow \boxed{\mathcal{M}} + \mathcal{O}(e^{-\Delta E(t_s-t_{\mathrm{ins}})}) + \mathcal{O}(e^{-\Delta E t_{\mathrm{ins}}})$$

Included in the two-state fit

Summation:

$$\sum_{t_{\mathrm{ins}}=a}^{t_s-a} R^{\mu\nu}(\Gamma;\vec{q}=\vec{0},t_s,t_{\mathrm{ins}}) \longrightarrow c + \boxed{\mathcal{M}} t_s + \mathcal{O}(e^{-\Delta E t_s})$$

L. Maiani, G. Martinelli, M. L. Paciello, and B. Taglienti, Nucl. Phys., B293: 420, 1987

Momentum fraction

N_f=2+1+1 twisted mass fermions with a clover term

- Lattice size 64^3 x 128
- a=0.08 fm
- m_π=139 MeV
- Lm_π=3.6

Statistics for connected contribution

	t_s/a	$N_{\rm cnfs}$	$N_{\rm srcs}$	$N_{\rm meas}$
0.64 fm	8	750	1	750
	10	750	2	1500
	12	750	4	3000
	14	750	6	4500
	16	750	16	12000
	18	750	48	36000
1.6 fm	20	750	64	48000

Needed for studying excited states

Increase statistics to keep approx. constant error

Statistics for disconnected contribution

Use hierarchical probing

no. of Hadamard vectors

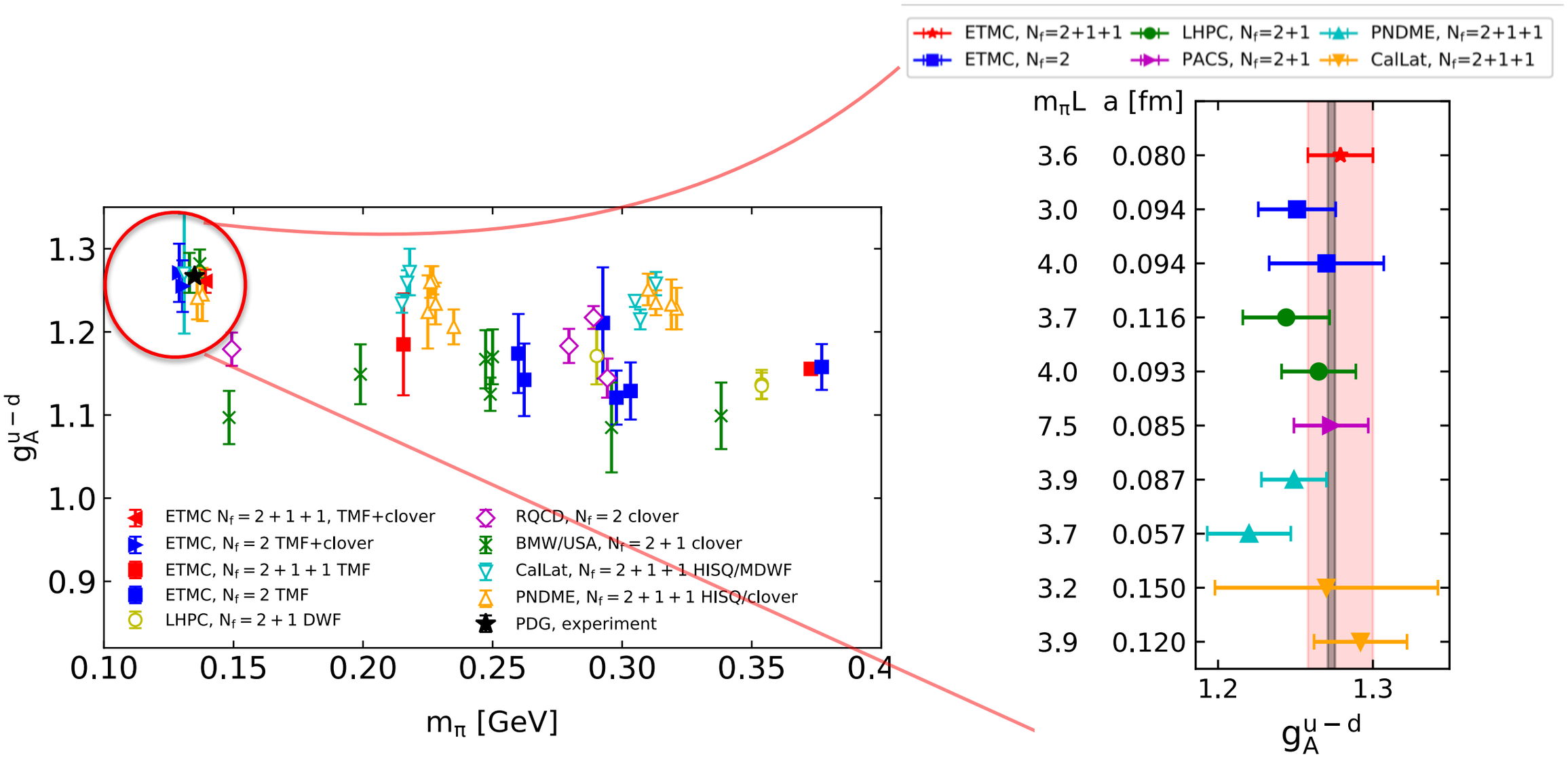
2pt	(u+d)-quark loop	s-quark loop	c-quark loop
600000	750×512 + deflation of 200 modes	750×512	9000×32

no. of stochastic vectors

Nucleon axial charge

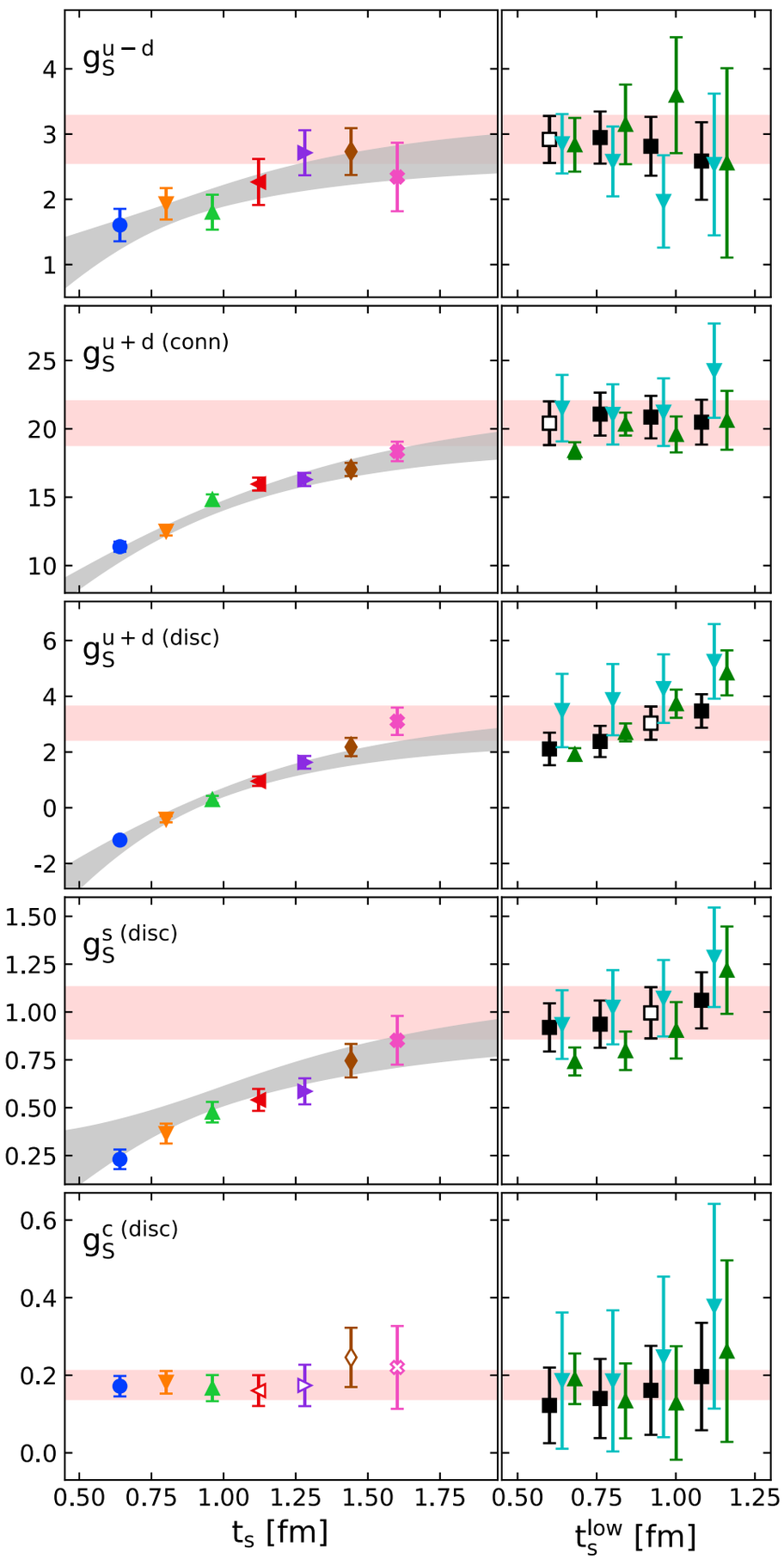
Comparison among lattice collaborations

- A number of calculations at the physical point
- Agreement with experimental value



Benchmark for lattice QCD computations of matrix elements

Nucleon σ-terms



❋Matrix element of scale operator

$$\sigma_q = m_q \underbrace{\langle N|\bar{\psi}_q \psi_q|N\rangle}_{g_S}, \quad q = u, d, s, c$$

❋ For u and d we have both connected and disconnected contributions

C. Alexandrou et al., PRD 102, 054517 (2020), arXiv: 1909.00485

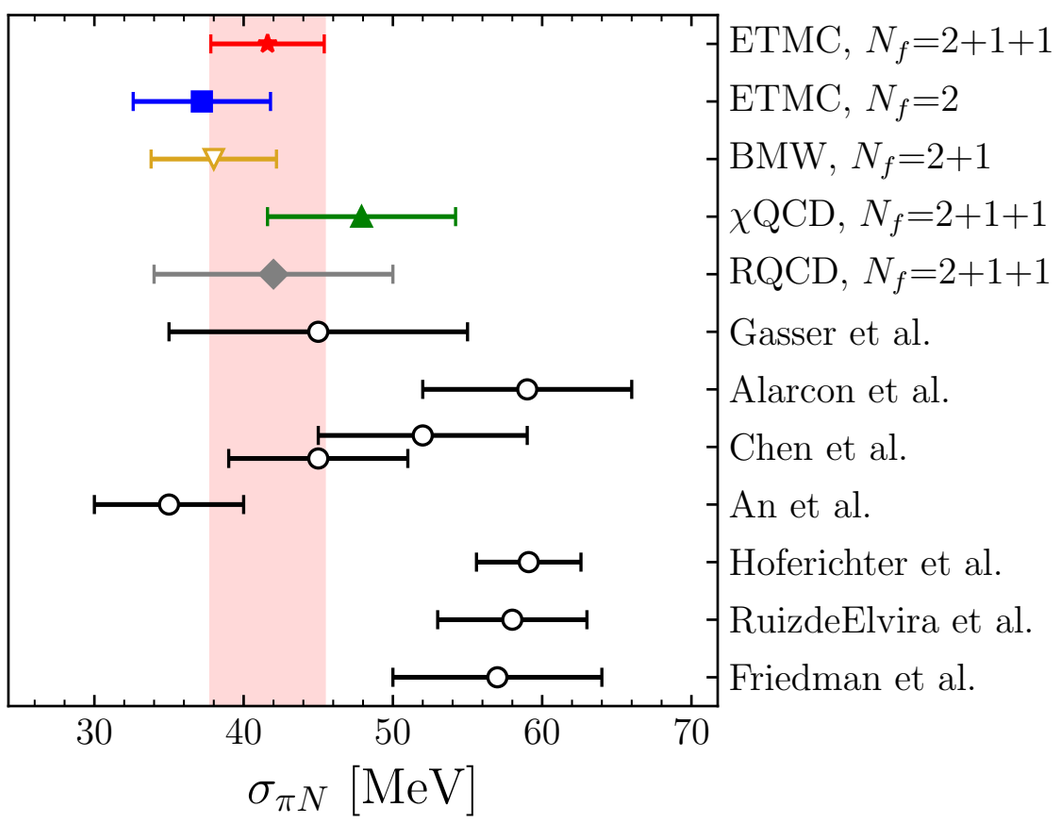
Nucleon σ-terms

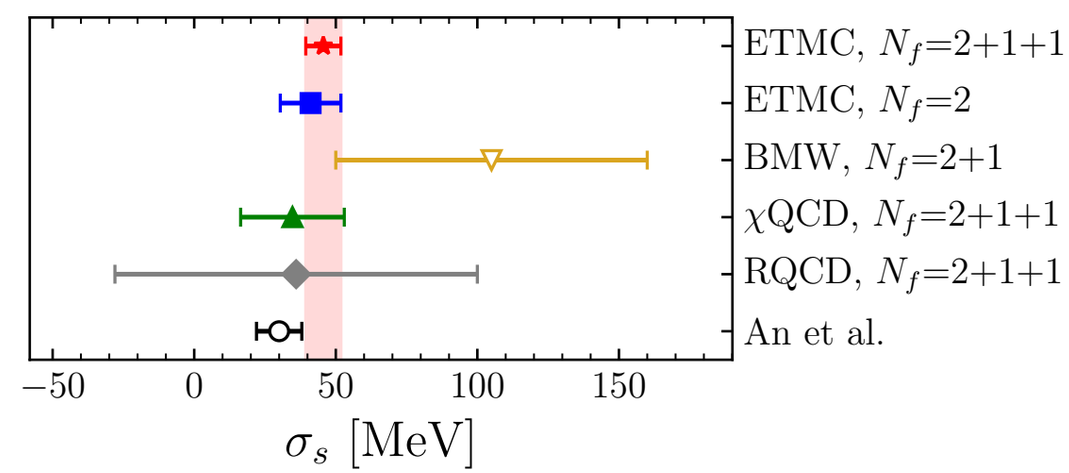
- Can extract directly at the physical point σ_q for u,d,s,c

Our values

	$u+d$	s	c
σ [MeV]	41.6(3.8)	45.6(6.2)	107(22)

In agreement with the value from χQCD





Nucleon momentum fraction

$$\langle N(p',s')|\mathcal{O}_{\rm V}^{\mu\nu}|N(p,s)\rangle = \bar{u}_N(p',s')\left[A_{20}(q^2)\gamma^{\{\mu P^\nu\}} + B_{20}(q^2)\frac{i\sigma^{\{\mu\alpha}q_\alpha P^{\nu\}}}{2m} + C_{20}(q^2)\frac{q^{\{\mu}q^{\nu\}}}{m}\right]u_N(p,s)$$

$$\mathcal{O}_{\rm V}^{\mu\nu} = \bar{q}\gamma^{\{\mu}iD^{\nu\}}q$$

$$J_q = \frac{1}{2}\left[A_{20}^q(0) + B_{20}^q(0)\right]$$

$$\langle x\rangle = A_{20}(0)$$

Ground-state dominance

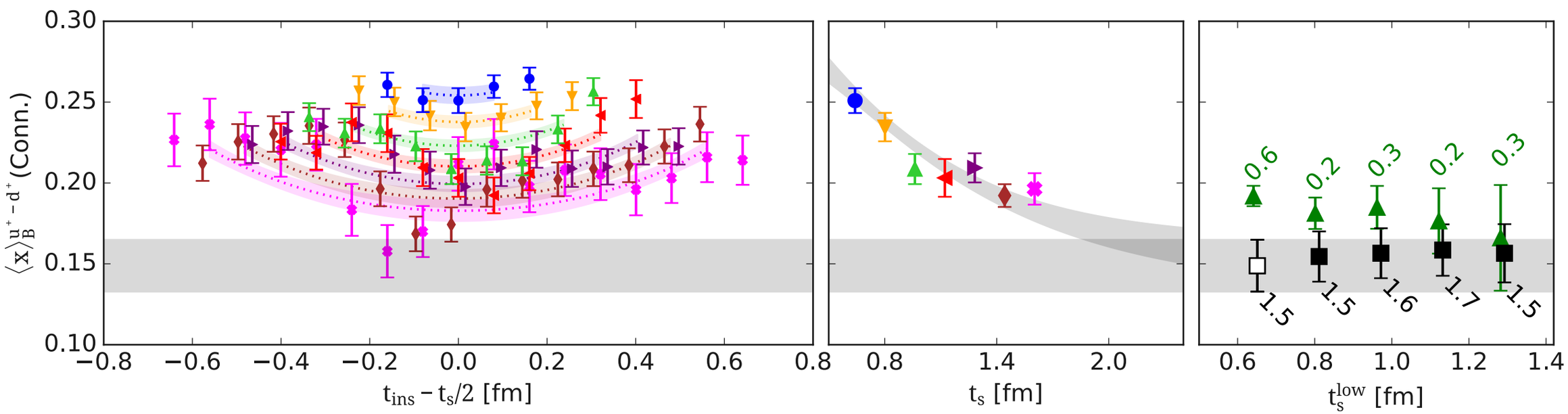
- Plateau - one state
- Two- state fits
- Summation

Isovector

$$\frac{C_{3pt}}{C_{2pt}}$$

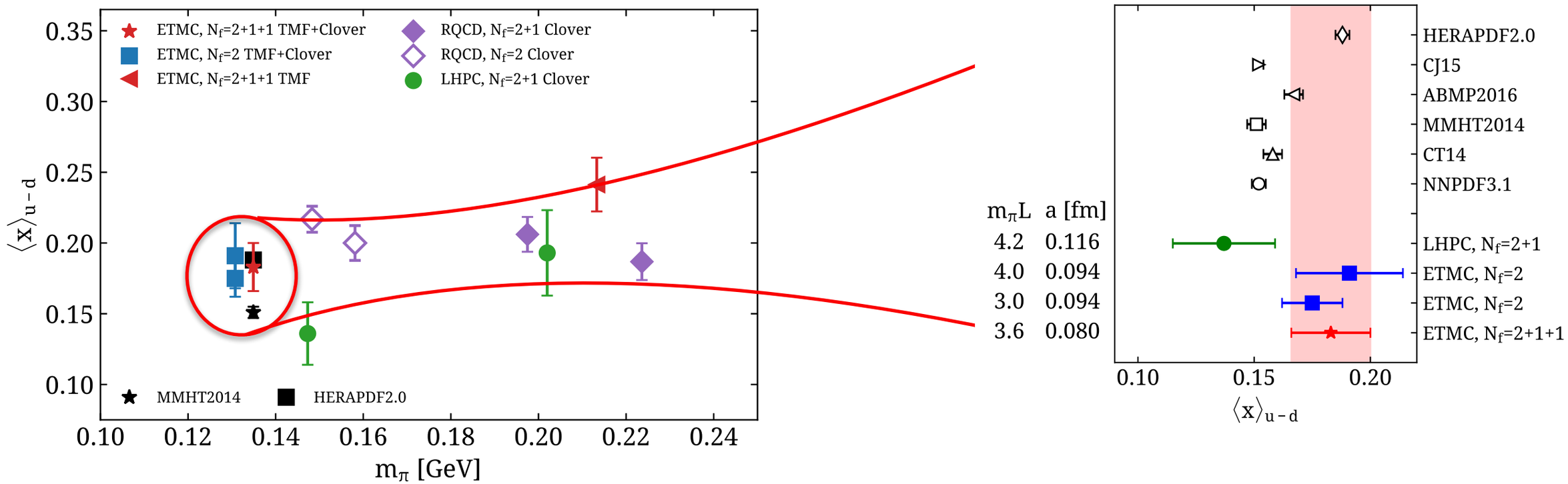
Plateau values

- 2 state fits
- summation



C. Alexandrou et al., PRD 101, 094513 (2020), arXiv: 2003.08486

Nucleon isovector momentum fraction results

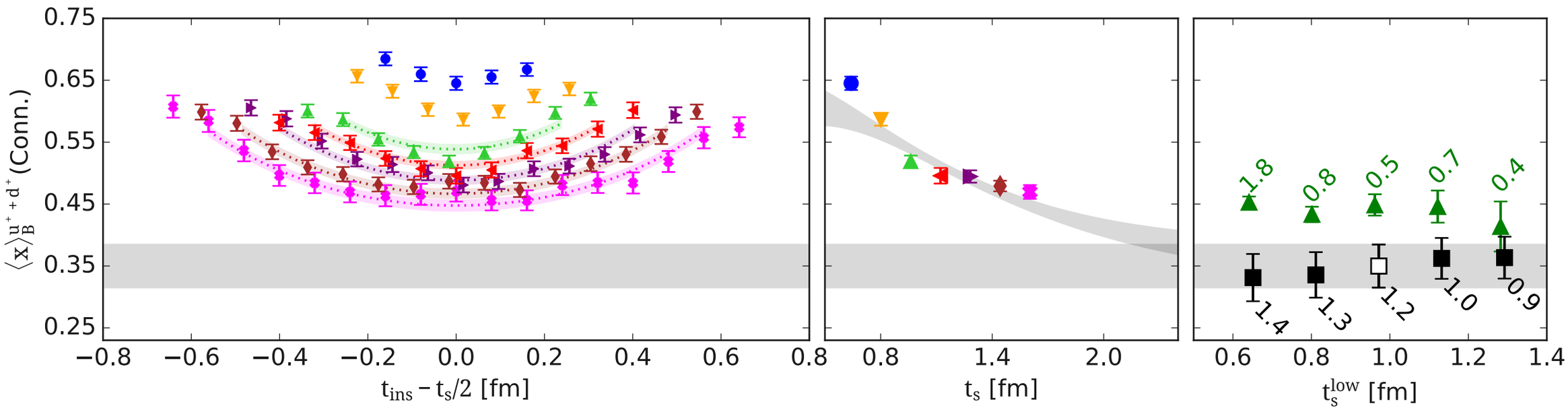


Comparison among lattice collaborations

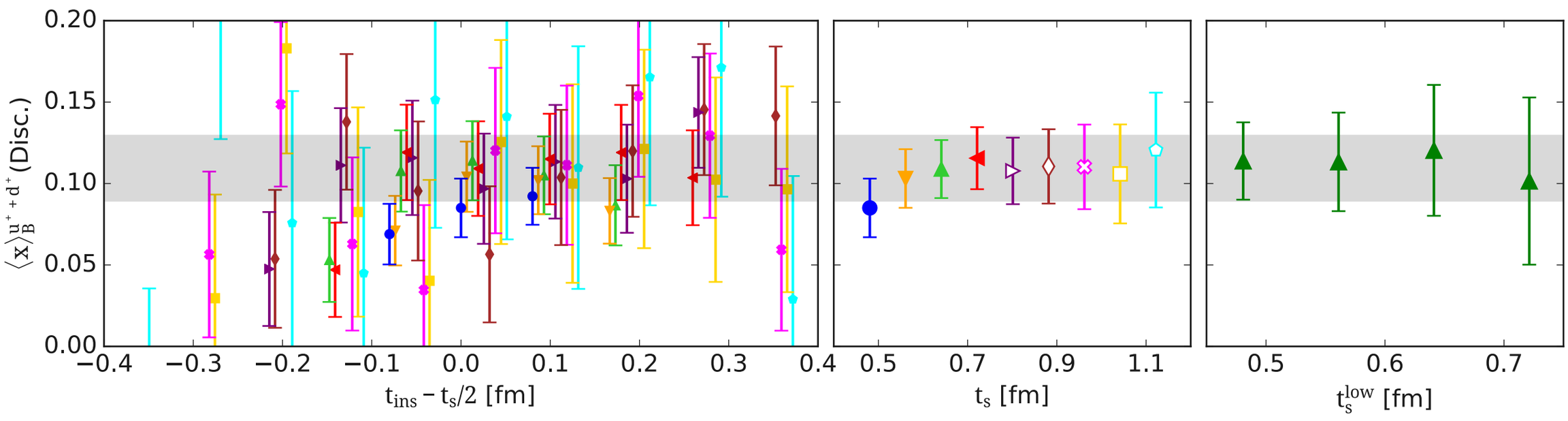
- Only a few calculations directly at the physical point
- Phenomenological determinations yield different values with spread compatible with the statistical error of lattice QCD

Nucleon isoscalar momentum fraction

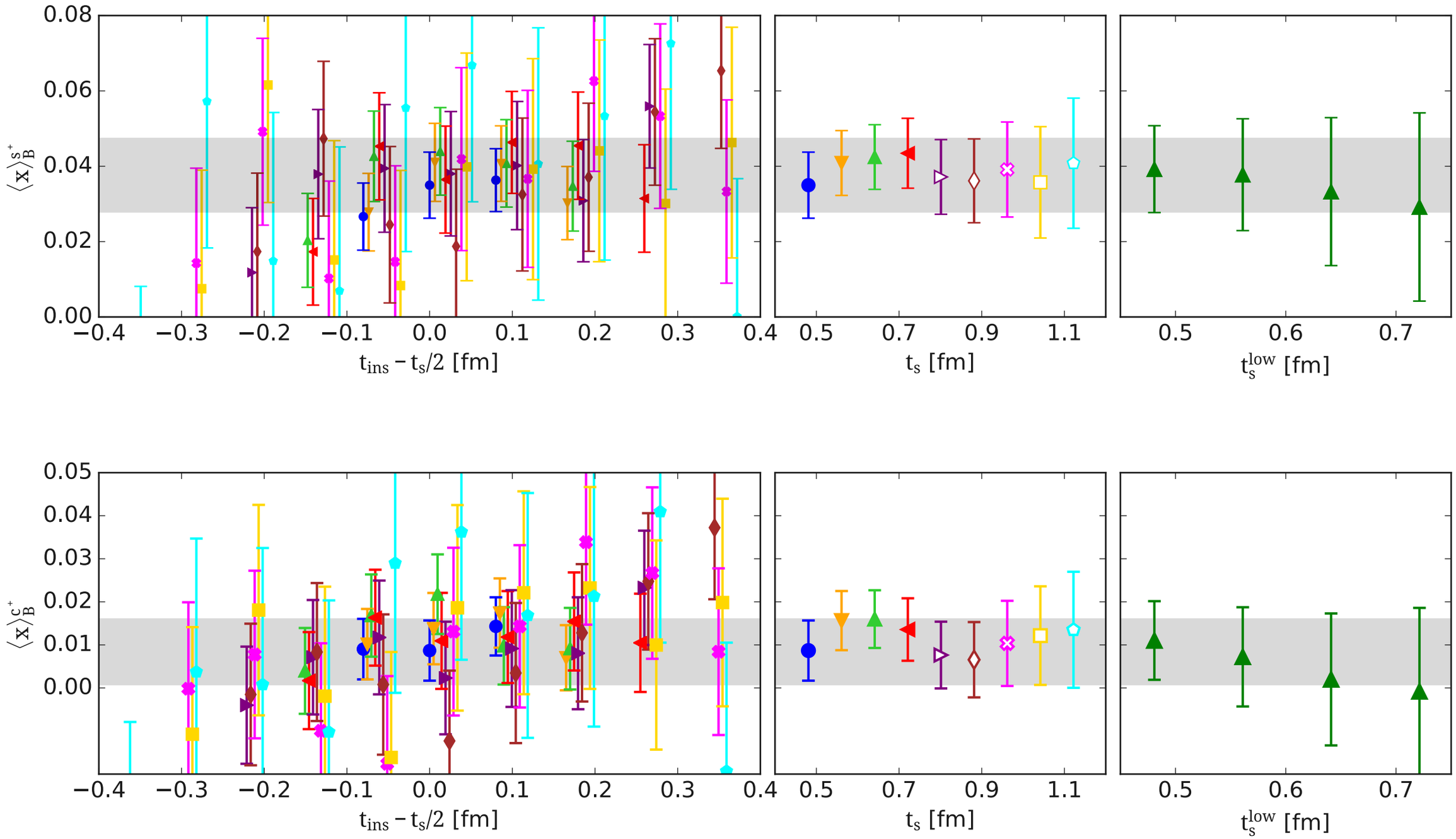
Connected



Disconnected



Charm and strange <x>$_q$



❋Non-zero signal for sea quark contribution

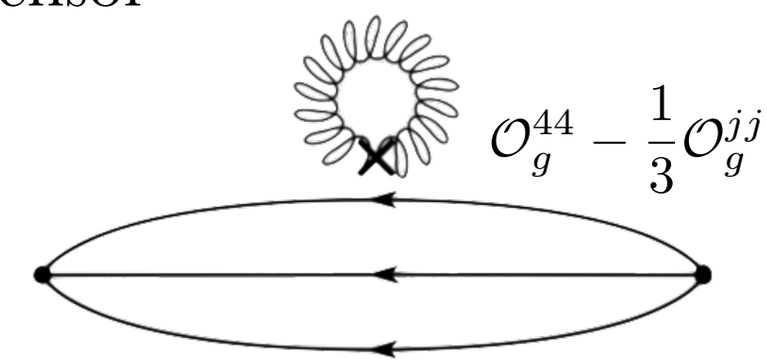
Gluon momentum fraction

$$\langle x \rangle_g = A^g_{20}(0)$$

$$\mathcal{O}^{\mu\nu}_g = 2\mathrm{Tr}\left[G^{\mu\rho}G^{\mu\rho}\right] \longleftarrow$$ Field strength tensor

In the rest frame of the nucleon

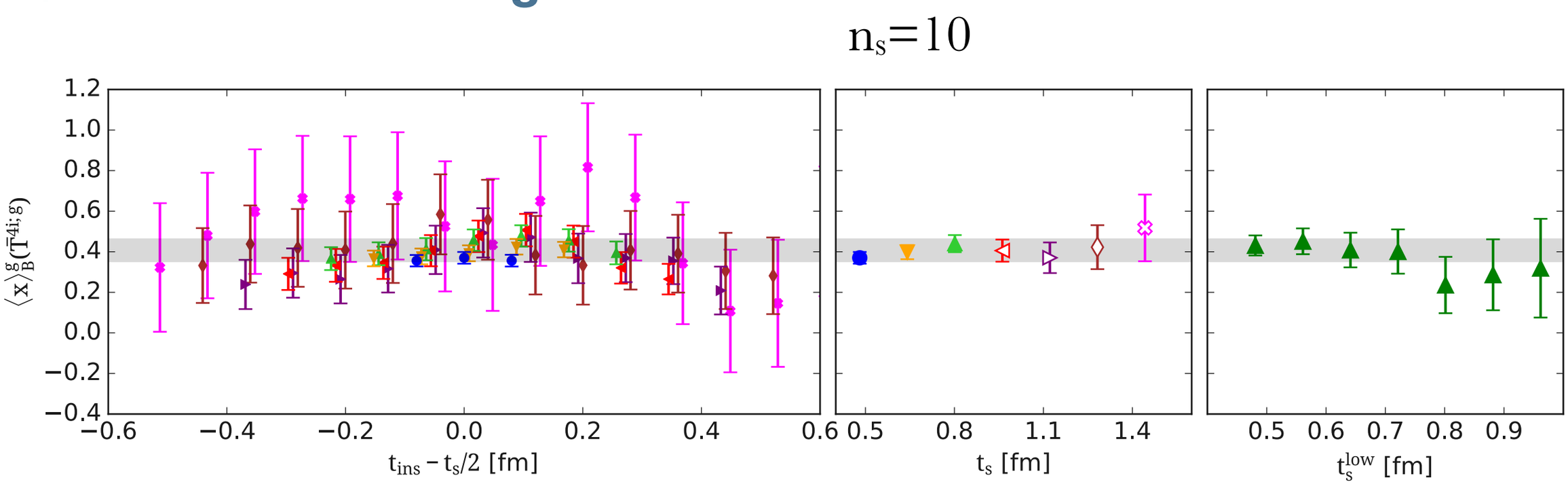
$$\frac{\langle N|\mathcal{O}^{44}_g - \frac{1}{3}\mathcal{O}^{jj}_g|N\rangle}{\langle N|N\rangle} = -2m_N < x >_g$$



In a moving frame

$$\frac{\langle N|\mathcal{O}^{4i}_g|N\rangle}{\langle N|N\rangle} = p_i < x >_g$$

✺Use stout smearing to reduce UV noise



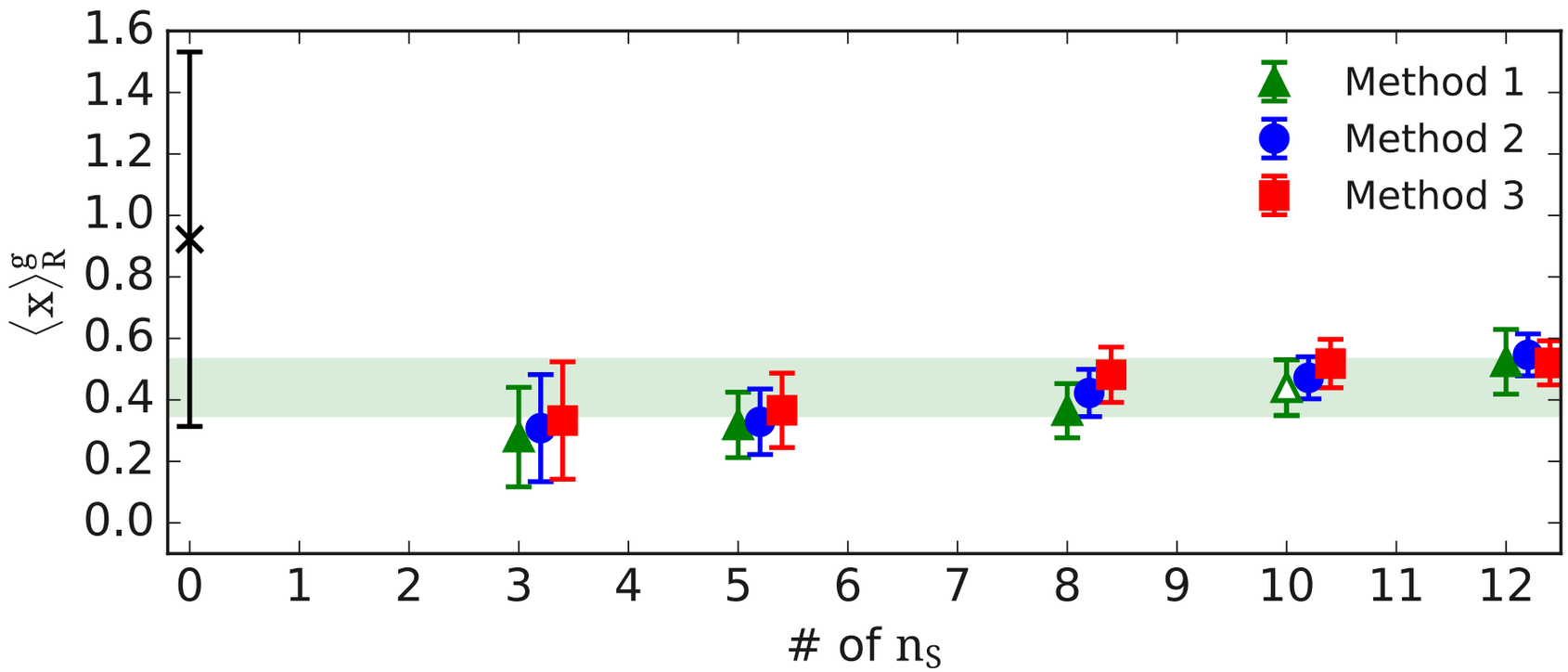
Excited state contributions are small for $<x>_g$

Renormalisation of gluon momentum fraction

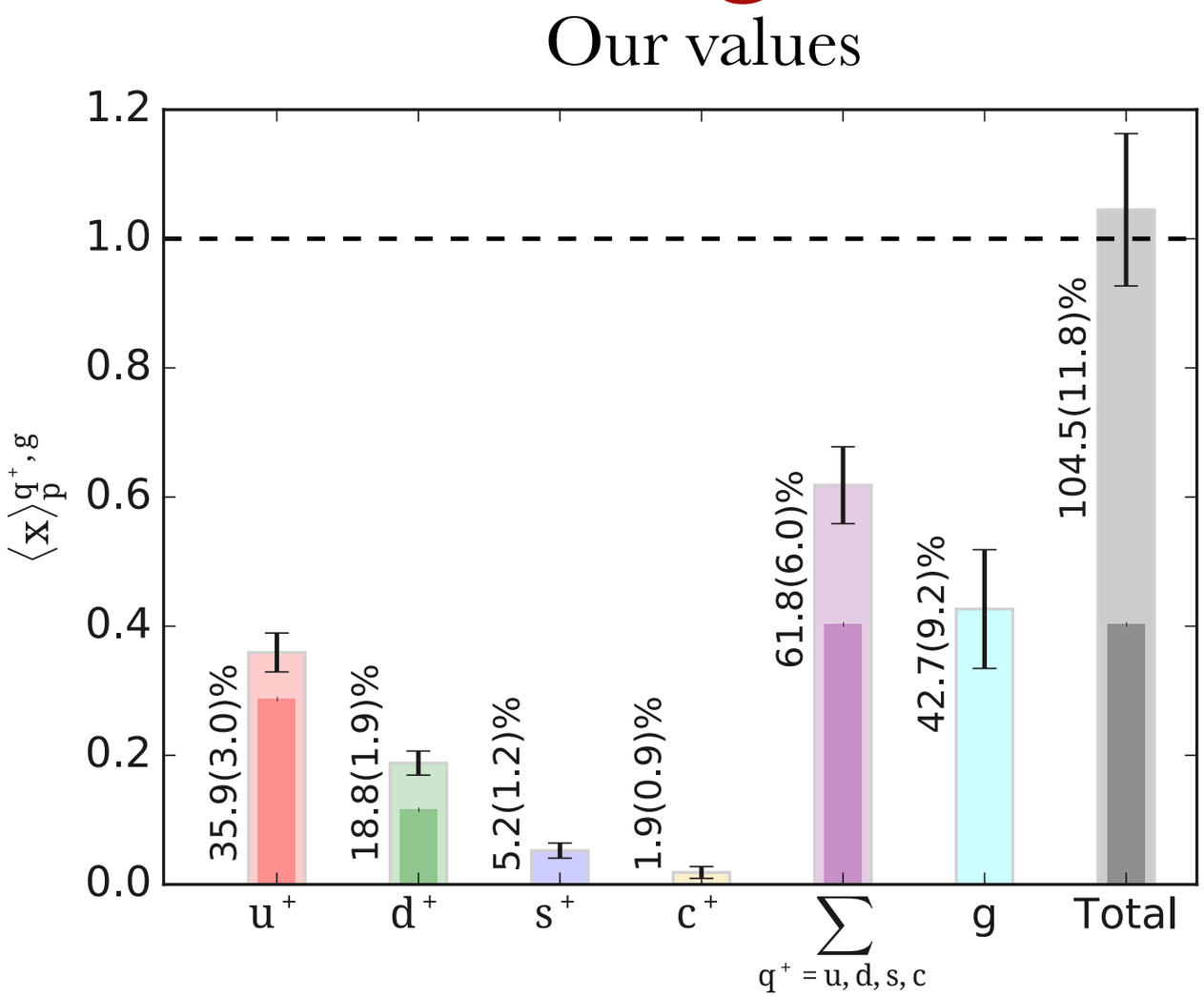
- There is mixing with quark momentum fraction —> need 2x2 matrix
- We employ non-perturbative renormalisation —> use three approaches to compute Z_{gg}

$$\langle x \rangle_g^R = Z_{gg} \langle x \rangle_g^B + Z_{gq} \sum_q \langle x \rangle_q^B$$

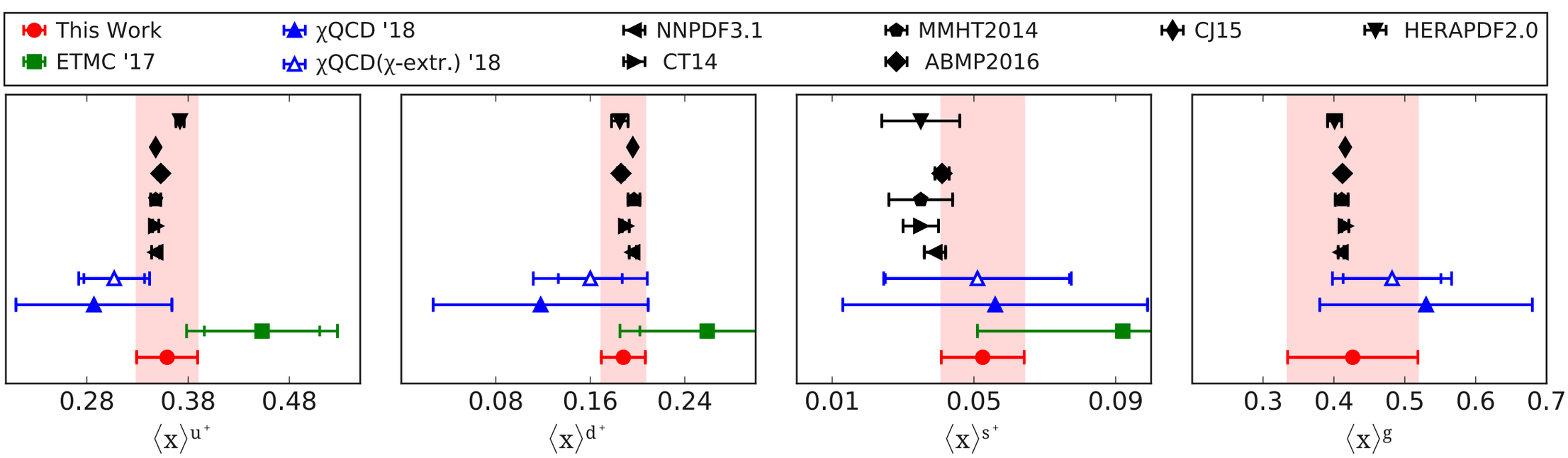
Computed in PT



Quark and gluon momentum fractions



- Good agreement with phenomenological extractions



Mass decomposition

❋ Use sum rule to obtain contribution of the trace anomaly

$$M = 0.939(4)\,\mathrm{GeV}$$

	$u+d$	s	c
σ [MeV]	41.6(3.8)	45.6(6.2)	107(22)

$$M_m = \langle H_m \rangle = \sum_q \sigma_q = 0.194(23)\,\mathrm{GeV}$$

	$\langle x \rangle$
u	0.359(30)
d	0.188(19)
s	0.052(12)
c	0.019(9)
g	0.427(92)
Tot.	1.045(118)

Use sum rule: to get M_a

$$M_a = \frac{1}{4}\langle H_a \rangle = \frac{1}{4}\left(M - \sum_q \sigma_q \right) = 0.186(23)\,\mathrm{GeV}$$

$$M_q = \langle H_q \rangle = \frac{3}{4}\left(M \sum_q \langle x \rangle_q - \langle H_m \rangle \right) = 0.290(38)\,\mathrm{GeV}$$

$$M_g = \langle H_g \rangle = \frac{3}{4} M \langle x \rangle_g = 0.301(65)$$

$\overline{MS}$ at $\mu = 2\,\mathrm{GeV}$

$$\boxed{M = M_q + M_g + M_m + M_a = 0.971(82)\,\mathrm{GeV}}$$

Mass decomposition

❋ Use sum rule to obtain contribution of the trace anomaly

$$M = 0.939(4)\,\mathrm{GeV}$$

	$u+d$	s	c
σ [MeV]	41.6(3.8)	45.6(6.2)	107(22)

	$\langle x \rangle$
u	0.359(30)
d	0.188(19)
s	0.052(12)
c	0.019(9)
g	0.427(92)
Tot.	1.045(118)

Instead use sum rule: to get M_a

$$M_a = M - M_q - M_g - M_m$$

$$M_m = \langle H_m \rangle = \sum_q \sigma_q = 0.194(23)\,\mathrm{GeV}$$

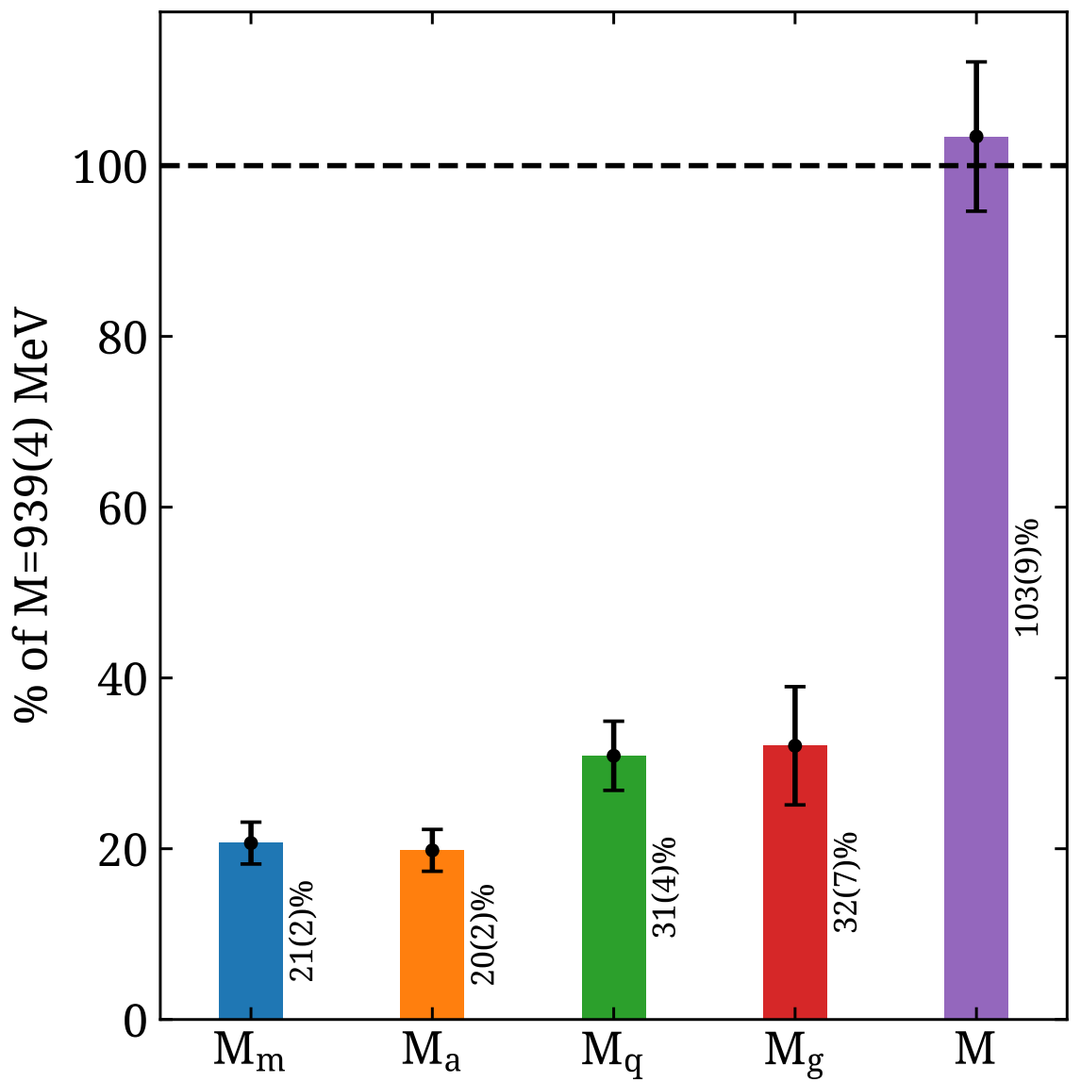
$$M_q = \langle H_q \rangle = \frac{3}{4}\left(M \sum_q \langle x \rangle_q - \langle H_m \rangle \right) = 0.290(38)\,\mathrm{GeV}$$

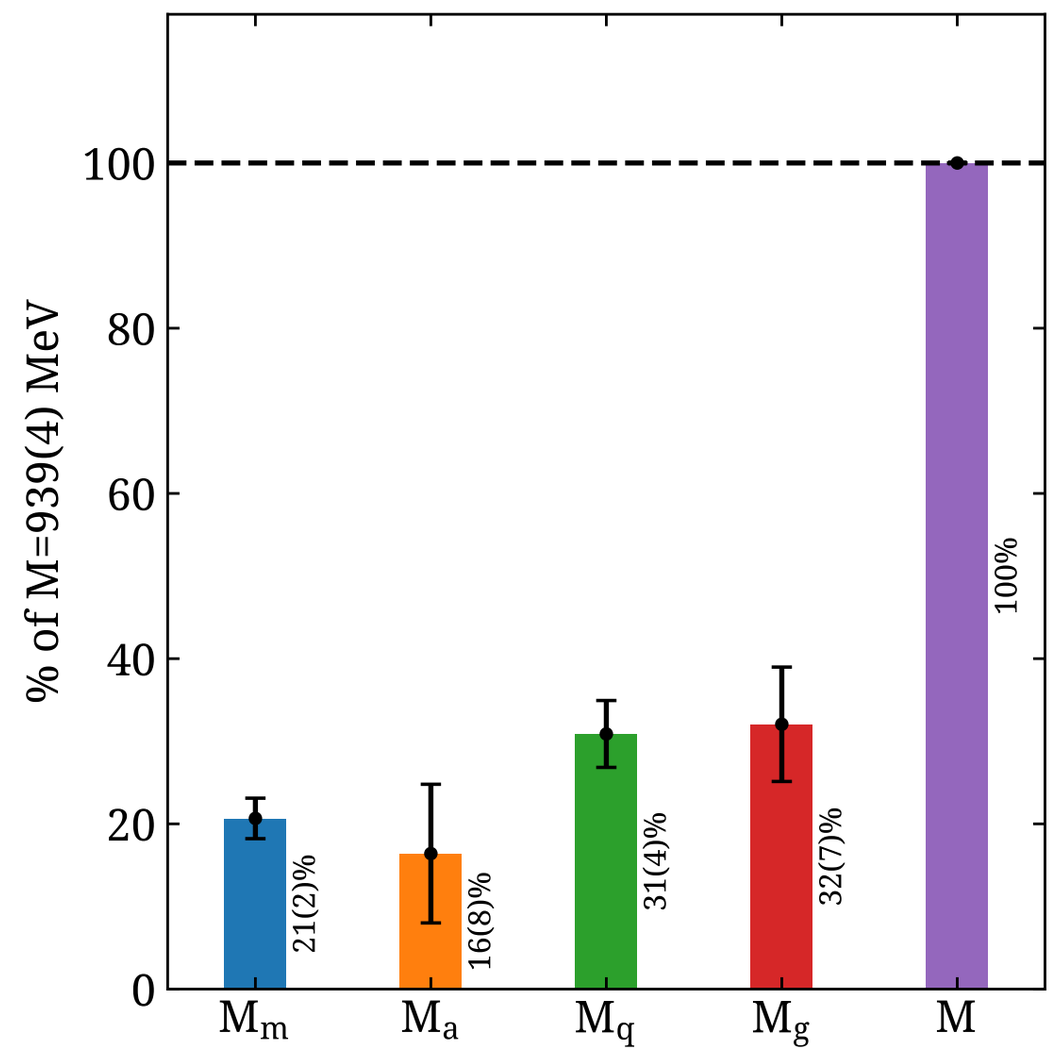
$$M_g = \langle H_g \rangle = \frac{3}{4} M \langle x \rangle_g = 0.301(65)$$

$\overline{MS}$ at $\mu = 2\,\mathrm{GeV}$

$$M_a = 0.154(79)\,\mathrm{GeV} \quad \text{compared to} \quad M_a = 0.186(23)\,\mathrm{GeV}$$

Mass decomposition of the proton





$\overline{MS}$ at $\mu = 2\,\mathrm{GeV}$

- M_a consistent using the two sum rules

Renormalisation of EMT

The components of the EMT have a complicated renormalization pattern involving mixing with several gauge-variant (GV) operators

S. Caracciolo et al., NPB 375 (1992) 195; G. Panagopoulos et al., arXiv:2010.02062

- **Although physical matrix elements of GV operators are zero, in a gauge-variant scheme such as RI/MOM, they contribute to the determination of the renormalization factors**

- **GV operators depend on ghost fields and gauge-fixing terms that are complicated to study non-perturbatively via lattice simulations**

- **Lattice QCD calculations use RI/MOM schemes with very promising outcomes, see e.g. recent results**

C. Alexandrou et al., PRD 96 (2017) 054503;Y.B. Yang et al., PRD 98 (2018) 074506; Y.B. Yang et al., PRL 121 (2018) 212001; P. Shanahan et al., PRD 99 (2019) 014511; C. Alexandrou et al., PRD 101 (2020) 094

$\Rightarrow$ **however, it is not a complete non-perturbative solution to the problem**

Gauge-invariant renormalisation scheme

Gauge-Invariant Renormalisation Scheme (GIRS)

- **We consider renormalisation conditions based on on-shell Green's functions of gauge-invariant operators in coordinate space extensions of which are used e.g. by the ALPHA collaboration and others**

K. Jansen (Alpha Collaboration), PLB 372 (1996) 275; V. Gimenez et al., PLB 598 (2004) 227

e.g. $\langle T^G_{\mu\nu}(x) T^F_{\mu\nu}(y) \rangle \quad (x \neq y)$

- **GIRS have several good features, e.g.**
  - **GV operators can be neglected in the renormalization procedure;**
  - **No need for gauge-fixing avoiding any issues with Gribov copies**
  - **Perturbative matching of GIRS and conversion to $\overline{\mathrm{MS}}$-scheme is doable,**

M. Costa, G. Karpasitis, G. Panagopoulos, H. Panagopoulos, T. Pafitis, A. Skouroupathis, G. Spanoudes

Coordinate gauge-invariant renormalisation scheme

✺ **First do for traceless components - Renormalisation problem on the lattice is analogous to the continuum**

$$\begin{pmatrix} \bar{T}^{G,R}_{\mu\nu} \\ \bar{T}^{F,R}_{\mu\nu} \end{pmatrix} = \begin{pmatrix} Z_{GG} & Z_{GF} \\ Z_{FG} & Z_{FF} \end{pmatrix} \begin{pmatrix} \bar{T}^{G}_{\mu\nu} \\ \bar{T}^{F}_{\mu\nu} \end{pmatrix}$$

✺**Renormalization conditions on the lattice:** *C. Alexandrou, M. Dalla Brida, K. Hadjiyiannakou, G. Spanoudes, S. Yamamoto*

$$\sum_{k\neq l}\sum_{\vec{x}} \left\langle \bar{T}^{G,R}_{kl}(x_0,\vec{x})\bar{T}^{G,R}_{kl}(0,\vec{0})\right\rangle \Big|_{\mu=|x_0|^{-1}} = \text{tree}$$

$$\sum_{k\neq l}\sum_{\vec{x}} \left\langle \bar{T}^{F,R}_{kl}(x_0,\vec{x})\bar{T}^{F,R}_{kl}(0,\vec{0})\right\rangle \Big|_{\mu=|x_0|^{-1}} = \text{tree}$$

$$\sum_{k\neq l}\sum_{\vec{x}} \left\langle \bar{T}^{G,R}_{kl}(x_0,\vec{x})\bar{T}^{F,R}_{kl}(0,\vec{0})\right\rangle \Big|_{\mu=|x_0|^{-1}} = \text{tree}$$

- 3 conditions can be obtained by considering 2-point functions of the EMT operators
- The sum over $\vec{x}$ reduces statistical and discretization errors

✺**A 4th condition can be obtained from 3-point functions among one EMT operator and a two lower-dimensional operators, e.g**

$$\sum_{k\neq l}\sum_{\vec{x},\vec{y}} \left\langle V^{a,R}_{k}(x_0,\vec{x})\bar{T}^{G,R}_{kl}(0,\vec{0})V^{a,R}_{l}(-x_0,\vec{y})^{\dagger}\right\rangle \Big|_{\mu=|x_0|^{-1}} = \text{tree}$$

✺**Challenges of GIRS on the lattice**

- **Window problem:** $\Lambda_{\text{QCD}} \ll \mu \ll a^{-1}, \qquad \mu = |x_0|^{-1}$
- **Statistical uncertainties of the relevant Green's functions in Monte Carlo simulations.**

✺**Requires study of the optimal values of x_0/a at the accessible lattice spacings a**

→ Currently under investigation

Trace-part of EMT?

✺A complete mass-decomposition and determination of the gluonic and fermionic contributions to the pressure inside the nucleon require the trace of the EMT.

Trace parts of $\hat{T}^{G,F}_{\mu=\nu}$: Very complicated renormalisation problem

The renormalisation pattern on the lattice is NOT as in the continuum. Additional operator mixing due to the breaking of Lorentz (Euclidean) invariance on the lattice

$$\begin{pmatrix} \mathcal{O}^R_{1,\mu\nu} - \langle \mathcal{O}^R_{1,\mu\nu} \rangle \\ \mathcal{O}^R_{2,\mu\nu} - \langle \mathcal{O}^R_{2,\mu\nu} \rangle \\ \mathcal{O}^R_{3,\mu\nu} - \langle \mathcal{O}^R_{3,\mu\nu} \rangle \\ \mathcal{O}^R_{4,\mu\nu} - \langle \mathcal{O}^R_{4,\mu\nu} \rangle \end{pmatrix} = \begin{pmatrix} Z_{11} & Z_{12} & Z_{13} & Z_{14} \\ Z_{21} & Z_{22} & Z_{23} & Z_{24} \\ Z_{31} & Z_{32} & Z_{33} & Z_{34} \\ 0 & 0 & 0 & Z_{44} \end{pmatrix} \begin{pmatrix} \mathcal{O}_{1,\mu\nu} - \langle \mathcal{O}_{1,\mu\nu} \rangle \\ \mathcal{O}_{2,\mu\nu} - \langle \mathcal{O}_{2,\mu\nu} \rangle \\ \mathcal{O}_{3,\mu\nu} - \langle \mathcal{O}_{3,\mu\nu} \rangle \\ \mathcal{O}_{4,\mu\nu} - \langle \mathcal{O}_{4,\mu\nu} \rangle \end{pmatrix}$$

We need 13 renormalization conditions, e.g. 10 conditions considering 2-point functions & 3 conditions considering 3-point functions.

Caracciolo et al., Annals of Physics, 197 (1990) 119

$$\mathcal{O}_{1,\mu\nu} \equiv \hat{T}^G_{\mu\nu} = \delta_{\mu\nu} \sum_{\rho\sigma} F_{\rho\sigma} F_{\rho\sigma}, \qquad \mathcal{O}_{2,\mu\nu} \equiv \delta_{\mu\nu} \sum_{\rho} F_{\mu\rho} F_{\mu\rho},$$

$$\mathcal{O}_{3,\mu\nu} \equiv \delta_{\mu\nu} \sum_{f} \bar{\psi}_f \gamma_\mu \overleftrightarrow{D}_\mu \psi_f, \qquad \mathcal{O}_{4,\mu\nu} \equiv \hat{T}^F_{\mu\nu} = \delta_{\mu\nu} \sum_{f} \bar{\psi}_f \psi_f$$

✺ Explore alternative strategies e.g. analogous to finite temperature computation of the trace

Conclusions

- Using sum rules to determine the trace anomaly gives a decomposition of the proton mass from lattice QCD data

  Scheme and scale independent contributions:

- The quark mass term M_m contributes ~20%
- The quark and gluon energy contributes ~2/3 - scheme and scale independent
- The rest about ~15% comes from the trace anomaly

- New ideas for the renormalisation of the ETM for lattice QCD are being explored