
Fermion Loops at the Physical Point For Nucleon Structure

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Giannis Koutsou

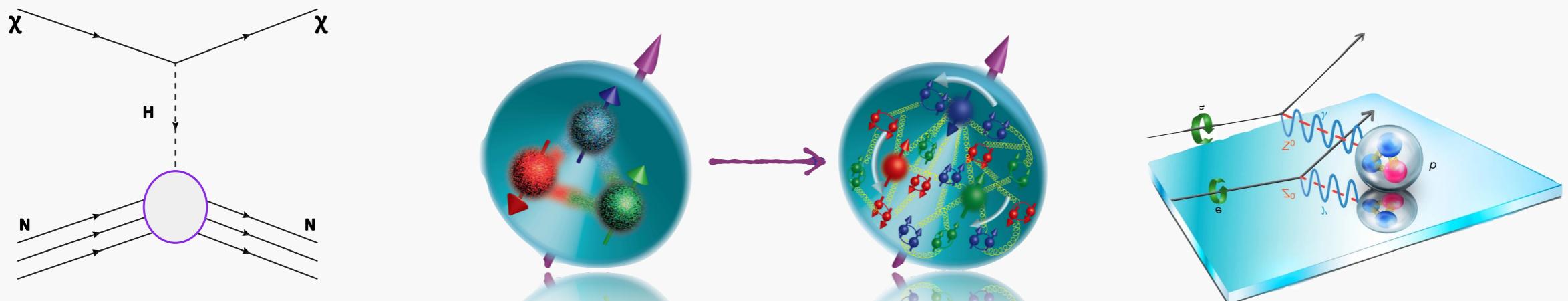
Computation-Based Science and Technology Research Centre (CaSToRC)
The Cyprus Institute

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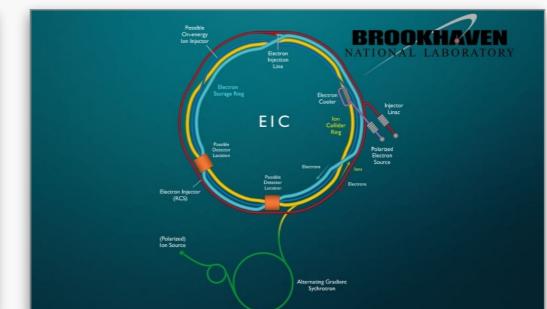
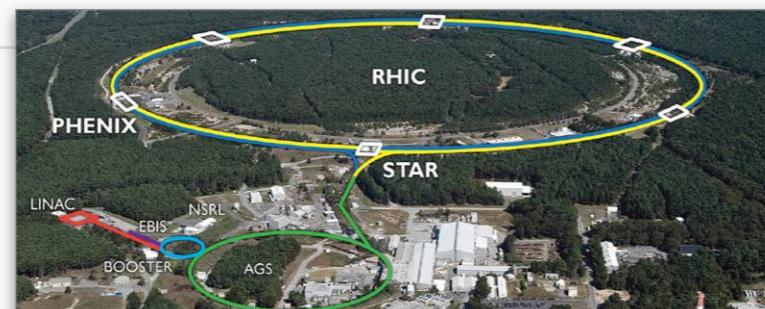
Nucleon Matrix Elements

- Scalar and tensor charges → novel interactions/dark matter searches
- Axial matrix elements → origin of nucleon spin
- Electromagnetic form factors → radii and moments well known experimentally
- Strange form factors → connect to weak charges and constraints on new physics
- Momentum fraction, moments of PDFs and GPDs, ...

Disconnected fermion loops are essential in precision calculations



JLab · Mainz · PSI · RHIC · Planned Electron Ion Collider



Nucleon Structure with Physical Point Ensemble

Outline

- $N_f=2+1+1$ ensembles at physical point (twisted mass + clover)
- Setup and statistics
- Excited states treatment
- Representative results including disconnected contributions
- Stochastic techniques
 - One-end trick; hierarchical probing; deflation



C. Alexandrou
S. Bacchio
J. Finkenrath
K. Hadjyiannakou



- Phys. Rev. D101 (2020) 094513 arXiv:2003.08486 • Phys. Rev. D101 (2020) 031501 arXiv:1909.10744
- Phys. Rev. D102 (2020) 054517 arXiv:1909.00485 • Phys. Rev. D100 (2019) 014509 arXiv:1812.10311

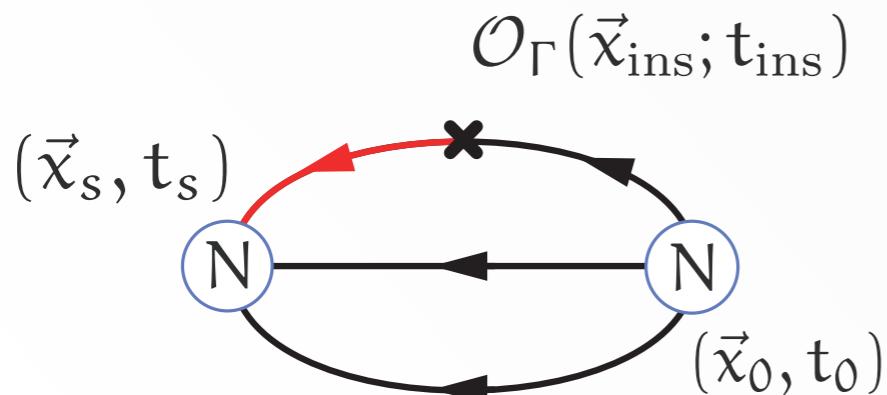
Matrix elements on the Lattice

General three-point function:

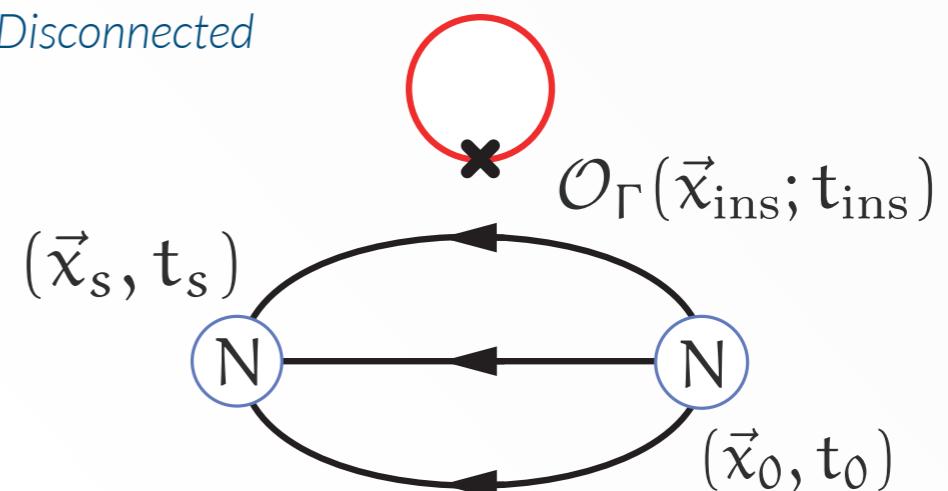
$$G_\Gamma(P; \vec{q}; t_s, t_{\text{ins}}) = \sum_{\vec{x}_s \vec{x}_{\text{ins}}} e^{-i\vec{q} \cdot \vec{x}_{\text{ins}}} P^{\alpha\beta} \langle \bar{\chi}_N^\beta(\vec{x}_s; t_s) | \mathcal{O}^\Gamma(\vec{x}_{\text{ins}}; t_{\text{ins}}) | \chi_N^\alpha(0; 0) \rangle$$

At quark level gives rise to both so-called connected and disconnected contributions

Connected



Disconnected

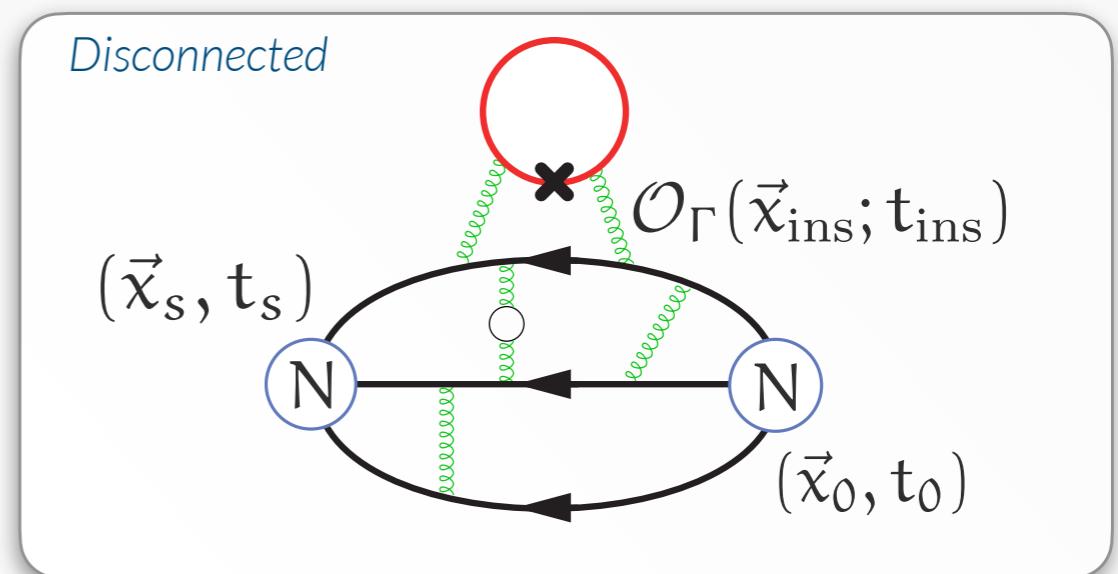
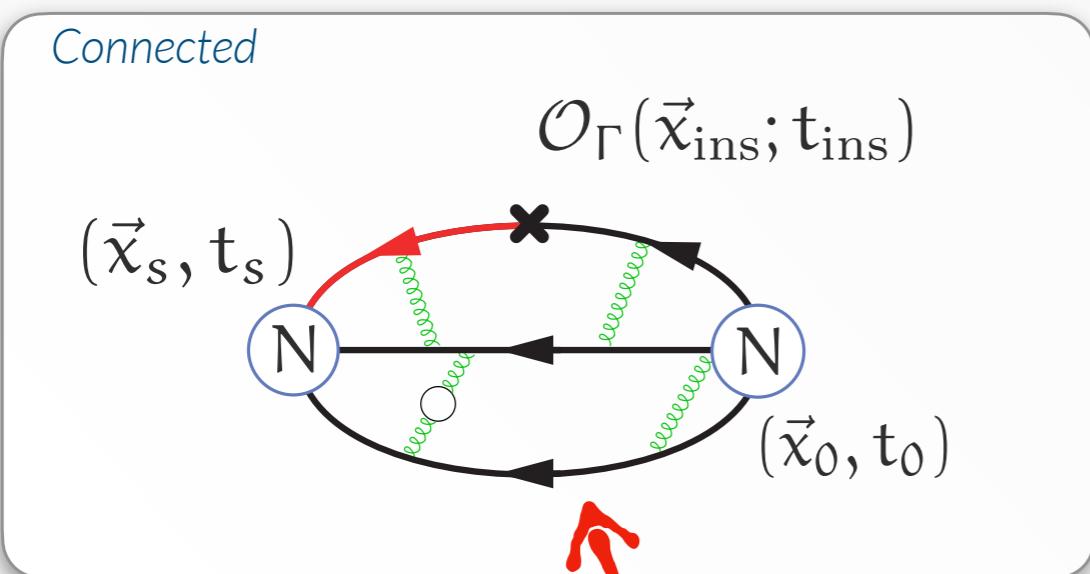


Matrix elements on the Lattice

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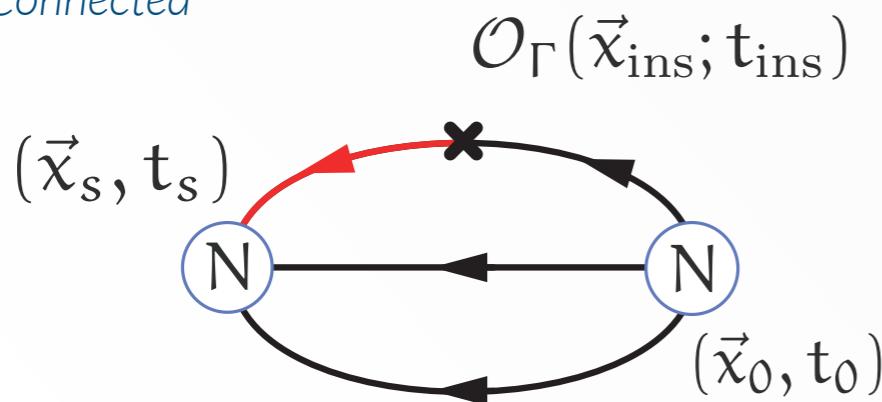


All gluon exchanges implied

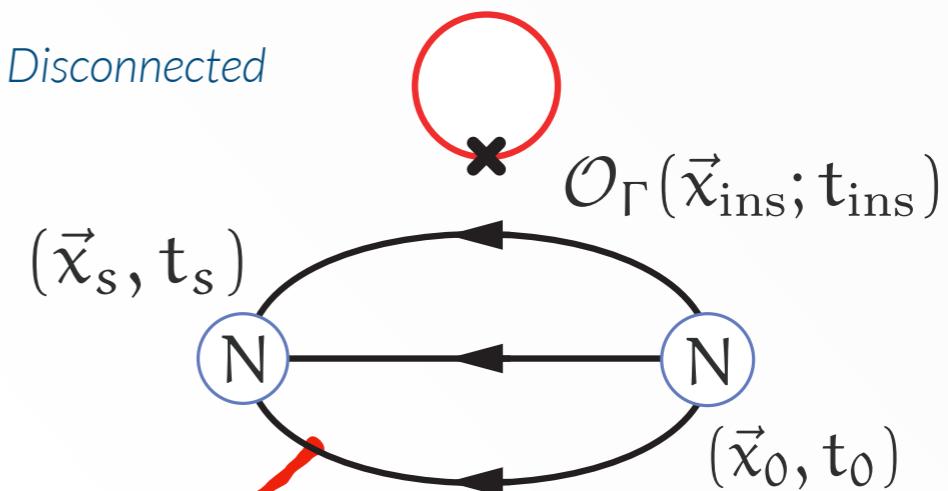
Matrix elements on the Lattice

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Connected



Disconnected

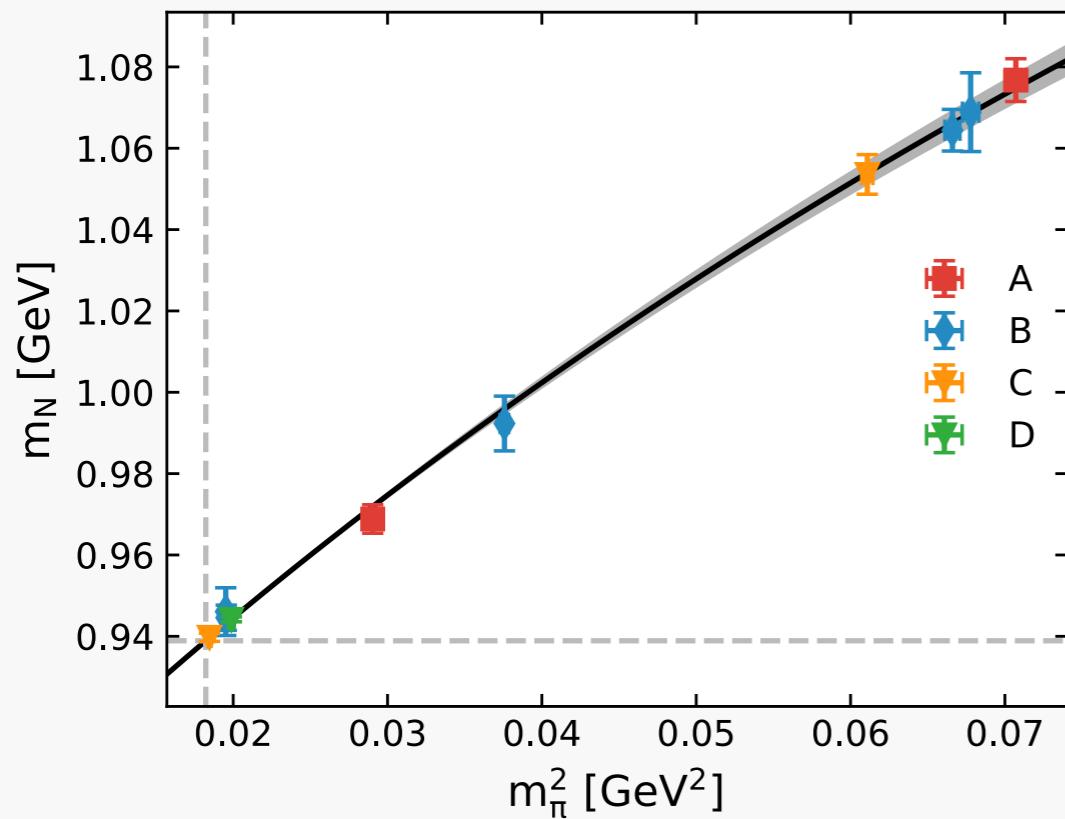


Disconnected

- Vanish in isovector matrix elements; $u - d$ combinations
- Enter in *isoscalar* matrix elements; $u + d$ combinations
- Combine with connected $u + d$ for individual up and down-quark combinations
- Individual quark, i.e. strange- (and charm-) quark contributions

Ensembles

Three $N_f=2+1+1$ ensembles at physical pion mass

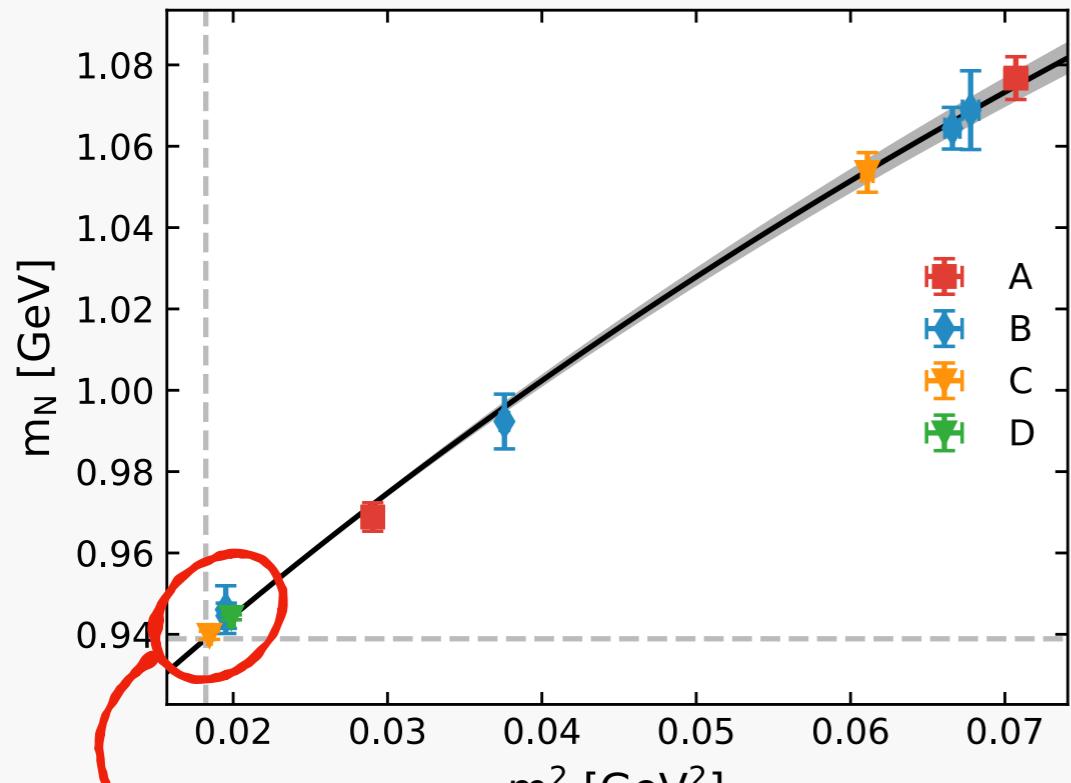


Ens. ID (abbrv.)	Vol.	a [fm]
cB211.072.64 (cB64)	64×128	0.080
cC211.060.80 (cC80)	80×160	0.068
cD211.054.96 (cD96)	96×192	0.057

- Three lattice spacings at physical point
- Several final analyses of coarsest
- Ongoing analysis of two finer

Ensembles

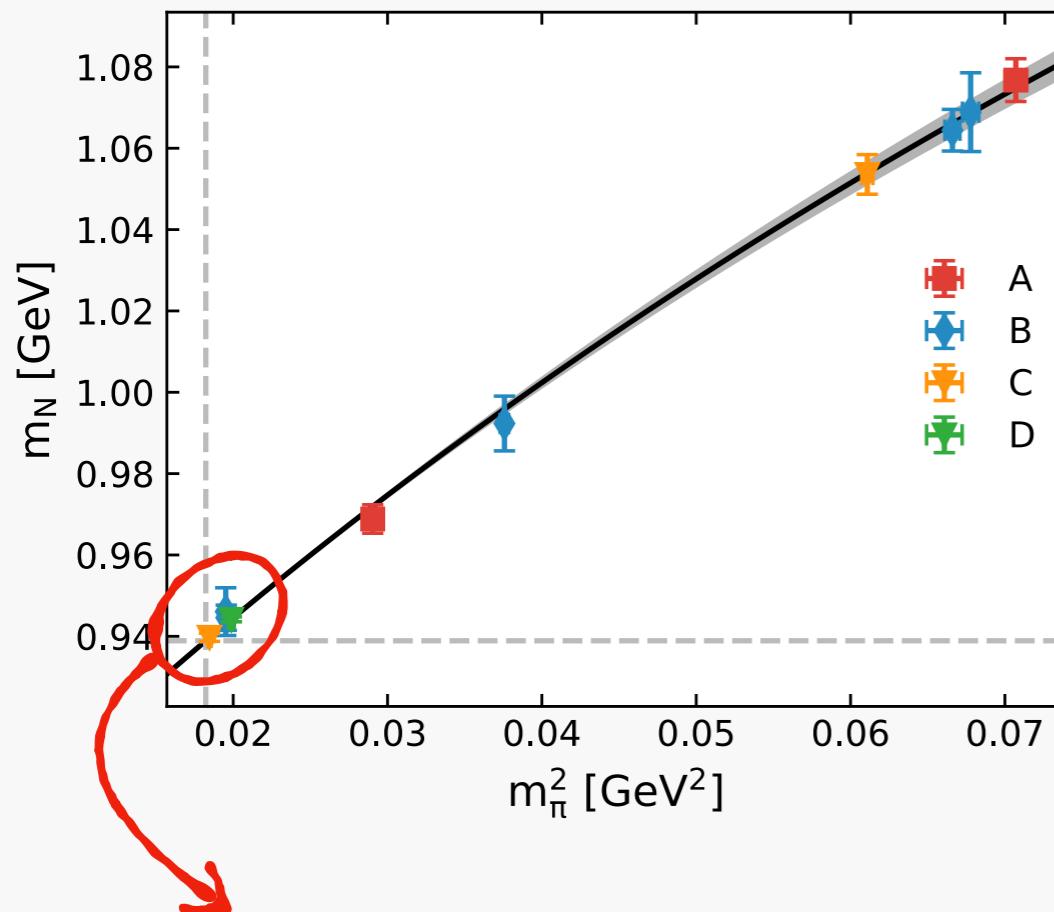
Three $N_f=2+1+1$ ensembles at physical pion mass



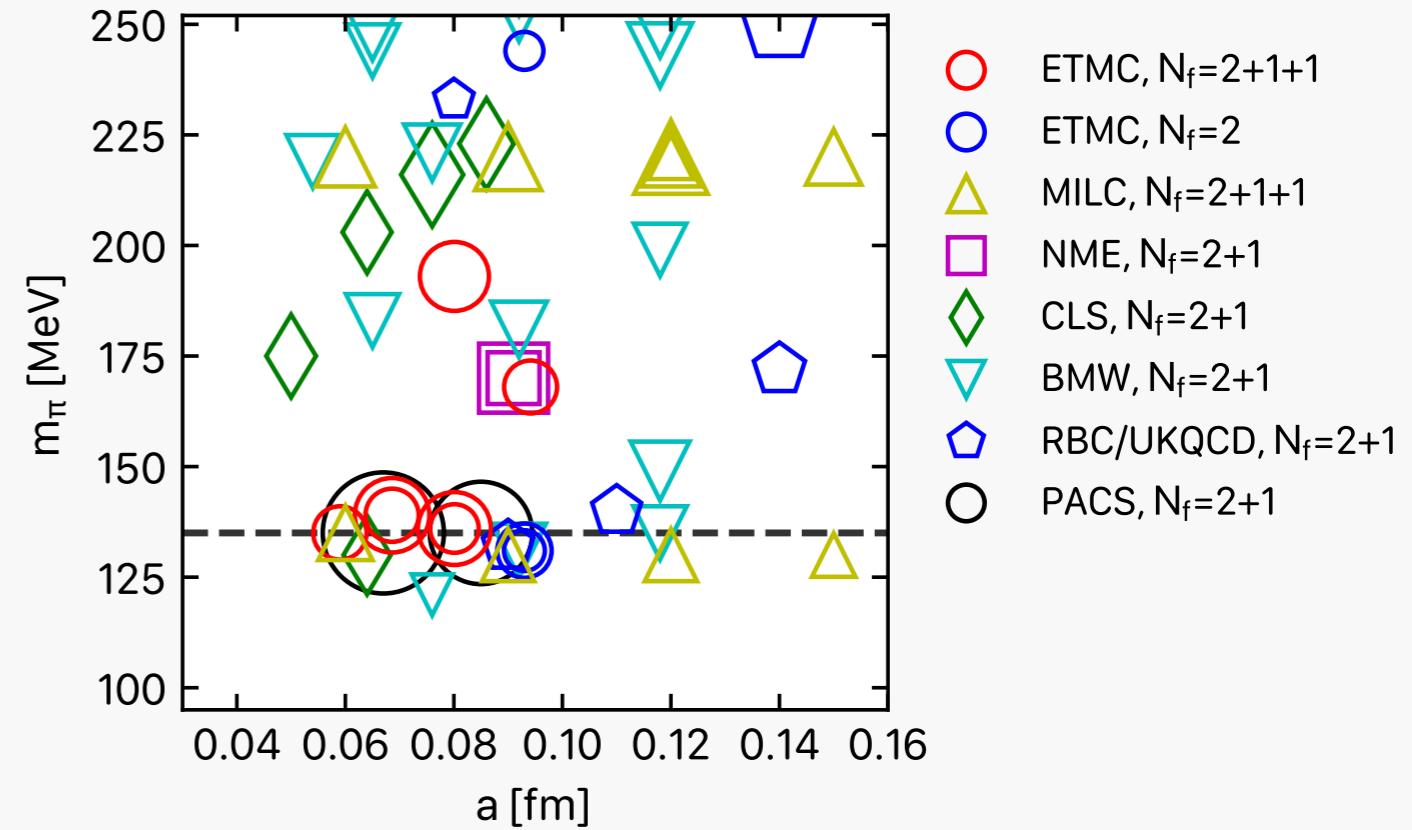
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Ensembles

Three $N_f=2+1+1$ ensembles at physical pion mass



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- Three lattice spacings at physical point
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Nucleon structure on the lattice

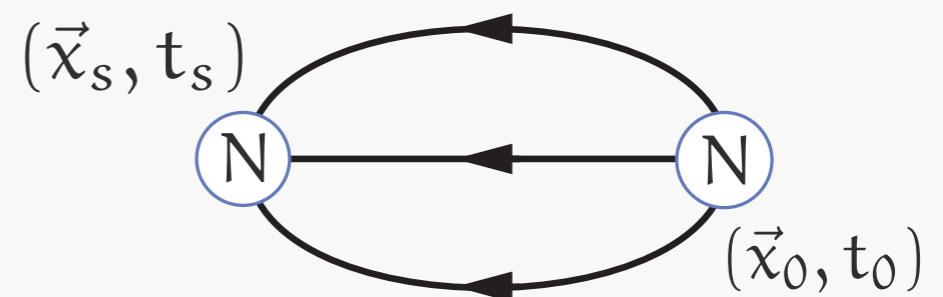
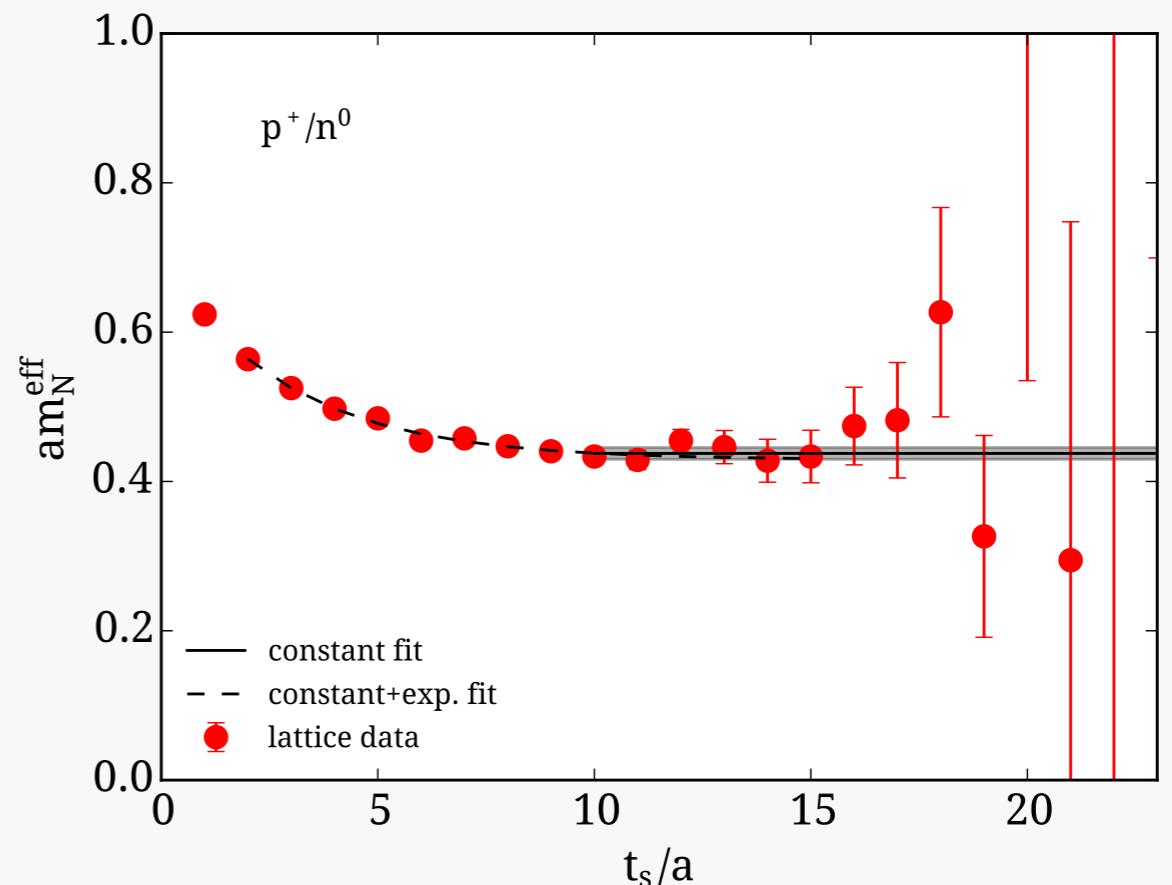
Two-point correlation functions

- Statistical error: $N^{-1/2}$ with Monte Carlo samples
- Correlation functions exponentially decay with time-separation

Systematic uncertainties

- Extrapolations: a , L , m_π
- Contamination from higher energy states

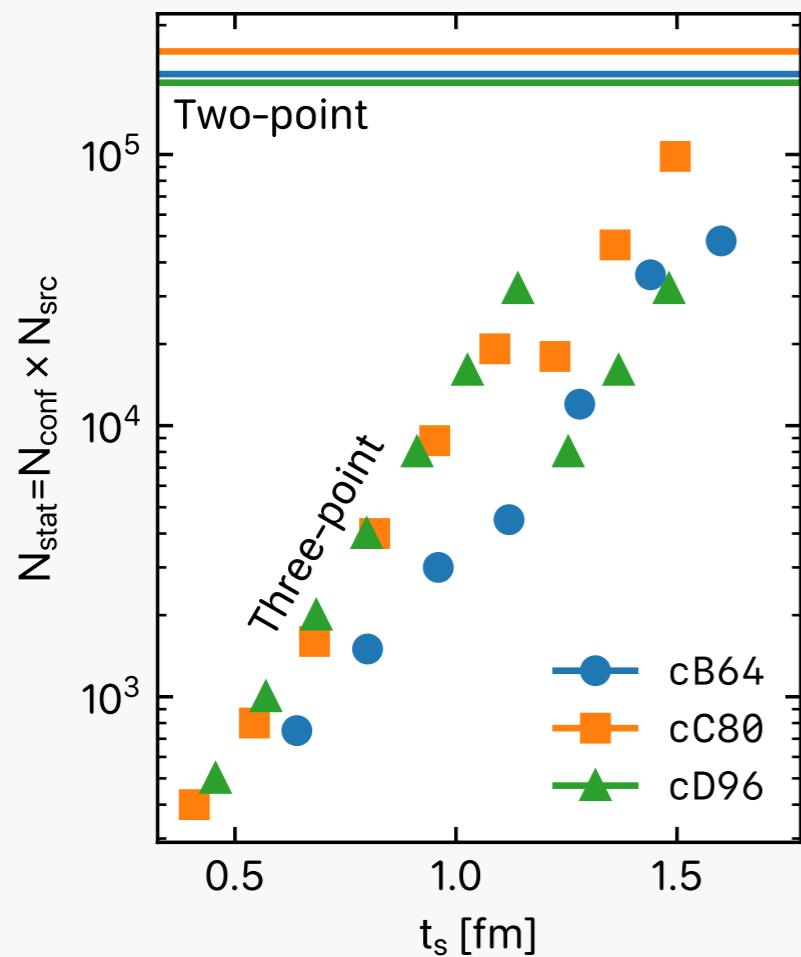
$$\sum_{\vec{x}_s} \Gamma^{\alpha\beta} \langle \bar{\chi}_N^\beta(x_s) | \chi_N^\alpha(0) \rangle = c_0 e^{-E_0 t_s} + c_1 e^{-E_1 t_s} + \dots$$



Statistics

$$R_\Gamma(P; \vec{q}; t_s; t_{ins}) = \frac{G_\Gamma(P; \vec{q}; t_s; t_{ins})}{G(\vec{0}; t_s)} \sqrt{\frac{G(\vec{p}; t_s - t_{ins}) G(\vec{0}; t_{ins}) G(\vec{0}; t_s)}{G(\vec{0}; t_s - t_{ins}) G(\vec{p}; t_{ins}) G(\vec{p}; t_s)}}$$

Connected: Increasing N_{src} with t_s



Ideally: Aim for constant statistical errors over all values of t_s of a given ensemble

- Robust analysis of excited states: summation method, two- or three-state fits, etc.

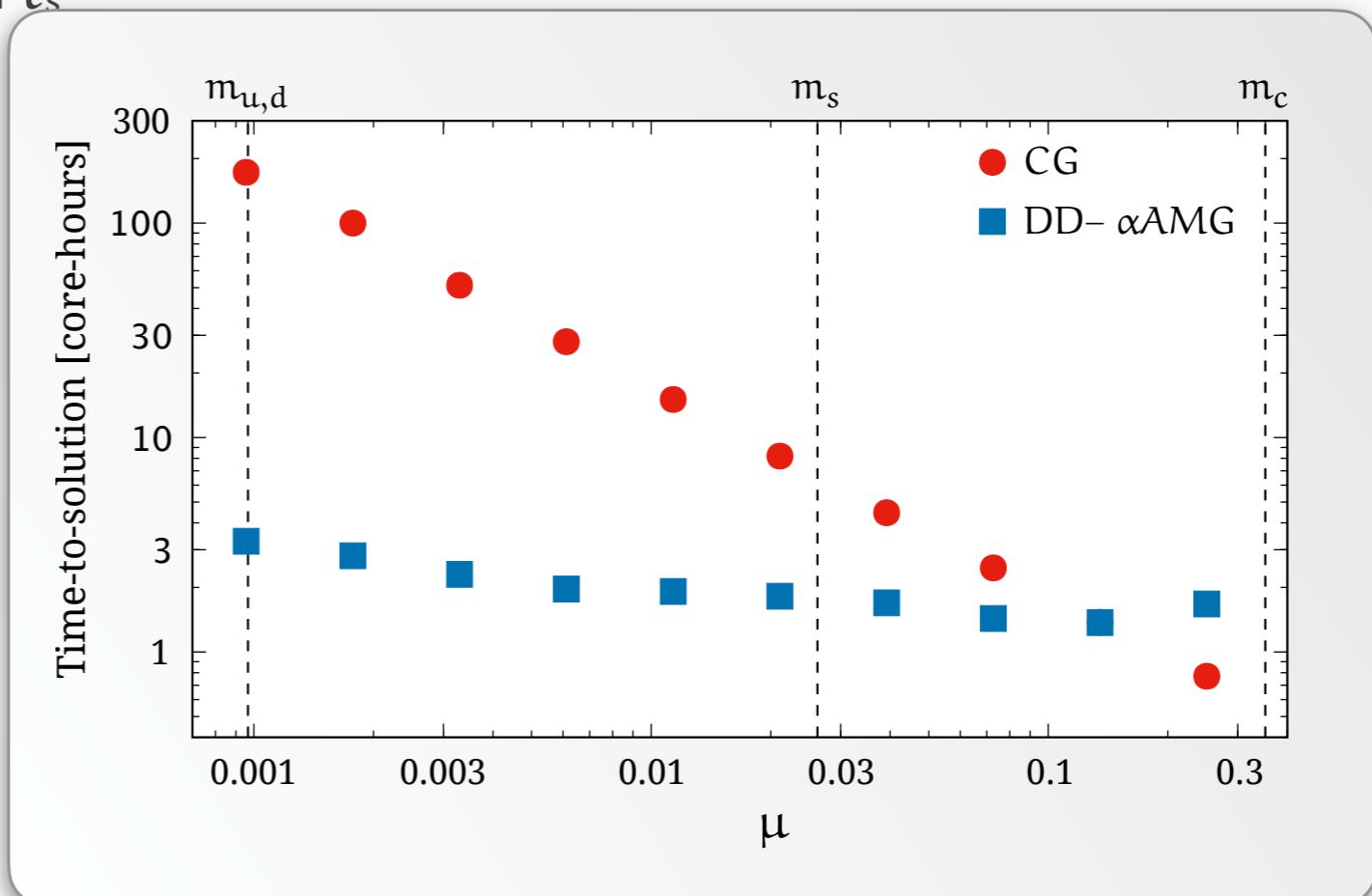
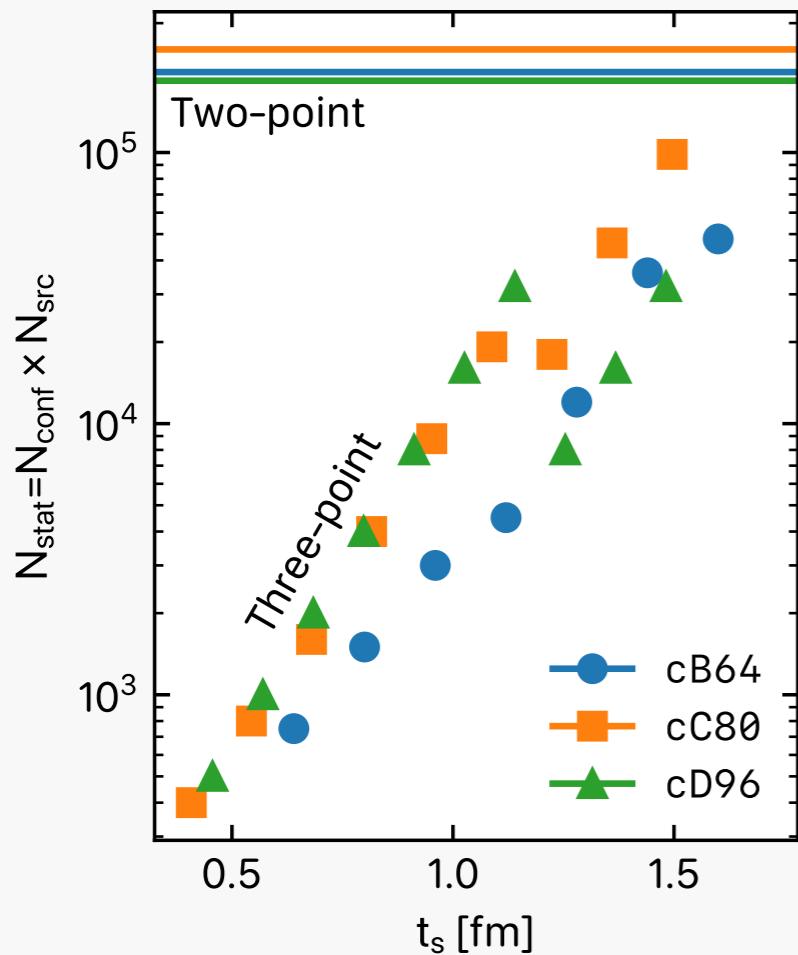
Two-point function: High number of sources per config

- Needed for disconnected contributions

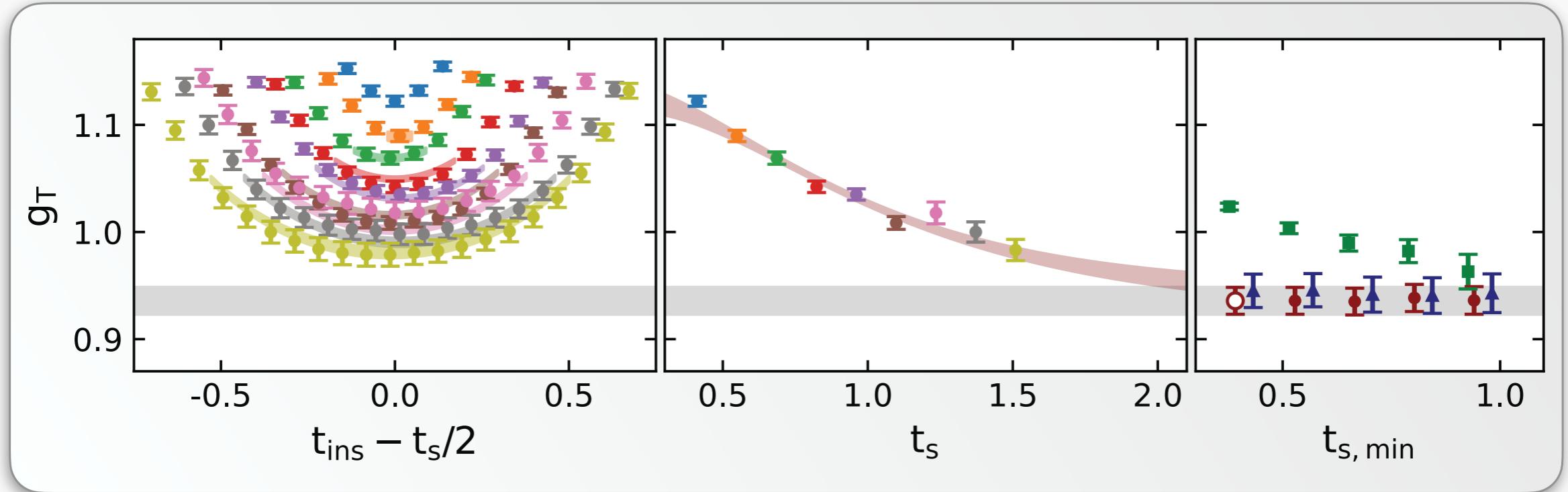
Statistics

$$R_\Gamma(P; \vec{q}; t_s; t_{ins}) = \frac{G_\Gamma(P; \vec{q}; t_s; t_{ins})}{G(\vec{0}; t_s)} \sqrt{\frac{G(\vec{p}; t_s - t_{ins}) G(\vec{0}; t_{ins}) G(\vec{0}; t_s)}{G(\vec{0}; t_s - t_{ins}) G(\vec{p}; t_{ins}) G(\vec{p}; t_s)}}$$

Connected: Increasing N_{src} with t_s

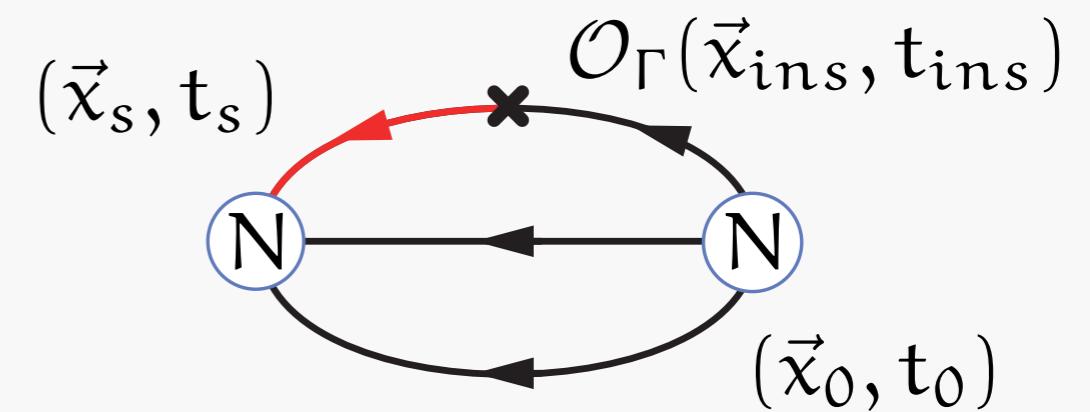


Treatment of excited states

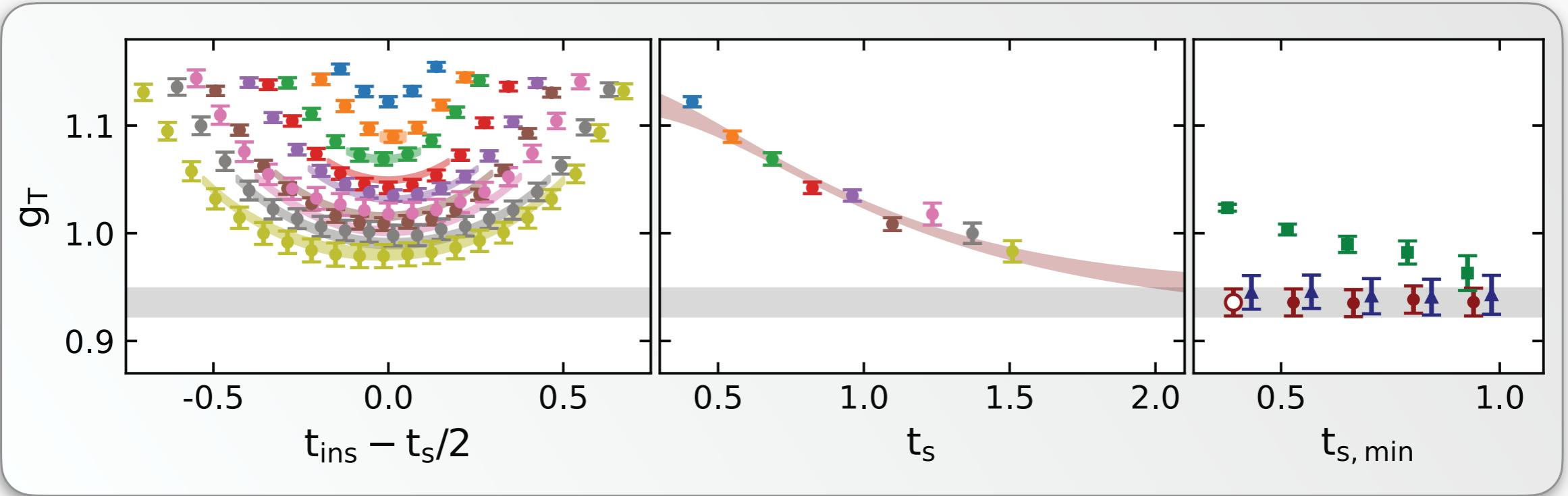


Example from intermediate α

- Isovector tensor charge (only connected)
- Increasing statistics with separation t_s
- Summation, two- and three-state fits



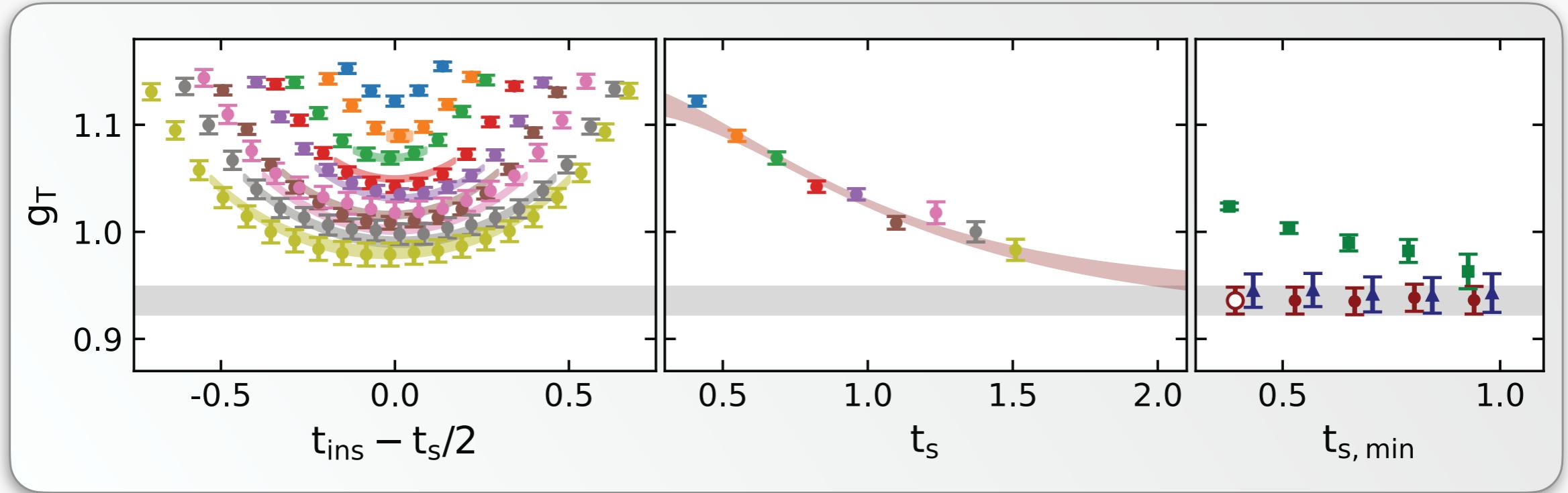
Treatment of excited states



Summation method

$$S_\Gamma(\vec{q}; t_s) = \sum_{t_{\text{ins}}=\tau}^{t_s-\tau} R_\Gamma(\vec{q}; t_s; t_{\text{ins}}) \rightarrow \mathcal{M}t_s + C$$

Treatment of excited states



Two-state fit

$$G_\Gamma(\vec{q}; t_s, t_{\text{ins}}) = \sum_{i=0}^1 \sum_{j=0}^1 c_{ij} e^{-E_i(0)(t_s - t_{\text{ins}})} e^{-E_j(\vec{q})t_{\text{ins}}}$$

$$\mathcal{M} = \frac{c_{00}}{\sqrt{a_0(\vec{0})a_0(\vec{q})}}$$

$$G(\vec{q}; t_s) = a_0(\vec{q})e^{-\varepsilon_0(\vec{q})t_s} + a_1(\vec{q})e^{-\varepsilon_1(\vec{q})t_s}$$

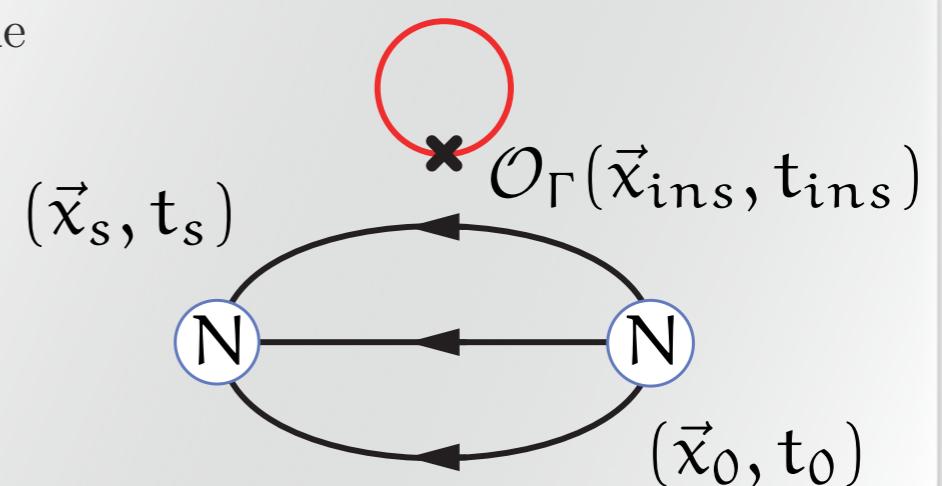
Statistics – Disconnected

$$R_\Gamma(P; \vec{q}; t_s; t_{ins}) = \frac{G_\Gamma(P; \vec{q}; t_s; t_{ins})}{G(\vec{0}; t_s)} \sqrt{\frac{G(\vec{p}; t_s - t_{ins}) G(\vec{0}; t_{ins}) G(\vec{0}; t_s)}{G(\vec{0}; t_s - t_{ins}) G(\vec{p}; t_{ins}) G(\vec{p}; t_s)}}$$

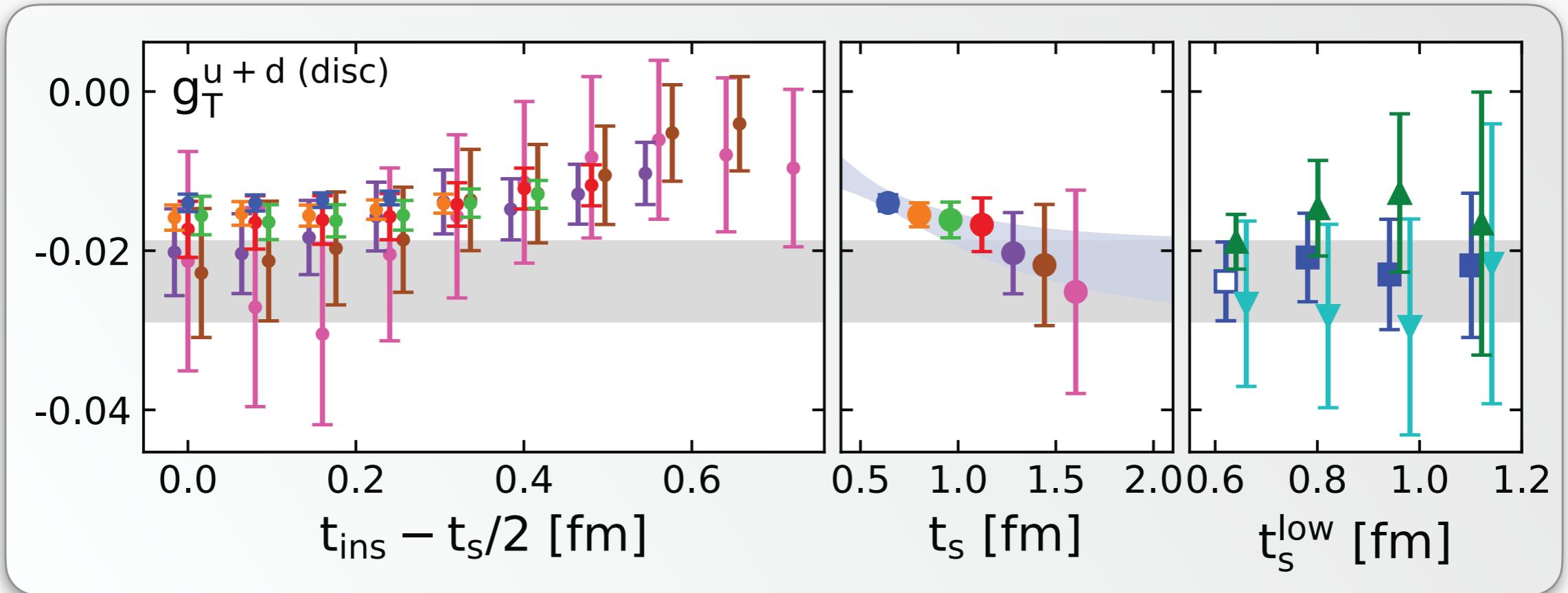
Disconnected: High number of sources per config. + hierarchical probing, color/spin dilution and exact of low-mode estimation of loops

Ens.	Light	
	Stochastic	Deflation
cB64:	$n_{vec} = 12_{col./spin} \times 512_{nhad.}$	$n_{ev} = 200$
cC80:	$n_{vec} = 12_{col./spin} \times 512_{nhad.}$	$n_{ev} = 450$
cD96:	$n_{vec} = 12_{col./spin} \times 512_{nhad.} \times 8_{stoch.}$	None

Ens.	Strange	
cB64:	$n_{vec} = 12_{col/spin} \times 12_{stoch.} \times 32_{nhad.}$	
cC80:	$n_{vec} = 12_{col/spin} \times 4_{stoch.} \times 512_{nhad.}$	
cD96:	$n_{vec} = 12_{col/spin} \times 4_{stoch.} \times 512_{nhad.}$	



Treatment of excited states



Example from intermediate α

- Disconnected contribution to isoscalar tensor charge
- Large number of two-point functions per configuration (here 650)
- All t_s obtained for same statistics
- Note small magnitude compared to connected

Scalar charge – σ -terms

- Pion nucleon σ -term: $\sigma_{\pi N} = m_{ud} \langle N | \bar{u}u + \bar{d}d | N \rangle$
- Strange σ -term: $\sigma_s = m_s \langle N | \bar{s}s | N \rangle$
- Enter super-symmetric candidate particle scattering cross sections with nucleon (e.g. neutralino through Higgs)

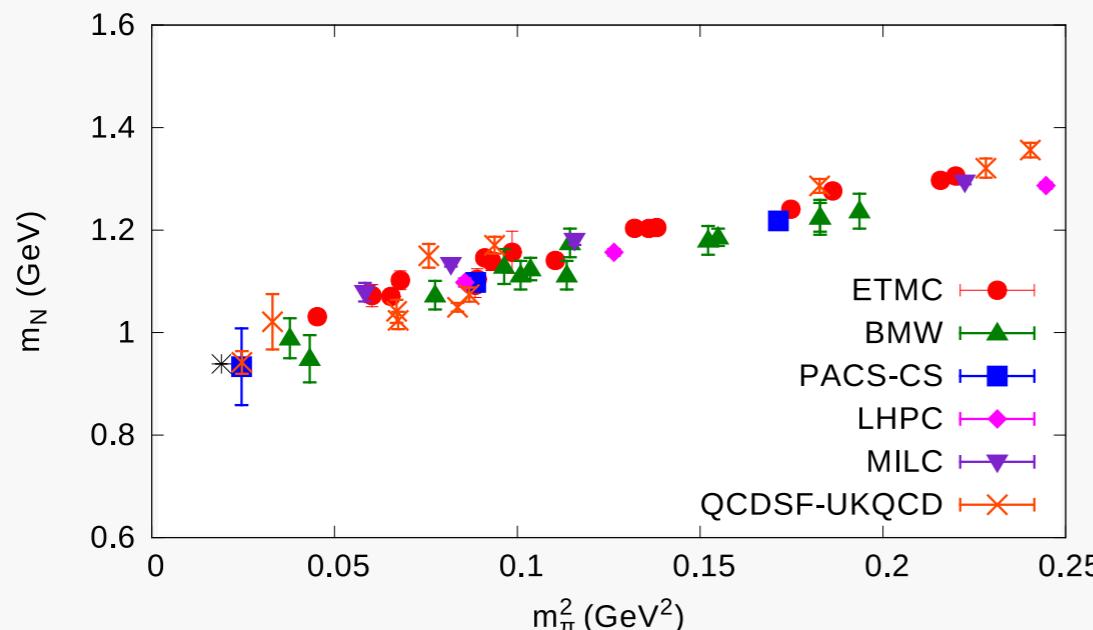
1. Direct calculation of matrix elements

Involves disconnected contributions

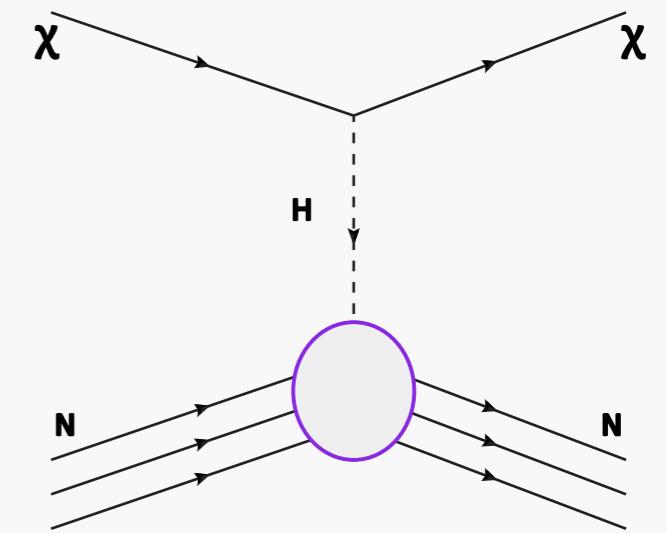
2. Through Feynman - Hellmann theorem:

$$\sigma_{\pi N} = m_{ud} \frac{\partial m_N}{\partial m_{ud}}$$

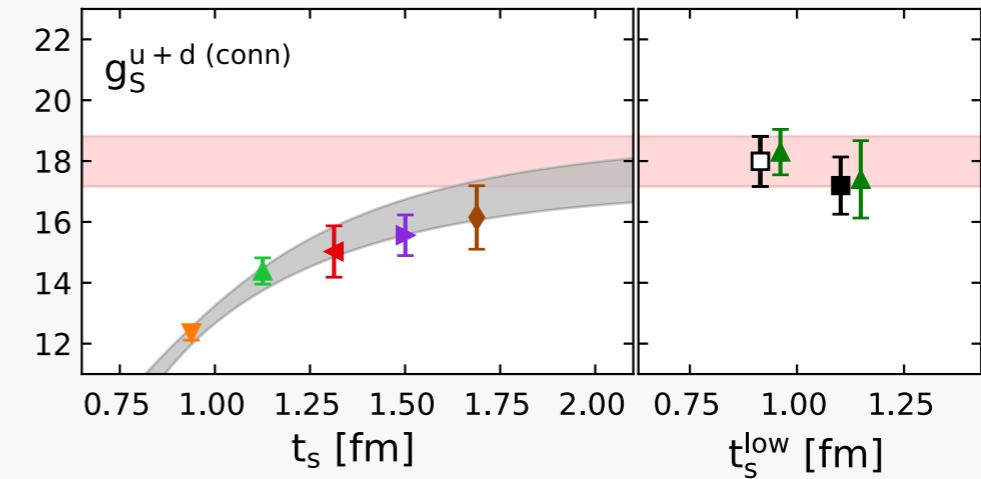
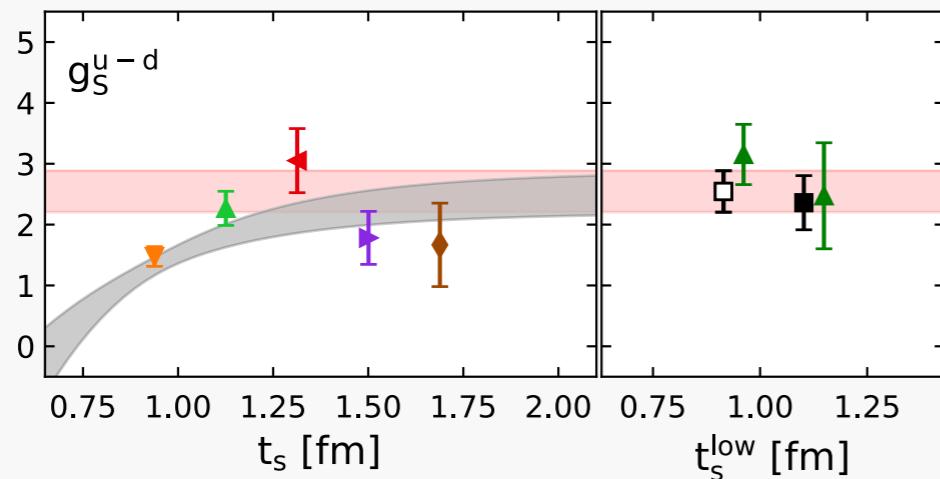
$$\sigma_s = m_s \frac{\partial m_N}{\partial m_s}$$



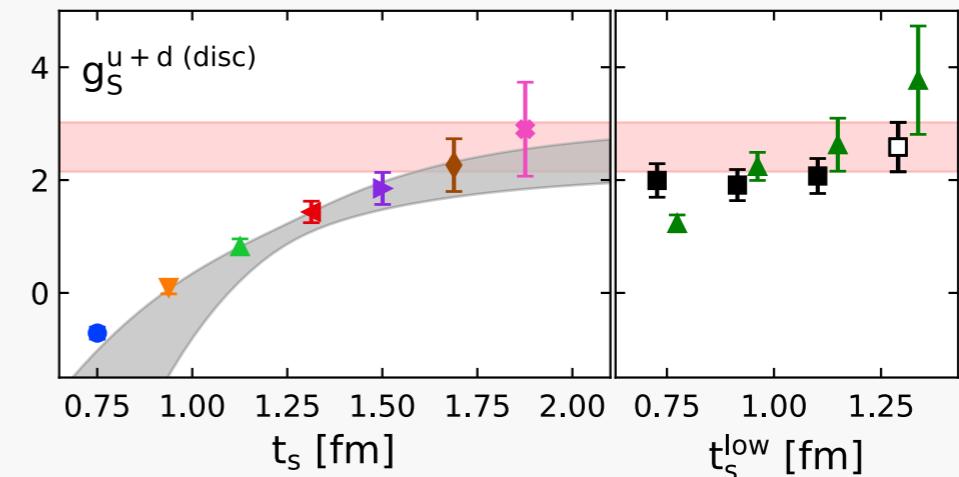
- Reliance on effective theories for dependence on m_π
- Weak dependence on m_s



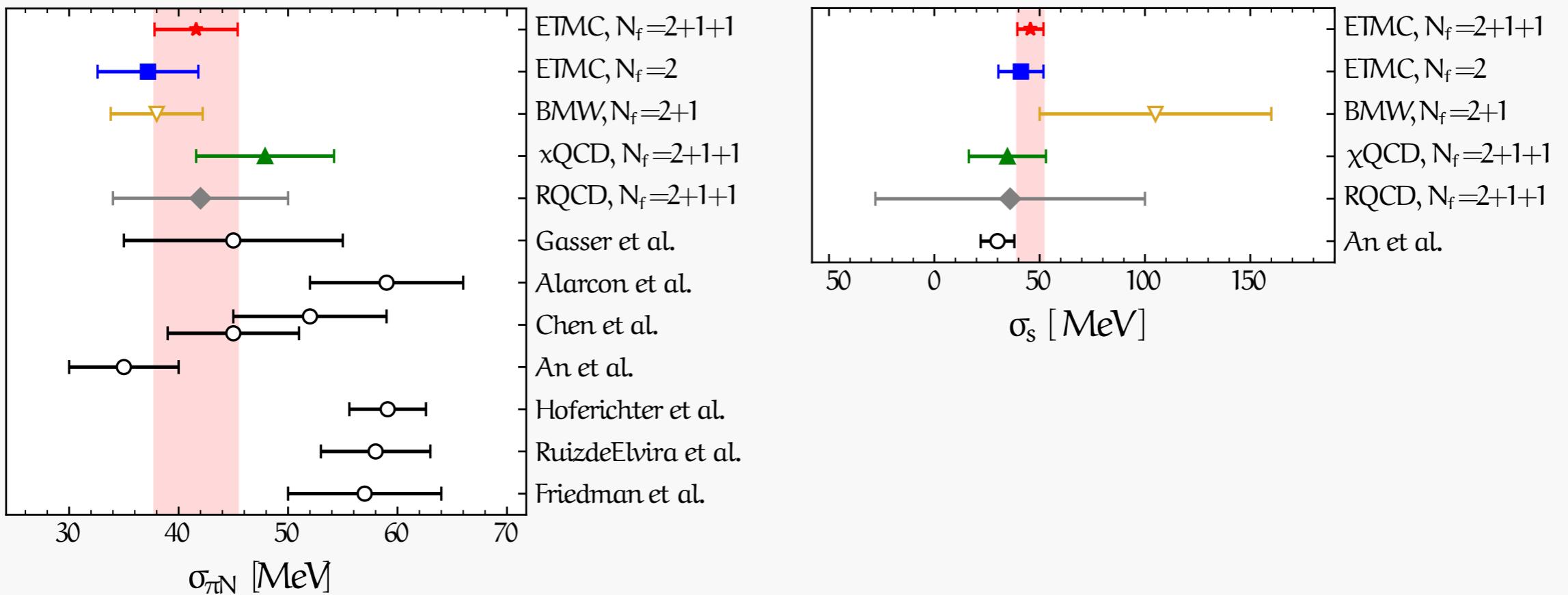
Scalar charge – σ -terms



- Showing coarsest lattice spacing
- Significant disconnected contribution
- Excited state effects require $t_s > 1.5$ fm



Scalar charge – σ -terms

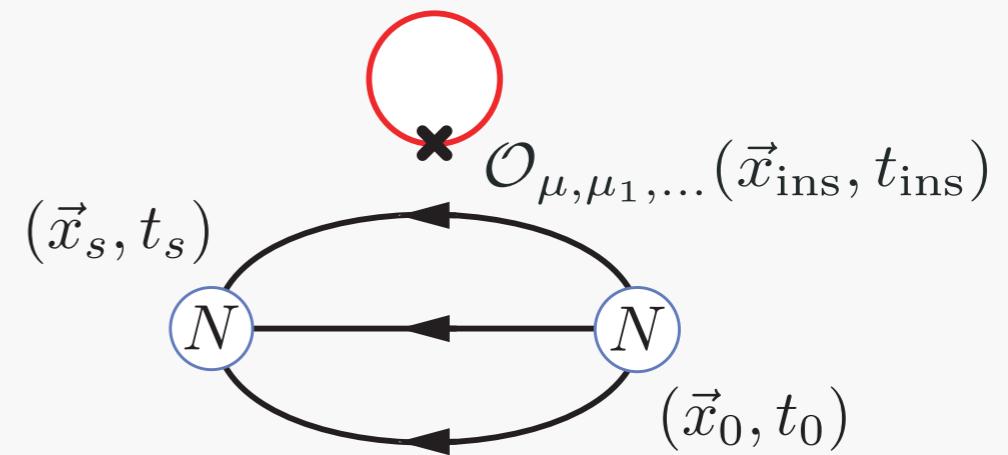
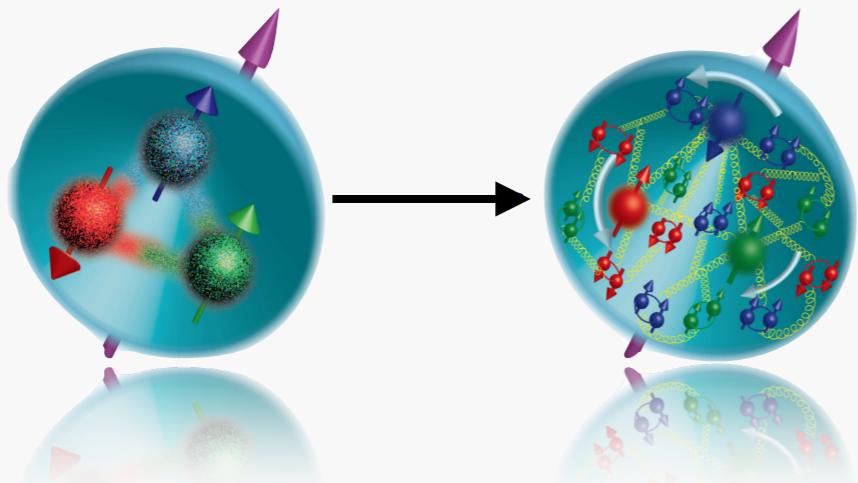


- Showing results which use physical point ensembles
- One result using FH method (BMW)
- Los Alamos group: 59.6(7.4) MeV, when explicitly including πN prior

Nucleon spin

Quark intrinsic spin contributions to nucleon spin

$$\frac{1}{2} \Delta \Sigma = \frac{1}{2} \sum_{q=u,d,s,\dots} g_A^q$$



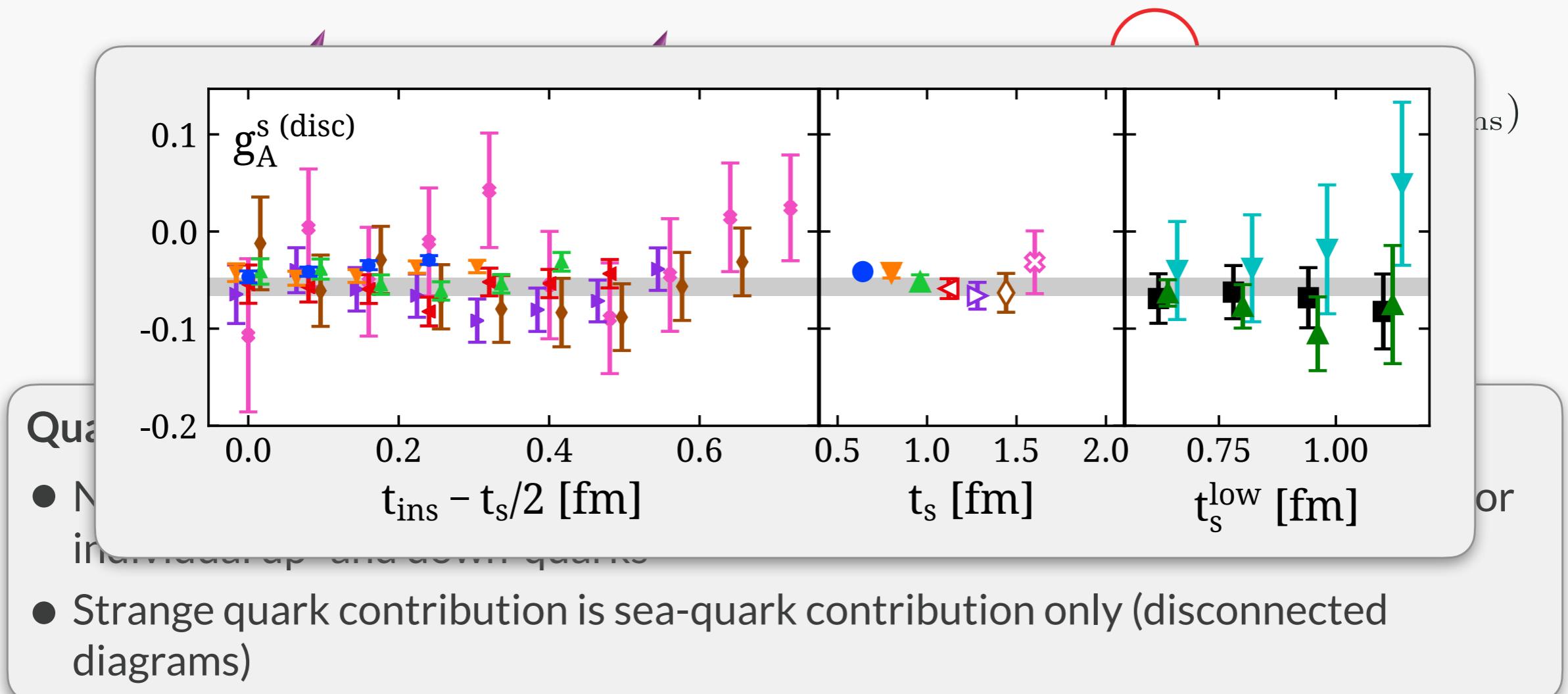
Quark intrinsic spin contributions to nucleon spin

- Need linear combination of isovector ($u-d$) and isoscalar ($u+d$) contributions for individual up- and down-quarks
- Strange quark contribution is sea-quark contribution only (disconnected diagrams)

Nucleon spin

Quark intrinsic spin contributions to nucleon spin

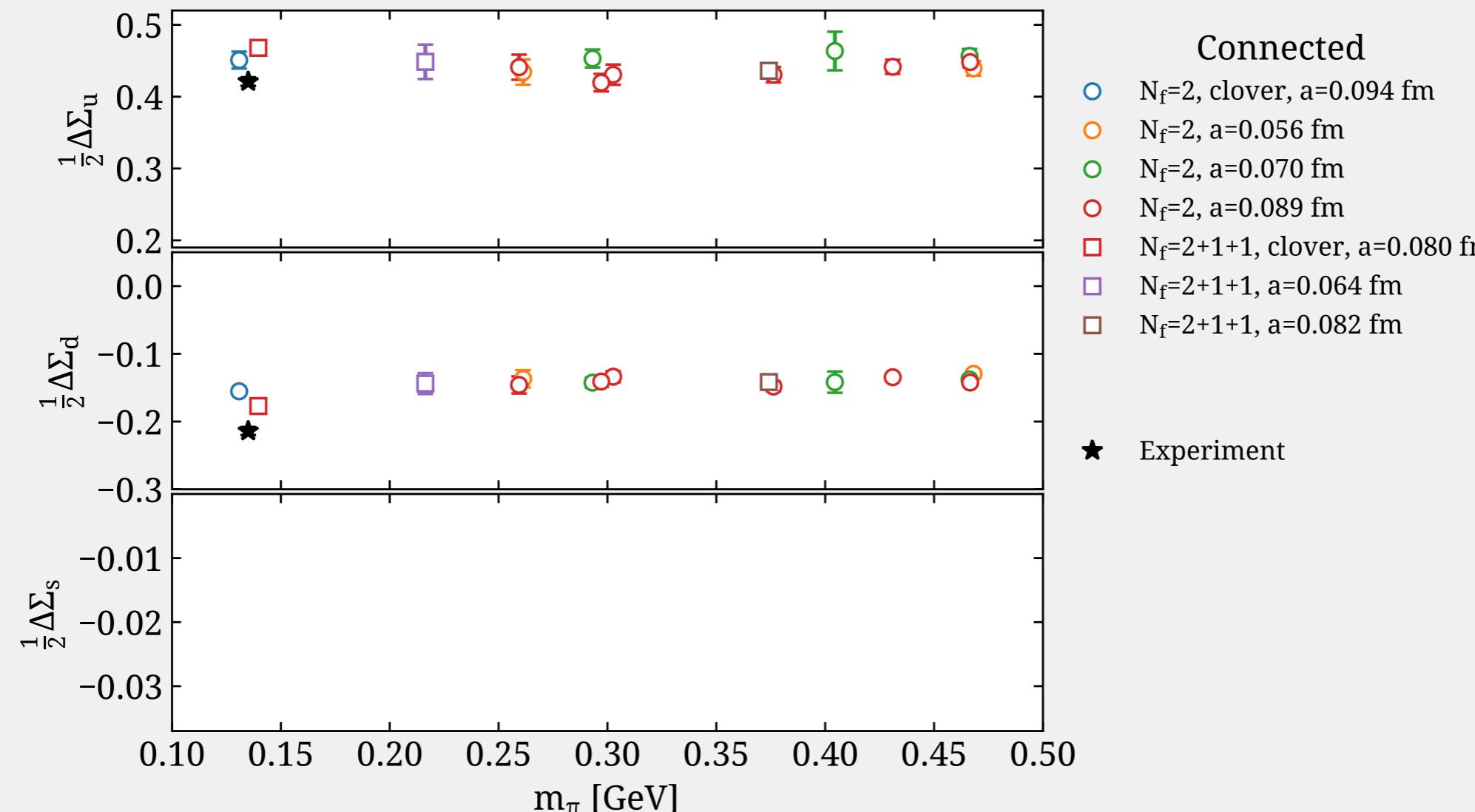
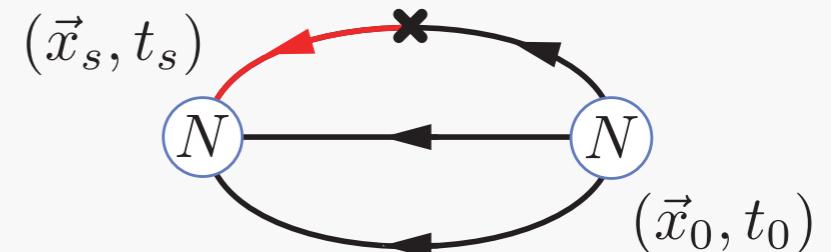
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Quark intrinsic spin contributions

Quark intrinsic spin contributions to nucleon spin

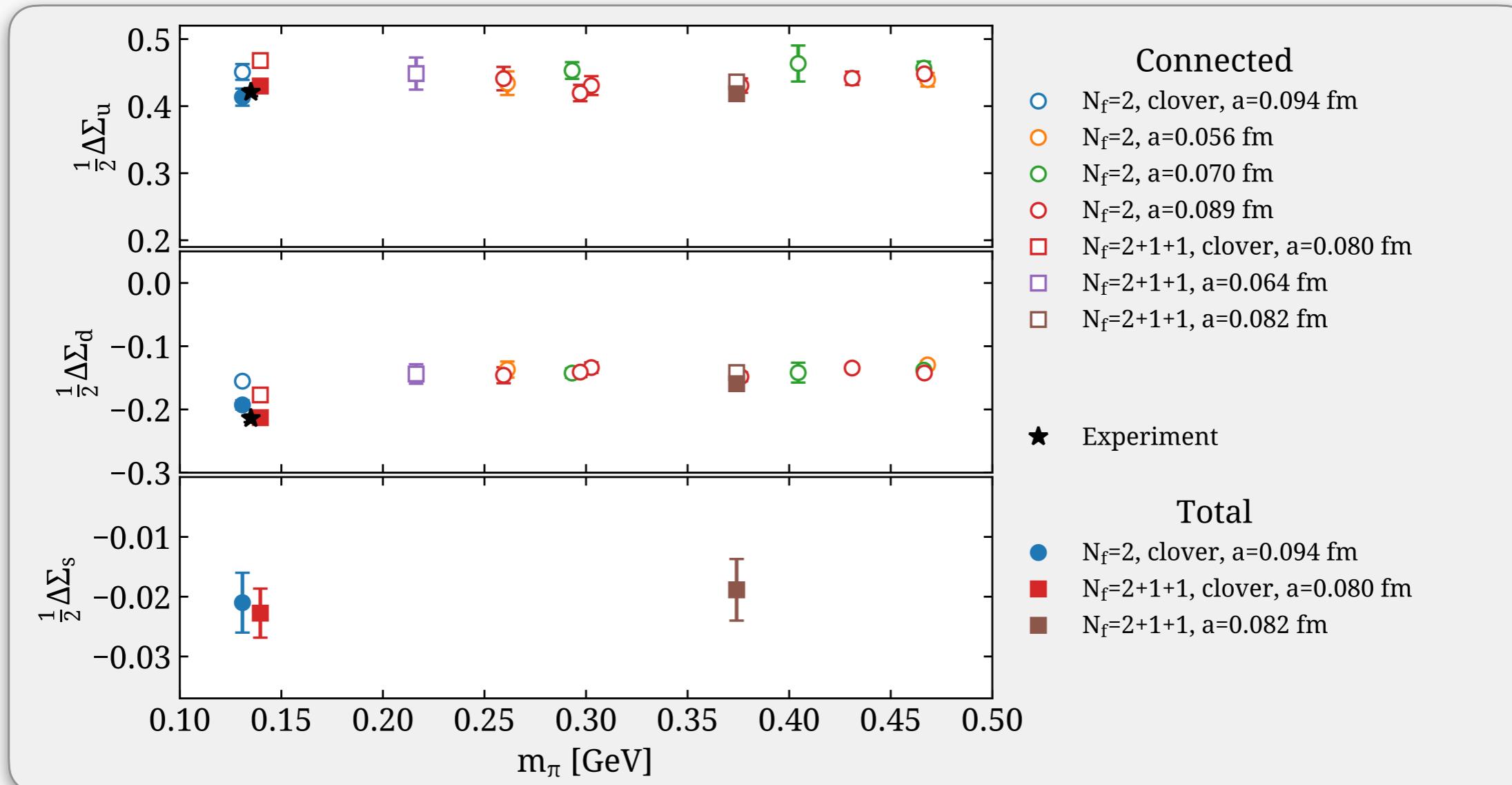
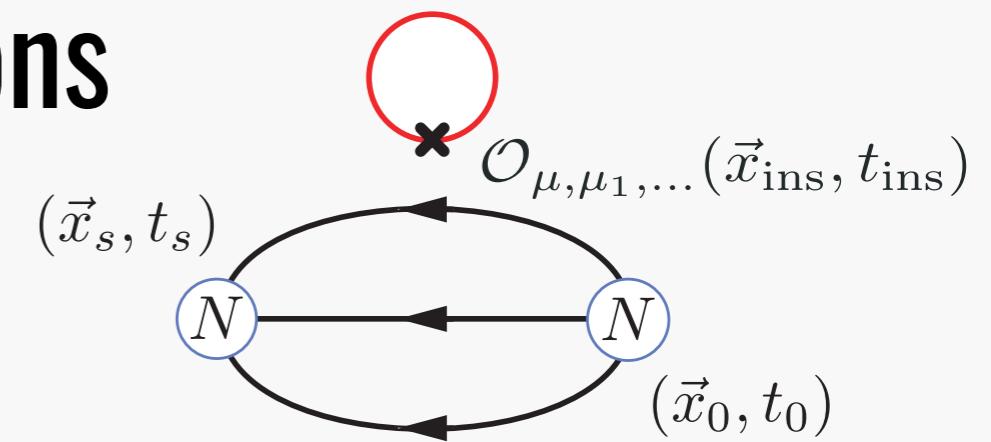
- Open symbols: connected only



Quark intrinsic spin contributions

Quark intrinsic spin contributions to nucleon spin

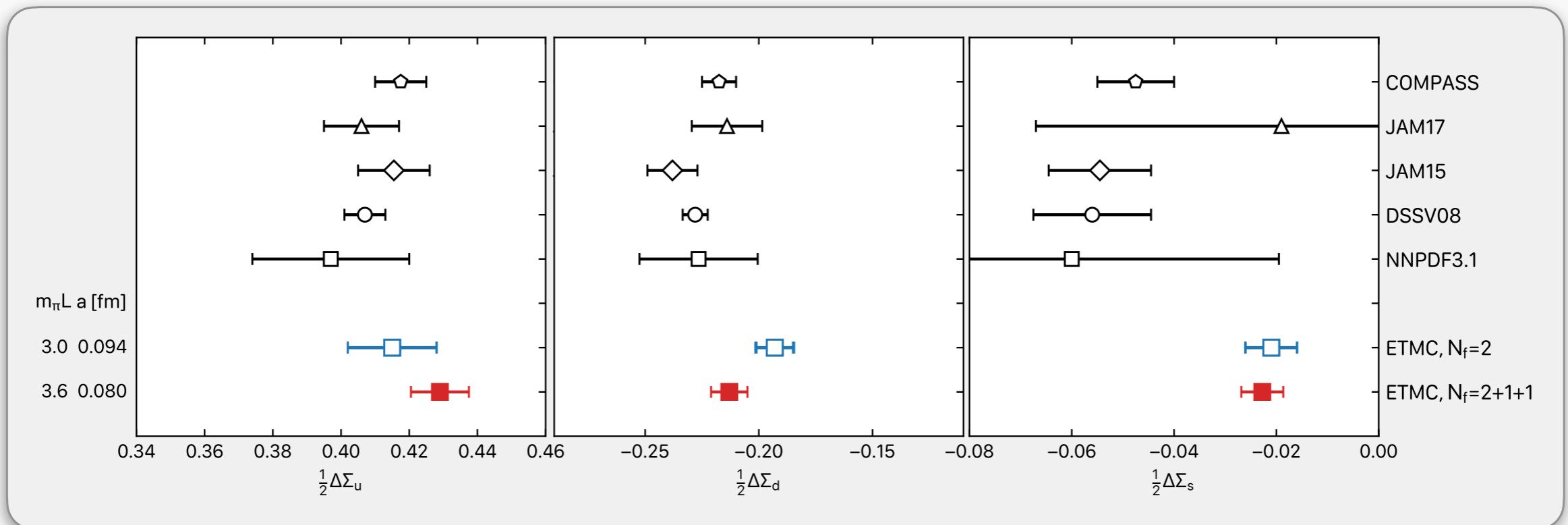
- Open symbols: connected only
- Filled symbols: disconnected added
- Of order 10–15%



Quark intrinsic spin contributions

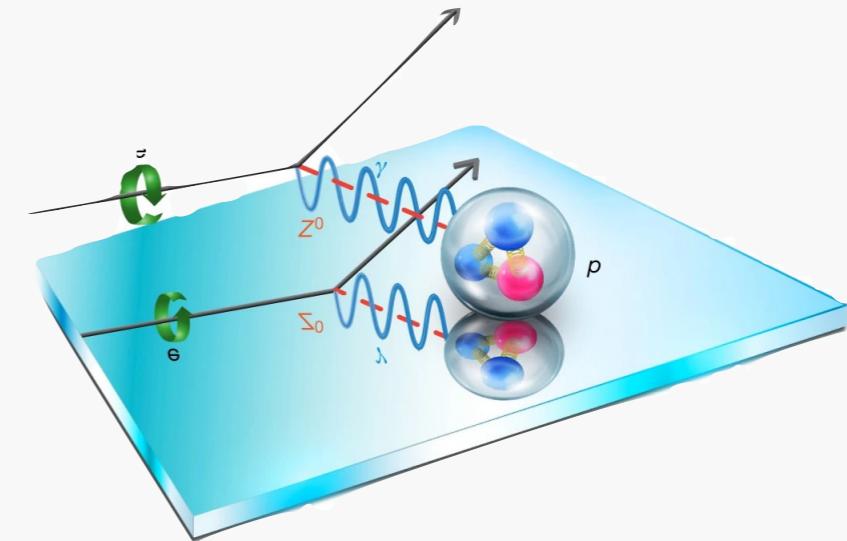
Quark intrinsic spin contributions to nucleon spin

- Individual up-, down-, and strange-quark intrinsic spin contributions to nucleon spin
- Lattice comparison to experiment



Nucleon Electromagnetic Form Factors

- Proton and neutron EM form factors → *radii and magnetic moments*
- Strange EM form factors → *strangeness, connect e.g. to QWeak*



Dirac and Pauli (F_1 and F_2) / Sachs Electric and Magnetic (G_E and G_M) form-factors:

$$G_E(q^2) = F_1(q^2) + \frac{q^2}{(2M_N)^2} F_2(q^2)$$

$$G_M(q^2) = F_1(q^2) + F_2(q^2)$$

Isovector & Isoscalar currents:

$$j_\mu^\nu = \bar{u}\gamma_\mu u - \bar{d}\gamma_\mu d,$$

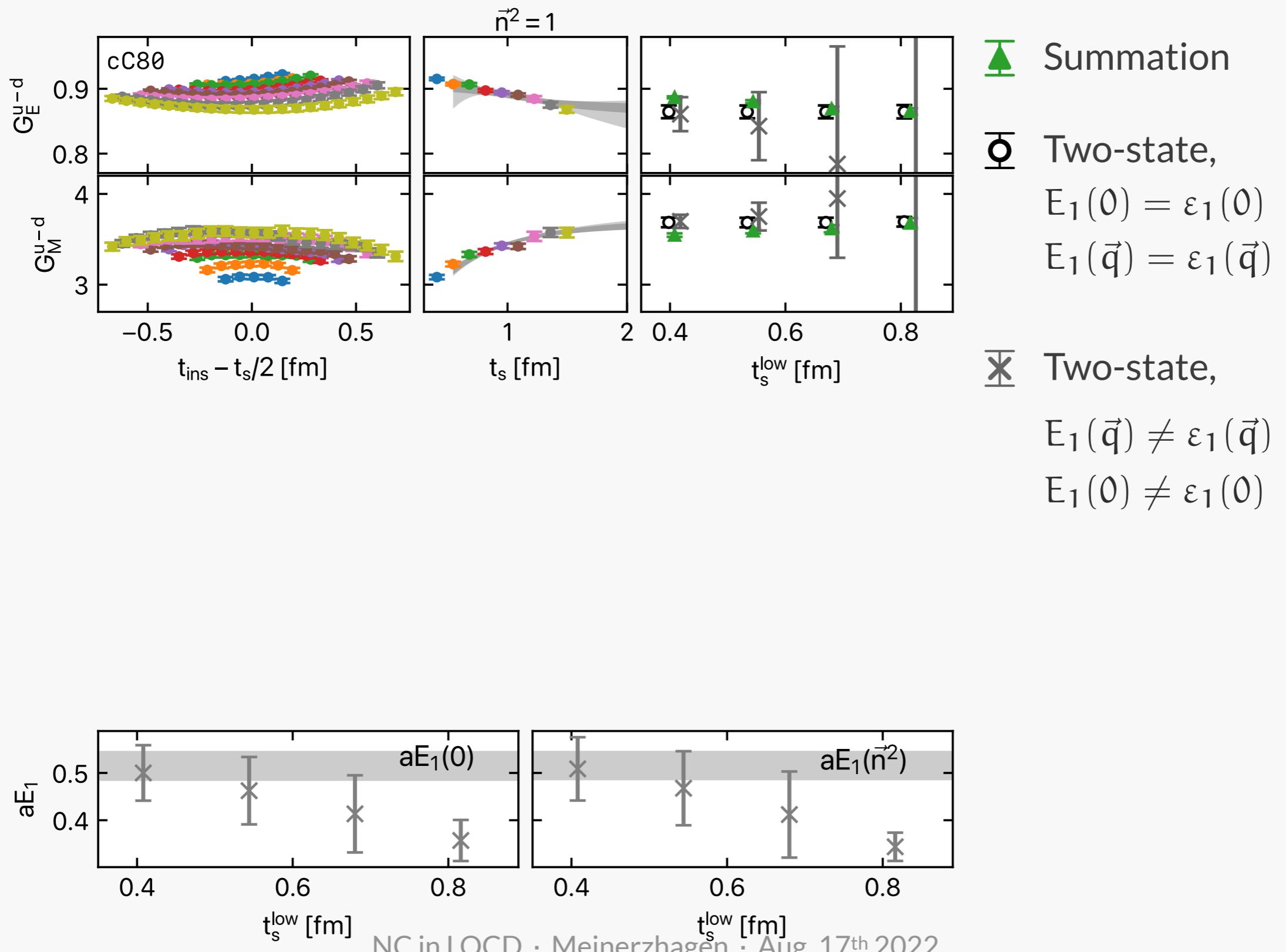
$$j_\mu^s = \bar{u}\gamma_\mu u + \bar{d}\gamma_\mu d$$

Assuming mass
degenerate up and
down quarks

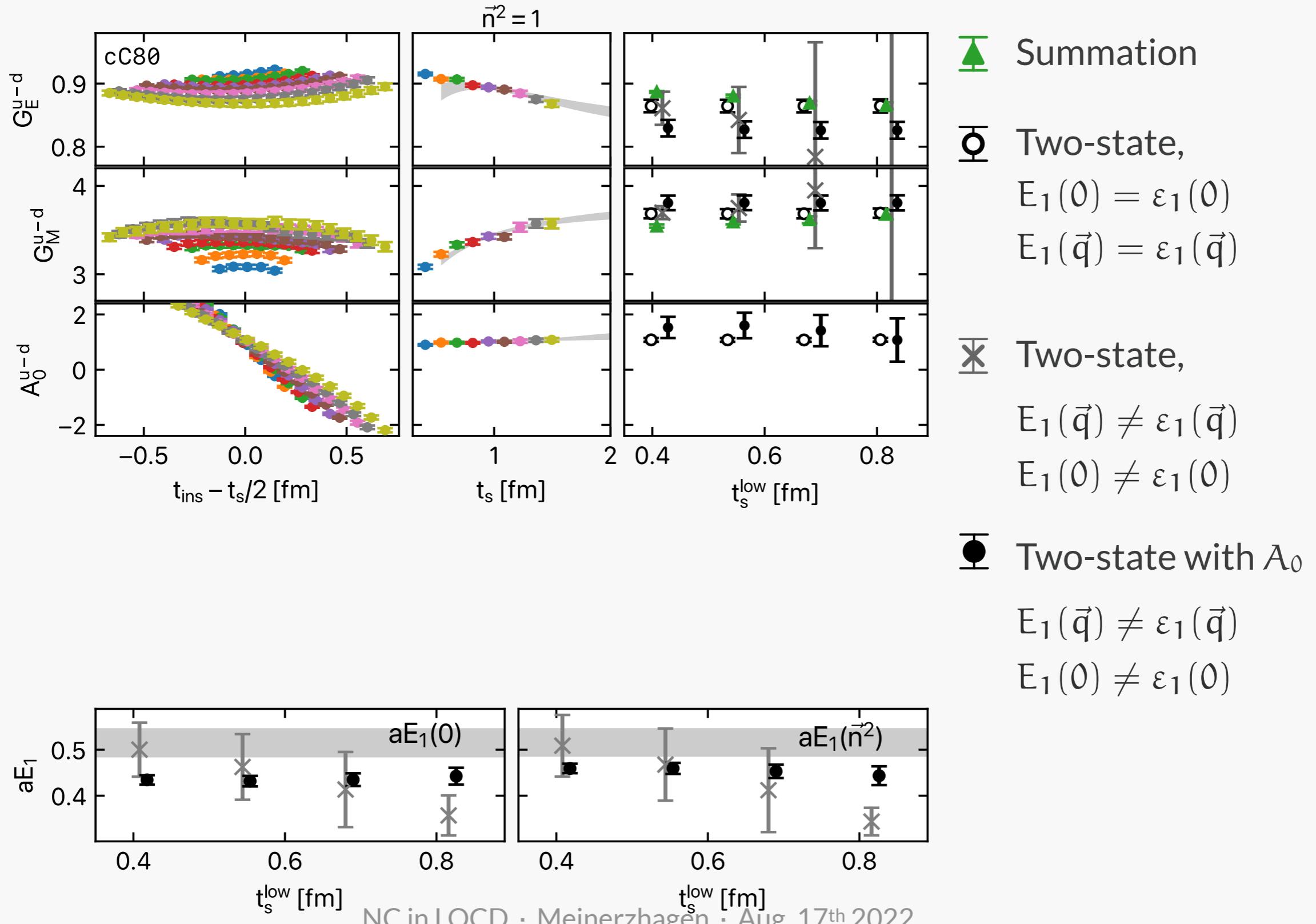
$$F^p - F^n = F^u - F^d$$

$$F^p + F^n = \frac{1}{3}(F^u + F^d)$$

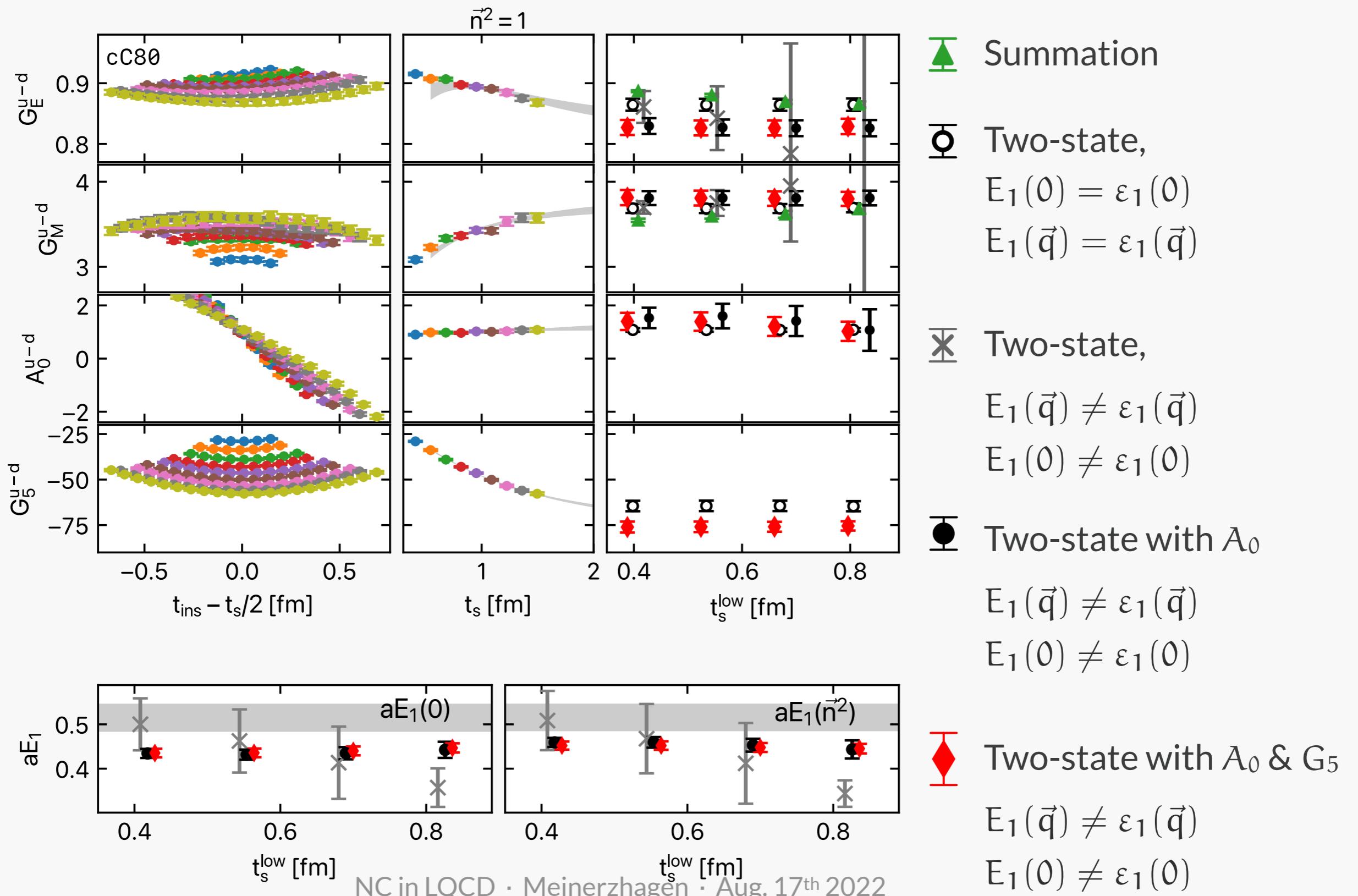
Treatment of excited states



Treatment of excited states

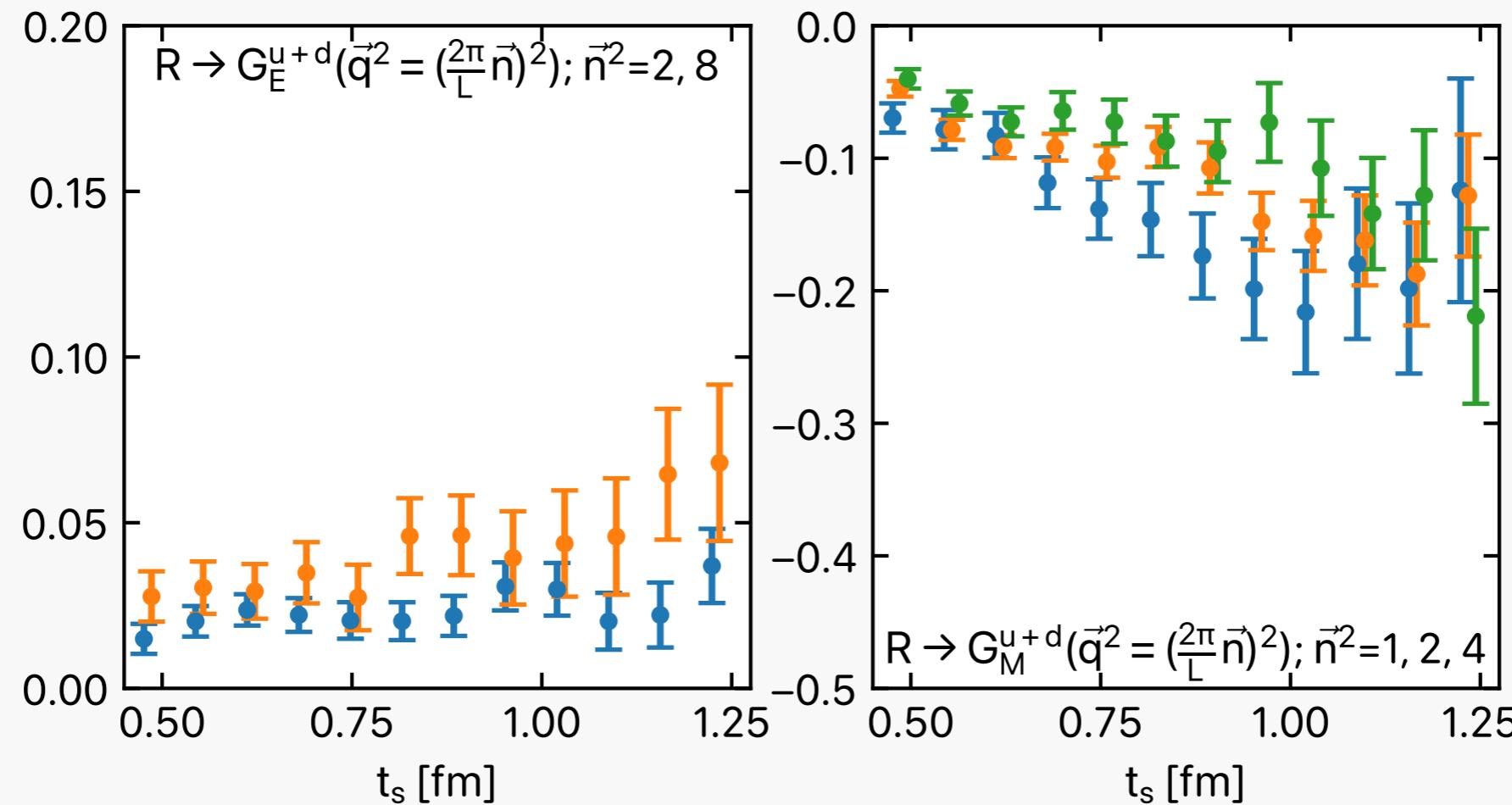


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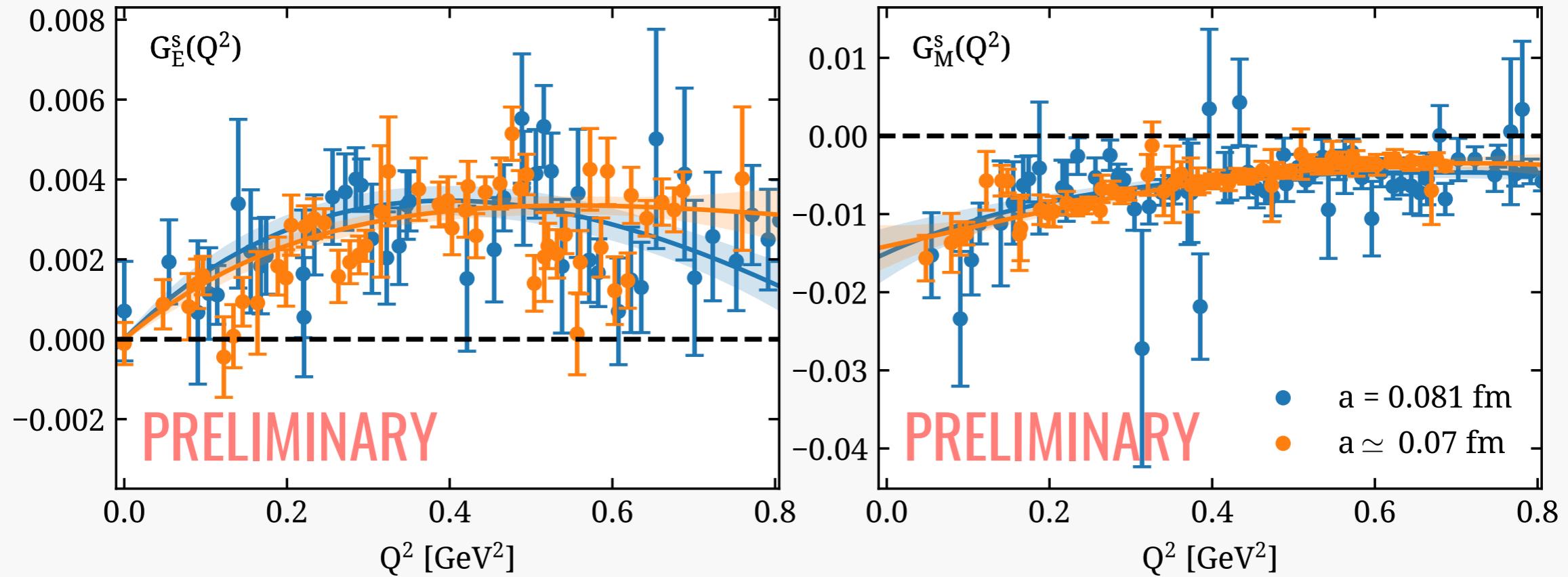


Disconnected EM form factors

Disconnected: High number of sources per config. + hierarchical probing, color/spin dilution and exact of low-mode estimation of loops



Strange quark contribution

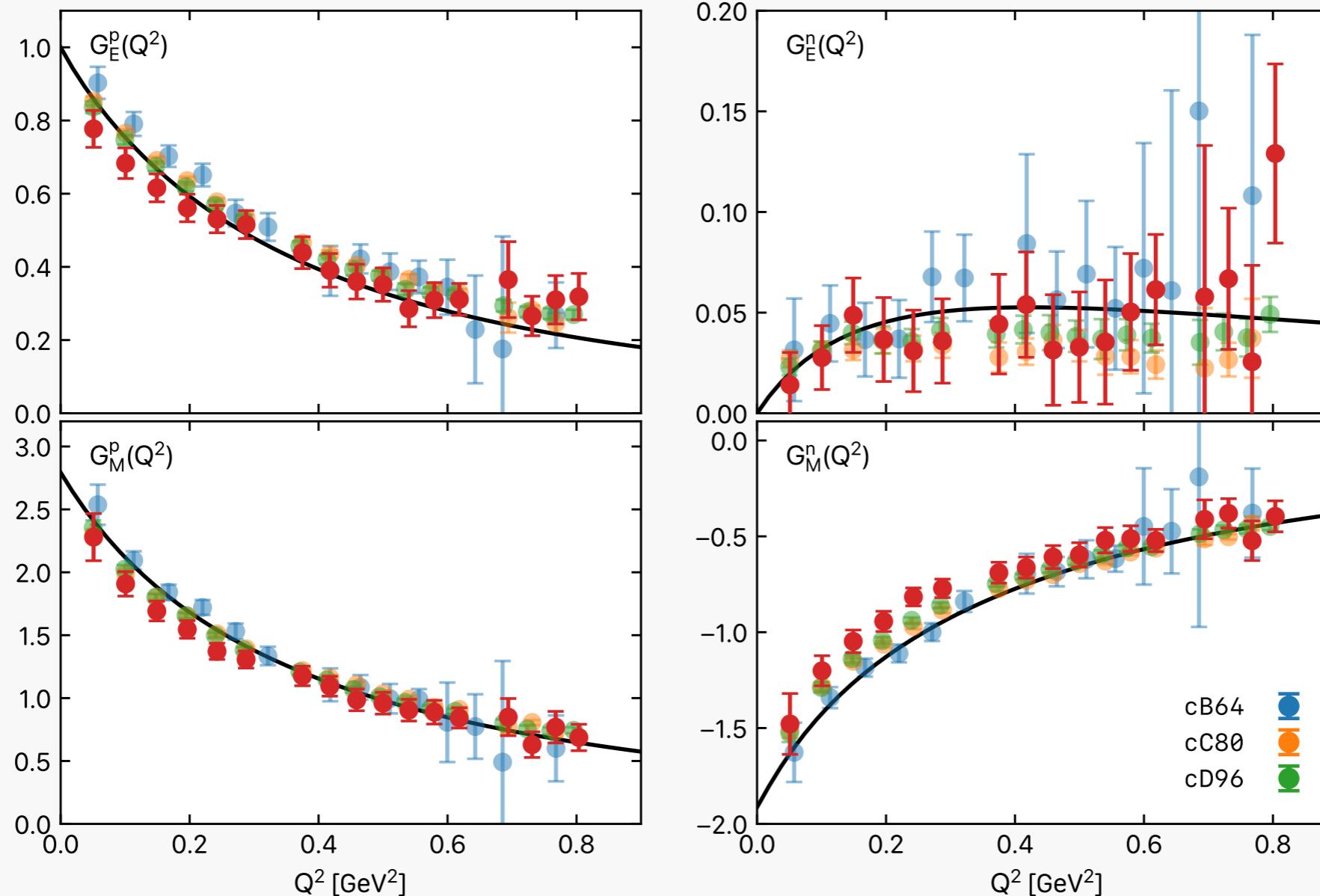


Phys. Rev. D101 (2020) 031501, arXiv:1909.10744 [hep-lat]

Strange EM form factors: not well known experimentally

- Preliminary finer lattice spacing $a=0.07 \text{ fm}$
- Compare to best experimental results so far:
 - HAPPEX: $G_M^s(Q^2 \sim 0.62 \text{ GeV}^2) = -0.070(67)$
 - A4: $G_E^s(Q^2 \sim 0.22 \text{ GeV}^2) = 0.050(38)(19)$
 $G_M^s(Q^2 \sim 0.22 \text{ GeV}^2) = 0.14(11)(11)$

Proton and Neutron (combining disc.)



- Preliminary continuum limit
 - Interpolate to Q^2 values of intermediate a
 - $G_{\text{lat}}(Q^2) = G_0(Q^2) + a^2 G_1(Q^2)$

Fermion Loop Techniques

One-end trick

- One-end trick: applicable to meson two-point functions

M Foster, C Michael, PRD 59 (99) 074503

- Can exploit a feature of TMFs to apply to disconnected loops

ETMC, CPC179 (2008) 695-715

Twisted mass Wilson operator: $M_{\pm} = M \pm i\gamma_5\mu$

Identity:

$$\begin{aligned} S_+(x; y) - S_-(x; y) &= \sum_{z,w} \frac{1}{M_+}(x; z)(M_- - M_+)(z; w)\frac{1}{M_-}(w; y) \\ &= -2i\mu \sum_z S_+(x; z)\gamma_5 S_-(z; y) \end{aligned}$$

The isovector combination can be written as:

$$\begin{aligned} Tr[\Gamma S_+(t; t)] - Tr[\Gamma S_-(t; t)] &= -i2\mu \sum_{\tau} Tr[\Gamma S_+(t; \tau)\gamma_5 S_-(\tau; t)] \\ &= -i2\mu \sum_{\tau} Tr[\gamma_5 \Gamma S_+(t; \tau) S_+^\dagger(t; \tau)] \end{aligned}$$

One-end trick

The isovector combination:

$$Tr[\Gamma S_+(t; t)] - Tr[\Gamma S_-(t; t)] = -i2\mu \sum_{\tau} Tr[\gamma_5 \Gamma S_+(t; \tau) S_+^\dagger(\tau; t)]$$

Can be computed via the one-end trick:

$$\langle \phi^\dagger(t) \gamma_5 \Gamma \phi(t) \rangle = \sum_{\tau \tau'} \langle \eta^\dagger(\tau) S_+^\dagger(\tau; t) \gamma_5 \Gamma S_+(t; \tau') \eta(\tau') \rangle = \sum_{\tau} Tr[\gamma_5 \Gamma S_+(t; \tau) S_+^\dagger(\tau; t)]$$

Variance of one-end trick:

$$\begin{aligned} & \langle |\phi^\dagger(t) \gamma_5 \Gamma \phi(t)|^2 \rangle - \langle \phi^\dagger(t) \gamma_5 \Gamma \phi(t) \rangle^2 = \\ & \sum_{\tau_1 \tau_2} Tr[S_+^\dagger(\tau_1; t) \Gamma S_+(t; \tau_2) S_+^\dagger(\tau_2; t) \Gamma S_+(t; \tau_1)] - \sum_{\tau \alpha} |S_+^\dagger(\tau; t) \Gamma S_+(t; \tau)|_{\alpha \alpha}^2 \end{aligned}$$

One-end trick

One-end trick applicable to the isovector combination:

$$Tr[\Gamma S_+(t; t)] - Tr[\Gamma S_-(t; t)] = -i2\mu \sum_{\tau} Tr[\gamma_5 \Gamma S_+(t; \tau) S_+^\dagger(\tau; t)]$$

Certain isoscalar observables that transform to isovector in twisted mass:

$$\bar{\psi} \Gamma \psi = \frac{1}{2} \bar{\chi} (1 + i\gamma_5 \tau_3) \Gamma (1 + i\gamma_5 \tau_3) \chi$$

$\Gamma = 1, \gamma_5, \sigma_{\mu\nu}$: transform to isovector

$\Gamma = \gamma_\mu, \gamma_5 \gamma_\mu$: remain isoscalar

For isoscalar observables transform to isoscalar in the twisted basis, a generalised version is applicable:

$$Tr[\Gamma S_+(t; t)] + Tr[\Gamma S_-(t; t)] = \sum_{\tau; \tau'} Tr[\gamma_5 \Gamma S_+(t; \tau) M(\tau; \tau') \gamma_5 S_+^\dagger(\tau'; t)]$$

M : Wilson operator at critical bare mass

Hierarchical probing

A. Stathopoulos *et al.*, arXiv:1302.4018

Use of Hadamard matrices for dilution basis:

$$H_1 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, H_{n+1} = \begin{pmatrix} H_n & H_n \\ H_n & -H_n \end{pmatrix}$$

with dimension $N=2^n$. Hierarchically add vectors as dilution basis expands (N),
e.g.:

$$\eta_1 = \begin{pmatrix} H_1 \\ H_1 \\ \vdots \\ H_1 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ 1 & 1 \\ 1 & -1 \\ \vdots & \vdots \end{pmatrix}, \eta_2 = \begin{pmatrix} H_2 \\ H_2 \\ \vdots \\ H_2 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

$V/N \in \mathbb{N}$

i.e. can reuse solutions from class- n Hadamard dilution for class- $n+1$

Hierarchical probing

Similar to colouring (even/odd or color/spin dilution):

$$\text{err} = \text{Tr}[A] - \text{Tr}[\eta_n^\top A \eta_n] = \text{Tr}[A(1 - \eta_n \eta_n^\top)]$$

$$\eta_n \eta_n^\top = \begin{pmatrix} \mathbb{1}_{2^n \times 2^n} & \mathbb{1}_{2^n \times 2^n} & \dots & \mathbb{1}_{2^n \times 2^n} \\ \mathbb{1}_{2^n \times 2^n} & \mathbb{1}_{2^n \times 2^n} & \dots & \mathbb{1}_{2^n \times 2^n} \\ \vdots & \vdots & \ddots & \vdots \end{pmatrix}$$

i.e. first contributions in the variance are between $N^{\text{th}} = (2^n)^{\text{th}}$ neighbours.

Hierarchical probing:

- Extending probing distance → reuse previous vectors (not the case in naive colouring)
- Matrix dimension (volume) must be divisible by Hadamard matrix length, which is restricted to 1, 2, 4 and $4k$ with k integer.
- Need to multiply Hadamard elements by noise vectors to create an unbiased estimator.

Stochastic Techniques

Disconnected: Hierarchical probing, color/spin dilution, and exact low-mode estimation of loops

Ens.	Light	
	Stochastic	Deflation
cB64:	$n_{\text{vec}} = 12_{\text{col./spin}} \times 512_{\text{nhad.}}$	$n_{\text{ev}} = 200$
cC80:	$n_{\text{vec}} = 12_{\text{col./spin}} \times 512_{\text{nhad.}}$	$n_{\text{ev}} = 450$
cD96:	$n_{\text{vec}} = 12_{\text{col./spin}} \times 512_{\text{nhad.}} \times 8_{\text{stoch.}}$	None

Ens.	Strange	
	Stochastic	Deflation
cB64:	$n_{\text{vec}} = 12_{\text{col/spin}} \times 12_{\text{stoch.}} \times 32_{\text{nhad.}}$	
cC80:	$n_{\text{vec}} = 12_{\text{col/spin}} \times 4_{\text{stoch.}} \times 512_{\text{nhad.}}$	
cD96:	$n_{\text{vec}} = 12_{\text{col/spin}} \times 4_{\text{stoch.}} \times 512_{\text{nhad.}}$	

Stochastic Techniques

Disconnected: Hierarchical probing, color/spin dilution, and exact low-mode estimation of loops

Ens.	Light		Also available without deflation ($n_{ev}=0$)
	Stochastic	Deflation	
cB64:	$n_{vec} = 12_{\text{col./spin}} \times 512_{\text{nhad.}}$	$n_{ev} = 200$	
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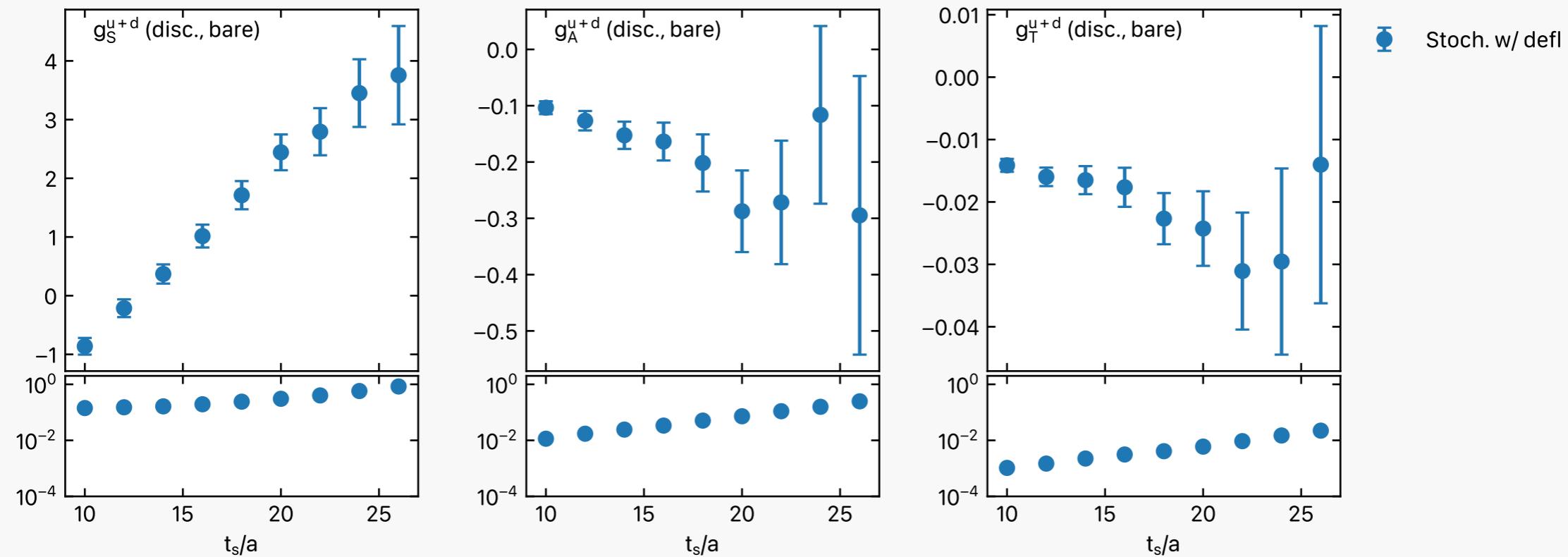
Stochastic Techniques

Disconnected: Hierarchical probing, color/spin dilution, and exact low-mode estimation of loops

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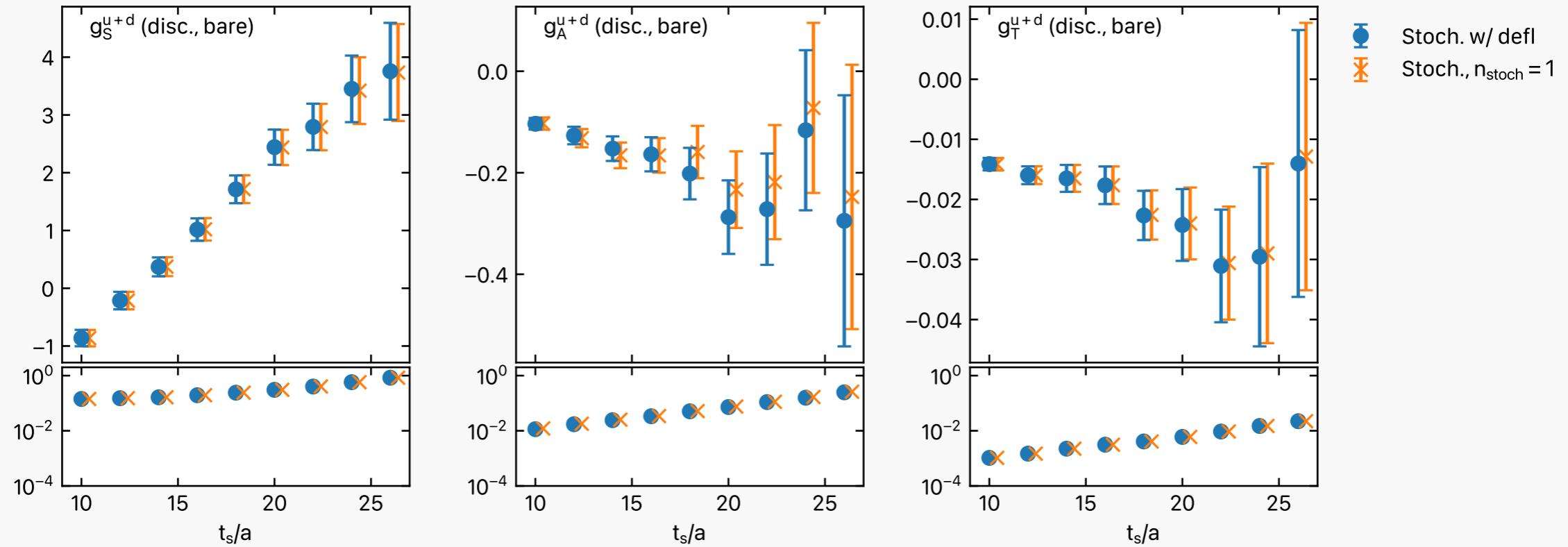
Ens.	Strange		Also available at next probing distance (512_{nhad})
	Stochastic	Deflation	
cB64:	$n_{vec} = 12_{\text{col/spin}} \times 12_{\text{stoch.}} \times 32_{\text{nhad.}}$		
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Stochastic Techniques



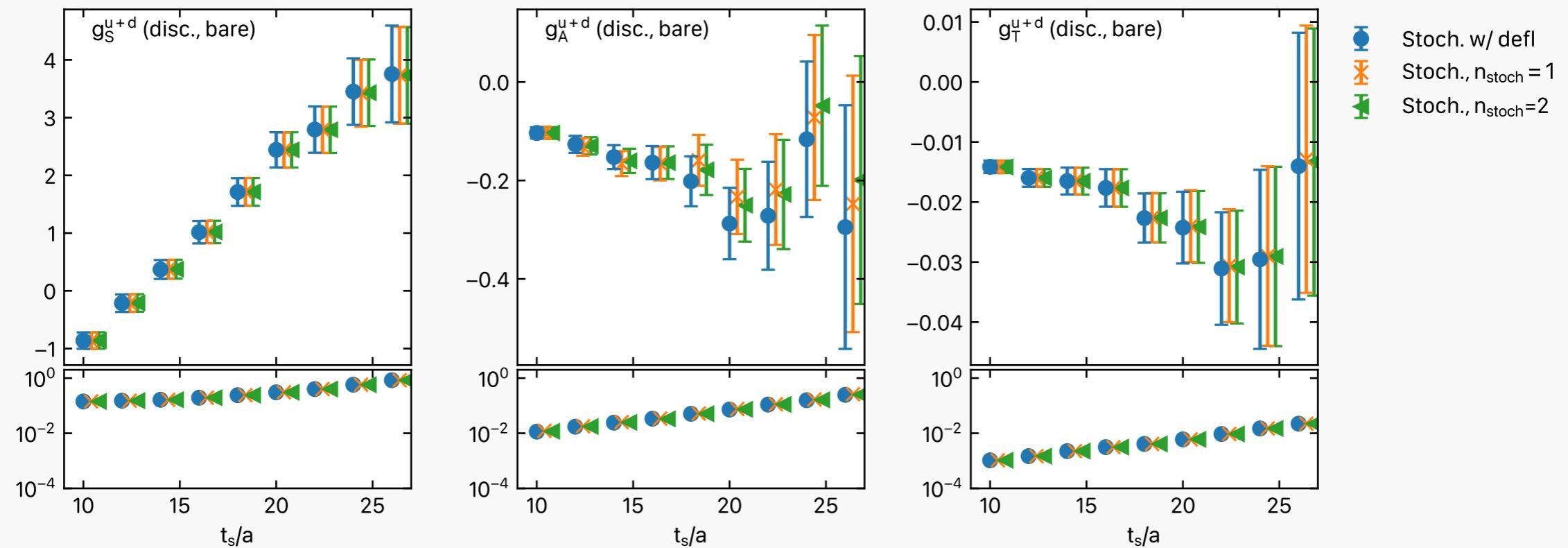
- Scalar, axial and tensor charges
- Intermediate lattice spacing ($a=0.07$ fm)
- Bottom row is error

Stochastic Techniques



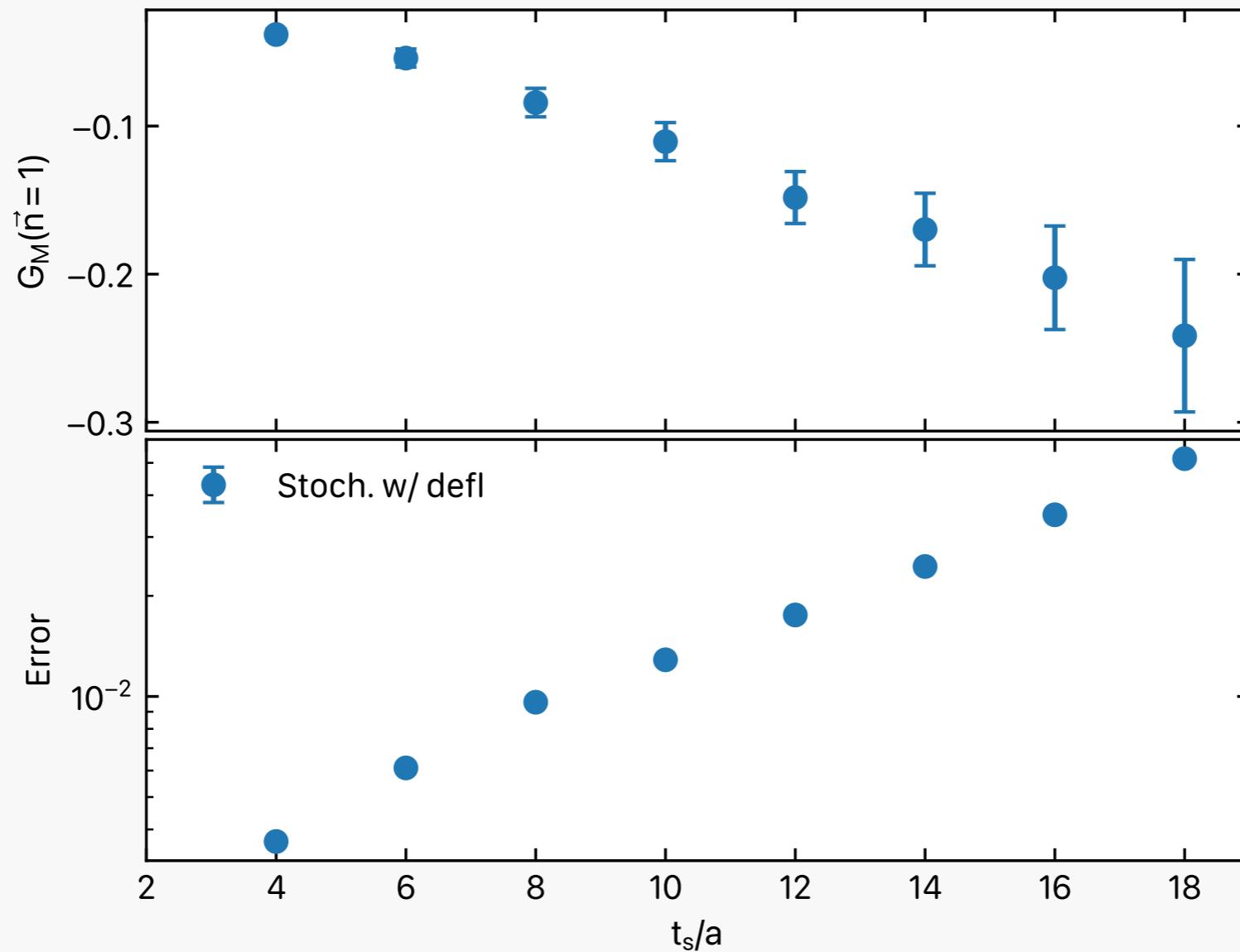
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Stochastic Techniques



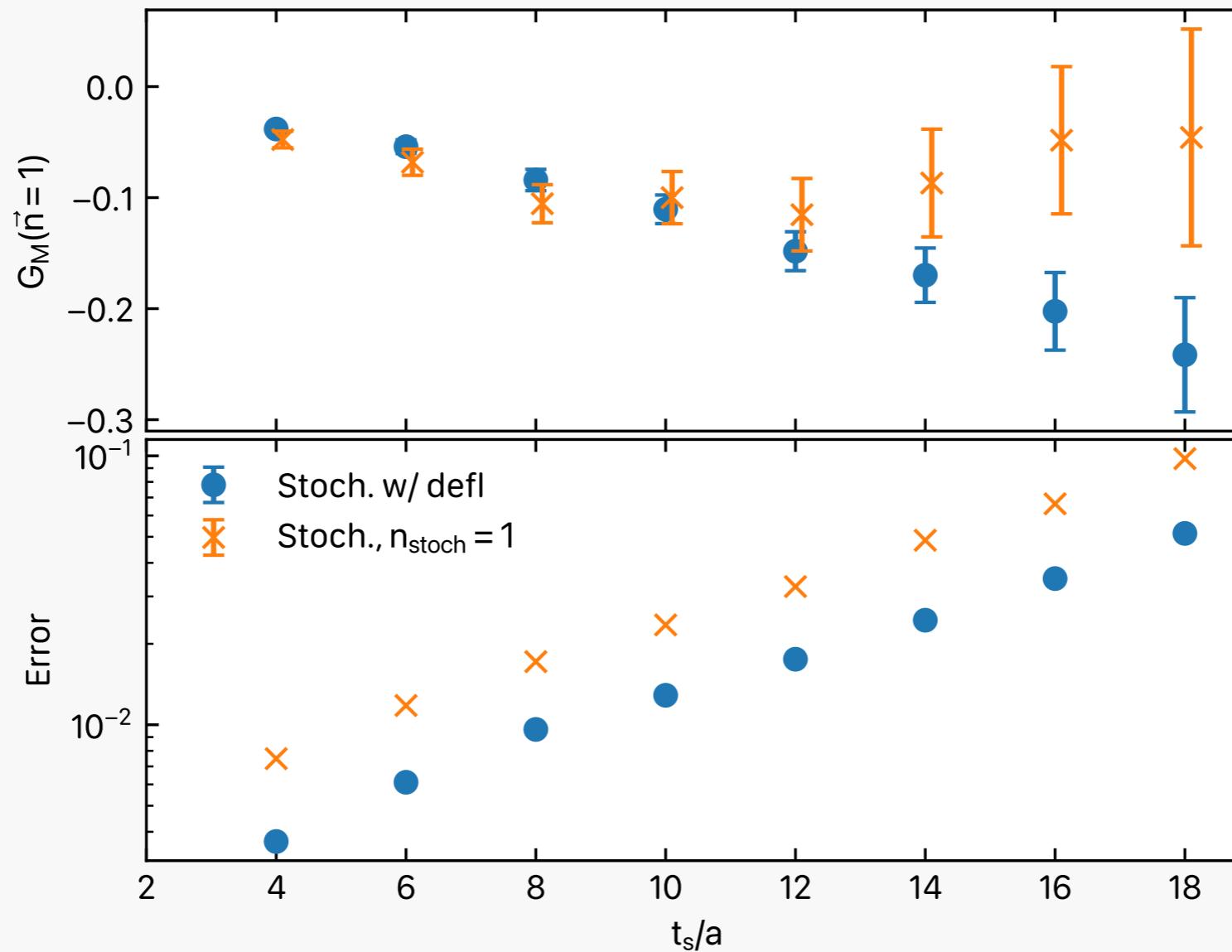
- Scalar, axial and tensor charges
- Intermediate lattice spacing ($a=0.07$ fm)
- Bottom row is error
- **Note:** in all cases, 512 Hadamard vectors \times 12 (spin/color dilution)

Stochastic Techniques



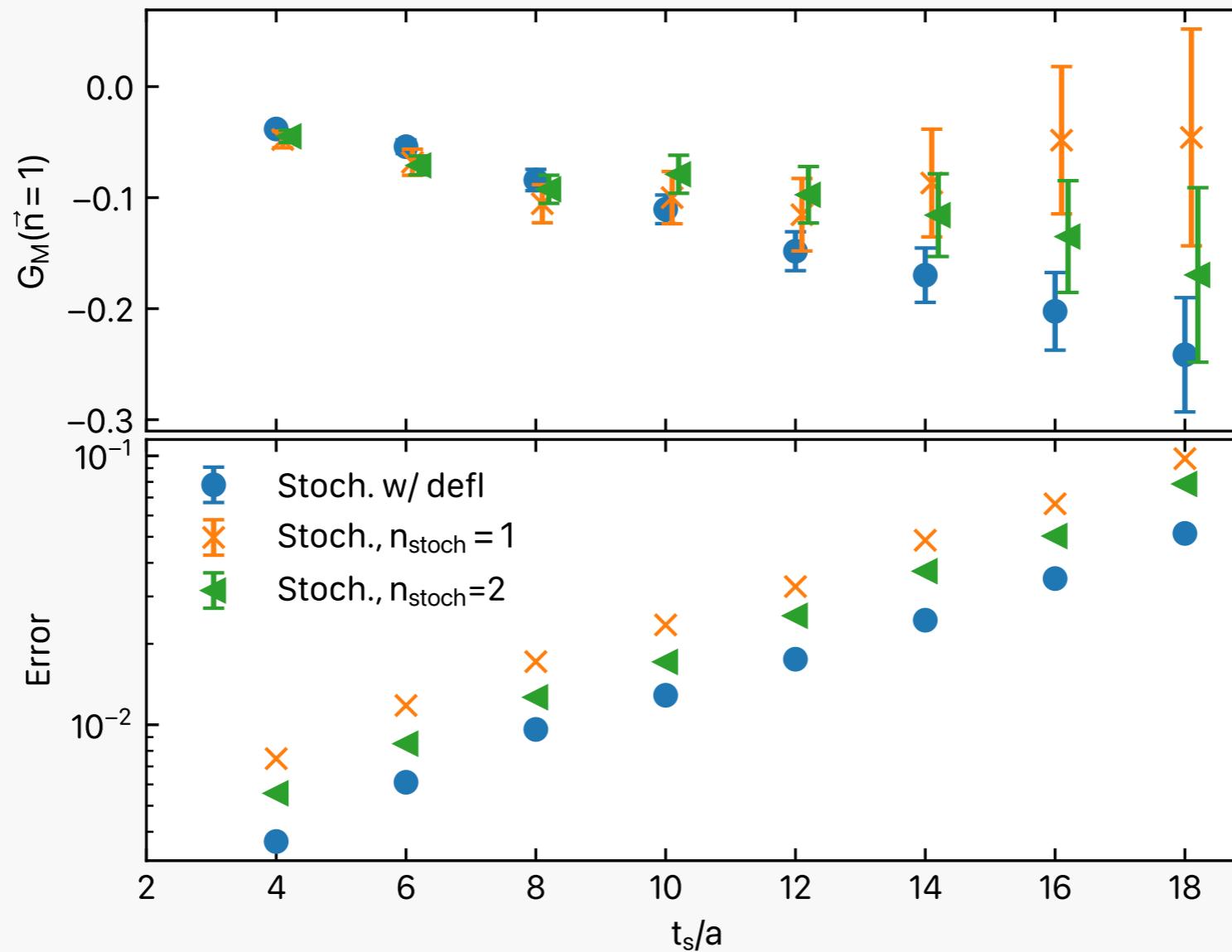
- Magnetic form factor at first non-zero momentum transfer
- Intermediate lattice spacing ($a=0.07$ fm)

Stochastic Techniques



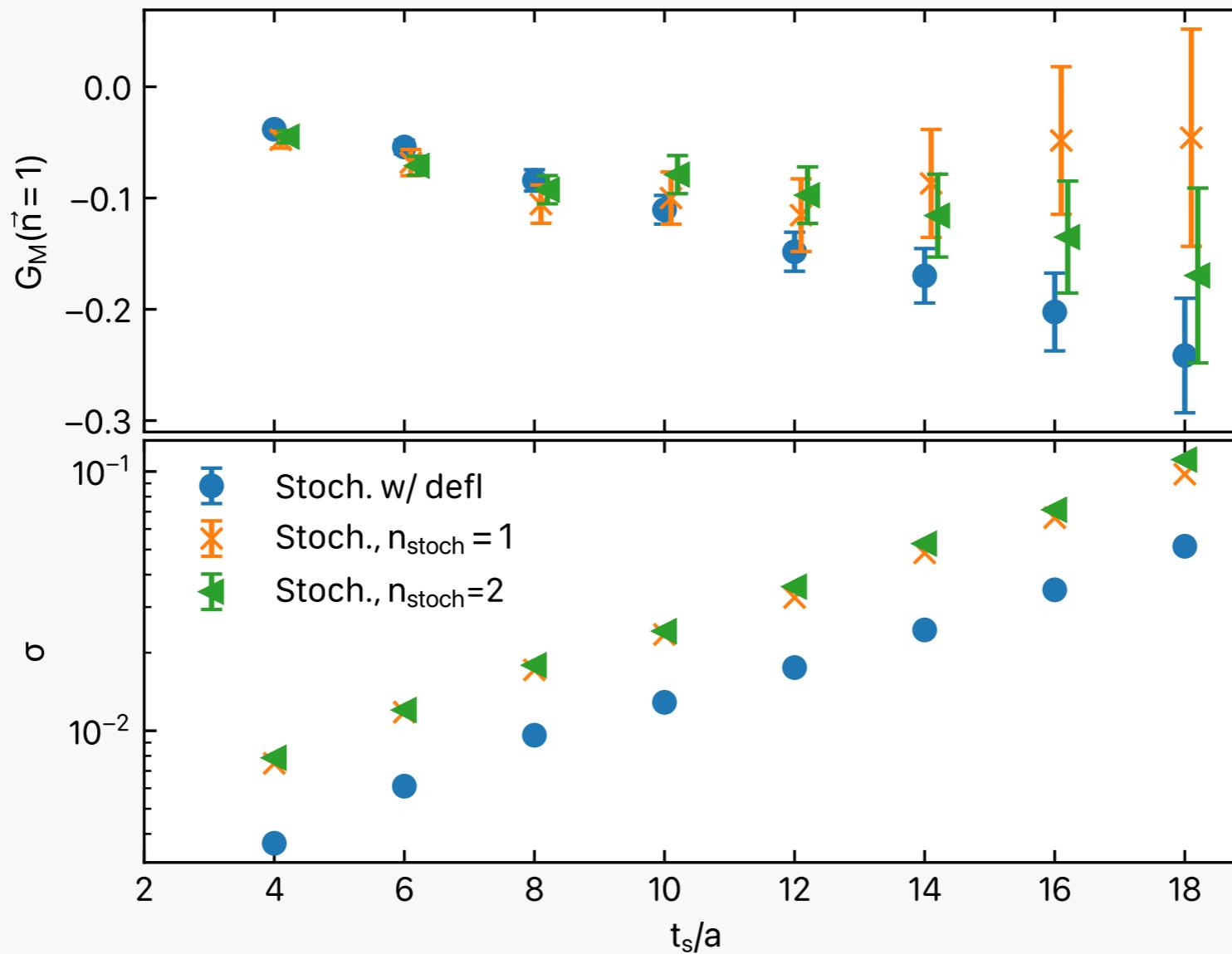
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Stochastic Techniques



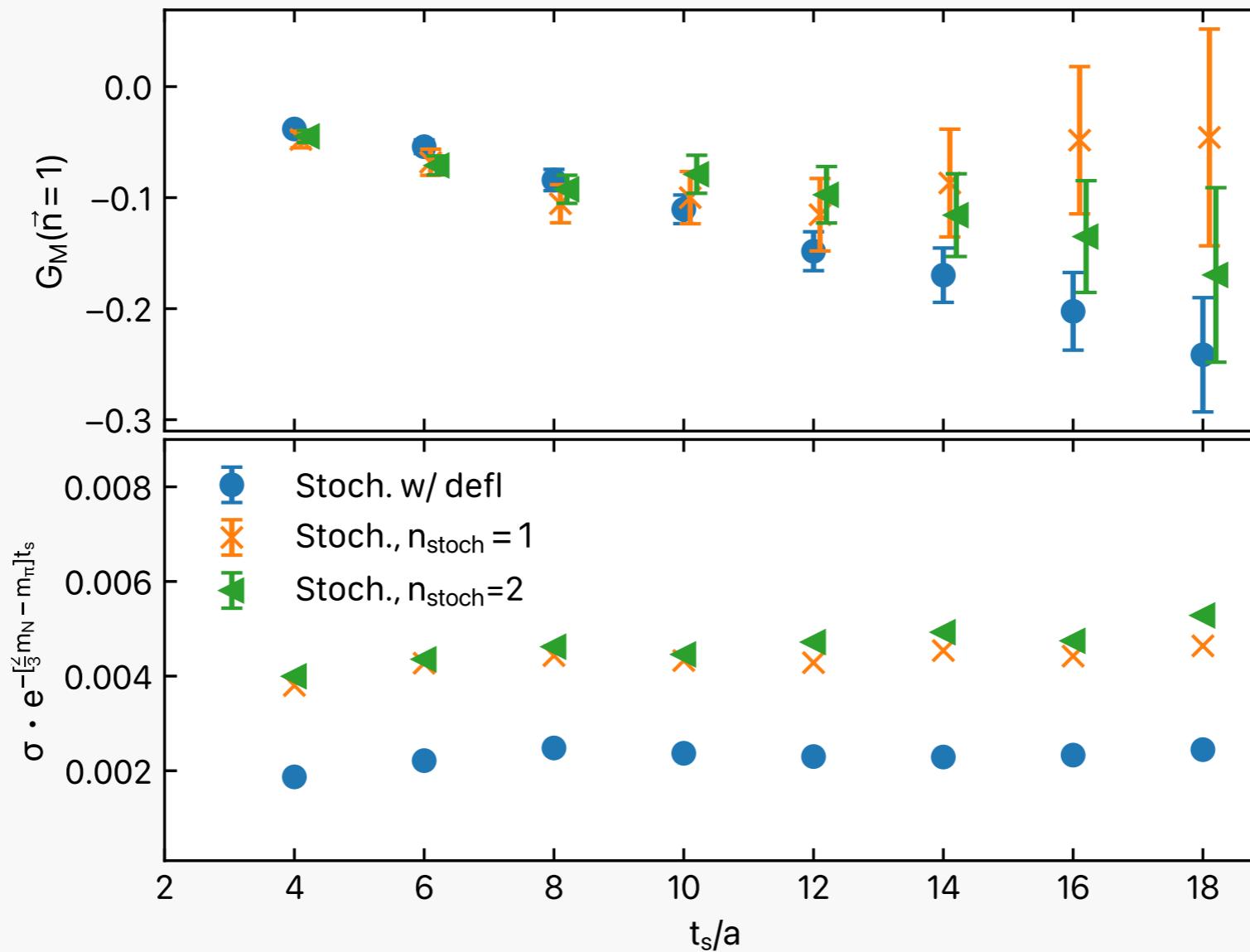
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Stochastic Techniques



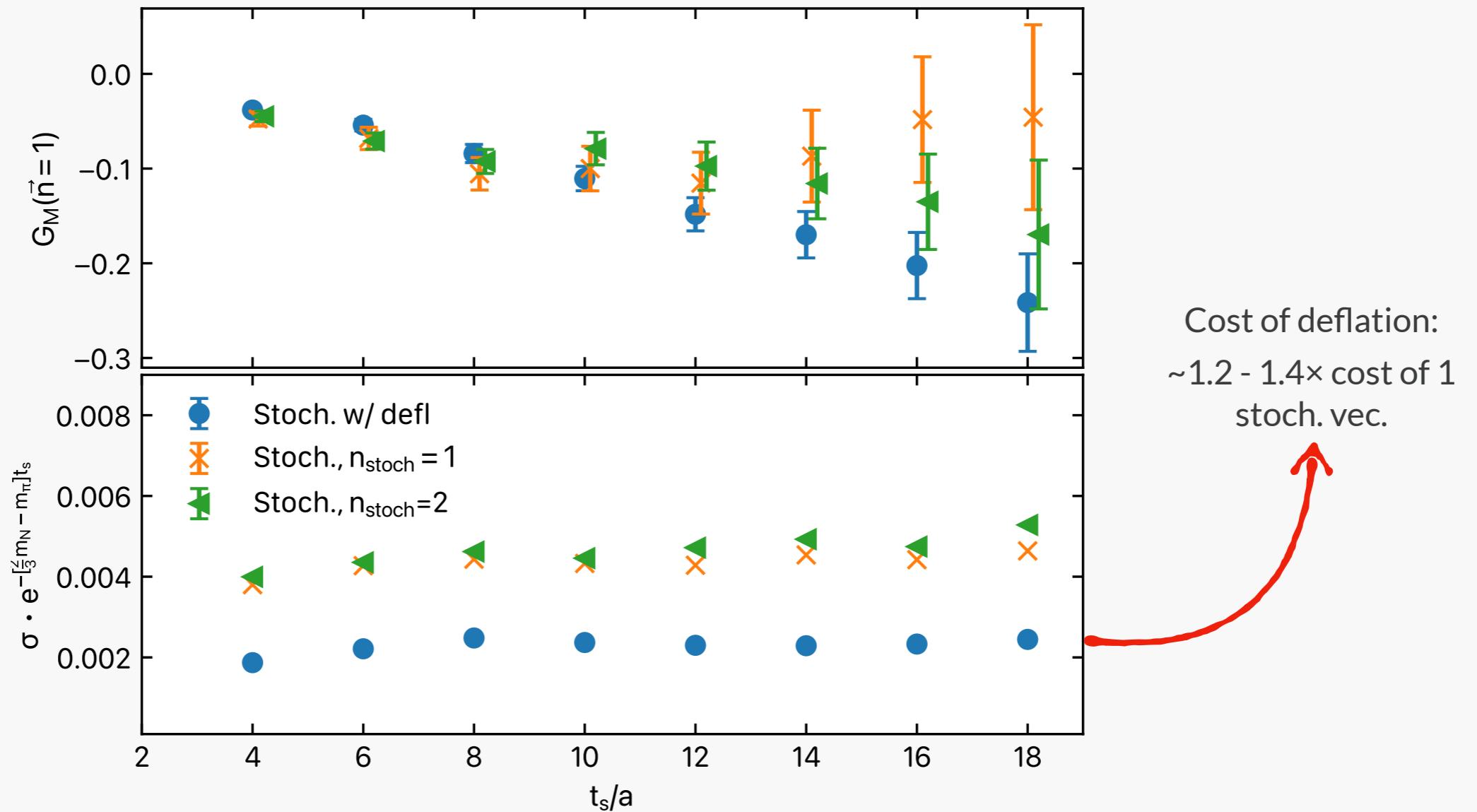
- Magnetic form factor at first non-zero momentum transfer
- Intermediate lattice spacing ($a=0.07$ fm)
- Expected scaling of error between 1 and 2 sources without deflation)

Stochastic Techniques



- Magnetic form factor at first non-zero momentum transfer
- Intermediate lattice spacing ($a=0.07$ fm)
- Expected scaling of error between 1 and 2 sources without deflation)
- Scaling with t_s as expected

Stochastic Techniques



- Magnetic form factor at first non-zero momentum transfer
- Intermediate lattice spacing ($a=0.07$ fm)
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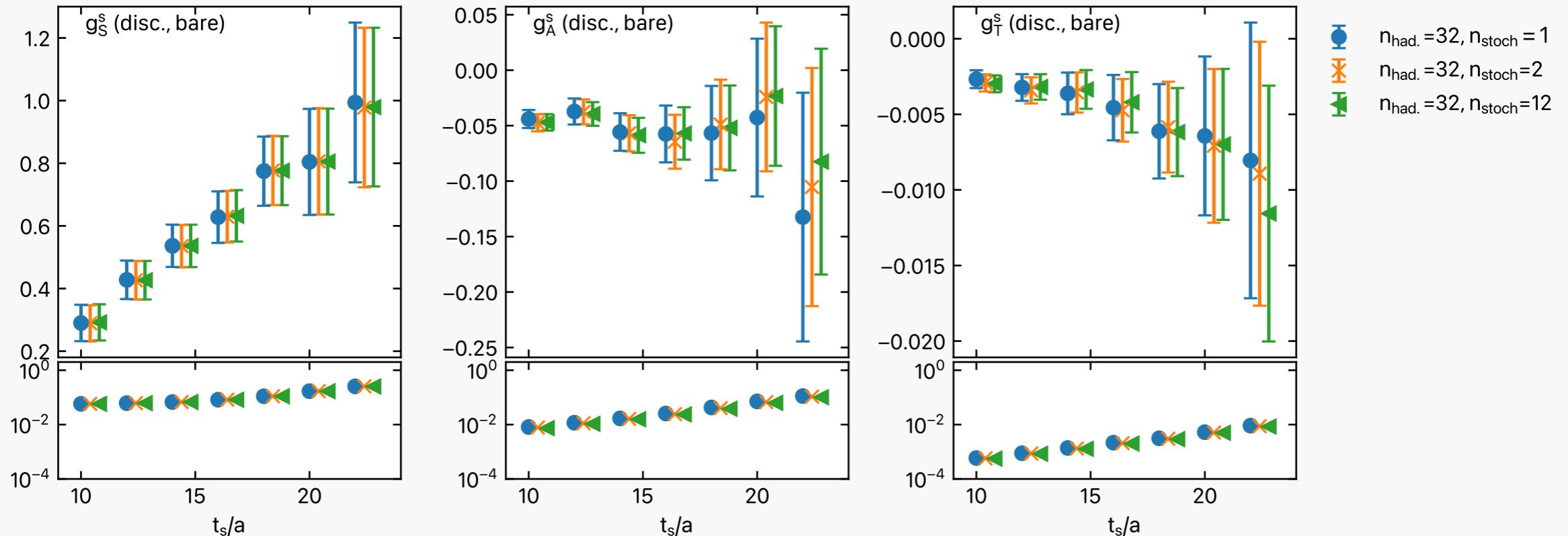
Stochastic Techniques

Disconnected: Hierarchical probing, color/spin dilution, and exact low-mode estimation of loops

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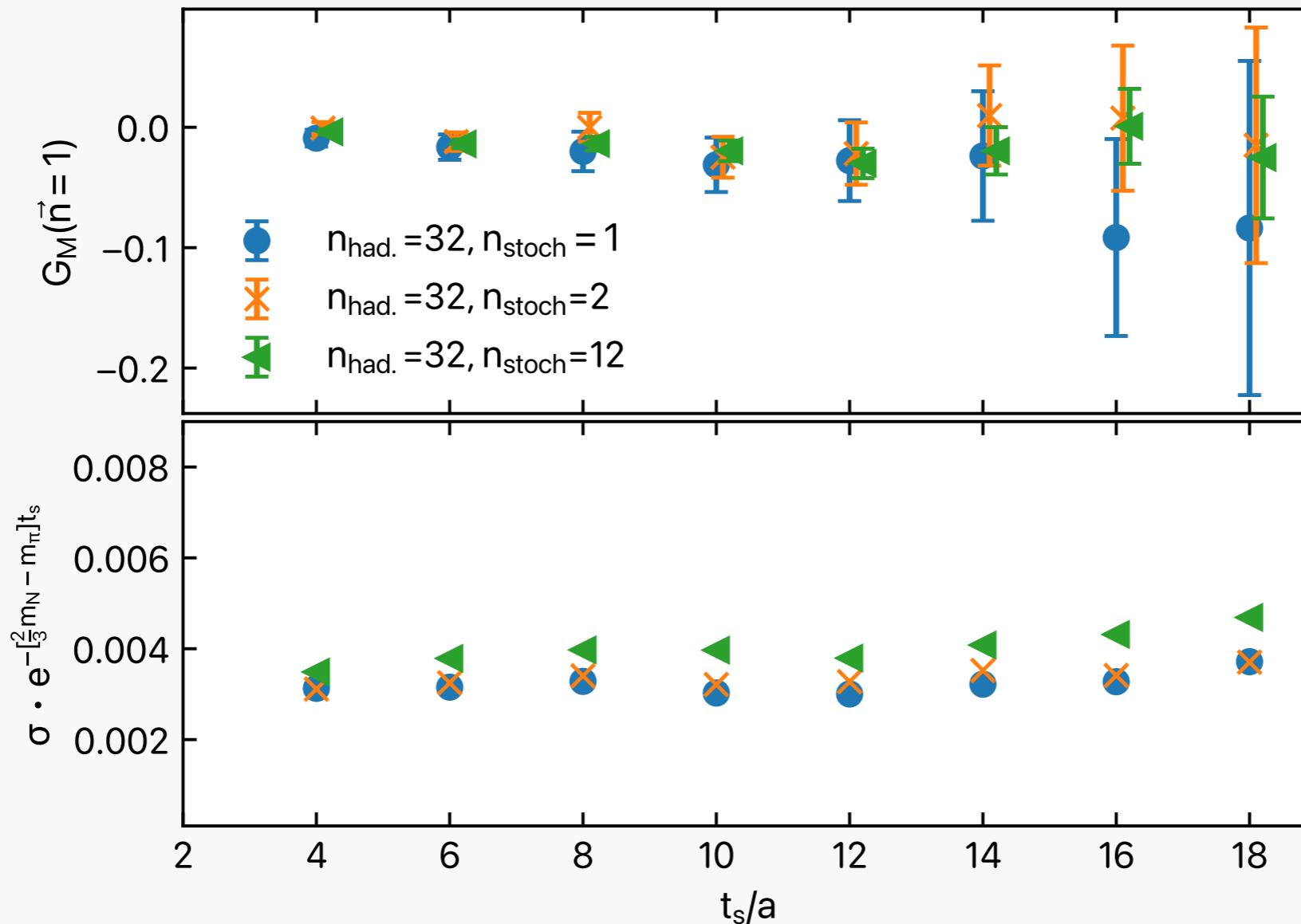
Ens.	Strange	
	Stochastic	Deflation
cB64:	$n_{vec} = 12_{col/spin} \times 12_{stoch.} \times 32_{nhad.}$	Also available at next probing distance (512_{nhad})
cC80:	$n_{vec} = 12_{col/spin} \times 4_{stoch.} \times 512_{nhad.}$	
cD96:	$n_{vec} = 12_{col/spin} \times 4_{stoch.} \times 512_{nhad.}$	

Stochastic Techniques



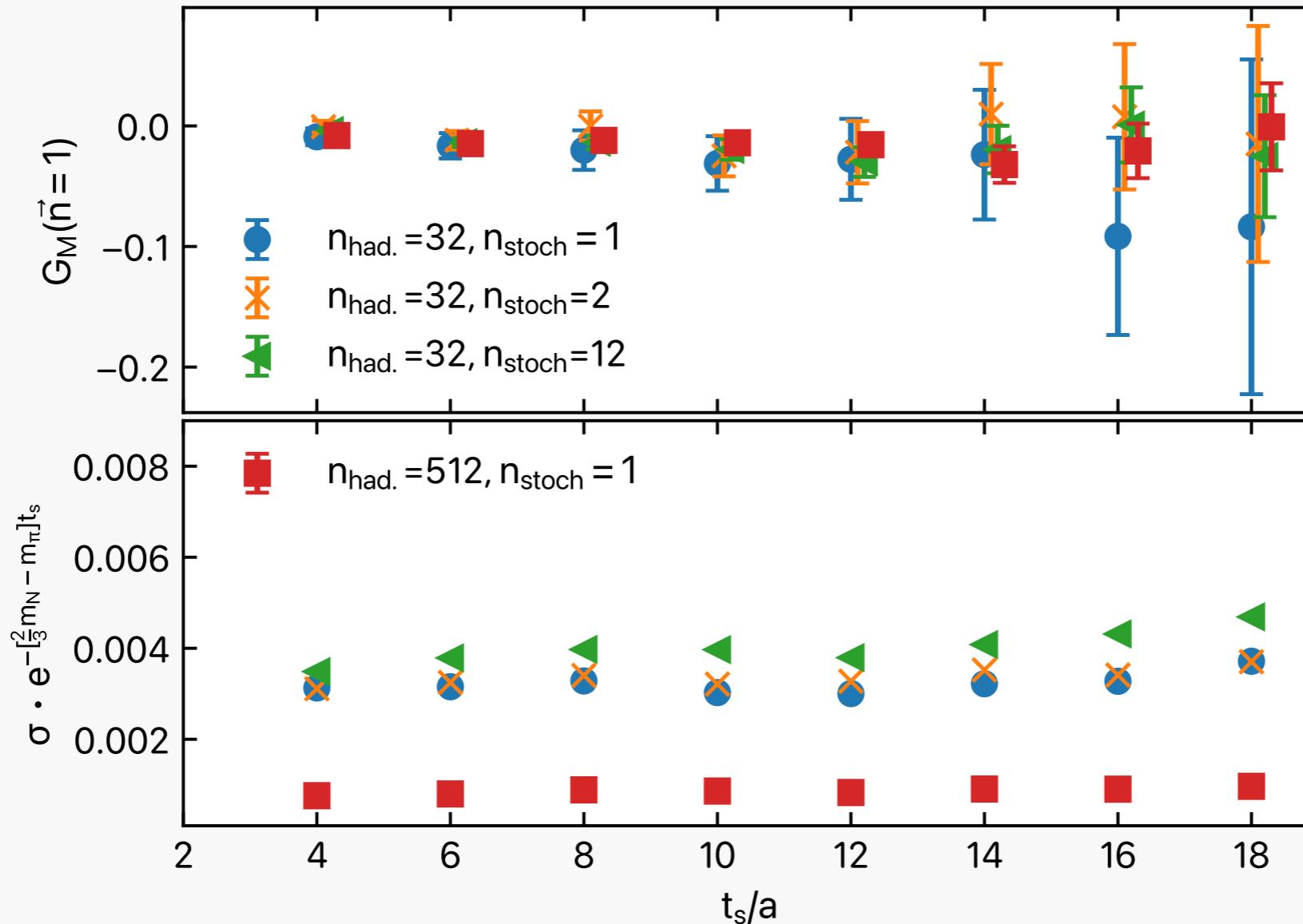
- No effect on local charges
- Coarsest lattice spacing ($a=0.08$ fm)

Stochastic Techniques



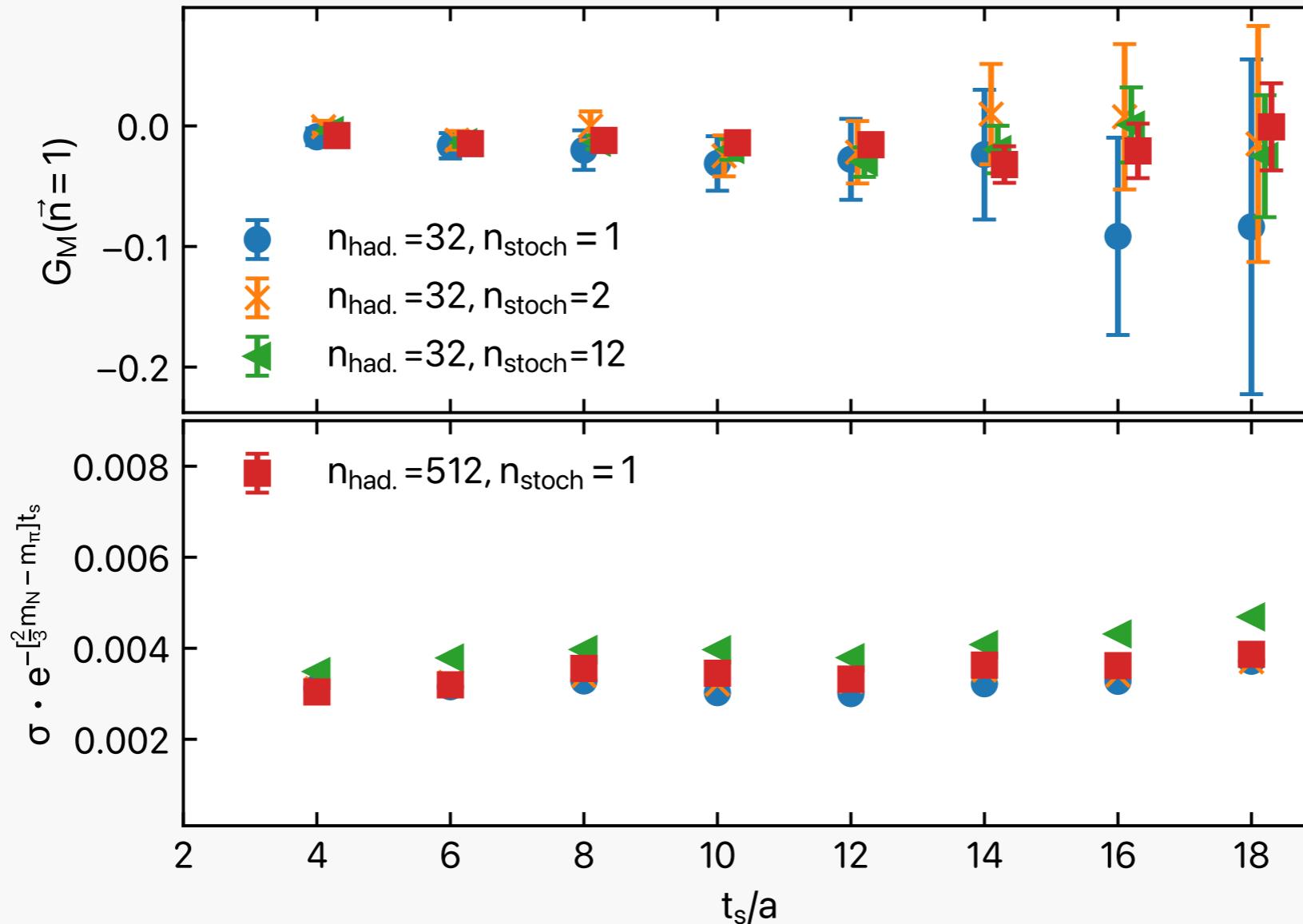
- Strange magnetic form factor at first non-zero momentum transfer
- Coarse lattice spacing ($a=0.08$ fm)
- At 12 sources, stochastic error seems to have saturated

Stochastic Techniques



- Strange magnetic form factor at first non-zero momentum transfer
- Coarse lattice spacing ($a=0.08$ fm)
- Increase in probing distance by one. But: 512 inversions compared to 32×12

Stochastic Techniques



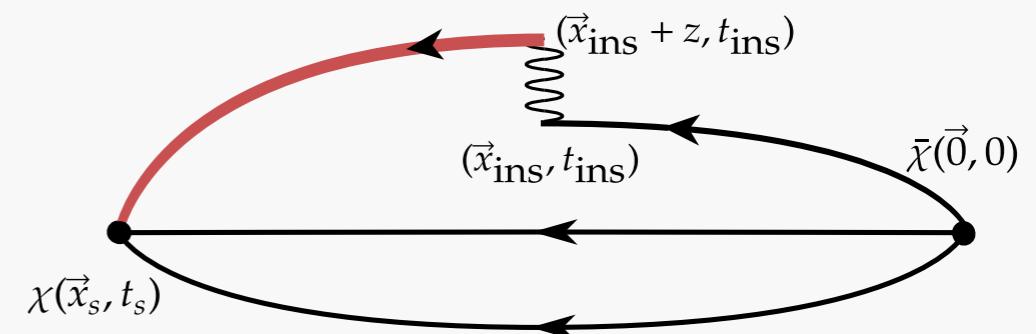
- Strange magnetic form factor at first non-zero momentum transfer
- Coarse lattice spacing ($a=0.08$ fm)
- Comparison ***at equal cost*** → larger distance wins slightly

Summary

- Multigrid solvers: $O(10^5)$ inversions for high statistics three-point functions
- Techniques for disconnected loops
 - Allow access to individual quark contributions to nucleon observables
 - Needed to high precision for contact to experiment
- Deflation and probing crucial at physical quark masses where the diagonal falls off slower

What I didn't cover

- Operators with derivatives
 - Access to e.g. moments of PDFs
 - Gauge-field dependence in loop current
- Operators with Wilson line
 - Access to quasi-PDFs
 - There, probing distance should be investigated w.r.t the displacement length



Acknowledgements



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POST-DOC/0718/0100