
The Structure of the Nucleon from Lattice QCD

Hartmut Wittig

Institute for Nuclear Physics, Helmholtz Institute Mainz, and PRISMA+ Cluster of Excellence,
Johannes Gutenberg-Universität Mainz

QCD on and off the Lattice
Universität Regensburg
18–20 September 2023



JOHANNES GUTENBERG
UNIVERSITÄT MAINZ



Connecting hadron/nuclear community with Lattice QCD

“Lattice Forum” (LatFor) Initiative (2001–2006)

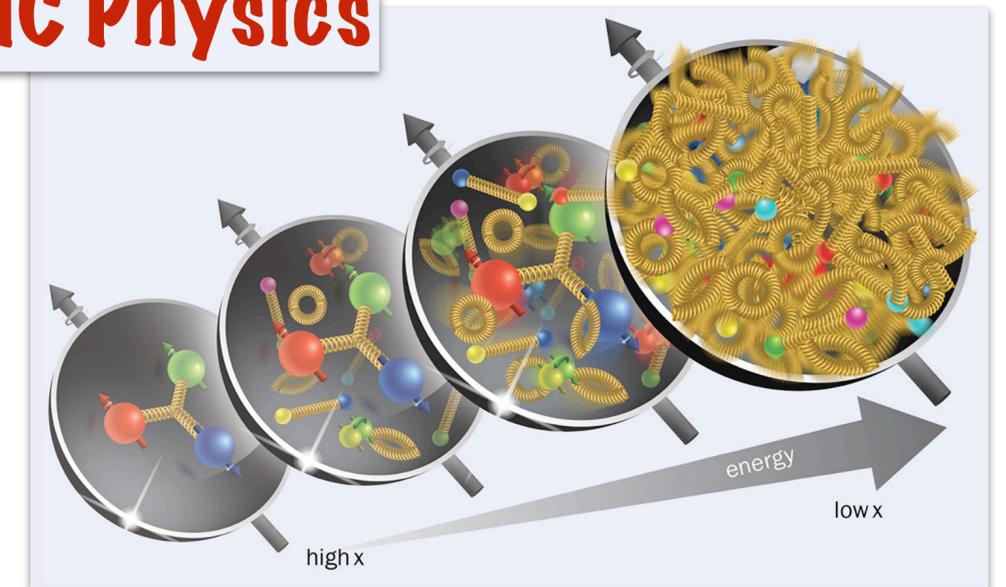
- Procure significant computing resources for hadron and particle physics in Germany
- Hardware platforms under discussion: QCDOC, apeNEXT, PC clusters
- Several meetings involving the lattice, hadron and nuclear communities
- Strong link to FAIR: PANDA, CBM



Nucleon Structure in Lattice QCD (1997 — ...)

- Structure functions
- Nucleon spin
- Strangeness in the nucleon
- Form factors, charges
- Generalised Parton Distributions
- Large-momentum Effective Theory — LaMET

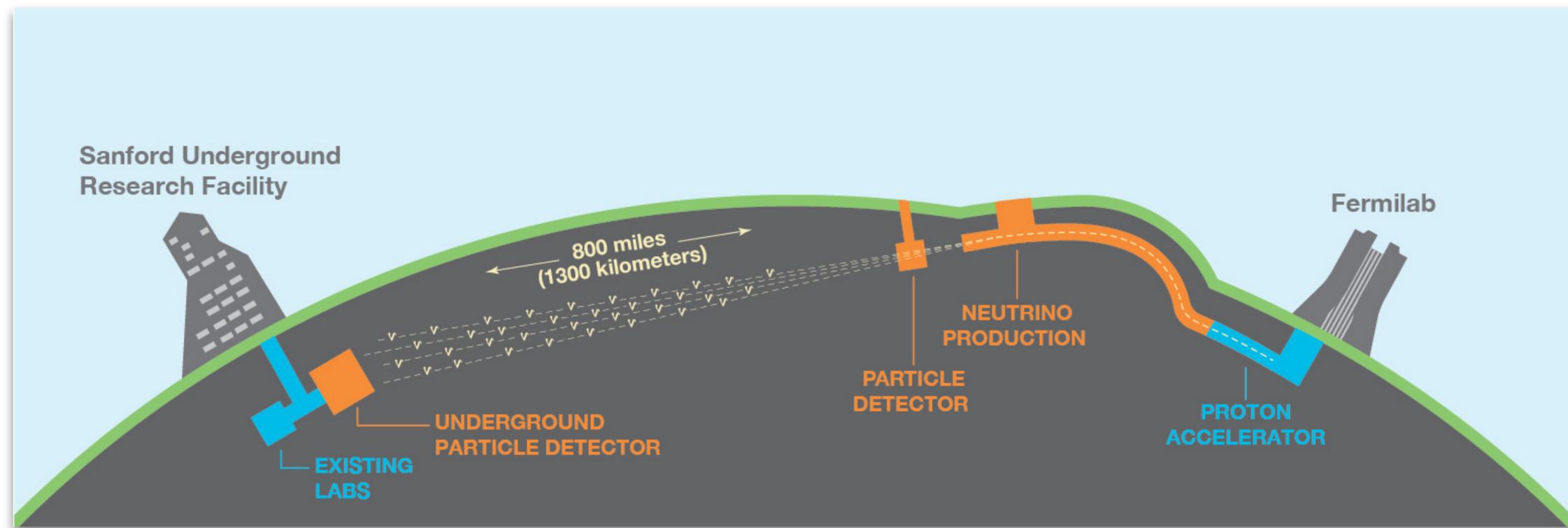
EIC Physics



Nucleon structure observables and BSM physics searches

Scattering experiments probe interactions of e^- , p , ν 's, DM particles with nuclear targets

DUNE — neutrino oscillation experiment: (anti-)neutrino beam onto **C, O, Ar** targets

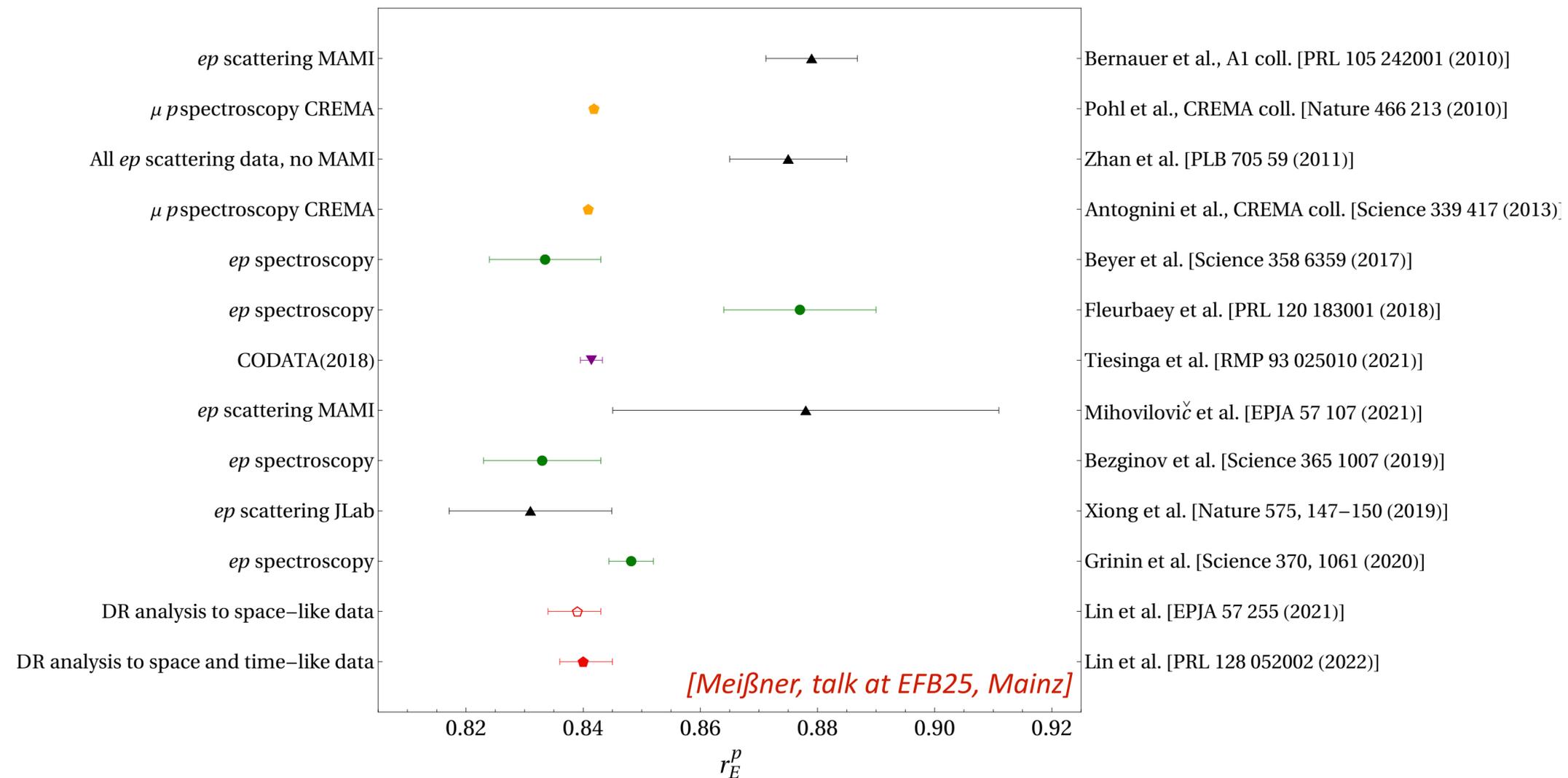


Neutrino-nucleus cross section dominates uncertainty

→ precise and bias-free theoretical predictions for axial form factor $G_A(Q^2)$ required

Is there a proton radius puzzle?

Discrepant measurements of r_E^p in muonic / electronic hydrogen and ep scattering

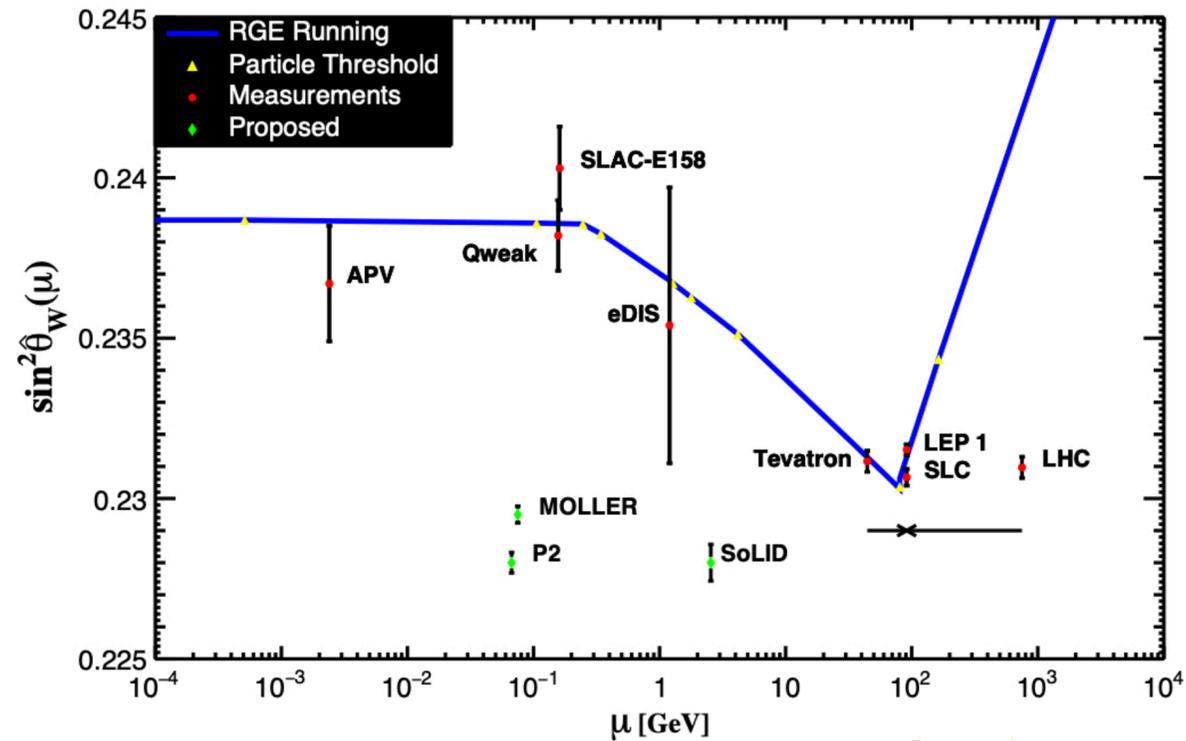


Signal for new physics or poorly understood systematic effects?

→ calls for *ab initio* calculation of the proton radius from QCD

Weak charge of the proton and the running of $\sin^2 \theta_W$

New particles (e.g. BSM gauge bosons) modify running of $\sin^2 \theta_W$ relative to SM prediction

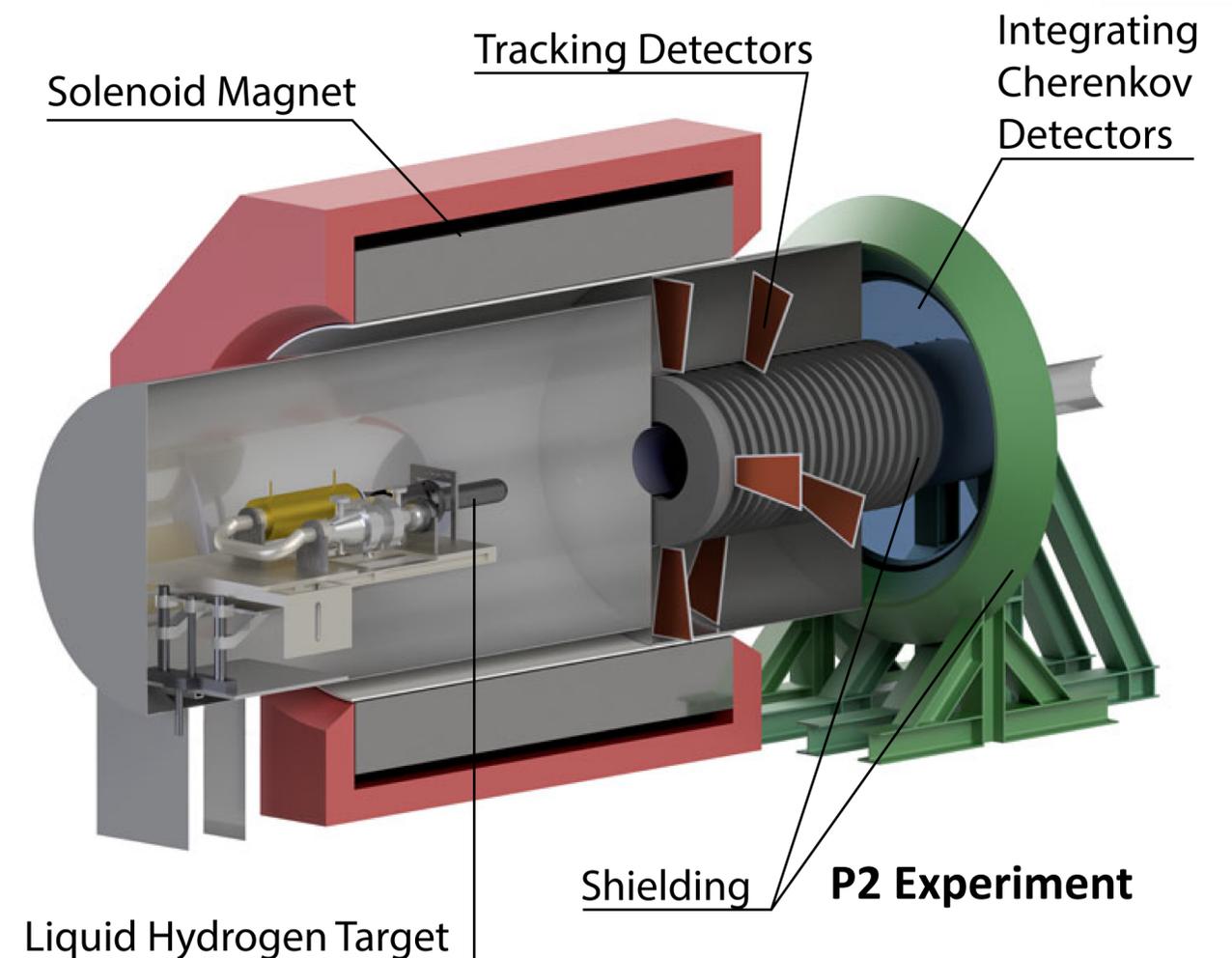


[J. Erler, 2105.00217]

P2@MESA: parity-violating ep scattering

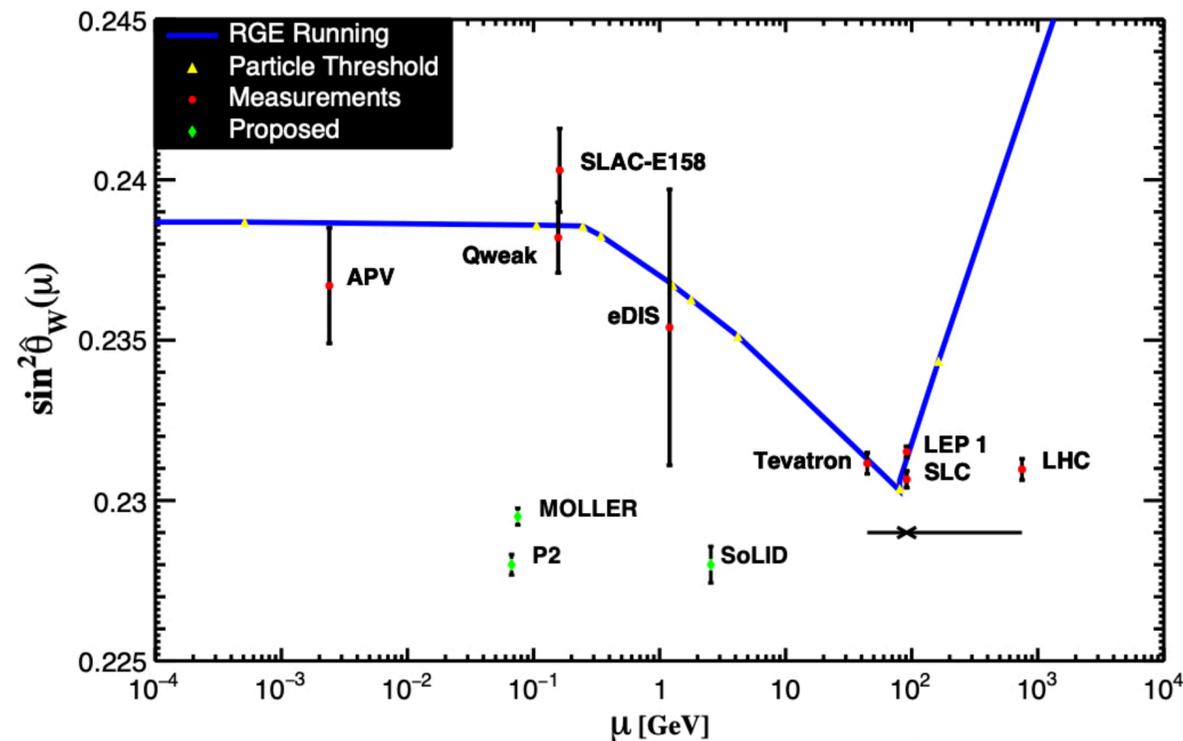
$$A_{LR} \equiv \frac{\sigma_L - \sigma_R}{\sigma_L + \sigma_R} = -\frac{G_F Q^2}{4\pi\sqrt{2}\alpha} (Q_W^P - F(Q^2)),$$

$$Q_W^P = 1 - 4 \sin^2 \theta_W \quad (\text{tree level})$$

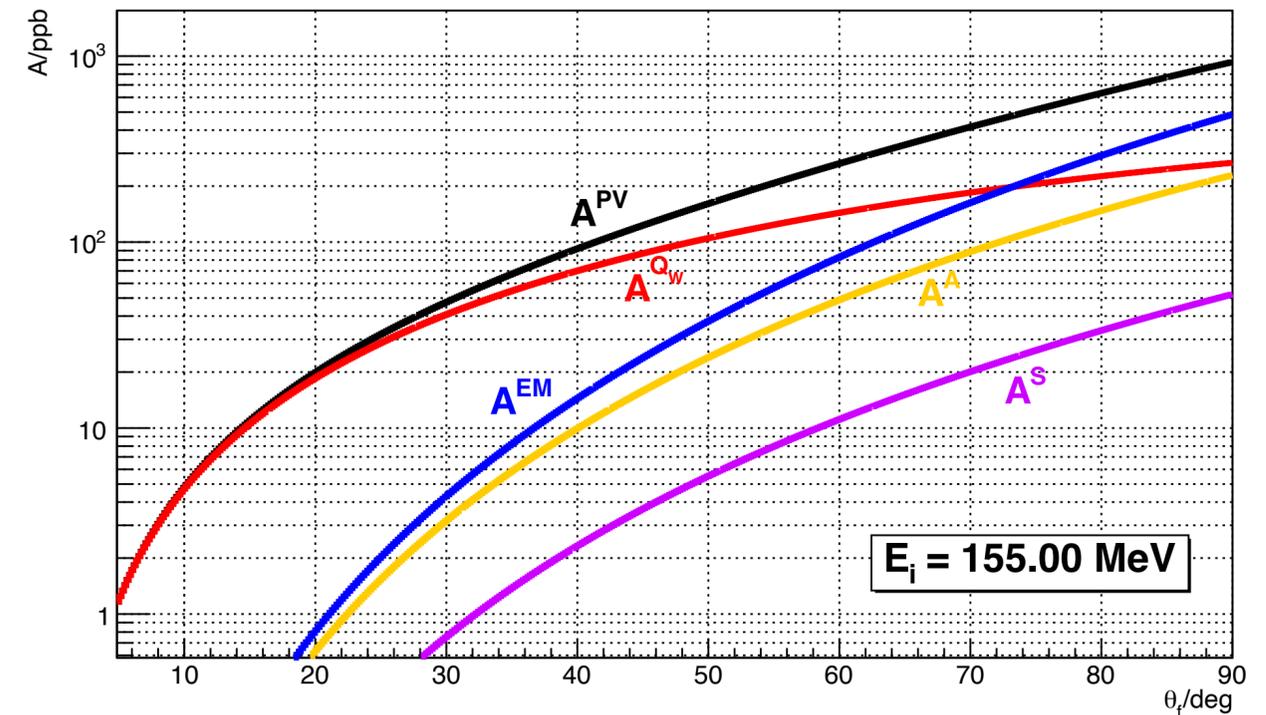


Weak charge of the proton and the running of $\sin^2 \theta_W$

New particles (e.g. BSM gauge bosons) modify running of $\sin^2 \theta_W$ relative to SM prediction



[J. Erler, 2105.00217]



[D. Becker et al., 1802.04759]

P2@MESA: parity-violating ep scattering

$$A_{LR} \equiv \frac{\sigma_L - \sigma_R}{\sigma_L + \sigma_R} = -\frac{G_F Q^2}{4\pi \sqrt{2}\alpha} \left(Q_W^P - F(Q^2) \right),$$

$$Q_W^P = 1 - 4 \sin^2 \theta_W \quad (\text{tree level})$$

Hadronic contributions

$$F(Q^2) = F_{EM}(Q^2) + F_A(Q^2) + F_{str}(Q^2)$$

$$Q^2 \approx 4E_i E_f \sin^2(\theta_f/2)$$

This talk

Methodology: The noise problem and excited states

Pion-nucleon σ -term

Axial form factor and radius

Electromagnetic form factors and the proton radius puzzle

Summary and Outlook

Challenges for lattice QCD: The noise problem

Signal deteriorates exponentially in baryonic correlators:

$$R_{\text{NS}}(t) \propto e^{(m_N - \frac{3}{2}m_\pi)t}$$

- Calculations of baryonic three-point functions limited to source-sink separations $t_s \lesssim 1.7 \text{ fm}$
- Potential bias from unsuppressed excited-state contributions

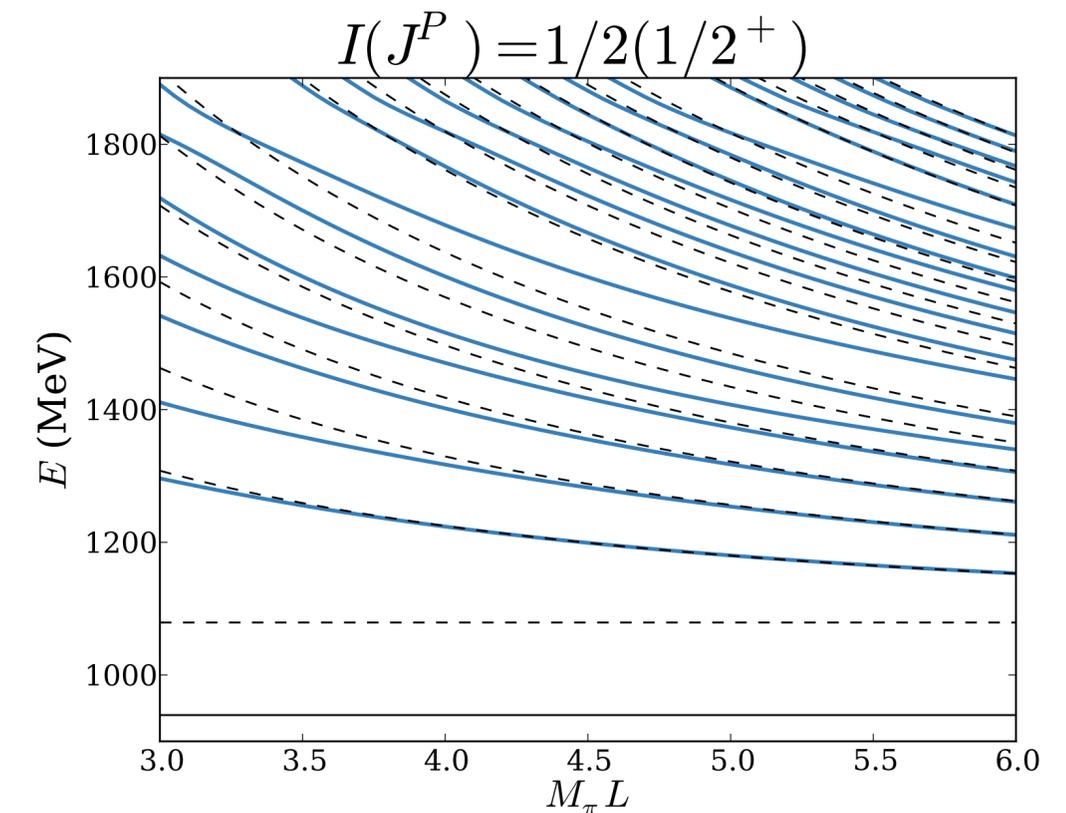
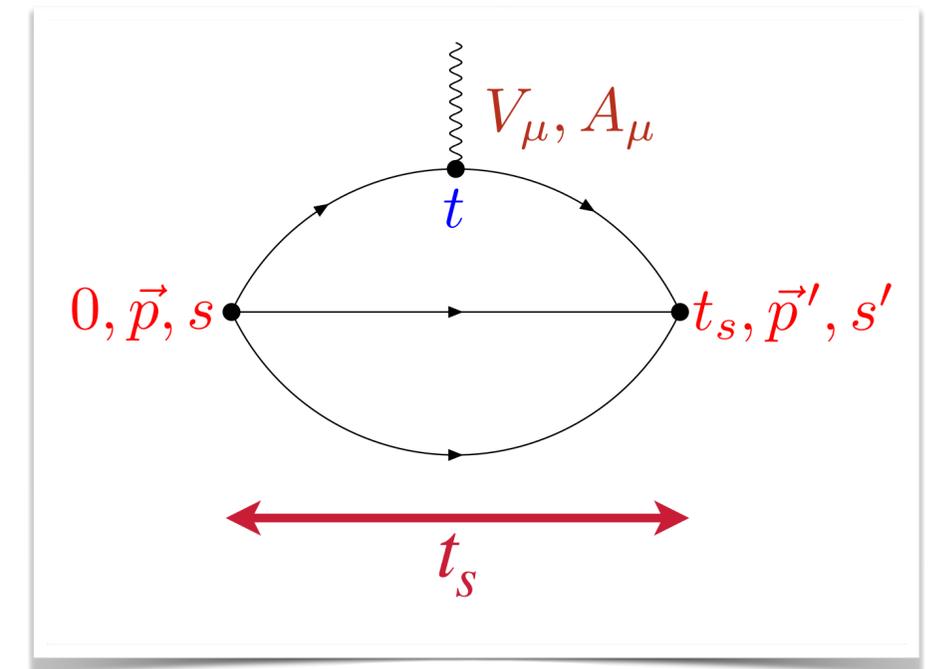
Nucleon charges from ratios of three- and two-point functions:

$$R_\Gamma(t, t_s) \equiv \frac{C_3^\Gamma(\mathbf{q} = 0; t, t_s)}{C_2(\mathbf{p} = 0; t_s)}$$

$$= g_\Gamma + c_{01} e^{-\Delta t} + c_{10} e^{-\Delta(t_s - t)} + c_{11} e^{-\Delta t_s} + \dots$$

$$\Delta = (E_1 - E_0), \quad \Gamma = A, S, T, \dots$$

Encounter dense spectrum of $N\pi, N\pi\pi, \dots$ states



[Hansen & Meyer, 1610.03843]

Challenges for lattice QCD: Quark-disconnected diagrams

Large inherent statistical noise

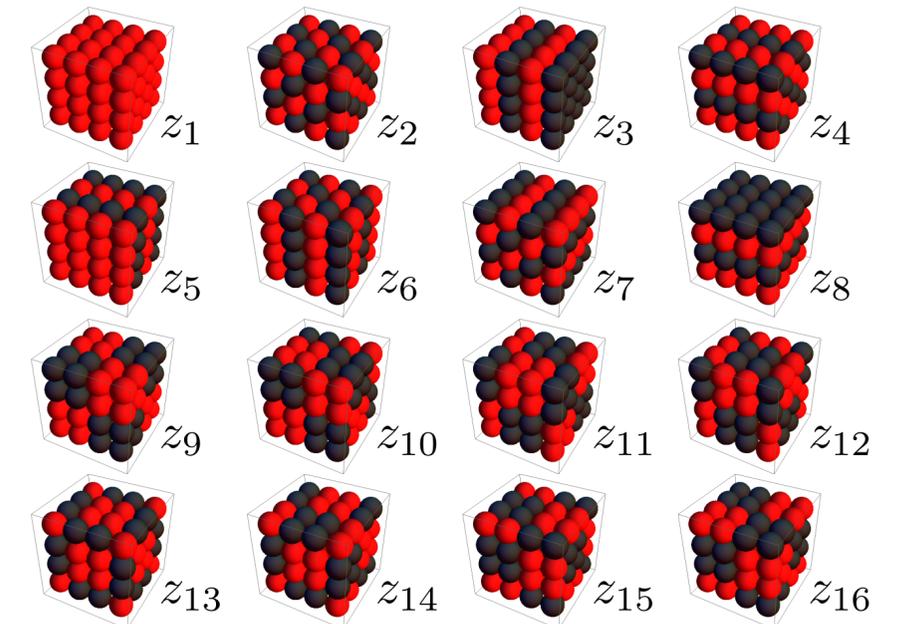
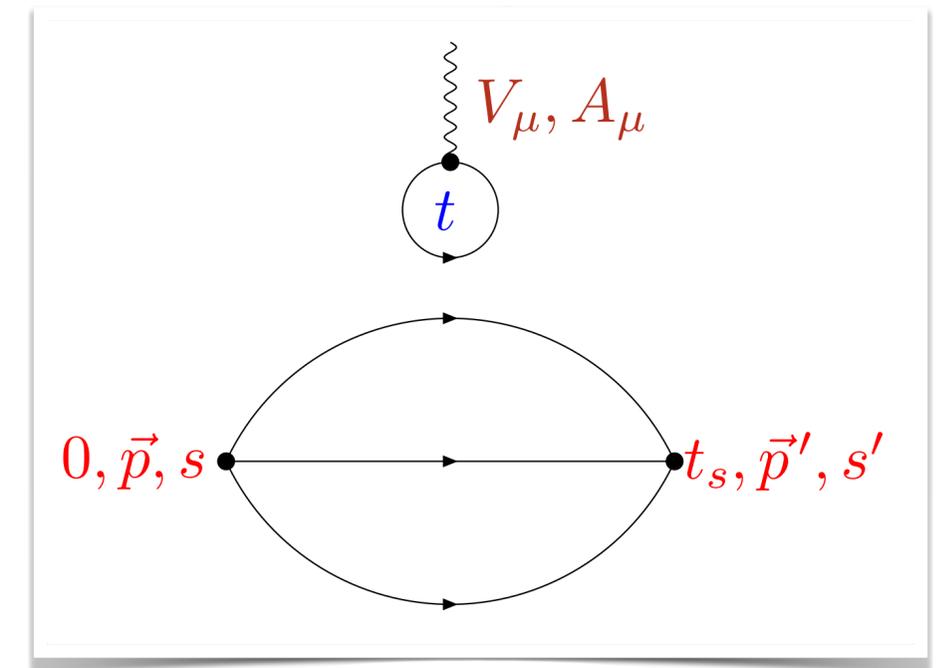
Contribute to isoscalar quantities and sigma-terms

Contribute exclusively to strange form factors

Computational techniques:

- Stochastic sources
- Hopping-parameter expansion
- Hierarchical probing / Hadamard vectors
- “One-end trick”
- Frequency splitting
- Stochastic noise cancellation in $u + d - 2s$

[Bali, Collins & Schäfer, 0910.3970; Dinter et al., 1202.1480;
Gülpers et al., 1411.7592; Stathopoulos et al., 1302.4018; Giusti et al., 1903.10447]



Fighting the noise problem

$$R_{\Gamma}(t, t_s) = g_{\Gamma} + c_{01} e^{-\Delta t} + c_{10} e^{-\Delta(t_s-t)} + c_{11} e^{-\Delta t_s} + \dots,$$

Multi-state fits

Include sub-leading terms in $R_{\Gamma}(t, t_s)$ or in individual two- and three-point functions with or without priors for the excitation spectrum

Summed operator insertions (“summation method”)

Excited-state contributions more strongly suppressed

$$S_{\Gamma}(t_s) \equiv \sum_{t=0}^{t_s-a} R_{\Gamma}(t, t_s) = K_{\Gamma} + (t_s - a) g_{\Gamma} + (t_s - a) e^{-\Delta t_s} d_{\Gamma} + e^{-\Delta t_s} f_{\Gamma} + \dots$$

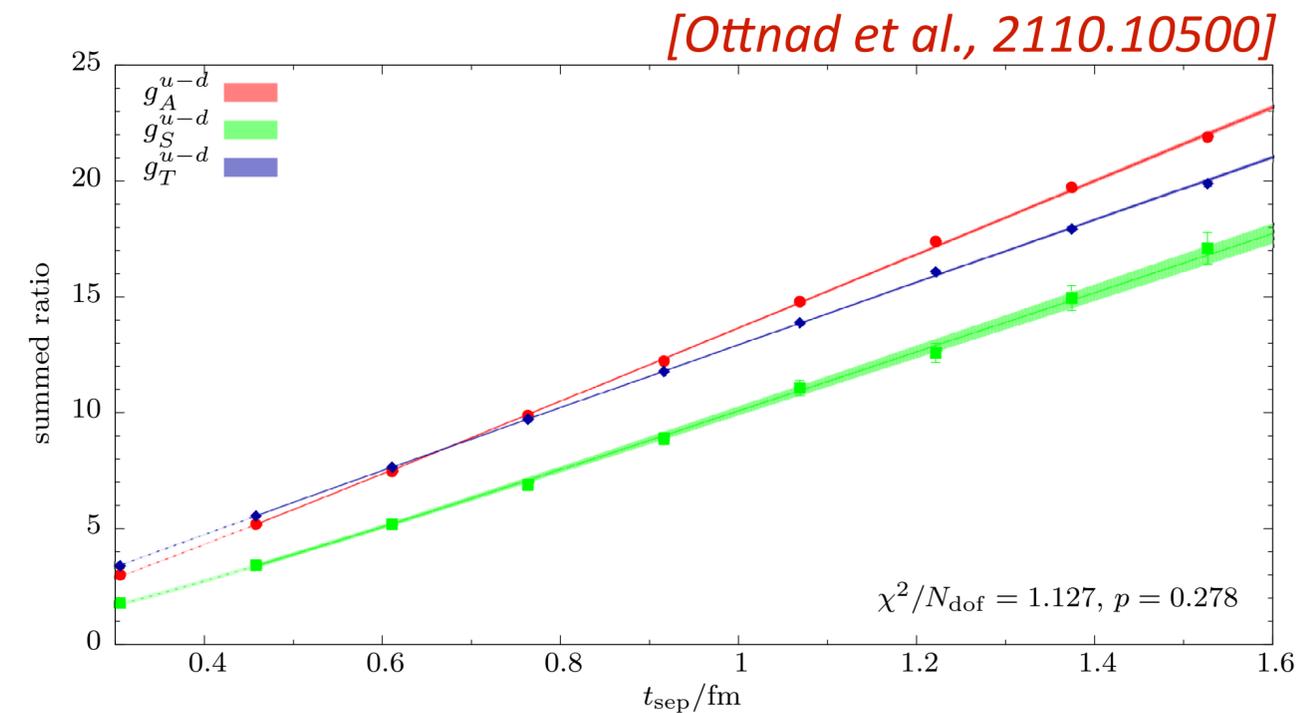
Variational approach

Compute correlator matrices; solve GEVP; optimise projection on ground state

Summation method

$$S_{\Gamma}(t_s) = K_{\Gamma} + (t_s - a) g_{\Gamma} + (t_s - a) e^{-\Delta t_s} d_{\Gamma} + e^{-\Delta t_s} f_{\Gamma} + \dots$$

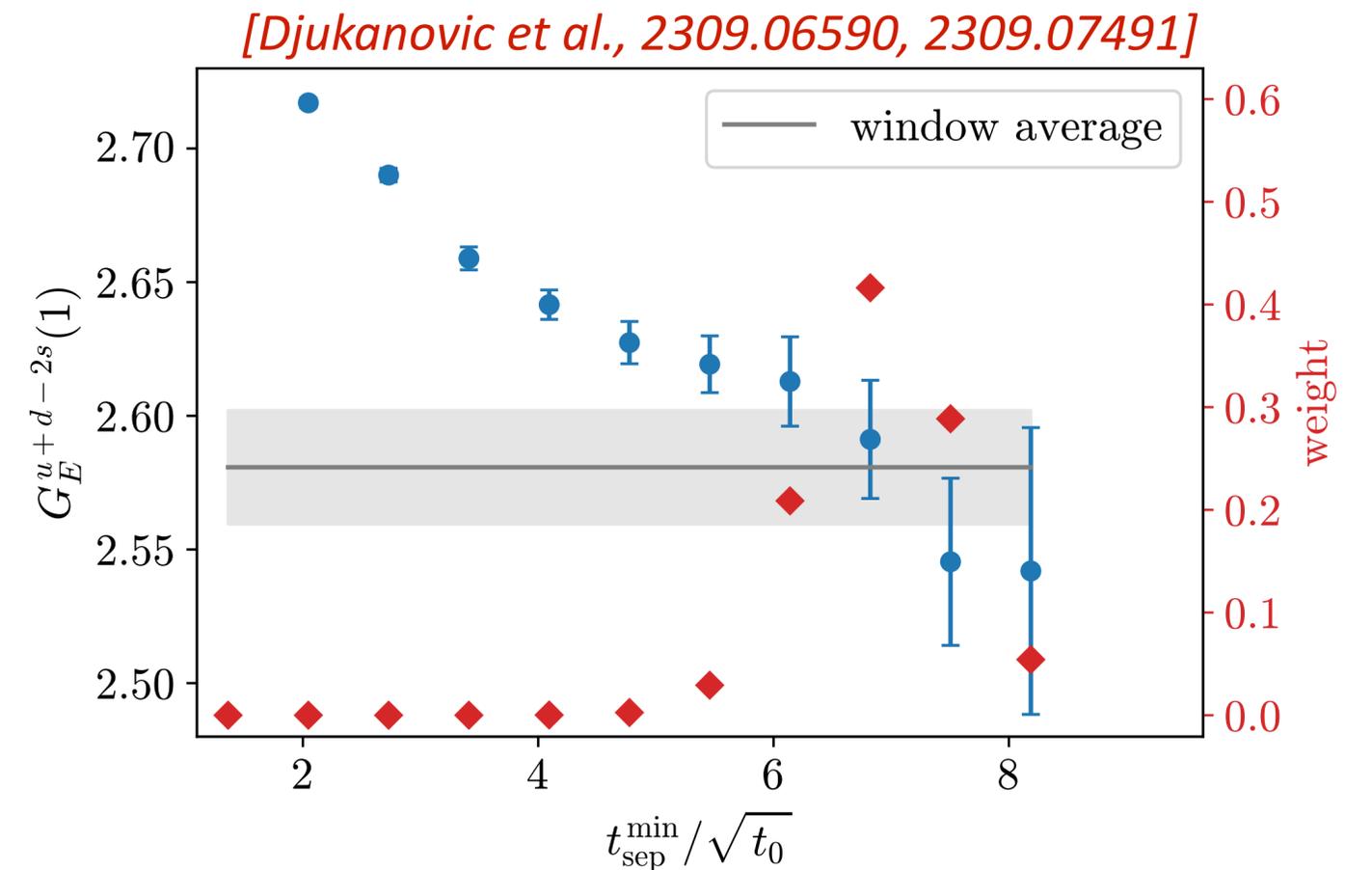
Isovector charges including sub-leading terms



Fit $S_{\Gamma}(t_s)$ over large interval in t_s including sub-leading terms

→ Improve statistical precision

Isoscalar electric form factor



Average slope over smoothed window in t_s^{min}

→ Reduce human bias

The Mainz nucleon structure project

Past and present members:

A. Agadjanov, S. Capitani, M. Della Morte, D. Djukanovic, T. Harris, G. von Hippel, J. Hua, B. Jäger, P. Junnarkar, B. Knippschild, J. Koponen, H.B. Meyer, D. Mohler, K. Ottnad, T.D. Rae, M. Salg, T. Schulz, J. Wilhelm, H. Wittig

- Recent publications based on CLS ensembles with $N_f = 2 + 1$ flavours of $O(a)$ improved Wilson quarks

Nucleon charges

[Harris et al., Phys Rev D 100 (2019) 034513]

Strange form factors

[Djukanovic et al., Phys Rev Lett 123 (2019) 212001]

Axial form factors

[Djukanovic et al., Phys Rev D 106 (2022) 074503]

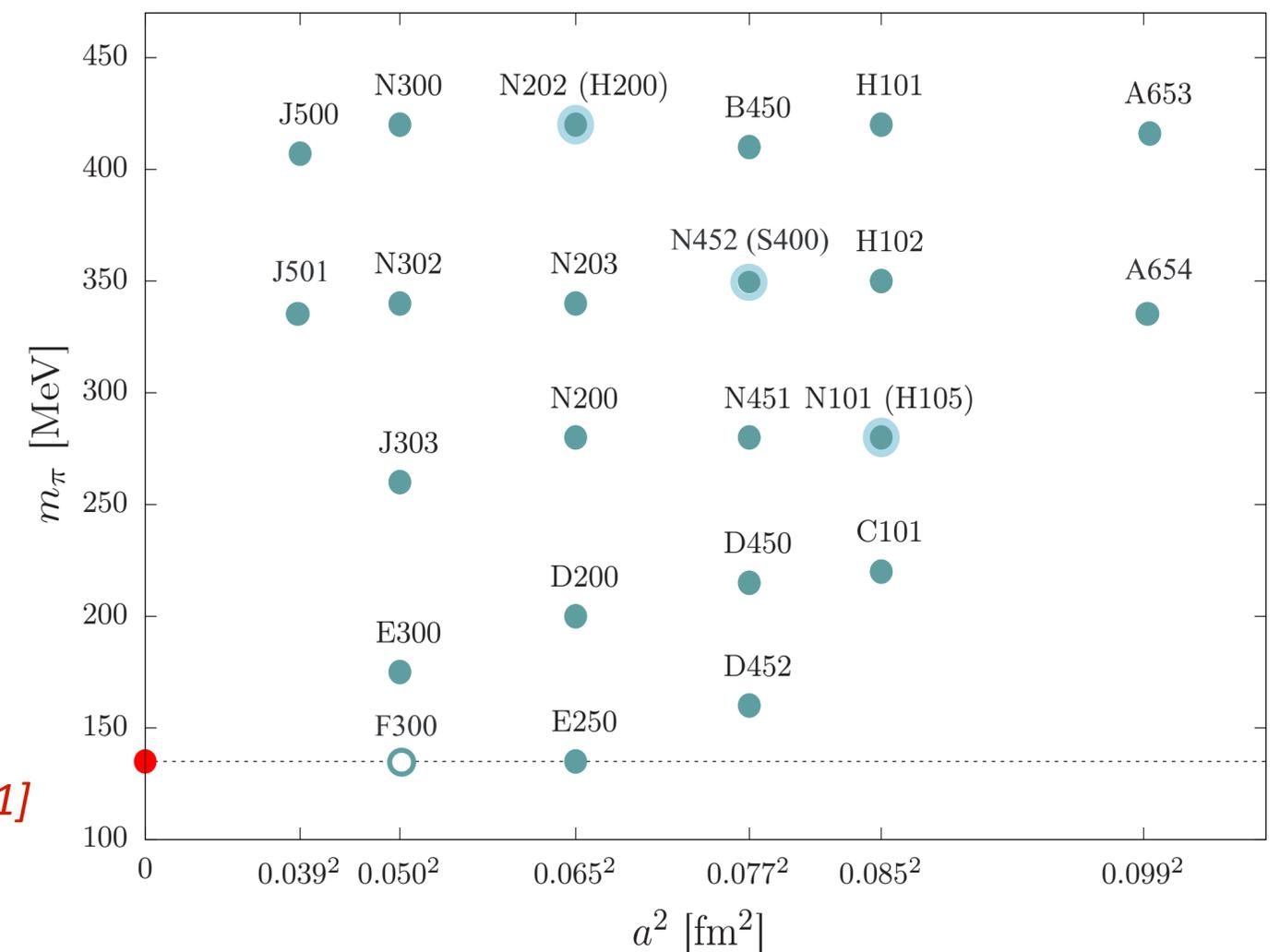
Nucleon sigma terms

[Agadjanov et al., arXiv:2303.08741]

Electromagnetic form factors

[Djukanovic et al., Phys Rev D 103 (2021) 094522; 2309.06590; 2309.07491]

- Same set of ensembles used by RQCD



Sigma-terms

Definitions:

$$\sigma_{\pi N} = m_{ud} \langle N | \bar{u}u + \bar{d}d | N \rangle = m_{ud} \frac{\partial m_N}{\partial m_{ud}}, \quad \sigma_s = m_s \langle N | \bar{s}s | N \rangle, \quad \sigma_0 = m_{ud} \langle N | \bar{u}u + \bar{d}d - 2\bar{s}s | N \rangle$$

“direct”
Feynman-Hellman

$\sigma_{\pi N}$ characterises coupling of DM particles to the nucleon

Lattice calculation: quark-disconnected diagrams contribute

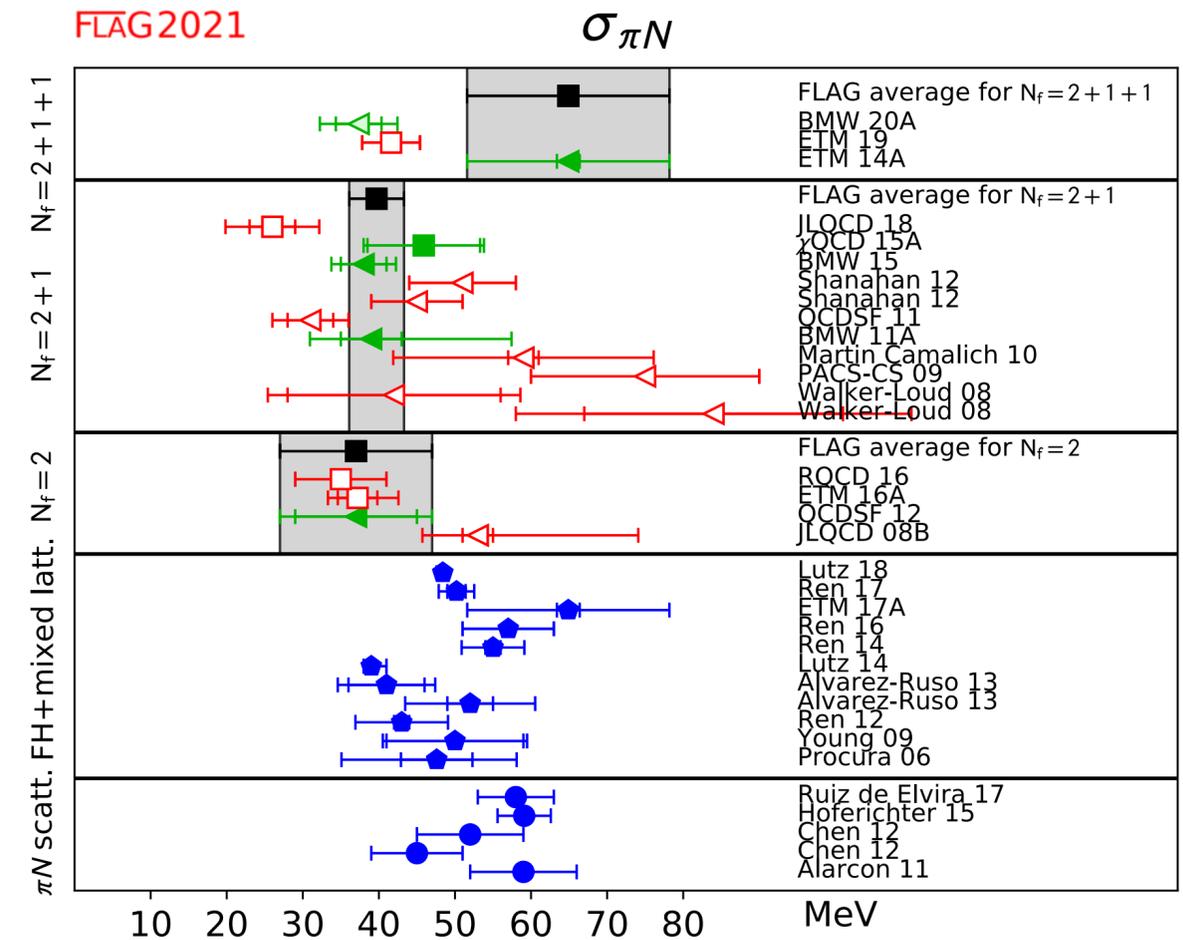
FLAG 5 average for $N_f = 2 + 1$: $\sigma_{\pi N} = (39.7 \pm 3.6) \text{ MeV}$

2.5σ tension with results from $N\pi$ -scattering, e.g.

$$\sigma_{\pi N} = (58 \pm 5) \text{ MeV} \quad [\text{Ruiz de Elvira et al., 1706.01465}]$$



Value depends on definition of isospin limit



Sigma-terms

Details of the calculation

[Agadjanov et al., 2303.08741]

- 16 CLS ensembles, 4 lattice spacings: $a = 0.050 - 0.087$ fm; Pion masses: 128 – 350 MeV

- Summation method / window average; cross-check using two-state fits

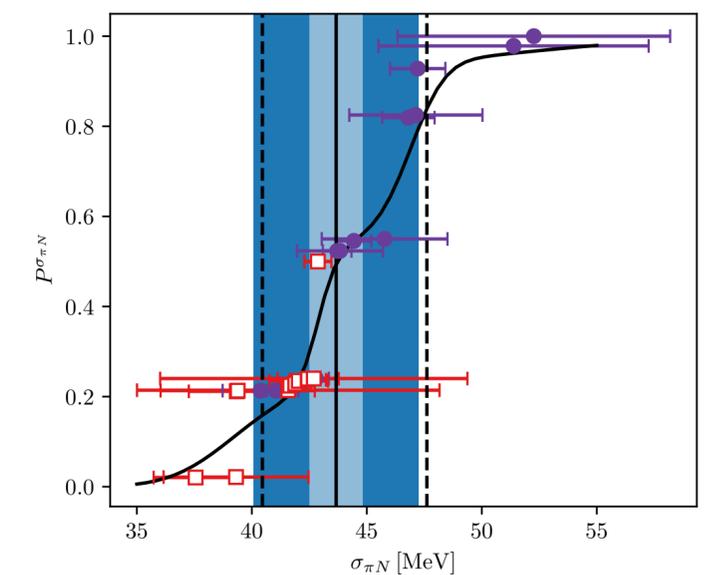
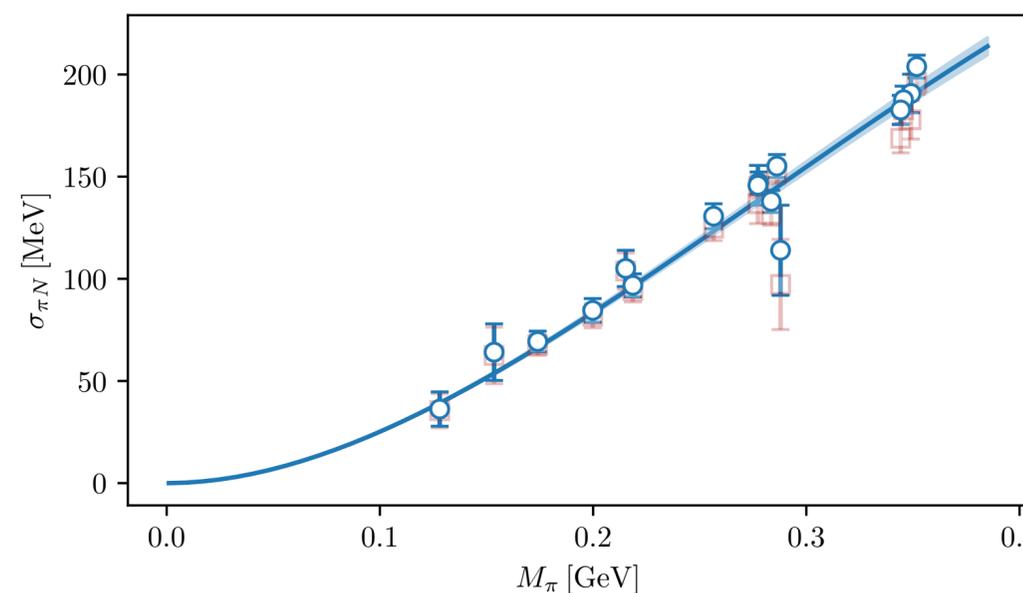
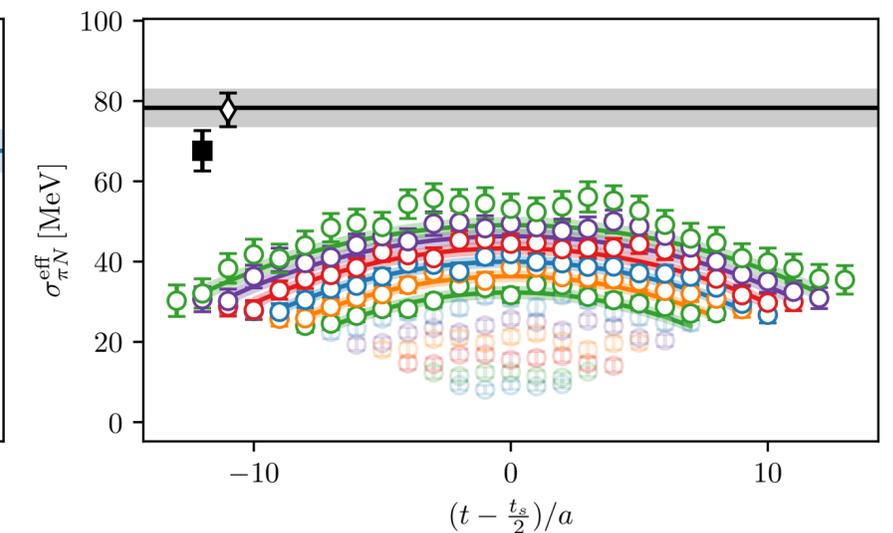
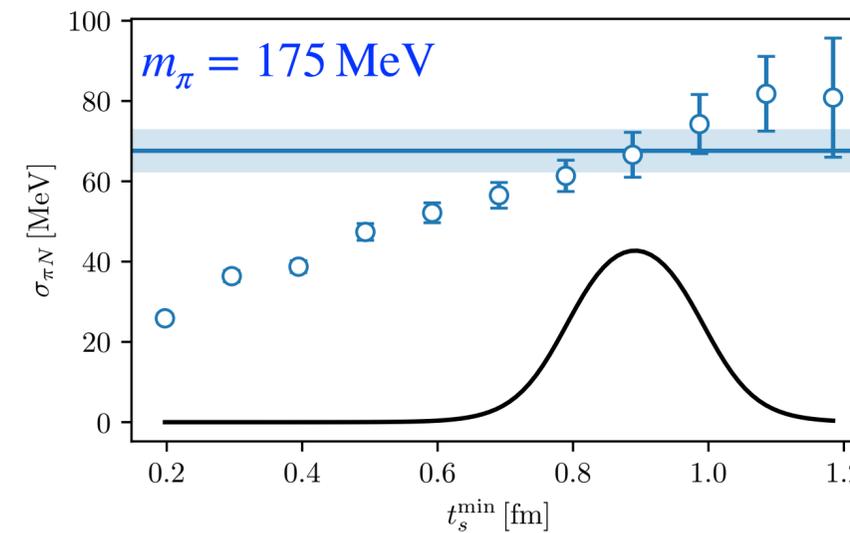
- Chiral + continuum extrapolation: *ansatz* derived from chiral expansion of nucleon mass via Feynman-Hellmann

- Final results from model average over fit variations / AIC

$$\sigma_{\pi N} = (43.7 \pm 1.2 \pm 3.4) \text{ MeV}$$

$$\sigma_s = (28.6 \pm 6.2 \pm 7.0) \text{ MeV}$$

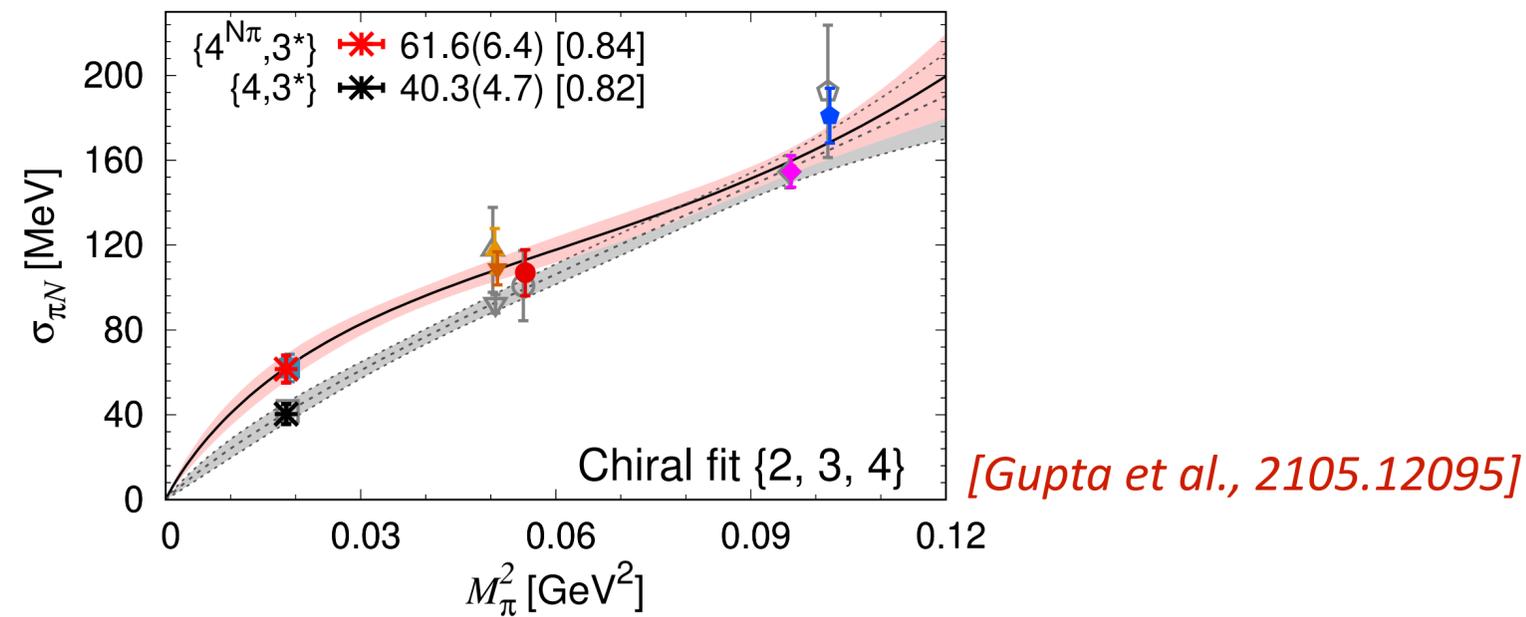
(excited-state treatment dominates error)



Sigma-terms: Comparison of results

$$\sigma_{\pi N} = (43.7 \pm 1.2 \pm 3.4) \text{ MeV} \quad (\text{Mainz/CLS})$$

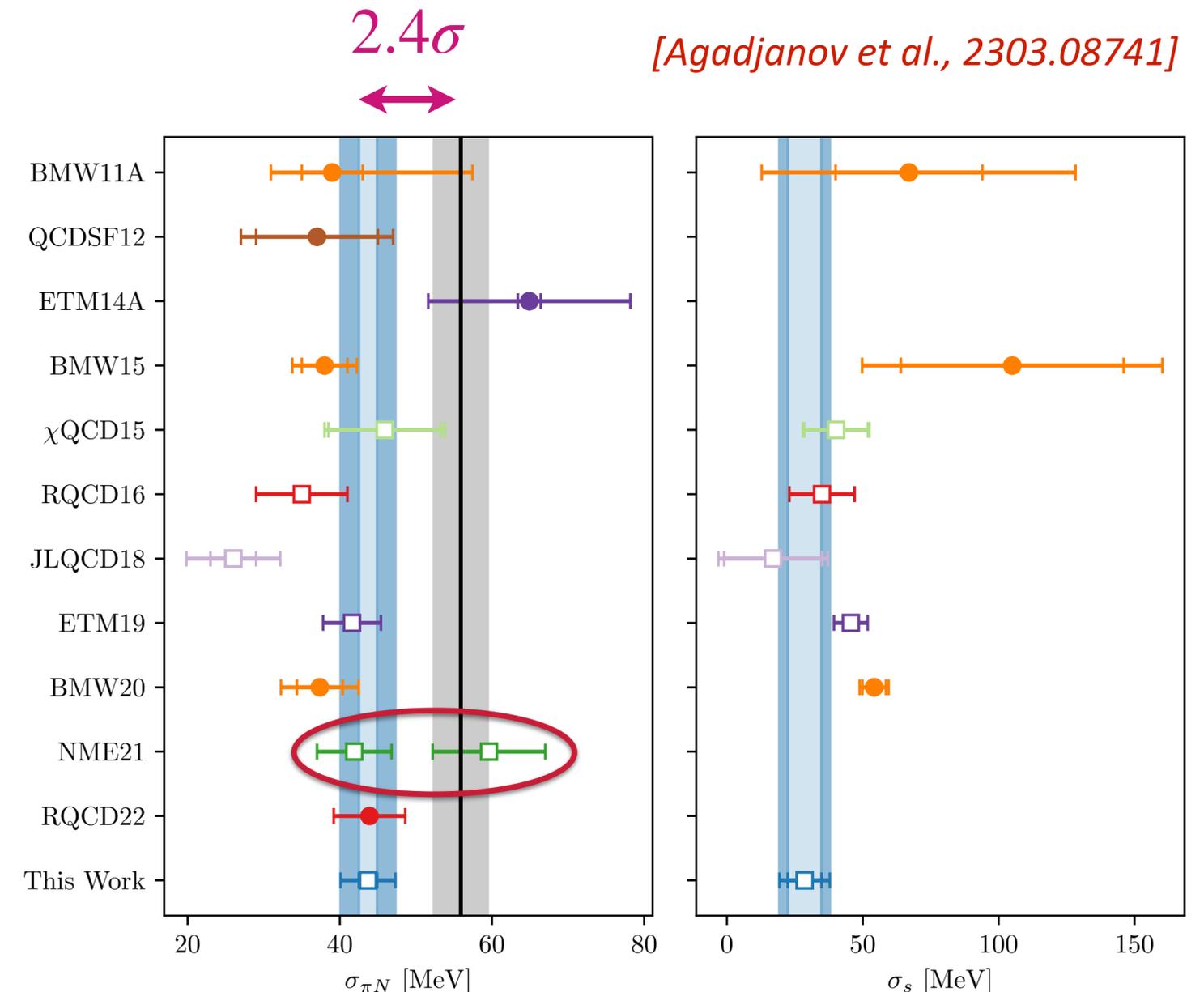
Bias from excited-state contributions?



$N\pi$ scattering: $\sigma_{\pi N} = (59.0 \pm 3.5) \text{ MeV}$
 [Hoferichter et al., 2305.07045]

Different conventions for isospin limit: m_{π^\pm} vs. m_{π^0}

→ apply shift of $\Delta\sigma_{\pi N} = (3.1 \pm 0.5) \text{ MeV}$: $\sigma_{\pi N} = (55.9 \pm 3.5) \text{ MeV}$



- “direct”
- “Feynman-Hellmann”

Nucleon form factors

Dirac and Pauli form factors:

$$\langle N(p', s') | J_\mu^{\text{em}}(0) | N(p, s) \rangle = \bar{u}(p', s') \left[\gamma_\mu F_1(Q^2) + \sigma_{\mu\nu} \frac{Q_\nu}{2m_N} F_2(Q^2) \right] u(p, s)$$

$$G_E(Q^2) = F_1(Q^2) - \frac{Q^2}{(am_N)^2} F_2(Q^2), \quad G_M(Q^2) = F_1(Q^2) + F_2(Q^2)$$

Axial and induced pseudoscalar form factors:

$$\langle N(p', s') | A_\mu(0) | N(p, s) \rangle = \bar{u}(p', s') \left[\gamma_\mu \gamma_5 G_A(Q^2) - i\gamma_5 \frac{Q_\mu}{2m_N} \tilde{G}_P(Q^2) \right] u(p, s)$$

Charge radii, magnetic moment, axial charge:

$$G_E(Q^2) = \left(1 - \frac{1}{6} \langle r_E^2 \rangle Q^2 + \mathcal{O}(Q^2) \right), \quad G_M(Q^2) = \mu \left(1 - \frac{1}{6} \langle r_M^2 \rangle Q^2 + \mathcal{O}(Q^2) \right)$$

$$G_A(Q^2) = g_A \left(1 - \frac{1}{6} \langle r_A^2 \rangle Q^2 + \mathcal{O}(Q^2) \right)$$

Nucleon form factors in Lattice QCD

Form factors computed for a discrete set of Q^2 -values, at a given value of m_π at non-zero lattice spacing and finite box size

- Describe the Q^2 -dependence: dipole fits or z -expansion *[Hill & Paz, PRD 82 (2010) 113005]*

$$G_\Gamma(Q^2) = \sum_k a_k^\Gamma z(Q^2)^k, \quad z(Q^2) = \frac{\sqrt{t_{\text{cut}} + Q^2} - \sqrt{t_{\text{cut}}}}{\sqrt{t_{\text{cut}} + Q^2} + \sqrt{t_{\text{cut}}}}$$

→ Fits yield electric, magnetic and axial charge radii, magnetic moment, axial charge

- Extrapolate to the physical point: continuum and infinite-volume limits, physical m_π
- Alternative 1: Direct fits to the dependence of form factors on Q^2 and m_π , supplemented by terms describing the a -dependence and finite-volume corrections
[Bauer et al., PRC 86 (2012) 065206; Capitani et al., 1504.04628, Djukanovic et al., 2102.07460]
- Alternative 2: Incorporate z -expansion into fits to the summation method, extrapolate coefficients a_k to the continuum limit *[Djukanovic et al., 2207.03440]*

Axial form factor and radius

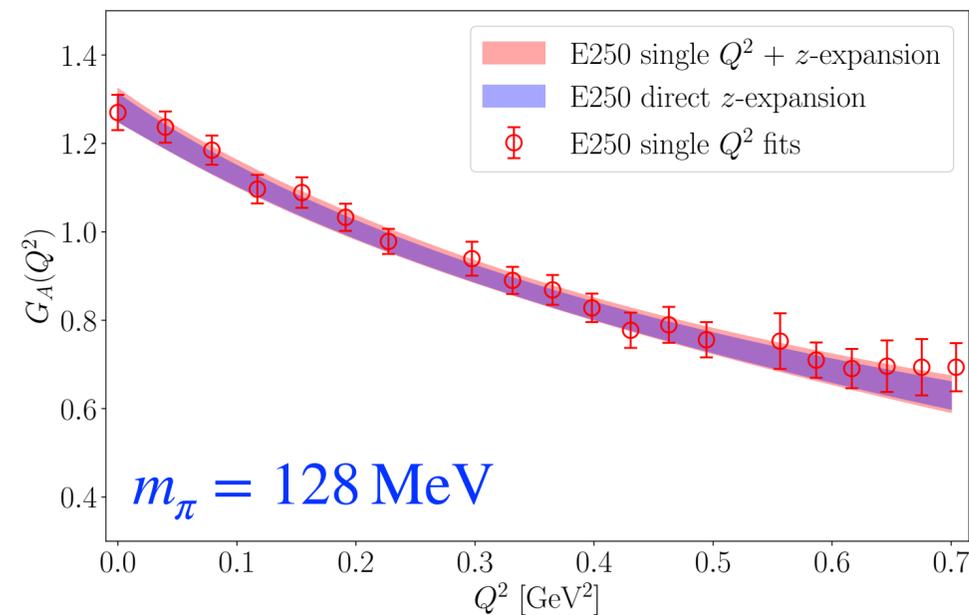
Details of the calculation

[Djukanovic et al., 2207.03440]

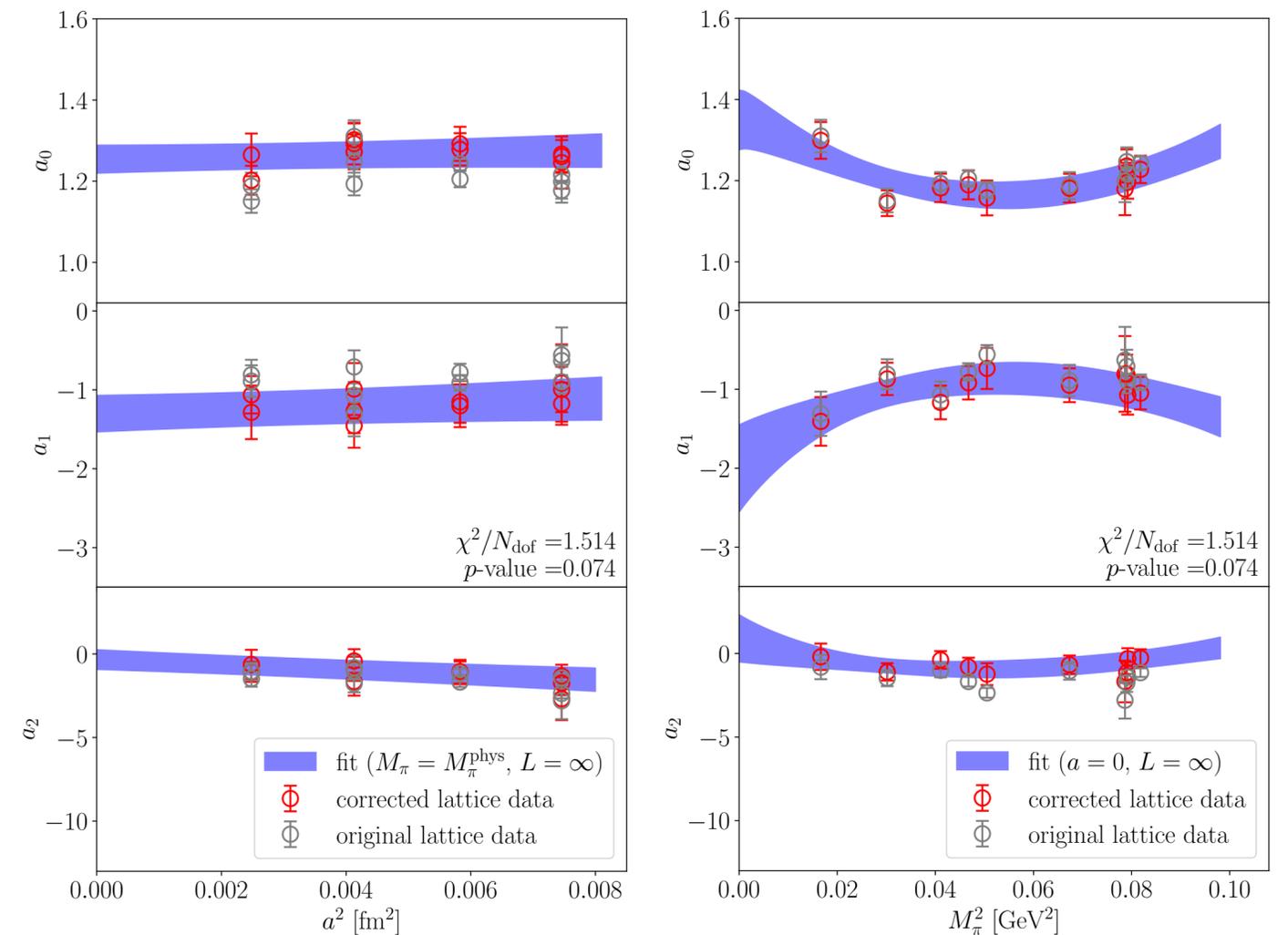
- 14 CLS ensembles, 4 lattice spacings: $a = 0.050 - 0.087$ fm; Pion masses: 128 – 350 MeV

$$S_A(t_s) \equiv \sum_{t=0}^{t_s-a} G_A^{\text{eff}}(t, t_s) = K_\Gamma + (t_s - a) \sum_{k=0}^{n_{\text{max}}} a_k z^k(Q^2) + \dots$$

- Consistency check with conventional treatment:



- Numerically robust; direct parameterisation of Q^2 -dependence



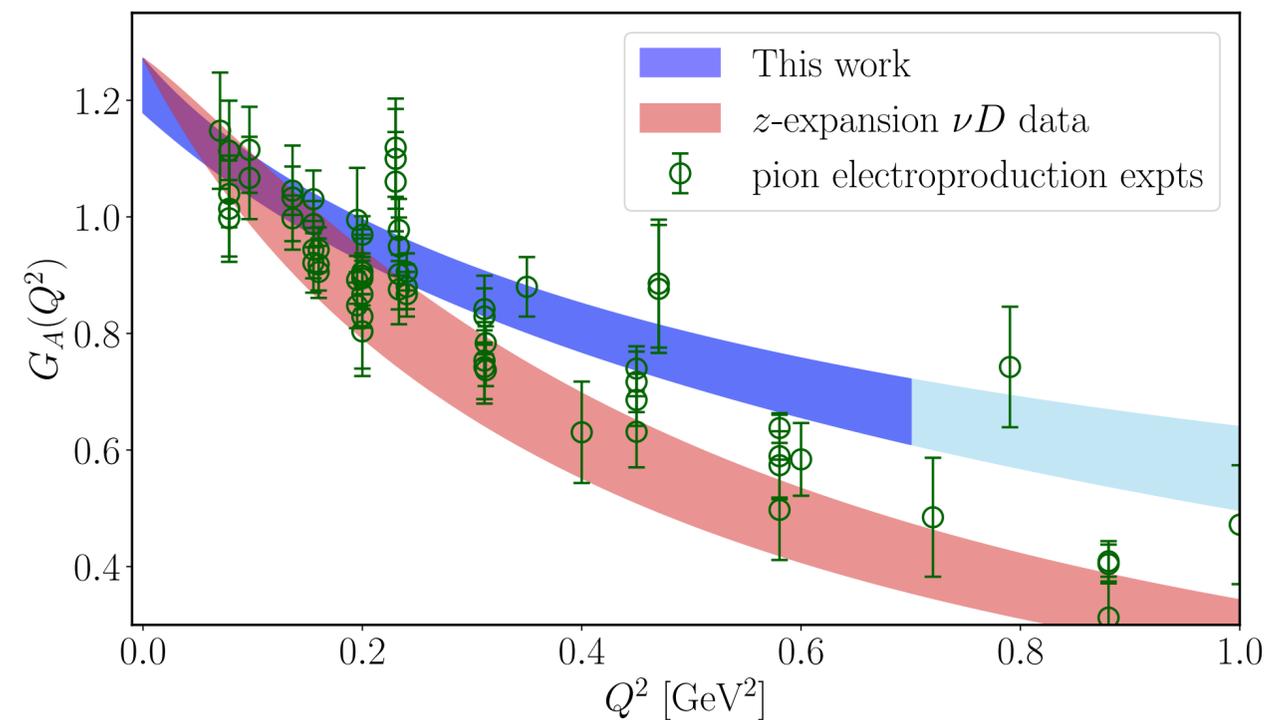
Axial form factor and radius: Results and comparison

$$a_0 = 1.225 \pm 0.039(\text{stat}) \pm 0.025(\text{syst}),$$

$$a_1 = -1.274 \pm 0.237(\text{stat}) \pm 0.070(\text{syst}),$$

$$a_2 = -0.379 \pm 0.592(\text{stat}) \pm 0.179(\text{syst})$$

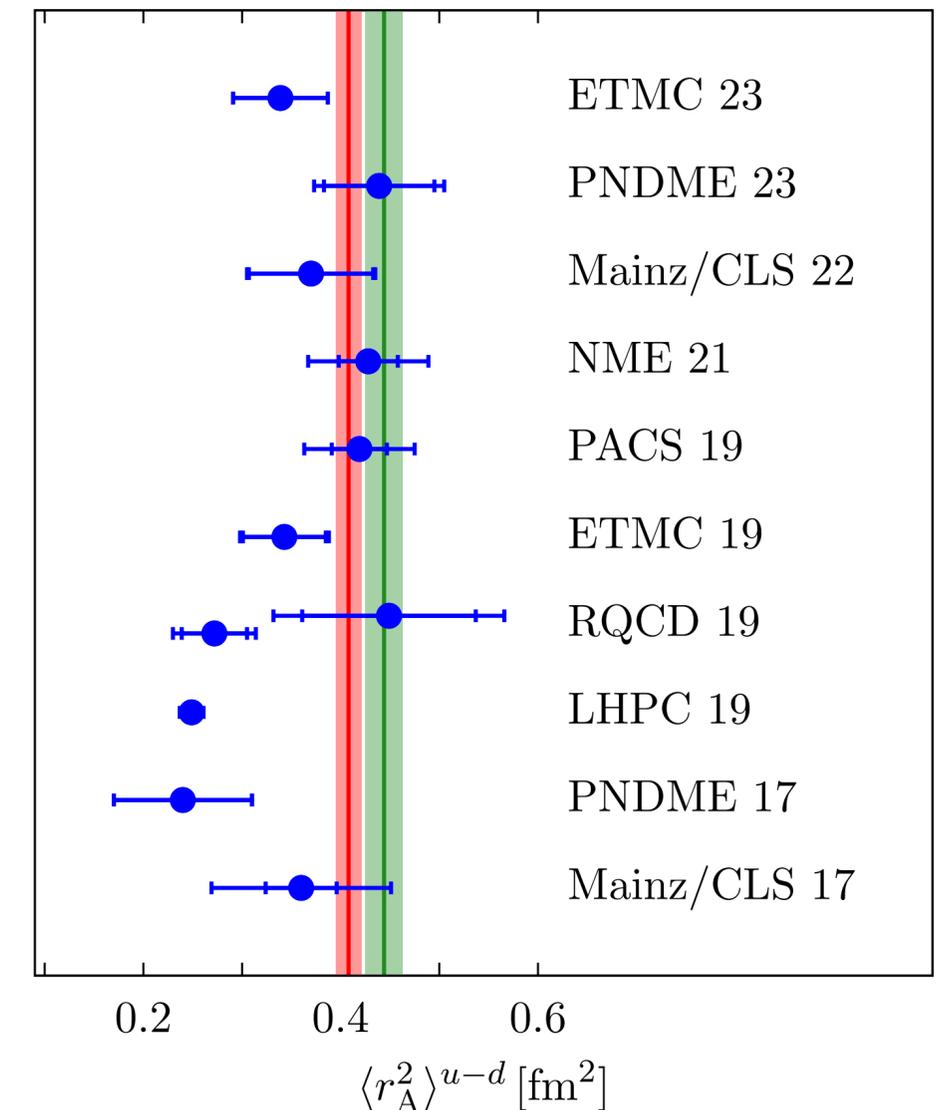
$$\Rightarrow \langle r_A^2 \rangle = (0.370 \pm 0.063 (\text{stat}) \pm 0.016 (\text{syst})) \text{ fm}^2$$



- Broad agreement on $\langle r_A^2 \rangle$ among lattice calculations
- Tension with νD scattering data at large Q^2

[Djukanovic et al., 2207.03440]

electroproduction ν scattering



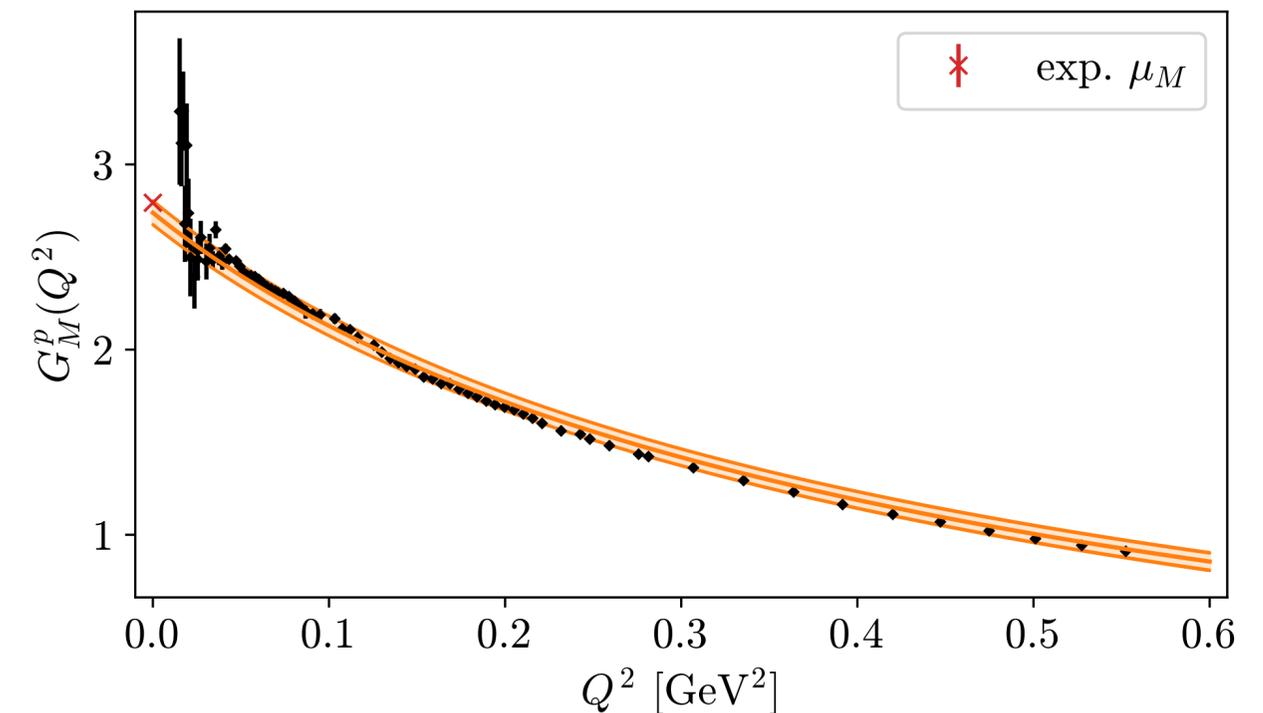
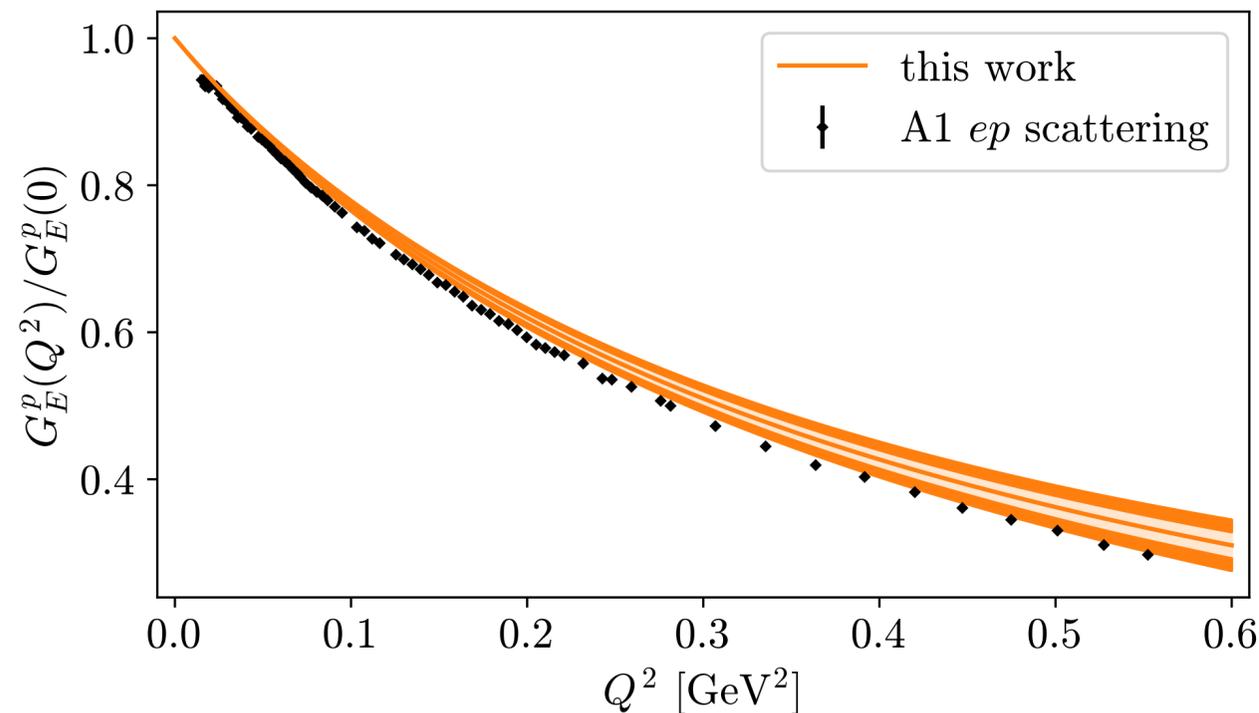
Electromagnetic form factors and the proton radius

Details of the calculation

[Djukanovic et al., 2309.06590, 2309.07491]

- 11 CLS ensembles, 4 lattice spacings: $a = 0.050 - 0.087$ fm; Pion masses: $128 - 300$ MeV
- Quark-connected and disconnected contributions — up to 400k individual measurements
- Compute isovector ($u - d$) and isoscalar ($u + d - 2s$) electromagnetic form factors
- “Direct” chiral and continuum fits using BChPT expressions + lattice artefacts, FV-corrections
- Final results from model average using AIC weights

Proton:



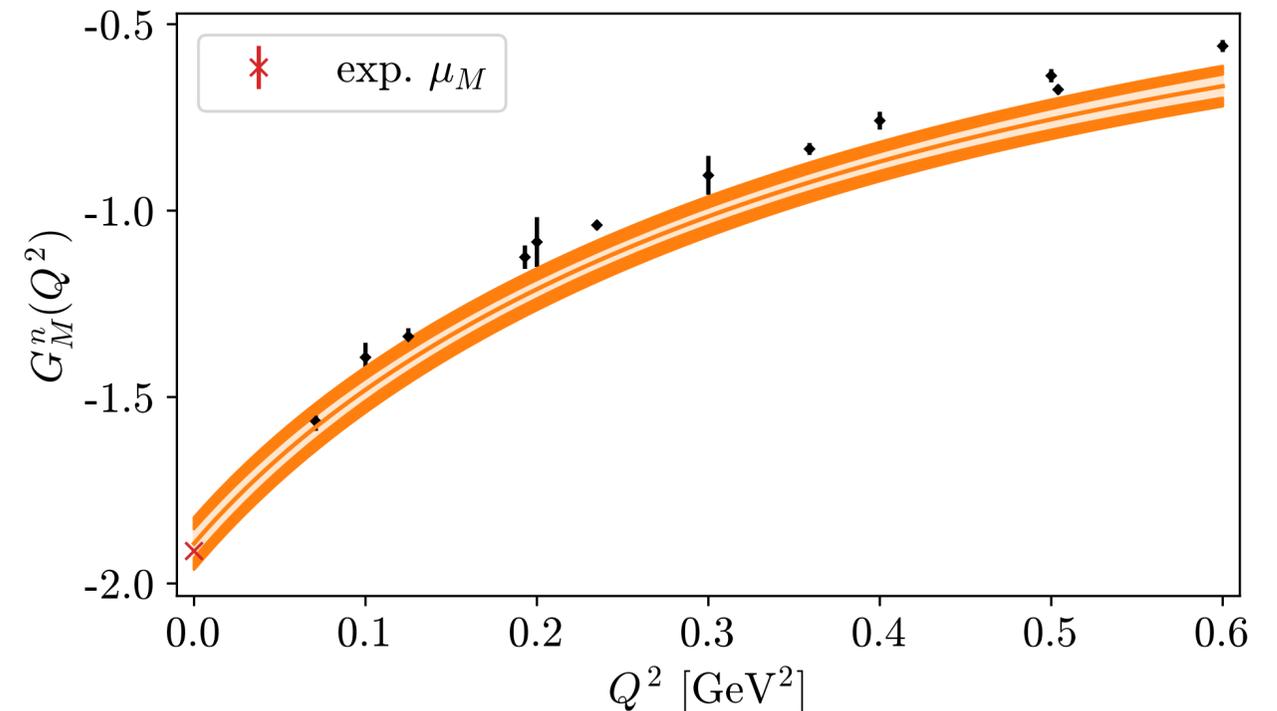
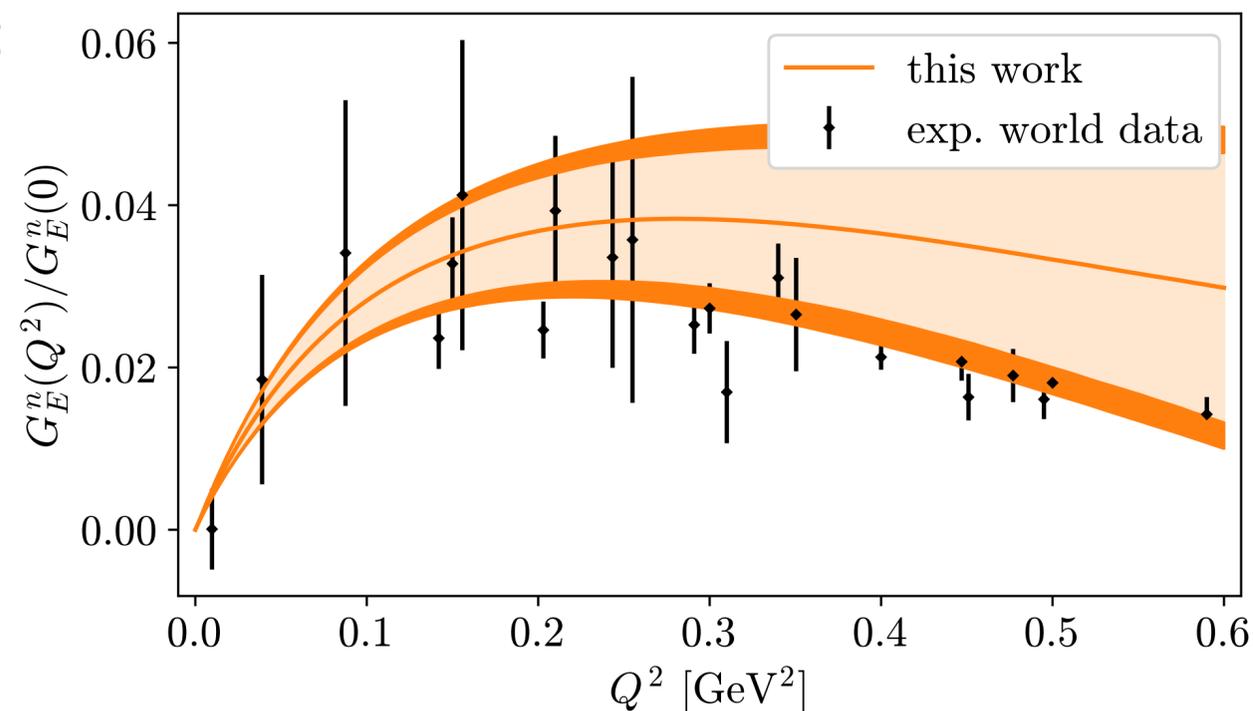
Electromagnetic form factors and the proton radius

Details of the calculation

[Djukanovic et al., 2309.06590, 2309.07491]

- 11 CLS ensembles, 4 lattice spacings: $a = 0.050 - 0.087$ fm; Pion masses: $128 - 300$ MeV
- Quark-connected and disconnected contributions — up to 400k individual measurements
- Compute isovector ($u - d$) and isoscalar ($u + d - 2s$) electromagnetic form factors
- “Direct” chiral and continuum fits using BChPT expressions + lattice artefacts, FV-corrections
- Final results from model average using AIC weights

Neutron:



Electromagnetic form factors and the proton radius

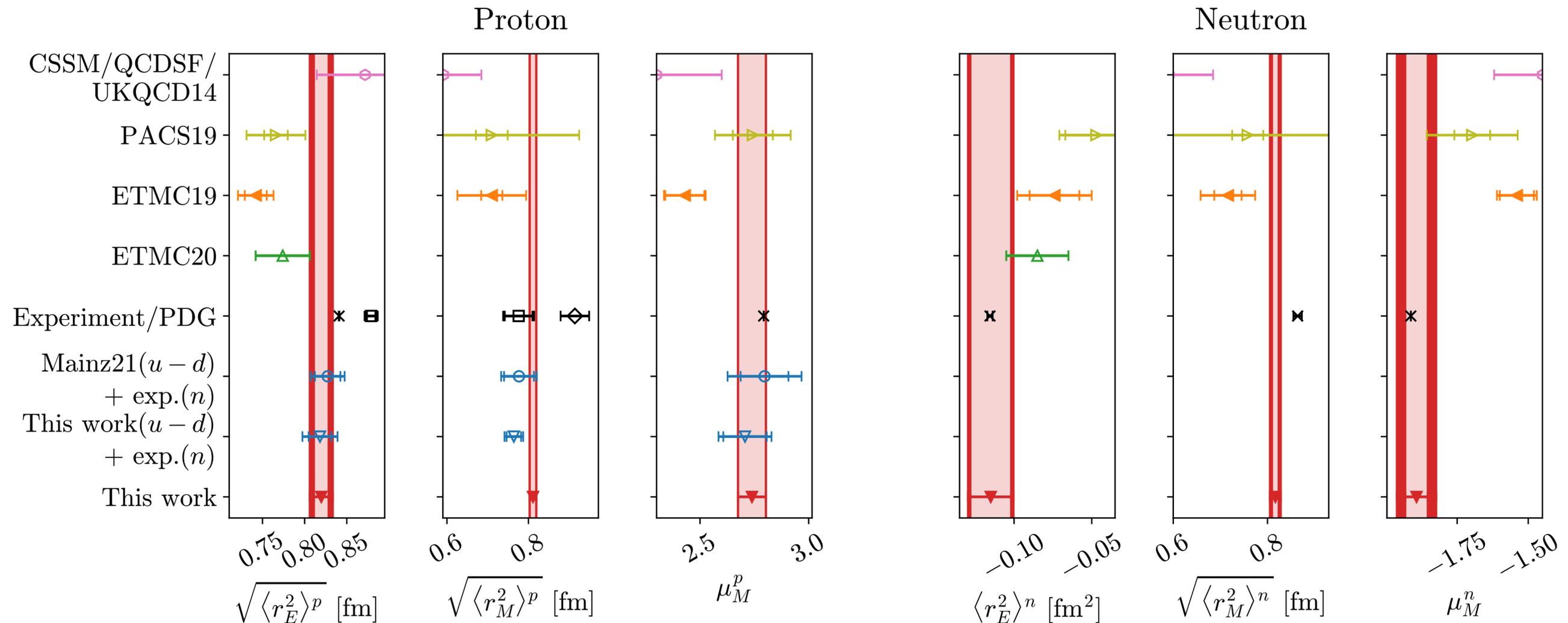
- Complete error budget

[Djukanovic et al., 2309.06590, 2309.07491]

- Proton's electric and magnetic radii obtained with 1.7% and 1.1%, respectively

→ Competitive with *ep*-scattering experiments

- Lattice calculation favours low value of the proton radius; Magnetic moments reproduced



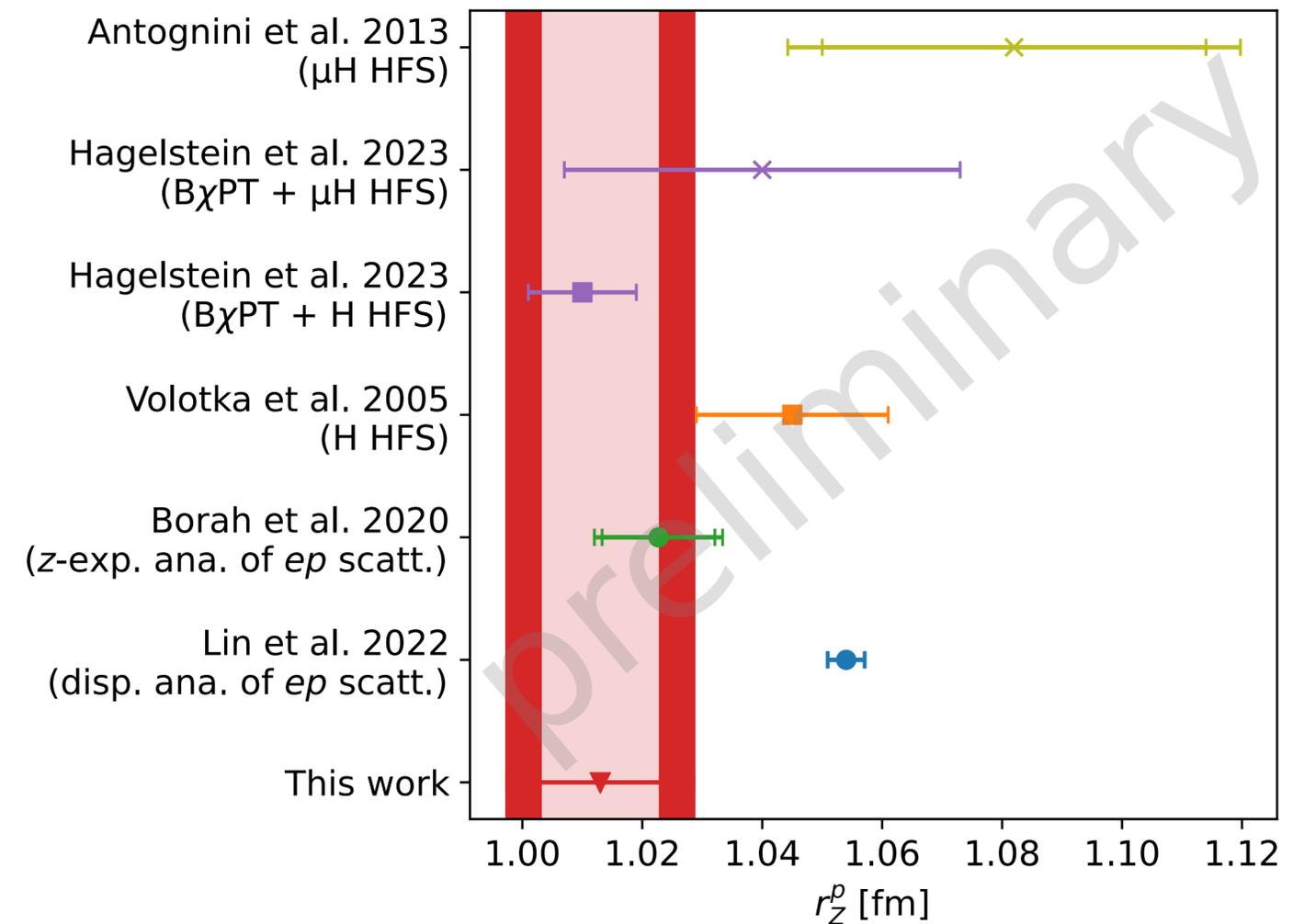
Hyperfine splitting and the Zemach radius

Electromagnetic structure of the proton affects the HFS of the s-state of hydrogen

Relevant parameter: Zemach radius

$$r_Z^p = -\frac{2}{\pi} \int_0^\infty \frac{dQ^2}{(Q^2)^{3/2}} \left(\frac{G_E^p(Q^2) G_M^p(Q^2)}{\mu_M^p} - 1 \right)$$

- Tail of the integrand suppressed:
Region above $Q^2 \gtrsim 0.6 \text{ GeV}^2$ contributes only 1%
- Extrapolate the BChPT fit to large Q^2 using the z -expansion
- Small result for r_Z^p consistent with correlation between r_Z^p and $\sqrt{\langle r_E^2 \rangle^p}$



[M. Salg @ Lattice 2023]

Summary

Lattice calculations of nucleon structural properties are entering the precision era

- Results precise enough to be confronted with phenomenological and experimental results:
Pion-nucleon σ -term, axial & electromagnetic form factors
- Lattice QCD contributes to resolving the proton radius puzzle: r_E^p , r_M^p , r_Z^p
- Results for strangeness form factors exceed experimental precision

Continue towards higher precision: improve control over excited-state contributions