Neutron electric dipole moment with lattice QCD

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Extended Twisted Mass Collaboration

STIMULATE
European Joint Doctorates

Neutron Electric Dipole Moment: from Theory to Experiment

ETC*, Trento, 1-5 August 2022

Outline

- **Introduction**
  - **State-of-the-art lattice QCD simulations**
  - **Approach to extract electromagnetic (EM) form factors**
- **Neutron electric dipole moment (nEDM) in lattice QCD**
  - **Evaluation of topological charge**
  - **Extraction of CP-odd form factor F_3**
  - **Discussion of results**
- **Conclusions**

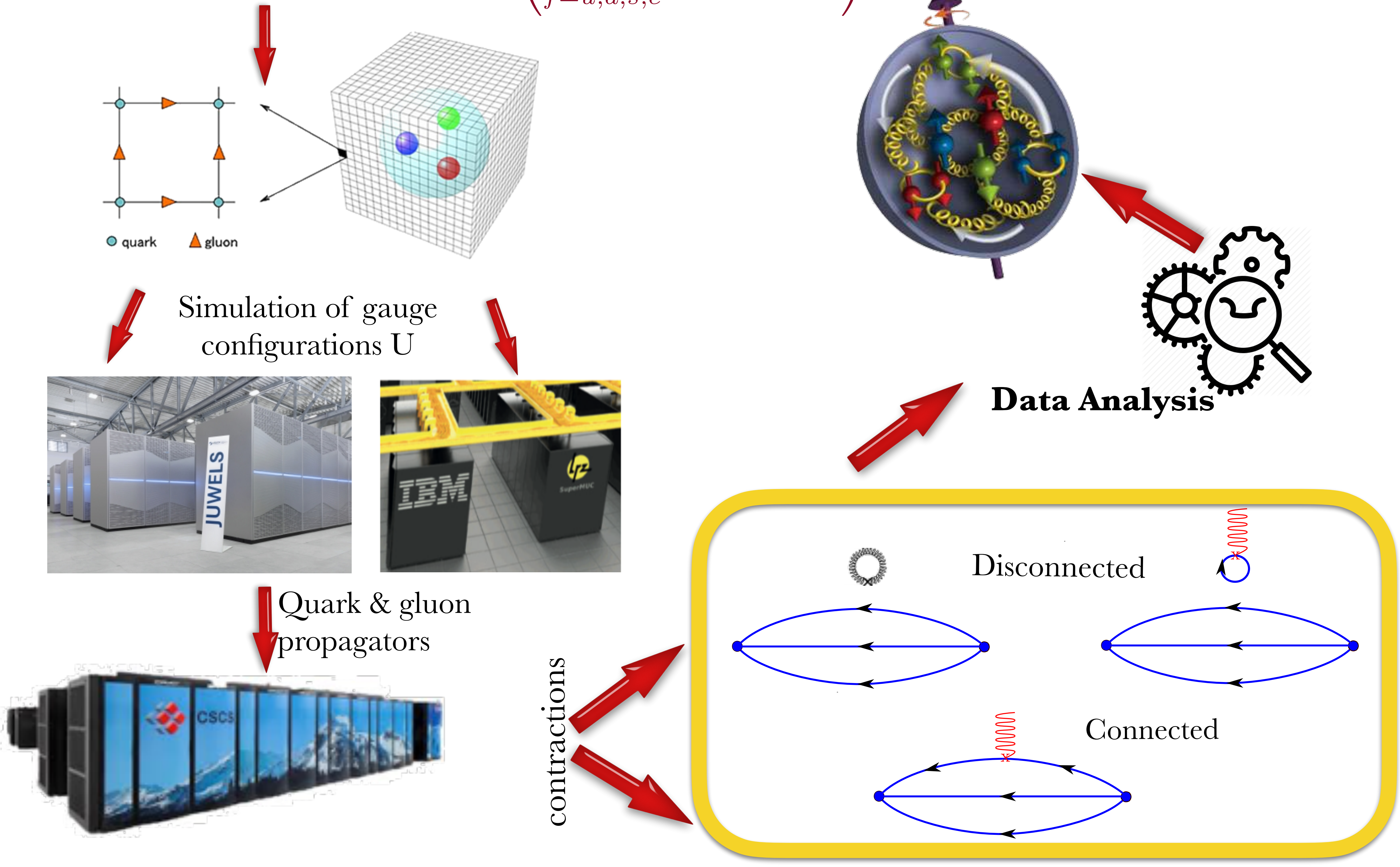
Collaborators:
A. Athenodorou, K. Hadjiyiannakou, A. Todaro

Extended Twisted Mass Collaboration

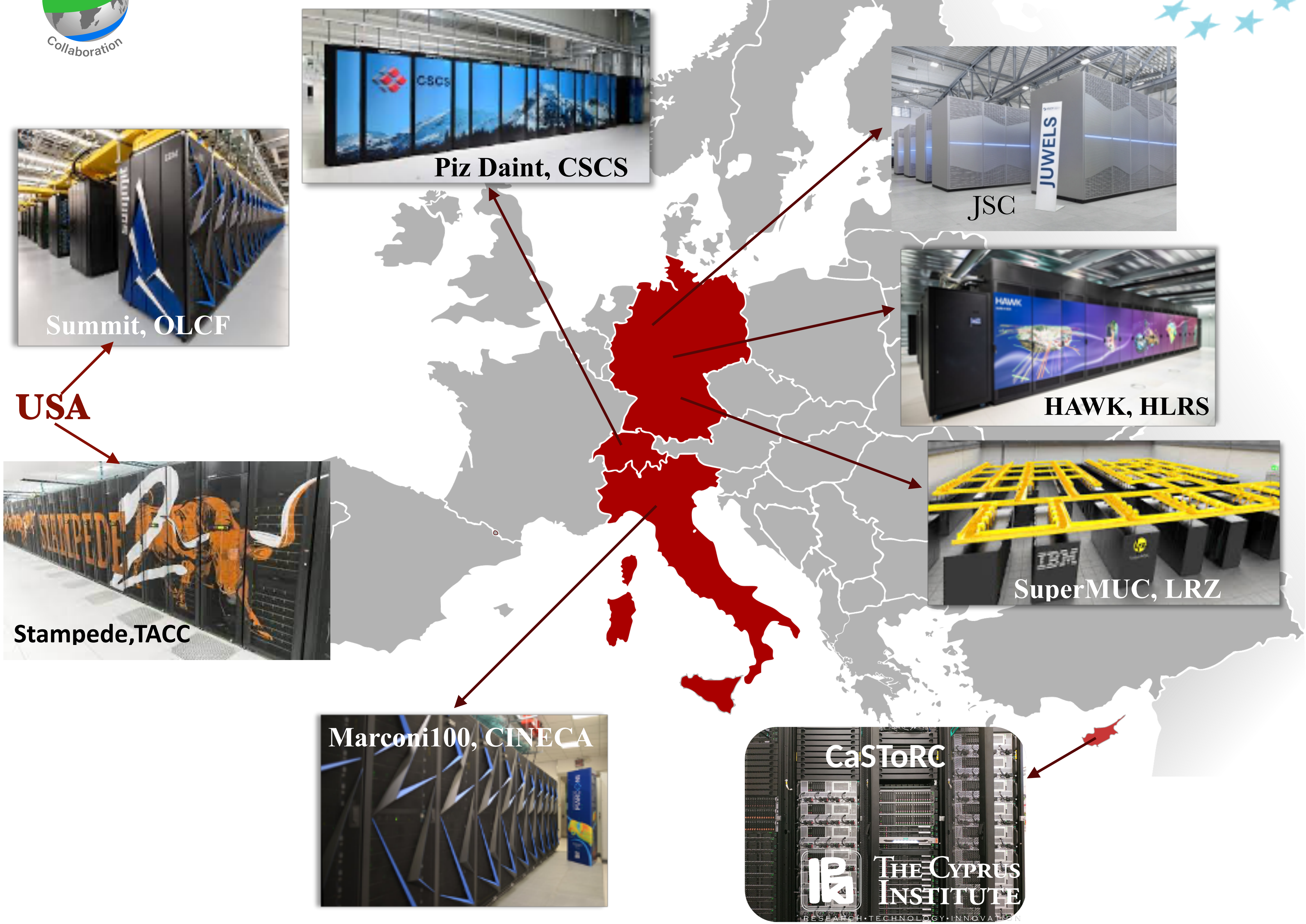
C.A., A. Athenodorou, K. Hadjiyiannakou and A. Todaro, Phys. Rev. D 103, 054501 (2021), arXiv: 2011.01084

Extraction of matrix elements in lattice QCD

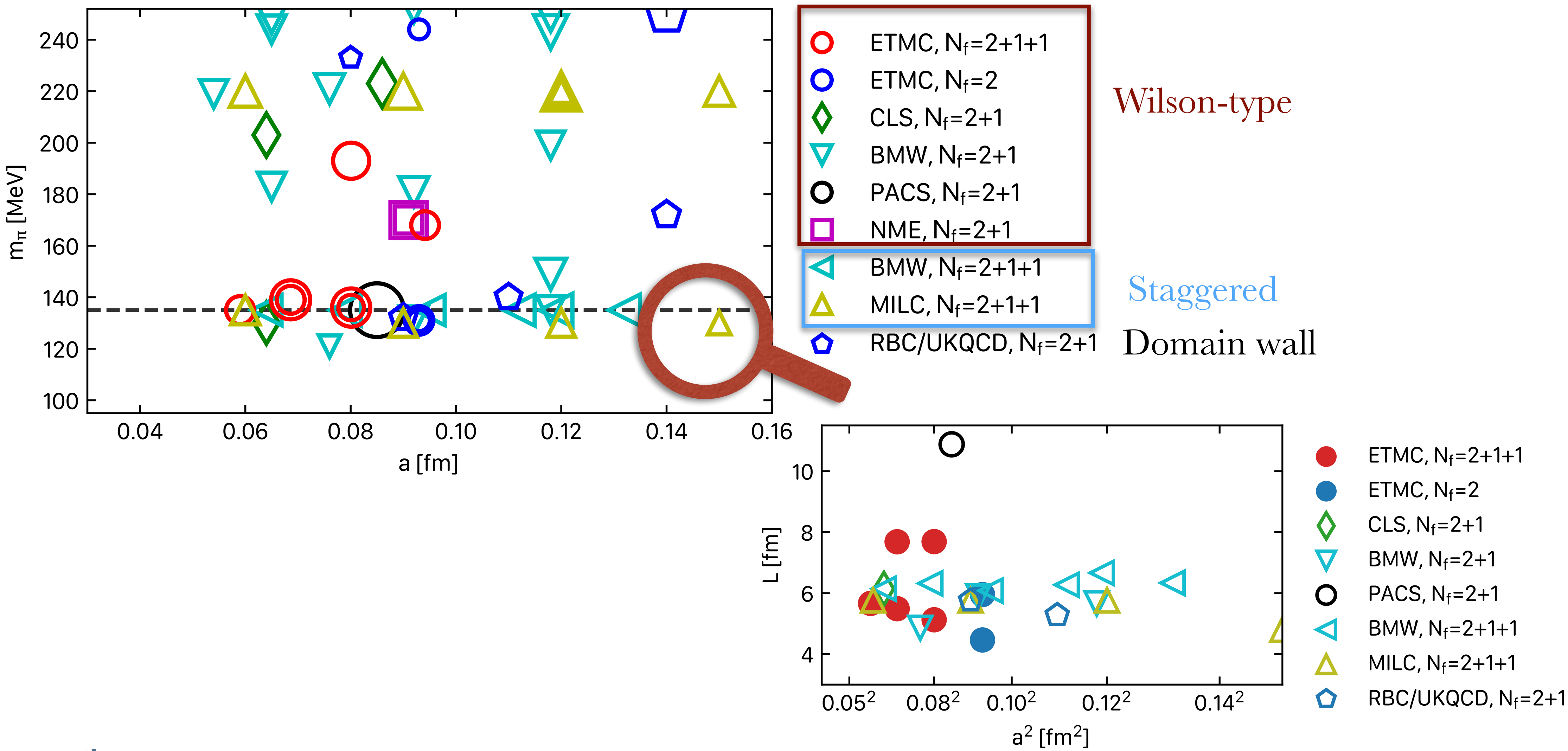
$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}[U] \mathcal{O}(D^{-1}[U], U) \left(\prod_{f=u,d,s,c} \mathrm{Det}(D_f[U]) \right) e^{-S_{\mathrm{QCD}}[U]}$$



Computational resources



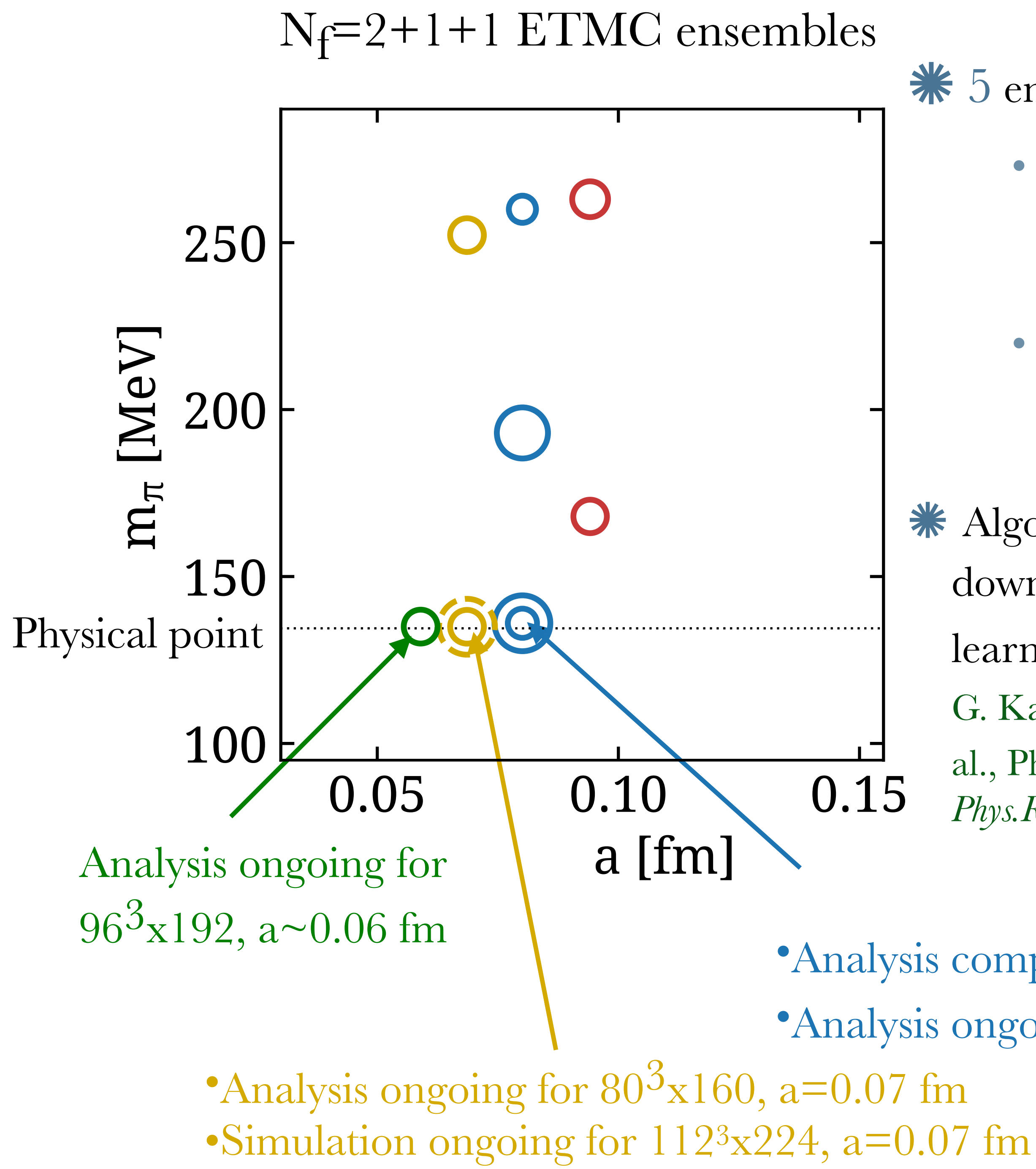
Status of current simulations



❋ A number of collaborations has physical point ensembles:

- Wilson-type: BMW, ETMC, CLS, PACS
  - BMW and ETMC have multiple lattice spacings 0.05<a<0.1 fm
  - PACS has a large volume ensemble at a single lattice spacing
- Staggered at physical point: MILC with 4 and BMW with 6 lattice spacings 0.05<a<0.15 fm
- Domain wall at physical point: RBC/UKQCD with 2 lattice spacings

Gauge ensembles generated by ETMC



- 5 ensembles at physical pion mass
  - 3 lattice spacings 0.05<a<0.1 fm —> take continuum limit **directly at the physical point** avoiding chiral extrapolation removing a major systematic error in the baryon sector
  - Two volumes at a=0.08 fm and 0.07 fm of Lm_π~3.6 (5.1 fm) and Lm_π ~5.4 (7.7 fm)
- Algorithmic improvements needed to go to a<0.05 fm due to critical slow down in HMC (long autocorrelations) —> new approaches e.g. Machine learning approaches using equivariant flows

G. Kanwar, et al., Phys. Rev. Lett. 125 (2020) 121601, arXiv:2003.06413; D. Boyda, et al., Phys.Rev.D 103 (2021) 074504, arXiv: 2008.05456; M. S. Albergo *et al.*, *Phys.Rev.D* 104 (2021) 114507, arXiv:2106.05934

C. A. *et al.* (ETMC), "Simulating twisted mass fermions at physical light, strange and charm quark masses" Phys. Rev. D98 (2018) 054518

Systematics & Challenges

- **Simulations directly at the physical point** ✓

  Systematic effects from chiral extrapolation are eliminated

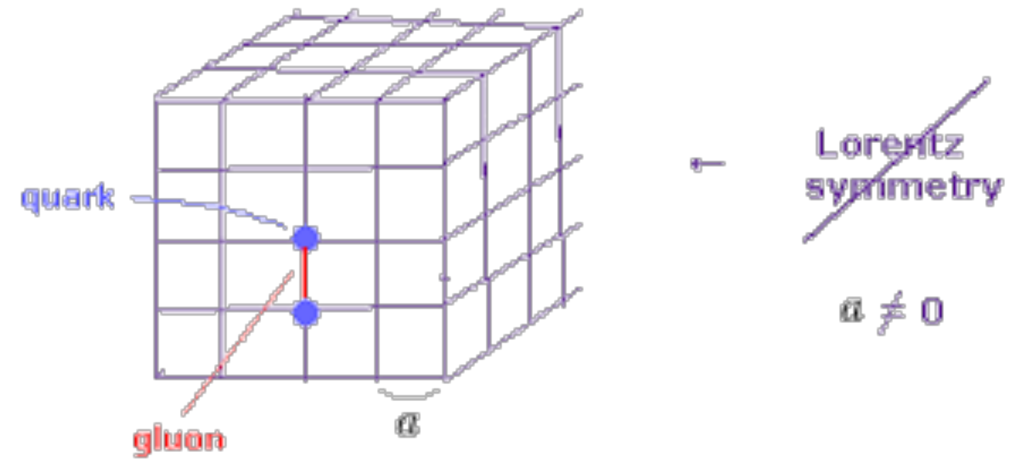
- **Discretisation effect:** Continuum limit

  —> need simulations for at least 3 lattice spacings

- **Finite volume effects:** Infinite volume limit

  —> need simulations for at least 3 volumes

Typically done using simulations for heavier than physical values of the pion mass



- **Ground-state identification**

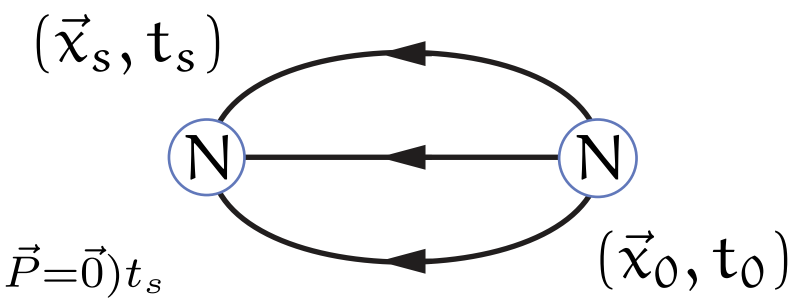
  Cross-check (one-, two- and three-state fits, summation), but two or more particle states create difficulties

- **Renormalisation**

  Non-perturbatively with improvements e.g using perturbative subtraction of lattice artefacts - more complicated for extended operators

- In what follows we assume **isospin symmetry** i.e. up and down quarks have equal mass, and **neglect EM effects**

Nucleon propagator

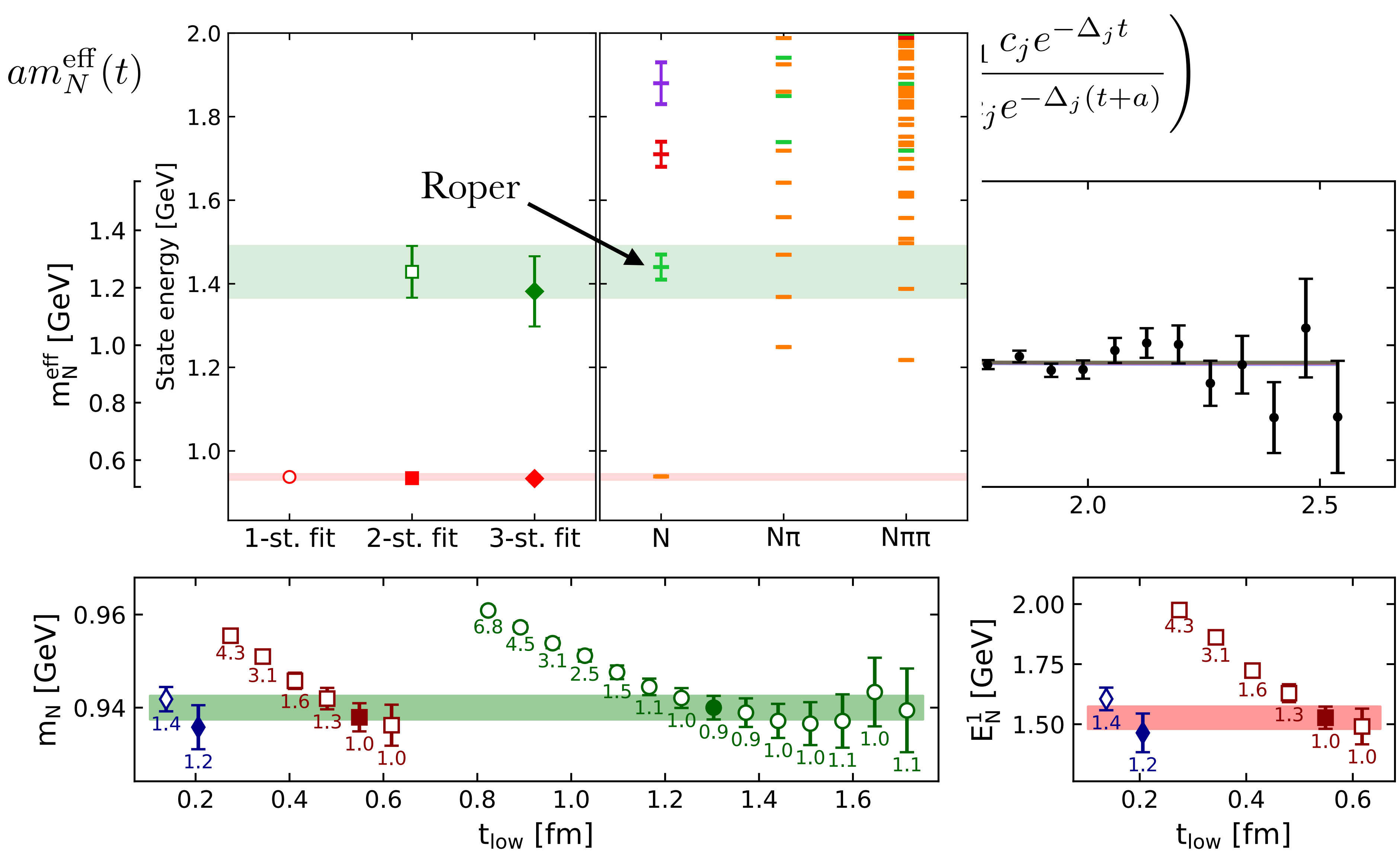


Analysis of two- and three-point functions C_{2pt} and C_{3pt}

$$C_{2\mathrm{pt}}(\Gamma_0;\vec{P}=\vec{0},t_s)=\sum_{\vec{x}_s}\mathrm{Tr}\left[\langle\Gamma_0 J_N(t_s,\vec{x}_s)\bar{J}_N(t_0,\vec{x}_0)\rangle\right]=\sum_{n=0}^{\infty}a_n e^{-E_n(\vec{P}=\vec{0})t_s}$$

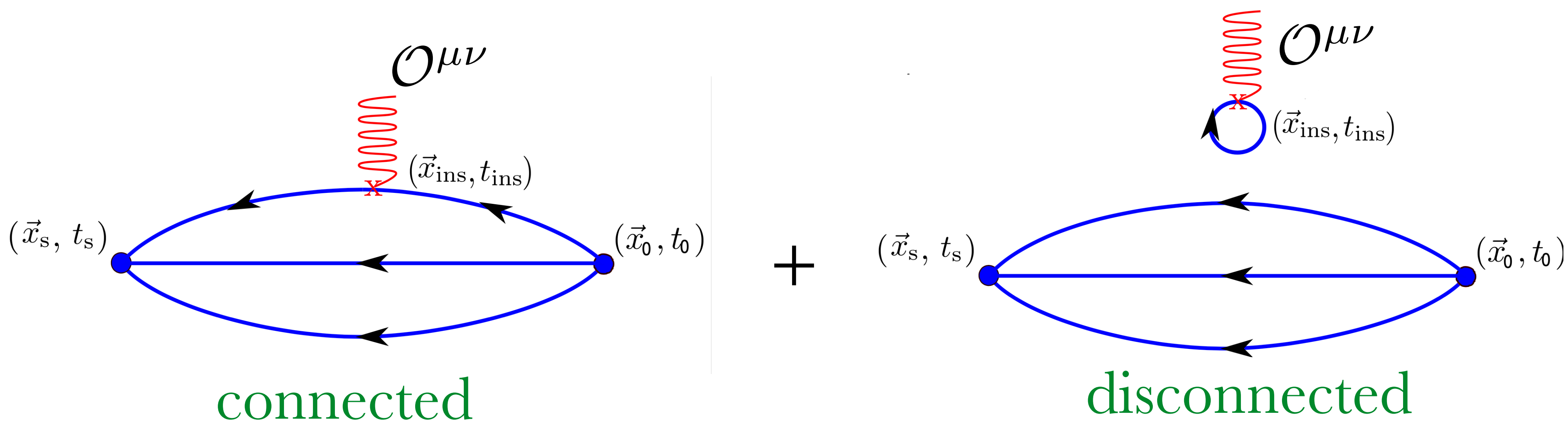
$$\xrightarrow{t_s\to\infty} a_0 e^{-m_N t_s}+\mathcal{O}\left(e^{-E_1(\vec{P}=\vec{0})t_s}\right)$$

Fit the nucleon two-point function or effective mass keeping up to two excited states



Nucleon matrix elements

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



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

Plateau and two-state fit:

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

Included in the two-state fit

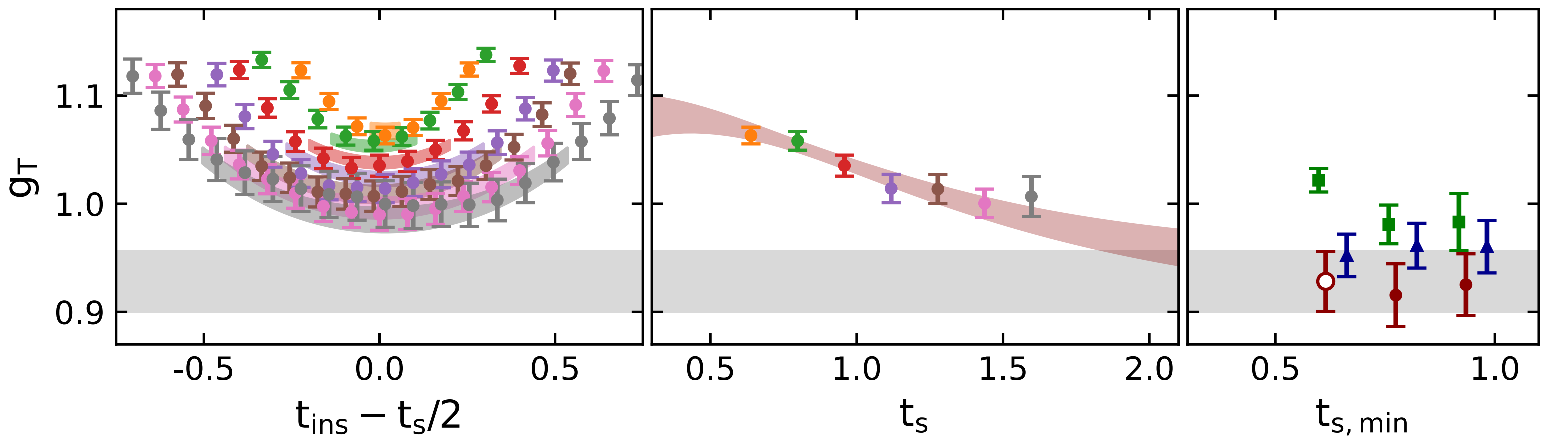
Summation:

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

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

Isovector tensor charge

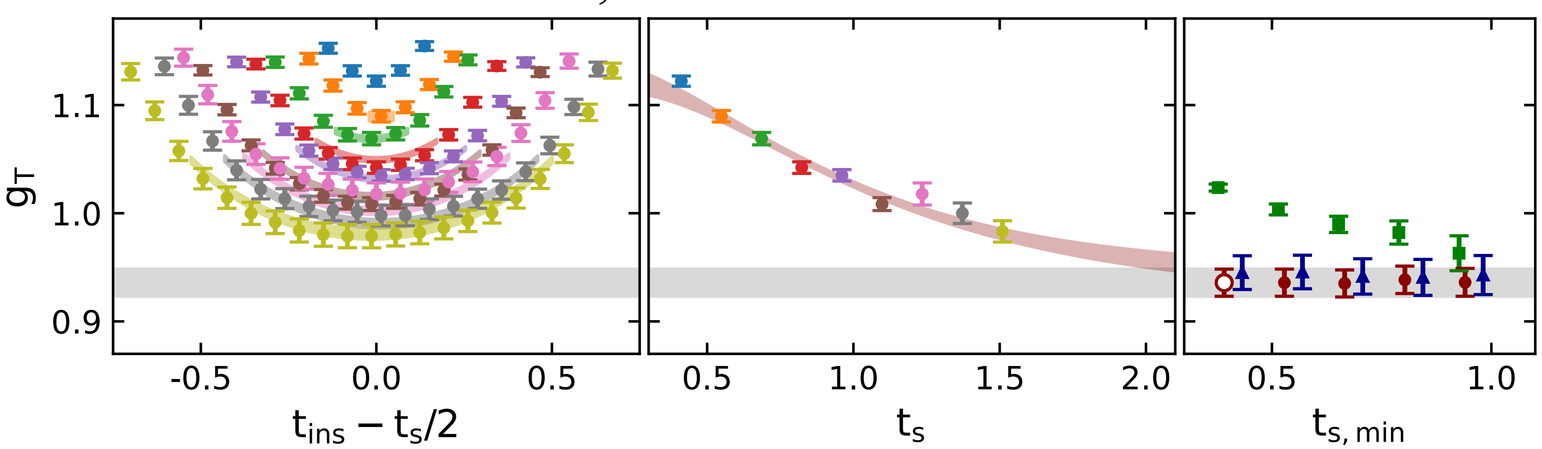
B-ensemble: $64^3 \times 128$, a~0.08 fm



t_s/a	t_s [fm]	n_{srcs}
8	0.64	1
10	0.80	2
12	0.96	4
14	1.12	6
16	1.28	16
18	1.44	48
20	1.60	64
2-point		264

x 750 configurations = **15 M** inversions!

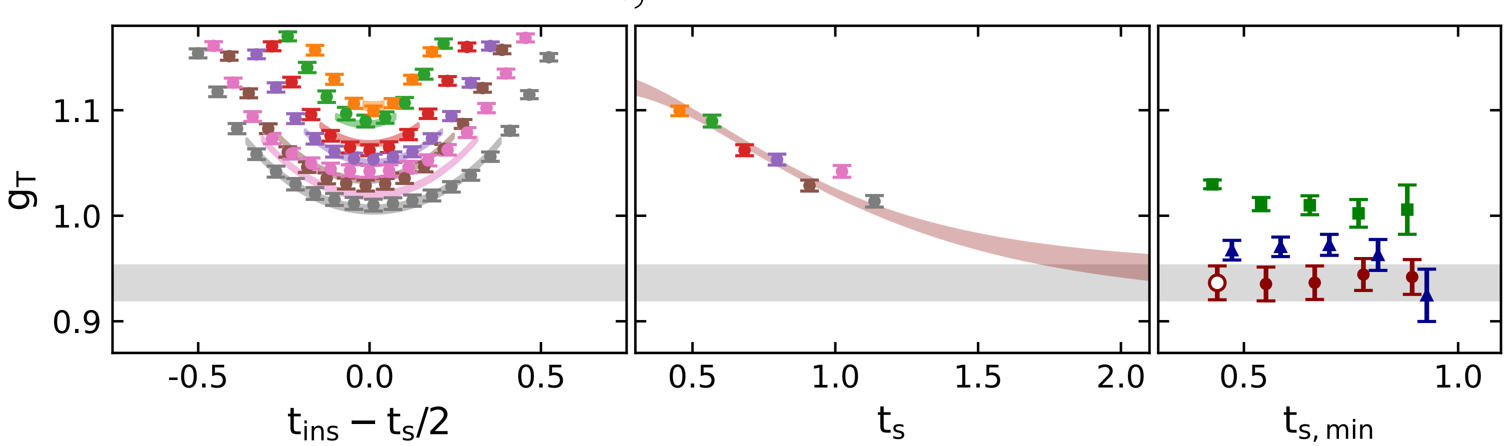
C-ensemble: $80^3 \times 160$, a~0.07 fm



t_s/a	t_s [fm]	n_{srcs}
8	0.549	1
10	0.686	2
12	0.823	5
14	0.961	11
16	1.098	24
18	1.235	45
20	1.372	116
22	1.509	246
2-point		650

x 401 configurations = **23.6 M** inversions!

D-ensemble: $96^3 \times 192$, a~0.06 fm



t_s/a	t_s [fm]	n_{srcs}
8	0.456	1
10	0.570	2
12	0.684	4
14	0.798	8
16	0.912	16
18	1.026	32
20	1.140	64
22	1.254	16
24	1.368	32
26	1.482	64
2-point		368

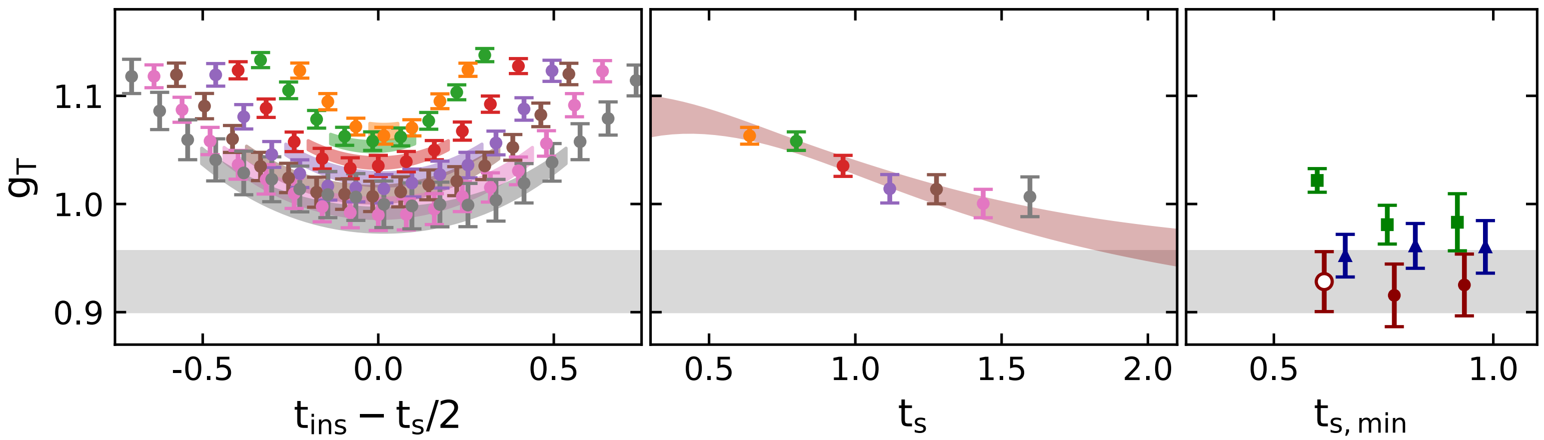
on-going

x 500 configurations = **15.9 M** inversions!

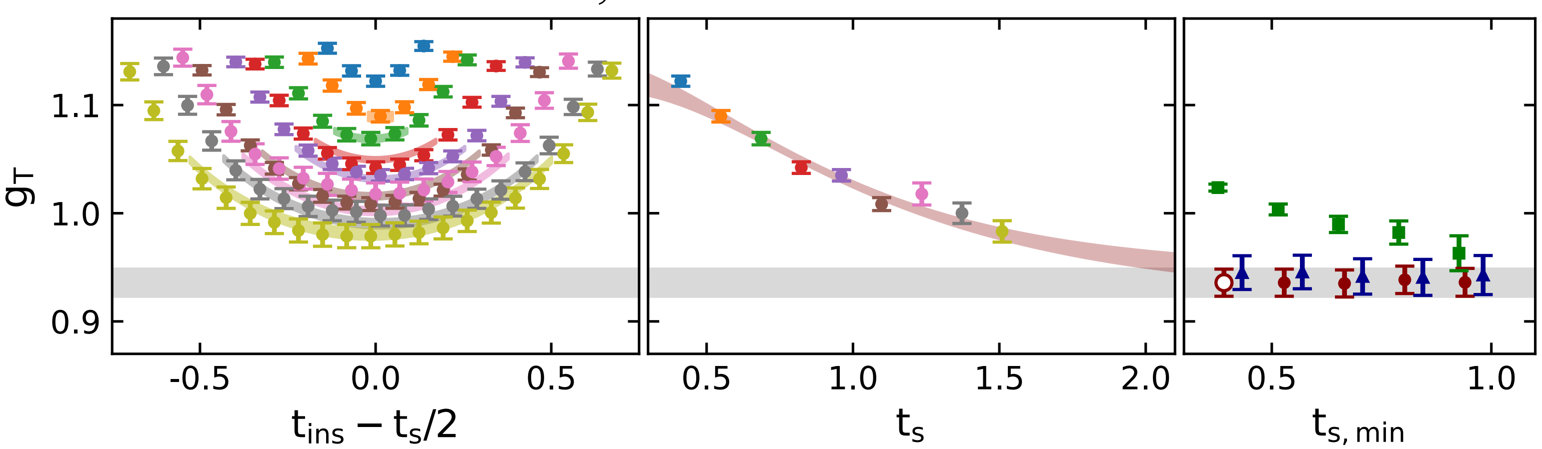
- Important to probe large t_s values keeping error approximately the same to reliably eliminate contributions from excited states

Isovector tensor charge

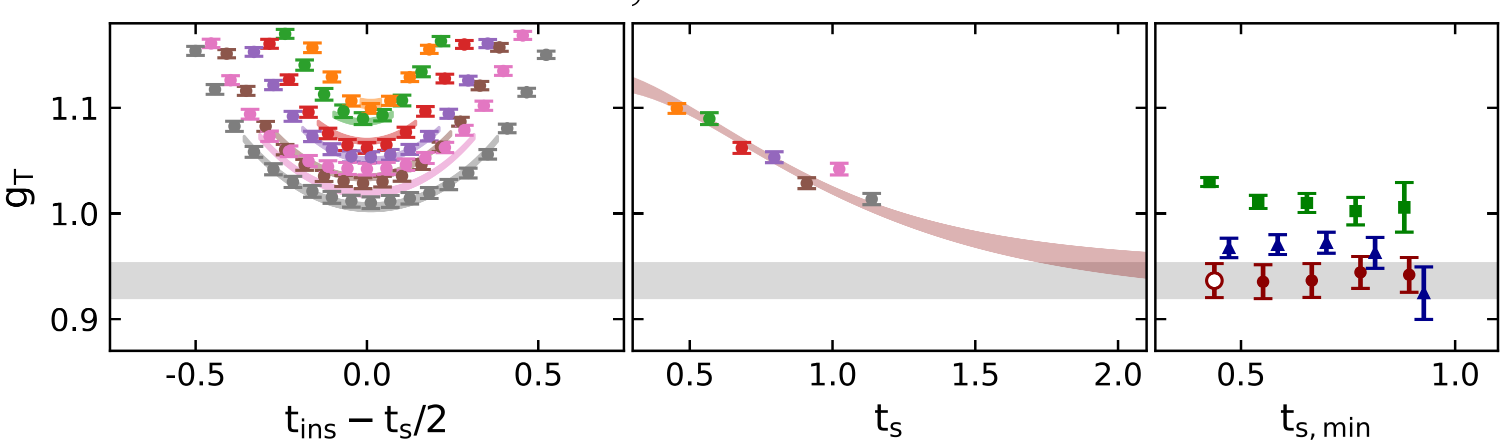
B-ensemble: 64^3 x 128, a~0.08 fm

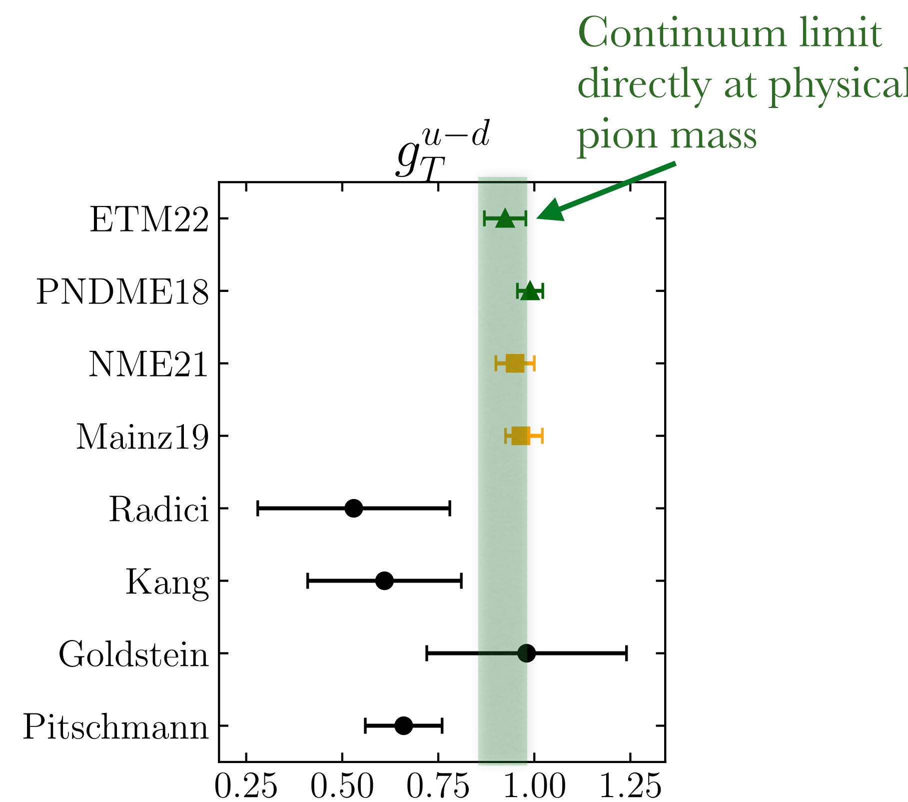


C-ensemble: 80^3 x 160, a~0.07 fm



D-ensemble: 96^3 x 192, a~0.06 fm





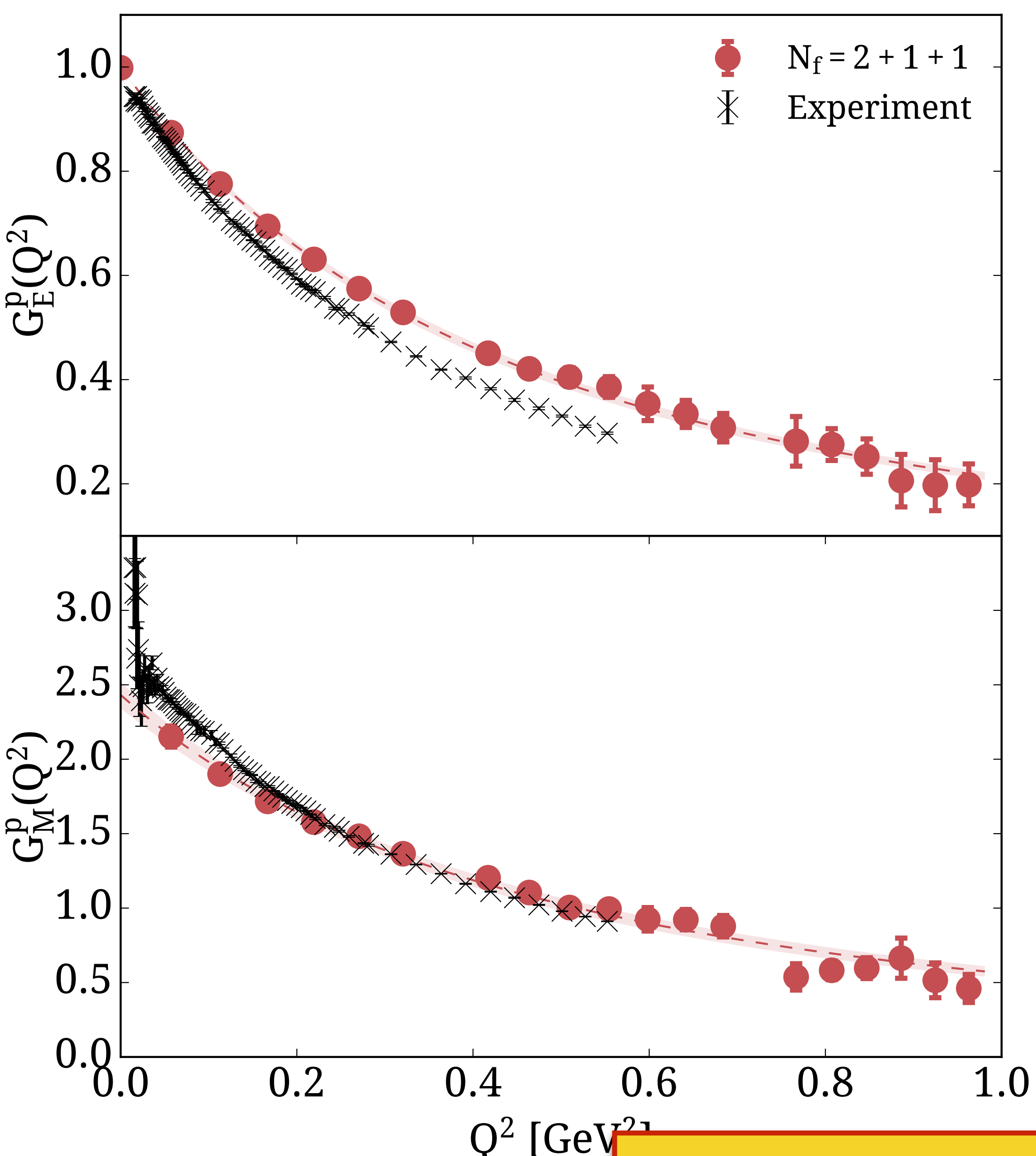
- Important to probe large t_s values keeping error approximately the same to reliably eliminate contributions from excited states

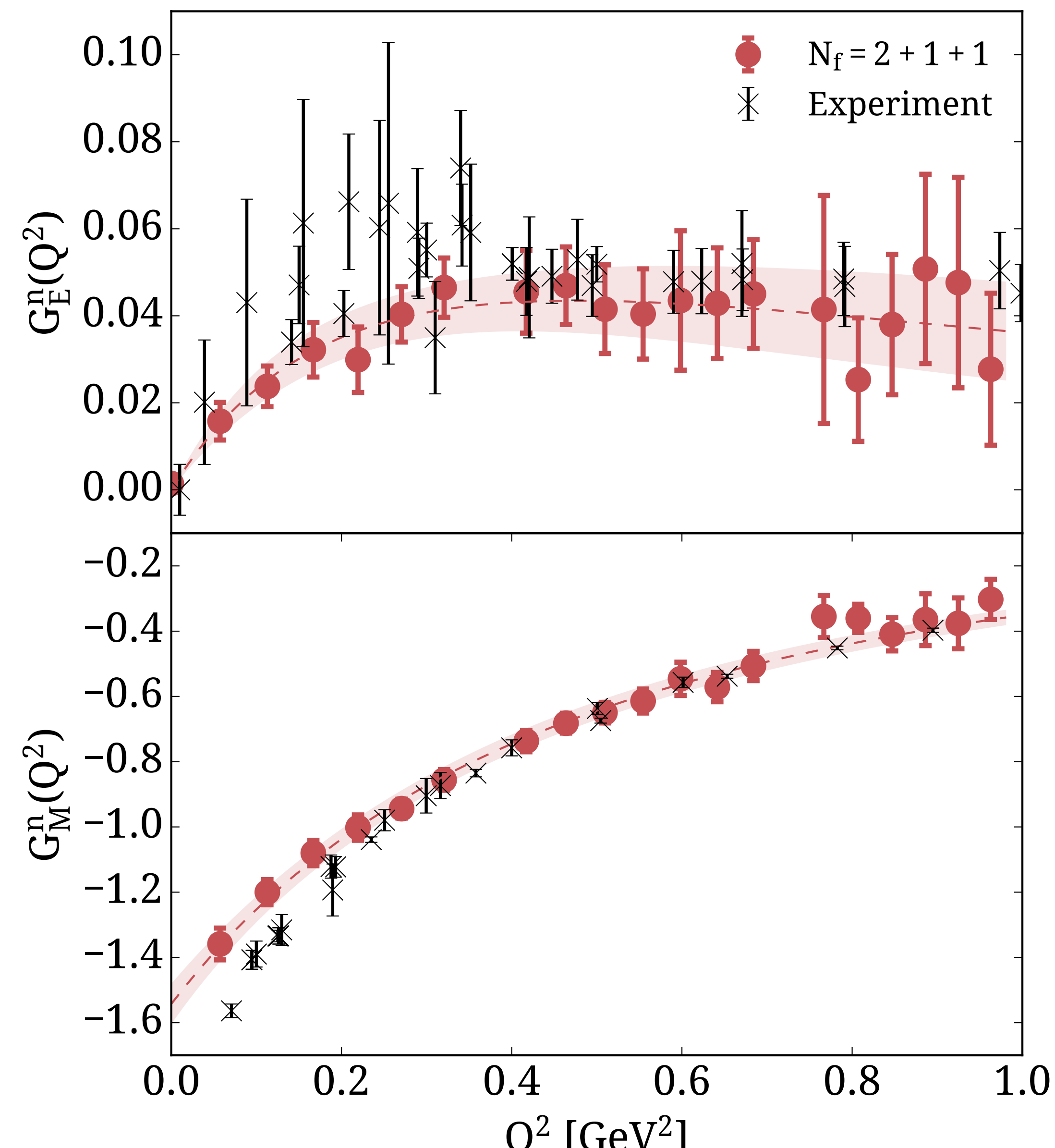
—> precision era of lattice QCD

Form factors

- Generalisation to non-zero momentum transfer to extract form factors
- EM form factors best studied

B-ensemble: 64^3 x 128, a~0.08 fm





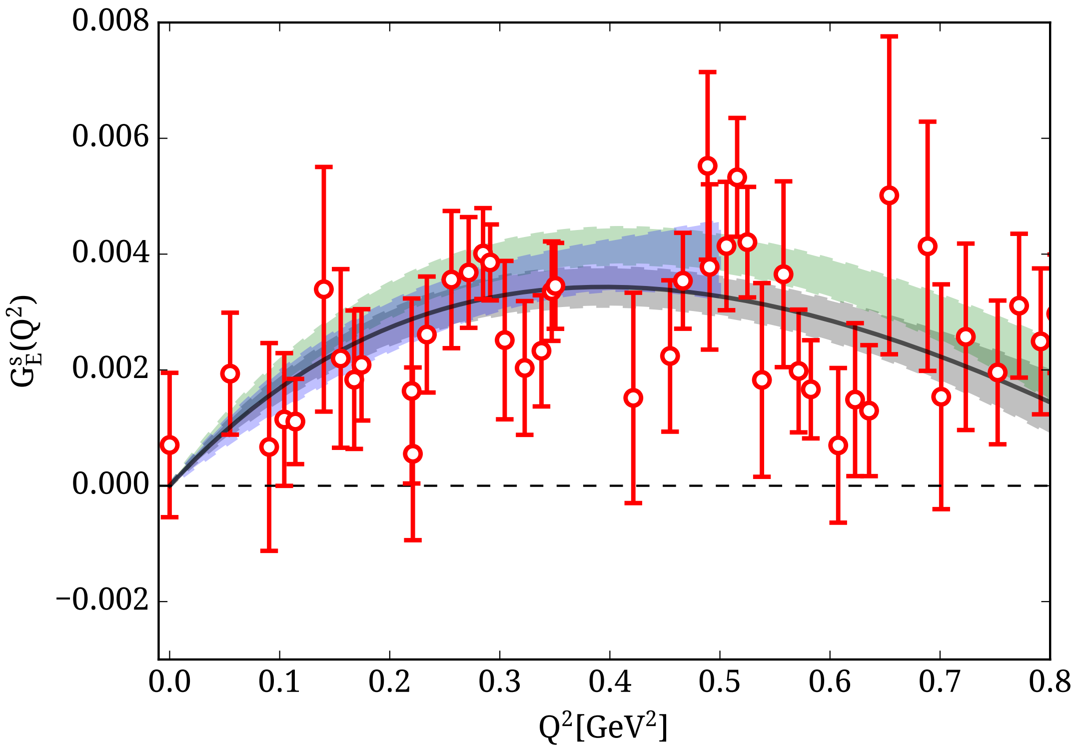
—> precision era of lattice QCD

TMC), Phys.Rev.D 100 (2019) 1, 014509,

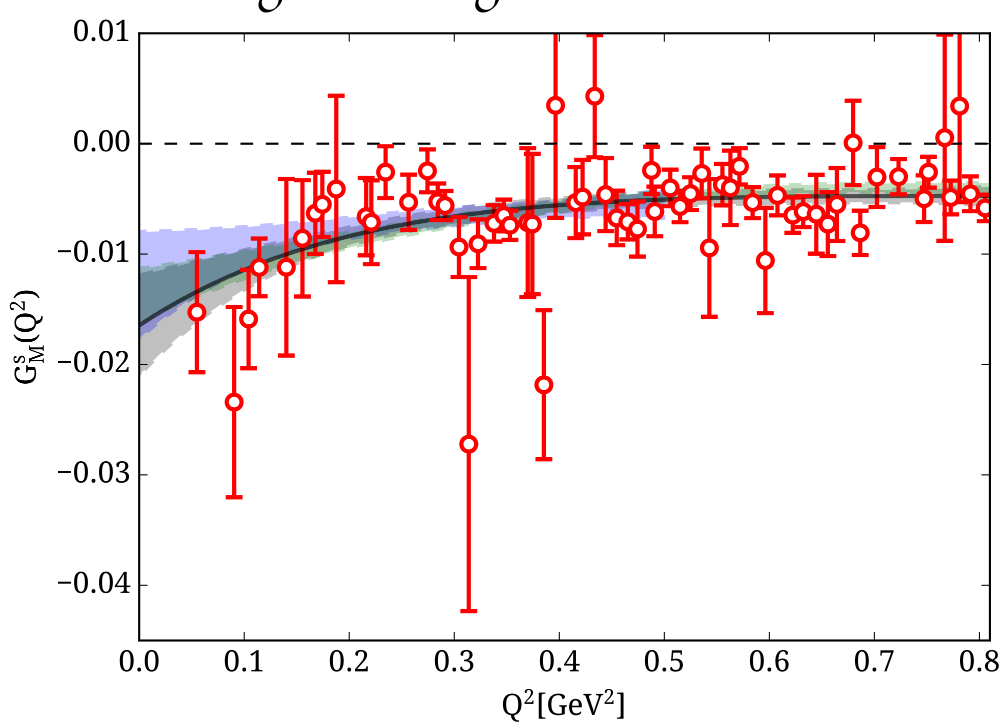
Strangeness of the nucleon

- Sea quark effects can be accurately determined —> provide precise input to experiments

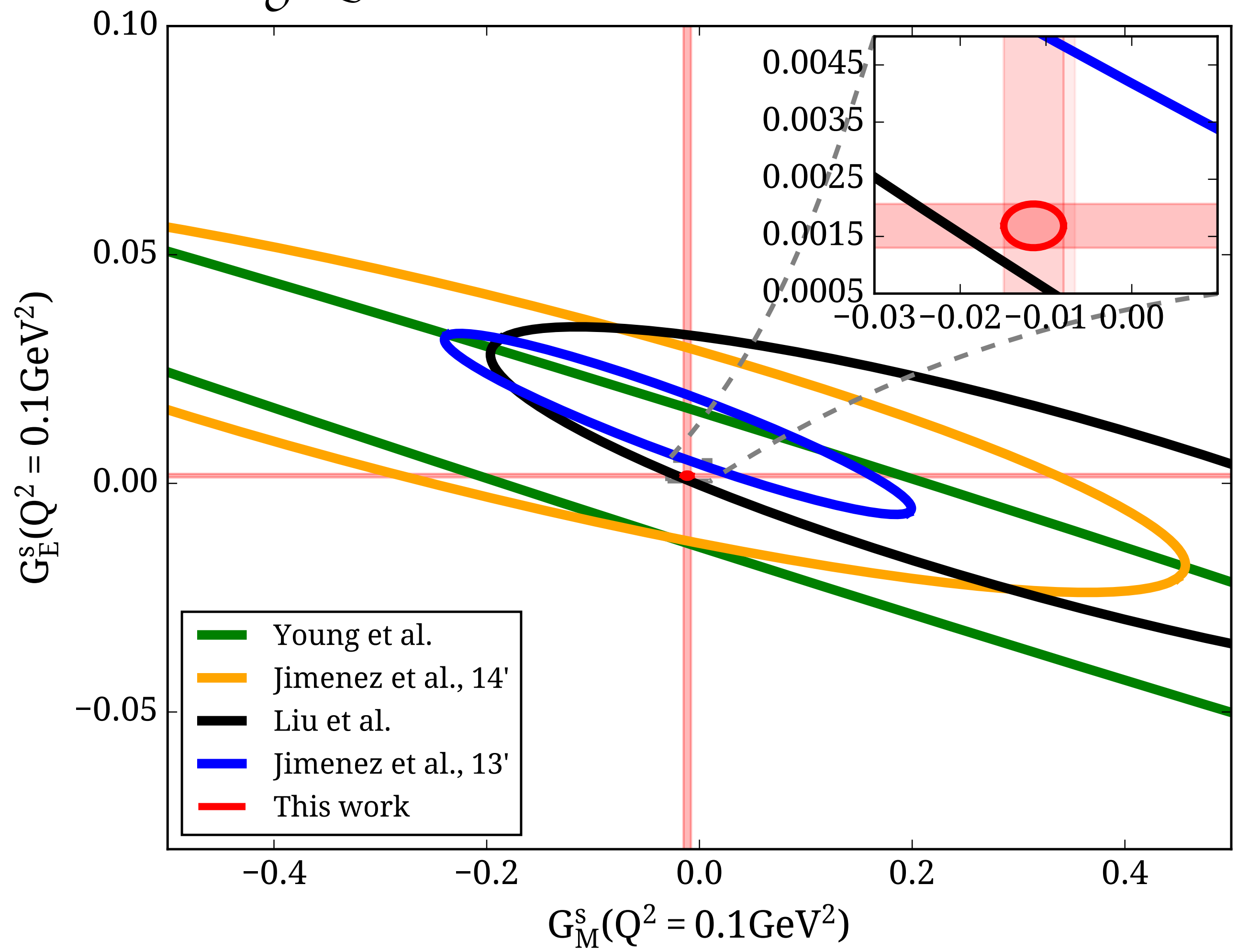
B-ensemble: 64^3 x 128, a~0.08 fm



Negative magnetic moment



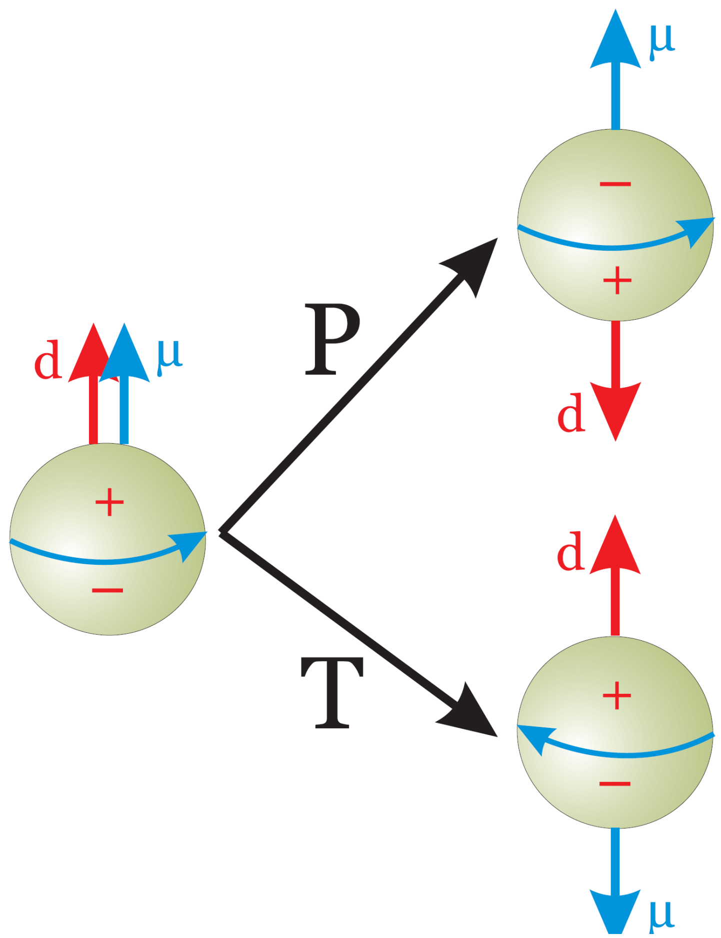
Significant input to experimental searches e.g Q-Weak, SolID, etc



C. A. *et al.*, Phys. Rev. D 101 (2020) 031501, arXiv:1909.10744

Neutron electric dipole moment

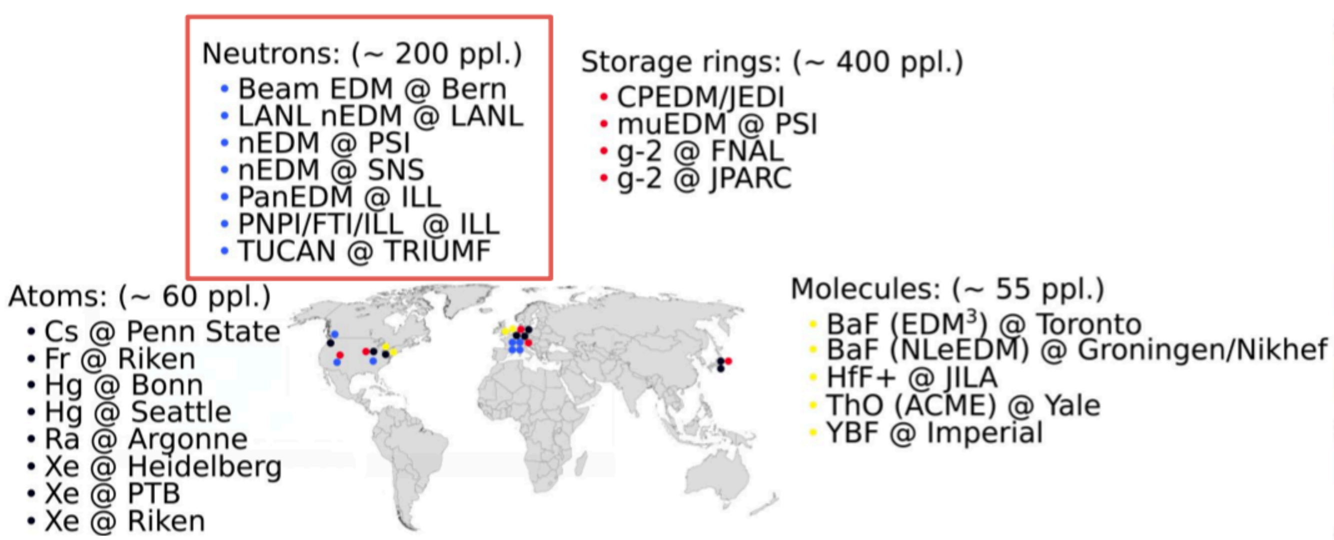
Motivation



- Possible detection of nEDM would break CP symmetry —> new source of CP violation within the Standard Model (SM)
- Despite experimental efforts over the last 70 years **no non-zero value has been measured**
- Best upper bound: $|d_N| < 1.8 \times 10^{-13}$ e fm

Abel *et al.*, Phys. Rev. Lett. 124, 081803 (2020)

New experiments are coming and plan to further improve current upper bound by 2 order of magnitude

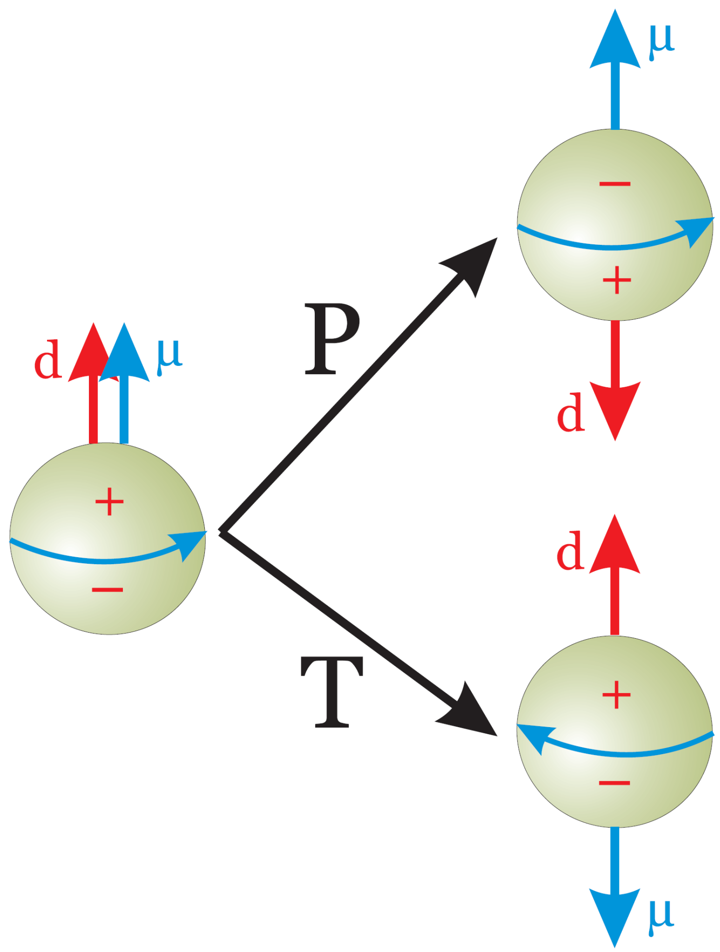


source: https://www.psi.ch/en/nedm/edms-world-wide

Experiment	Features	Status
PSI	spallation so-D_2, magnetic fields	analysis/upgrading
PanEDM (ILL/Munich)	reactor He-II, 1st MSR	commissioning
ILL/PNPI/Gatchina	dual cell, 2nd best nEDM meast	upgrading source
LANL	spallation so-D_2 UCN source	2021-
TUCAN (Japan/Canada)	spallation He-II, MSR	upgrading, 2022-
SNS	fully cryogenic source/experiment	2022-
ILL/ESS n-beam	intense pulsed neutron beam	R&D, 2025-
J-PARC crystal	high E in crystal	R&D

source: [*J.W. Martin, J. Phys.: Conf. Ser. 1643 012002 (2020)*]

Motivation



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Abel *et al.*, Phys. Rev. Lett. 124, 081803 (2020)

Standard model prediction

- **Electroweak sector:** phase in quark mass from Yukawa coupling with Higgs field

  $|d_N| \sim O(10^{-19})$ e fm

- **Strong sector:** a QCD Lagrangian invariant under *C*, *P* and *T* transformations does not permit nEDM
  Include the *CP*-violating Cherns-Simons (CS) term:

$$\mathcal{L}_\theta(x) = -i\theta \frac{1}{32\pi^2} F^a_{\mu\nu}(x)\tilde{F}^{\mu\nu,a}(x) = -i\theta q(x)$$

Topological charge: $\mathcal{Q} = \frac{1}{32\pi^2}\int d^4x F^a_{\mu\nu}(x)\tilde{F}^{\mu\nu,a}(x)$

General approach

$$\mathcal{L}_{\rm QCD}(x) = \frac{1}{2g^2}\mathrm{Tr}\left[F_{\mu\nu}(x)F^{\mu\nu}(x)\right] + \sum_f \overline{\psi}_f(x)(i\gamma_\mu D^\mu + m_f)\psi_f(x)$$

- $\mathcal{L}_{\rm QCD}$ invariant under C, P and T transformations —> cannot induce a non-vanishing nEDM.
- Insert the CP-violating Cherns-Simons (CS) term —> $\mathcal{L}(x) = \mathcal{L}_{\rm QCD}(x) + \underbrace{\mathcal{L}_\theta(x)}_{-i\theta q(x)}$
- Compute expectation values including CS-term: $\langle \mathcal{O}(x_1,...,x_n)\rangle_\theta = \frac{1}{Z_\theta}\int d[U]d[\psi_f]d[\bar{\psi}_f]\; \mathcal{O}(x_1,...,x_n)\; e^{-S_{\rm QCD}+i\theta\int q(x)d^4x}$
- Sign problem: CS-term makes the action complex
  - Measure the neutron energy in an external electric field
  - Simulate with imaginary θ as done by e.g. QCDSF, Guo *et al.* 2015
  - Since θ is small expand keeping only first order terms

Correlation with topological charge

$$\langle \mathcal{O}(x_1,...,x_n)\rangle_\theta = \langle \mathcal{O}(x_1,...,x_n)\rangle_{\theta=0} + \langle \mathcal{O}(x_1,...,x_n)(i\theta\mathcal{Q})\rangle_{\theta=0} + O(\theta^2)$$

- Measure the neutron CP-violating electromagnetic form factor $F_3(Q^2)$ and extract $F_3(0)$ —> $|d_N| = \frac{F_3(0)}{2m_N}$
- We can only calculate $F_3(Q^2)$ and need to take Q^2 —>0

Nucleon matrix for nEDM

Form factor decomposition for the nucleon electromagnetic form factor:

$$\langle N^\theta(\vec{p_f}, s)|J_\mu^{\rm EM}|N^\theta(\vec{p_i}, s')\rangle = \bar{u}_N^\theta(\vec{p_f}, s)\Gamma_\mu^\theta(q)u_N^\theta(\vec{p_i}, s')$$

$$\Gamma^\theta(q) = F_1(Q^2)\gamma_\mu + \left(F_2(Q^2) + i\gamma_5 F_3^\theta(Q^2)\right)\frac{\sigma_{\mu\nu}q_\nu}{2m_N^\theta}\,; \qquad F_3^\theta = \theta F_3^{(1)} + O(\theta^3) \qquad m_N^\theta = m_N + O(\theta^2)$$

- Compute the 3-point function:

$$\langle J_N(\vec{p_f}, t_s)J_\mu^{\rm EM}(\vec{q}, t)\bar{J}_N(\vec{p_i}, 0)\rangle_\theta \sim |Z_N^\theta|^2 e^{-E_N^f(t_s - t)}e^{-E_N^i t}e^{i\alpha^\theta\gamma_5}\Lambda_{\frac{1}{2}}^\theta\Gamma_\mu^\theta\Lambda_{\frac{1}{2}}^\theta e^{i\alpha^\theta\gamma_5}$$

$$\alpha^\theta = \theta\alpha^{(1)} + O(\theta^3) \qquad Z_N^\theta = Z_N + O(\theta^2)$$

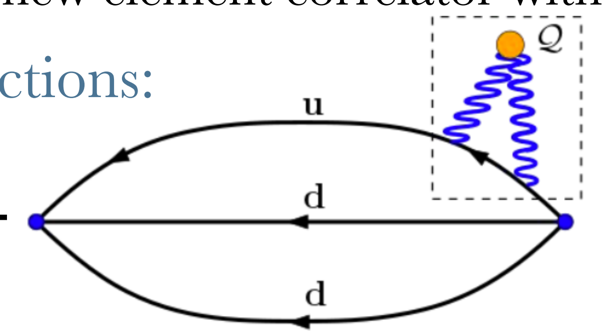
$$\langle J_N(\vec{p_f}, t_s)J_\mu^{\rm EM}(\vec{q}, t)\bar{J}_N(\vec{p_i}, 0)e^{i\theta\mathcal{Q}}\rangle = \underbrace{\langle J_N(\vec{p_f}, t_s)J_\mu^{\rm EM}(\vec{q}, t)\bar{J}_N(\vec{p_i}, 0)\rangle}_{C_{3pt}} + i\theta\underbrace{\langle J_N(\vec{p_f}, t_s)J_\mu^{\rm EM}(\vec{q}, t)\bar{J}_N(\vec{p_i}, 0)\mathcal{Q}\rangle}_{C_{3pt,\,Q}} + O(\theta^2)$$

C_{3pt}

$C_{3pt,\,Q}$ new element correlator with topological charge

- Need to determine $\alpha^{(1)}$ —> extracted from nucleon 2-point functions:

$$C_{2pt} = \langle J_N(\vec{p}_f, t_f)\bar{J}(\vec{0}, 0)\rangle\,, \qquad C_{2pt,\mathcal{Q}} = \langle J_N(\vec{p}_f, t_f)\mathcal{Q}\bar{J}(\vec{0}, 0)\rangle$$



$$\longrightarrow \quad \frac{C_{2\rm pt,\mathcal{Q}}}{C_{2\rm pt}} \to \alpha^1$$

- To extract matrix element take ratio of 3- and 2-point functions:

$$\Pi_{3pt,\mathcal{Q}}^{\mu k}(q) \equiv \lim_{t_f, t\to\infty}\frac{C_{3pt,\mathcal{Q}}}{C_{2pt,\mathcal{Q}}}R_{2pt} \qquad \text{e.g.} \qquad \Pi_{3pt,\mathcal{Q}}^{0k}(q) = \frac{iq_kC}{2m_N}\left(a^{(1)}G_E(Q^2) - \frac{F_3^{(1)}(Q^2)}{2m_N}(E_N + m_N)\right)$$

Topological charge

- CP-odd EM form factor F_3 much less studied
- Need topological charge for the computation of the matrix element - need an appropriate discretisation
  - Field theoretic definition - Di Vecchia *et al.*, Nucl. Phys. B192, 392 (1981)
  - Fermionic definition using spectral projectors - Giusti and Luescher, J. High Energy Phys. 03 (2009)
- In the continuum the two definitions are equivalent

Field theoretic definition: $\mathcal{Q} = \frac{1}{32\pi^2} \int d^4x \, \epsilon_{\mu\nu\rho\sigma} \mathrm{Tr}\left[F_{\mu\nu}(x) F_{\rho\sigma}(x)\right]$

- Discretize $F_{\mu\nu}$ - use $O(a^2)$ improved definition by using Clover and rectangular Wilson loops
- Smooth out the ultraviolet fluctuations —> use gradient flow

$$\dot{V}_\mu(x,\tau) = -g_0^2 \left[\partial_{x,\mu} S_G(V(\tau))\right] V_\mu(x,\tau)$$
$$V_\mu(x,0) = U_\mu(x)$$

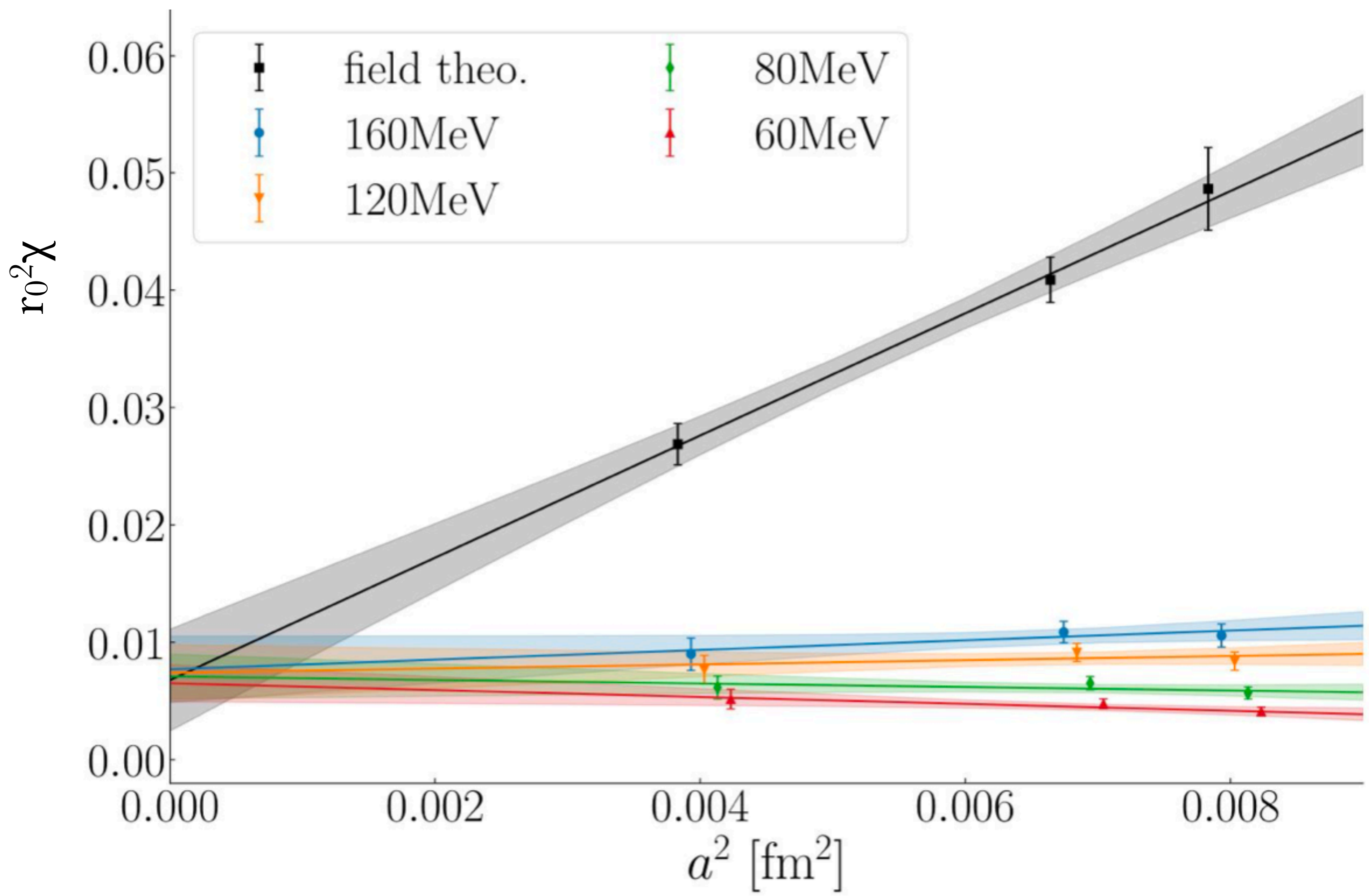
Spectral projector definition:

- Write in terms of the eigenmodes of the Wilson-Dirac operator

$$\mathcal{Q} = \frac{Z_S}{Z_P} \sum_i^{\lambda_i < M_{\mathrm{thr}}} u_i^\dagger \gamma_5 u_i \,, \qquad \left(D_W^\dagger D_W\right) u_i = \lambda_i u_i$$

Comparison of two definitions of topological charge (I)

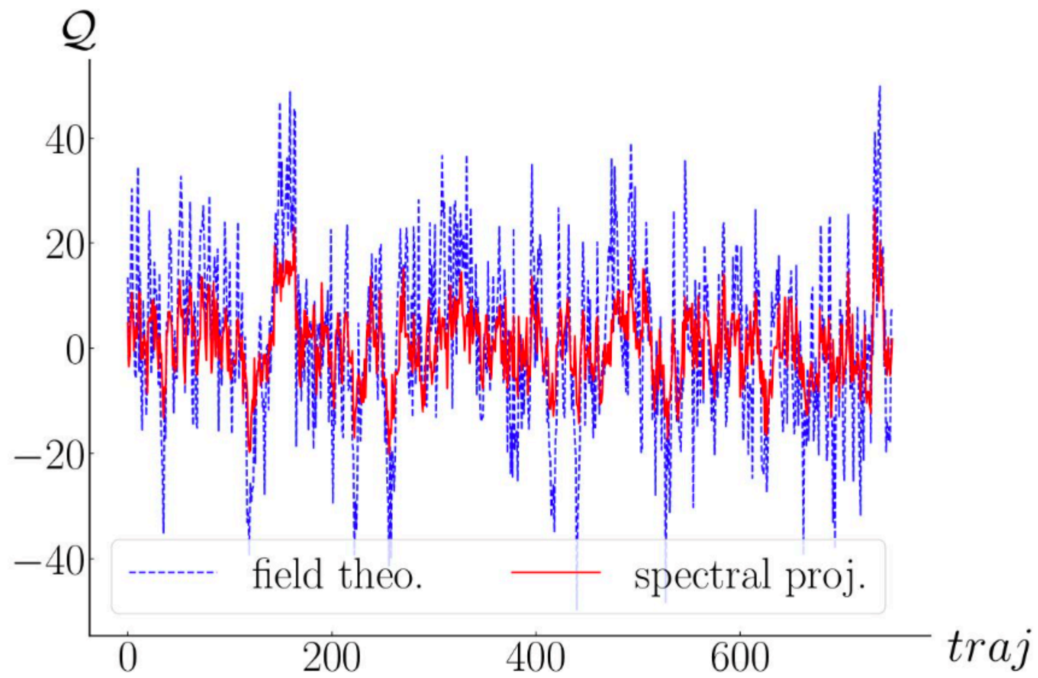
❋Topological susceptibility $\chi = \langle Q^2 \rangle / V$

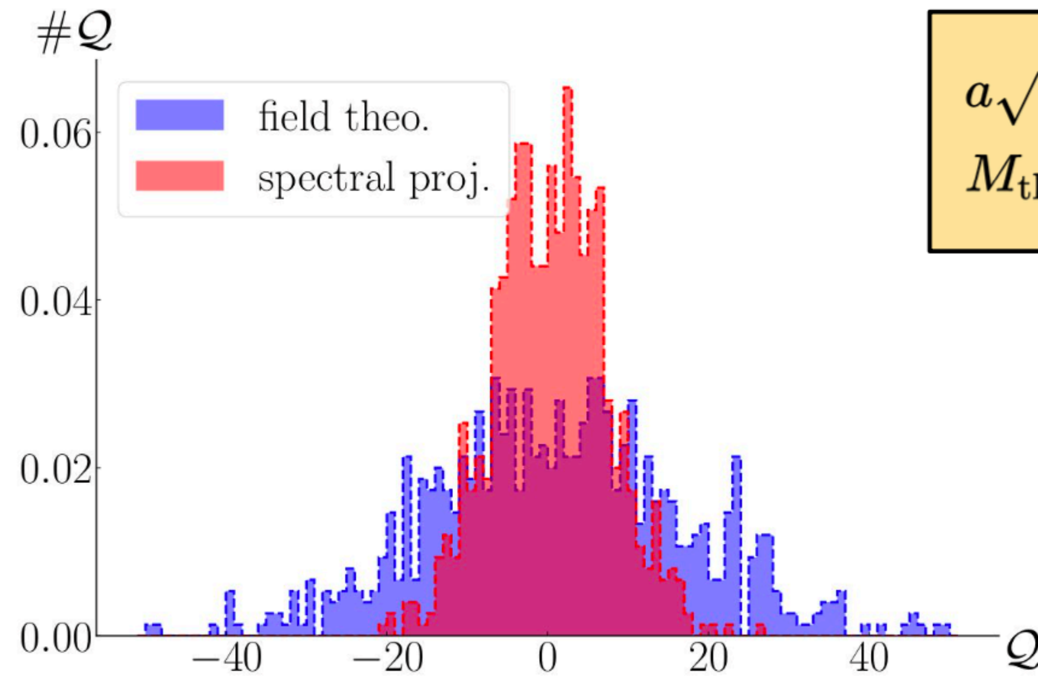


❋Topological susceptibility via spectral projectors shows milder cutoff effects as compared to the field theoretical definition

❋The choice oice of the threshold M_{thr} doesn't affect the continuum extrapolation

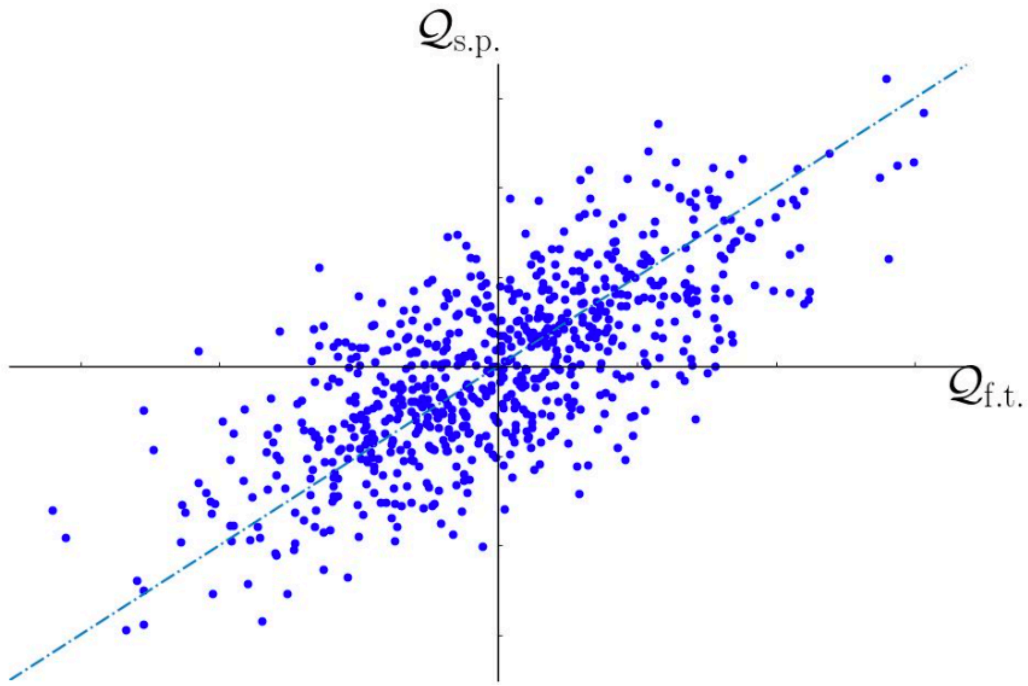
Comparison of two definitions of topological charge (II)





$a\sqrt{\tau_{\text{flow}}} = 0.15$ fm

$M_{\text{thr}} = 65$ MeV



	Field Theoretical	Spectral Projectors
$< Q >$	1.2(1.4)	0.46(54)
$< Q^2 >$	254(22)	49.1(4.6)
Pearson Correlation Coefficient		72(2) %

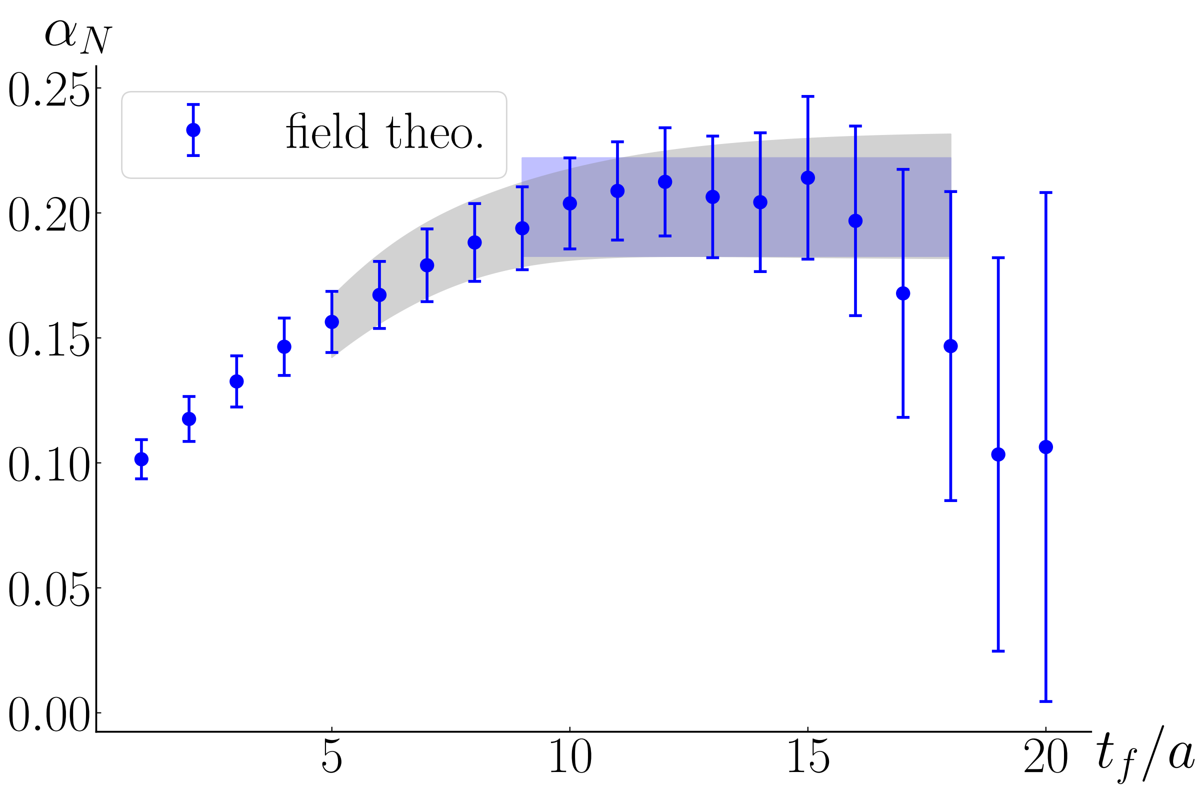
C.A., A. Athenodorou, K. Hadjiyiannakou and A. Todaro, Phys. Rev. D 103, 054501 (2021), arXiv: 2011.01084

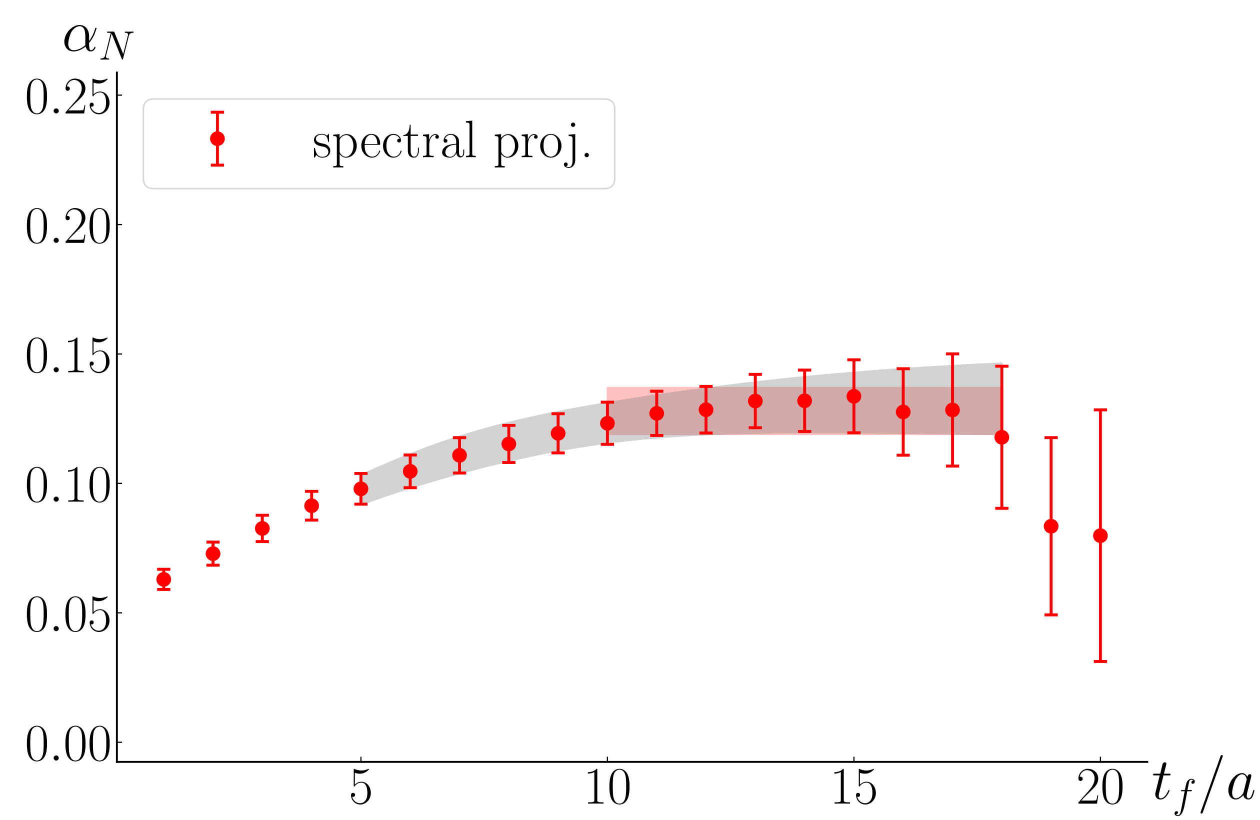
Determination of the mixing angle $\alpha^{(1)}$

Nf=2+1+1 twisted mass fermions with a clover term: B-ensemble

- Lattice size 64^3 x 128
- a=0.08 fm determined from the nucleon mass
- m_π=139 MeV
- Lm_π=3.6

$$\alpha^1 = \lim_{t_f \to \infty} \frac{C_{2\mathrm{pt},\mathcal{Q}}}{C_{2\mathrm{pt}}}$$

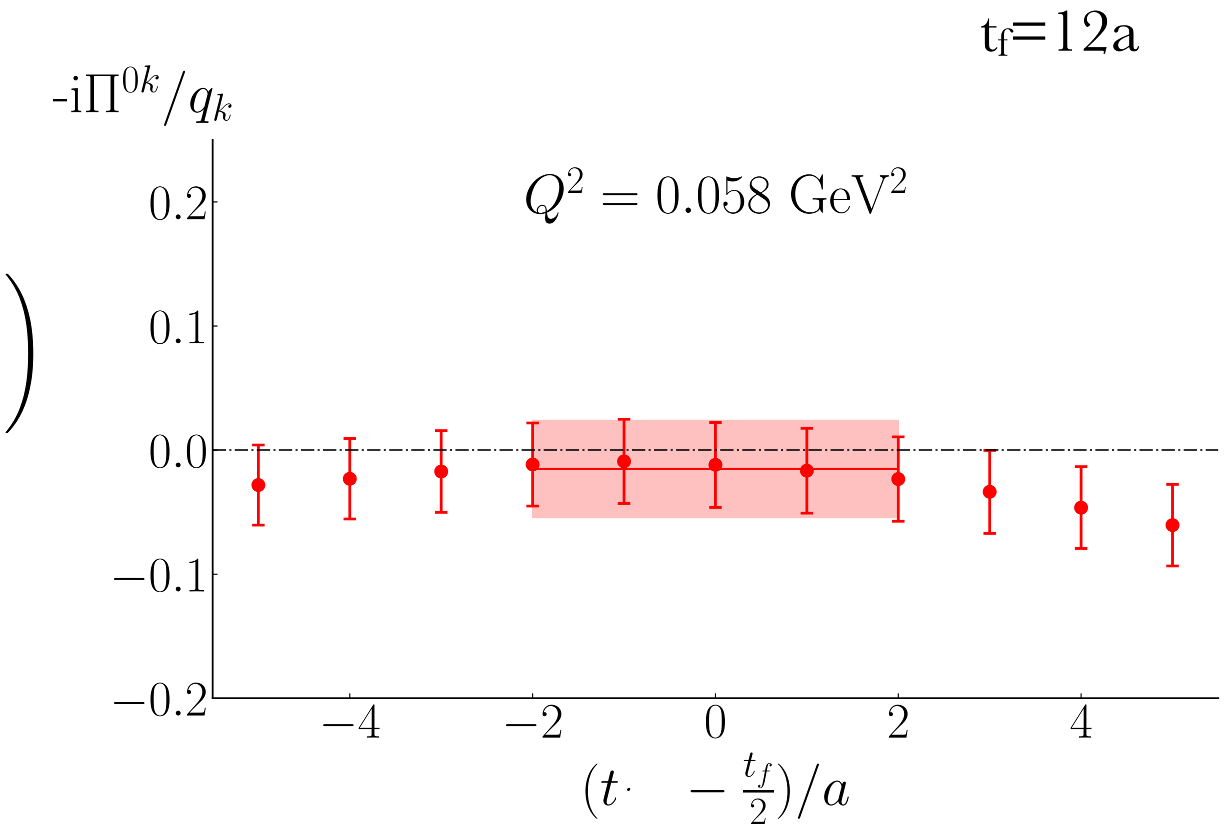




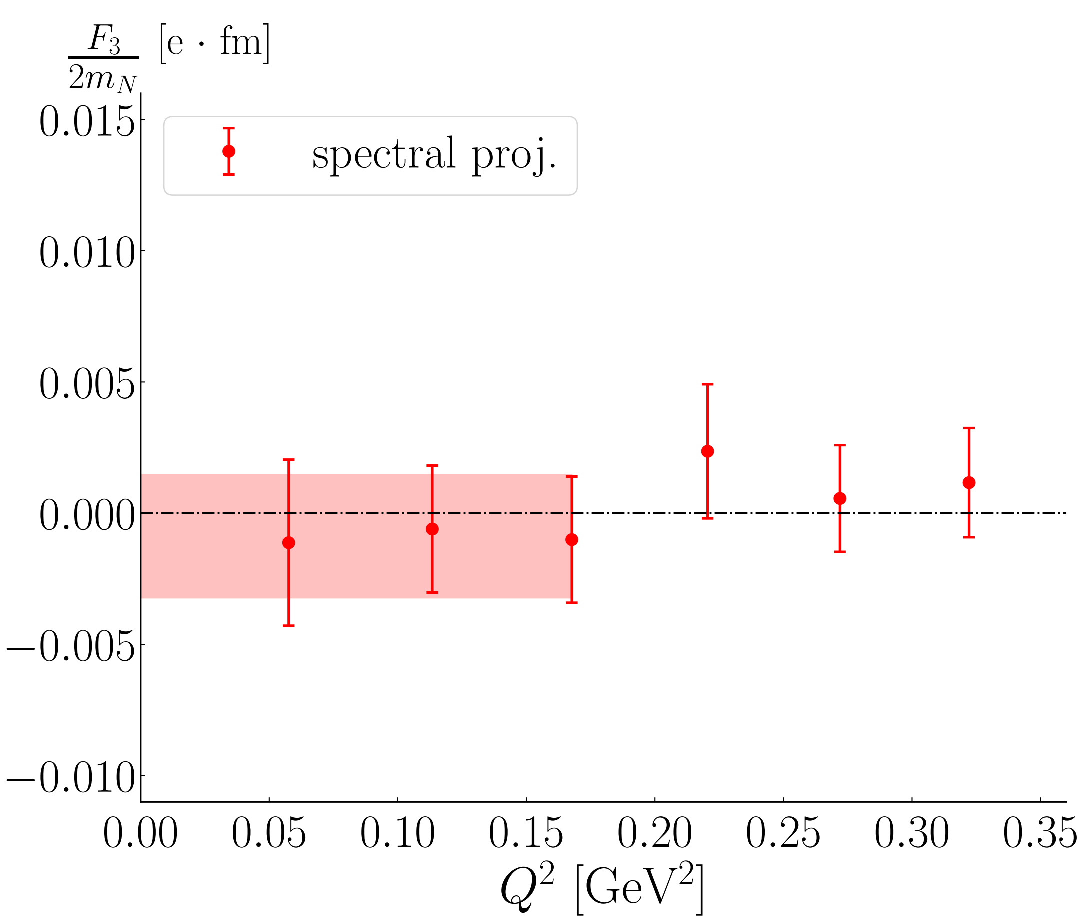
Determination of CP-odd F_3

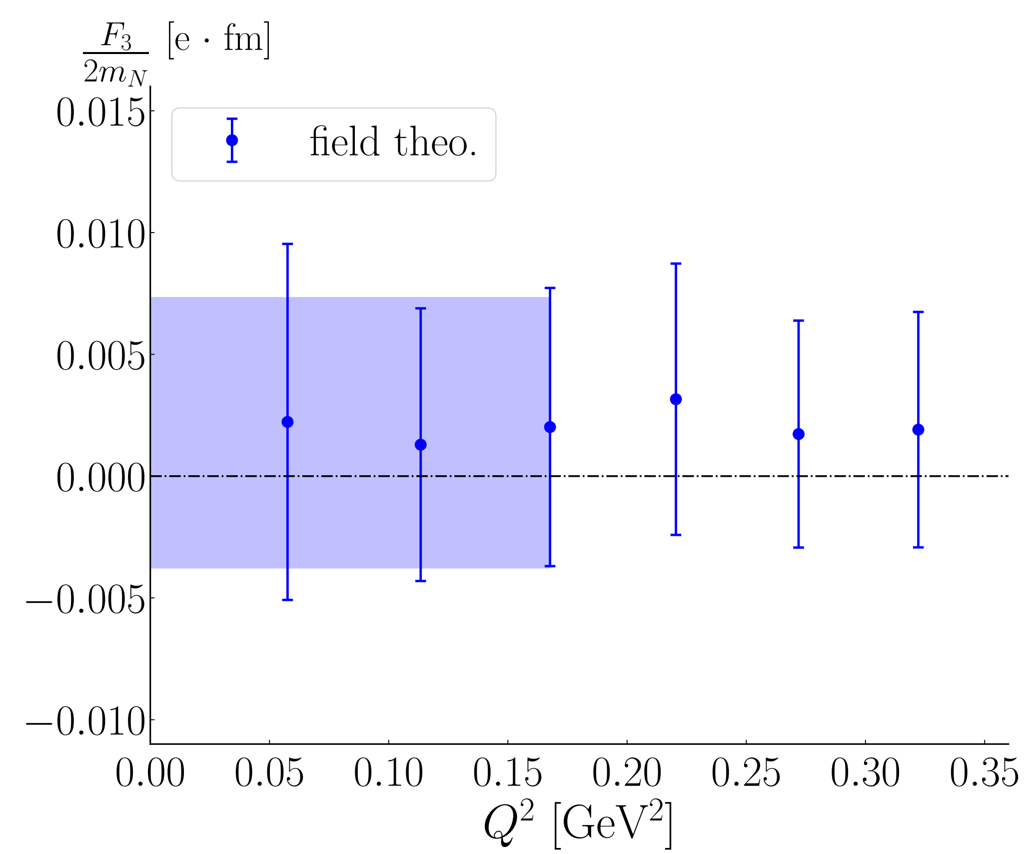
$$\Pi^{\mu k}_{3pt,\mathcal{Q}}(q) \equiv \lim_{t_f, t \to \infty} \frac{C_{3pt,\mathcal{Q}}}{C_{2pt,\mathcal{Q}}} R_{2pt}$$

$$\Pi^{0k}_{3pt,\mathcal{Q}}(q) = \frac{i q_k C}{2m_N} \left(a^{(1)} G_E(Q^2) - \frac{F_3^{(1)}(Q^2)}{2m_N}(E_N + m_N) \right)$$

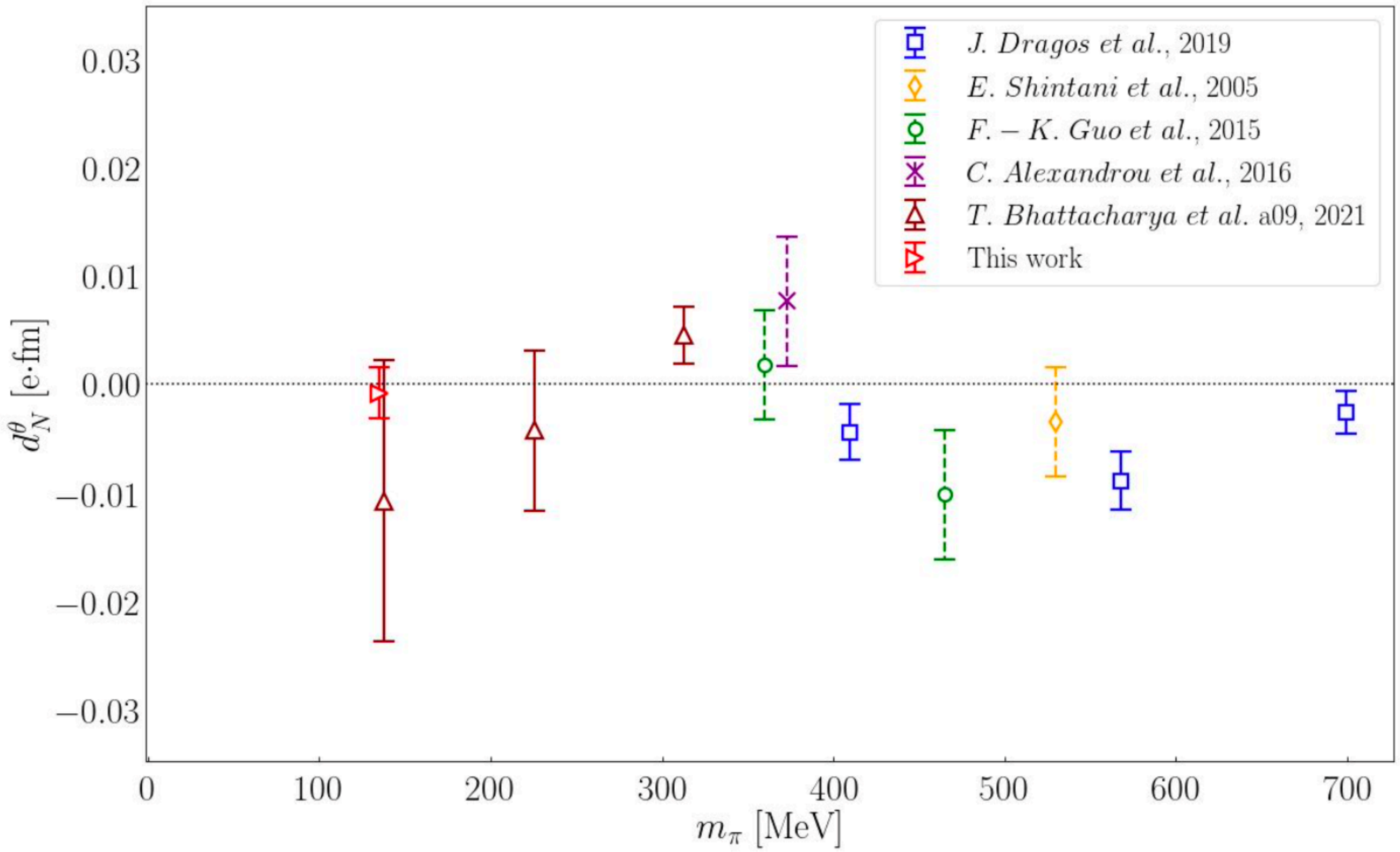


- Extract at finite momentum and take $Q^2 \to 0$





Results for nEDM



Chiral & continuum extrapolation

Paper	Neutron EDM
J.Dragos et al. (2019)	-0.00152(71)
T.Bhattacharya et al. (2021)	-0.003(7)(20)
T.Bhattacharya et al. (2021) with Nπ	-0.028(18)(54)
This work	-0.0009(24)

❋Results shown with dashed error bars are corrected by subtracting spurious contribution

Abramczyk et al., Phys. Rev. D 96, 014501 (2017)

Conclusions

- Using spectral projections improved signal by 2x
- Obtain lattice determination of nEDM directly at the physical pion mass to unprecedented accuracy

$$d_N^{\theta} = -0.0009(24)\theta \, e \, fm$$

- Ruling out a zero value would require at least 2-orders-of-magnitude increase in statistics
- Alternative approaches of extracting θ-nEDM highly desirable e.g. simulating ensembles at imaginary θ
- Exascale computing plus new ideas !!

Extended Twisted Mass Collaboration