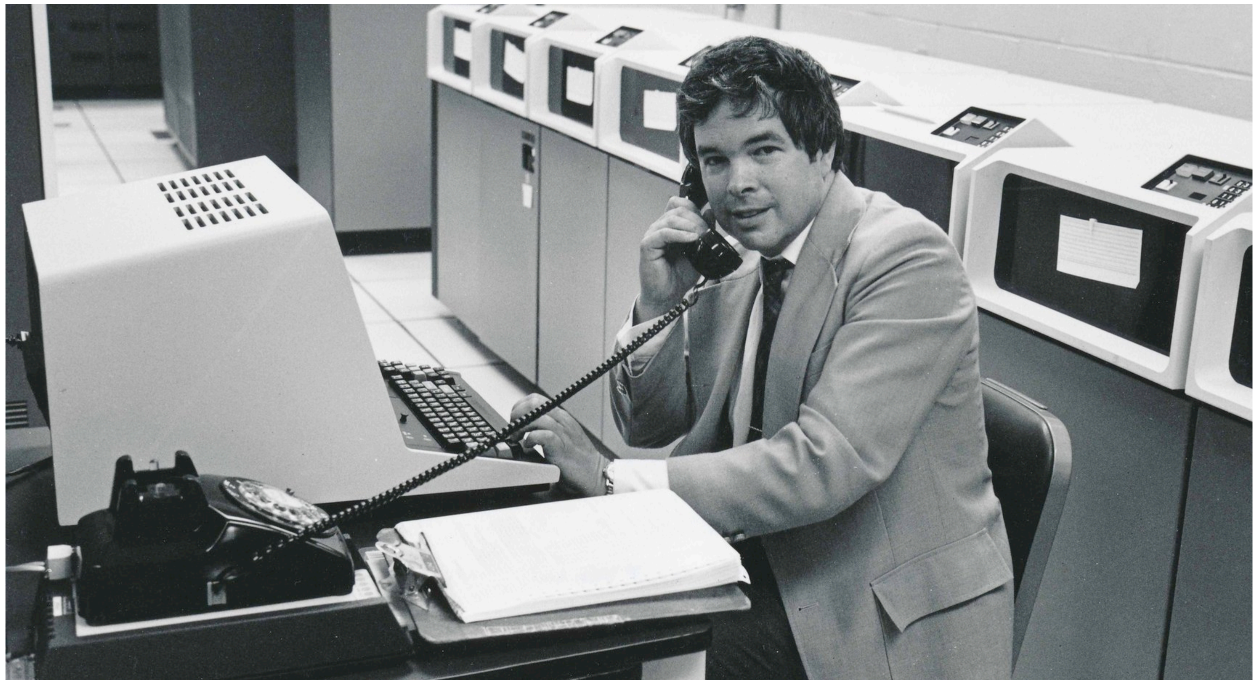
Quantum fluctuations of quarks and gluons in nuclei



2024 Ken Wilson Award acceptance

Michael Wagman

41th International Symposium on Lattice Field Theory
University of Liverpool - August 1, 2024

Fermilab

Thanks to all my collaborators, mentors, and friends

Special thanks to my colleagues

University of Washington: *Martin Savage (advisor),*
Silas Beane, Raúl Briceño, Mike Buchoff,
Zohreh Davoudi, Dorota Grabowska, Max Hansen,
David Kaplan, Steve Sharpe, Jesse Stryker

MIT: *Will Detmold, Phiala Shanahan,*
Anthony Grebe, Gurtej Kanwar, David Murphy,
Andrew Pochinsky, Yong Zhao

Fermilab: *George Fleming, Dan Hackett, Andreas Kronfeld,*
Will Jay, Hank Lamm, Jim Simone, Hersh Singh,
Ruth Van de Water, Judah Unmuth-Yockey

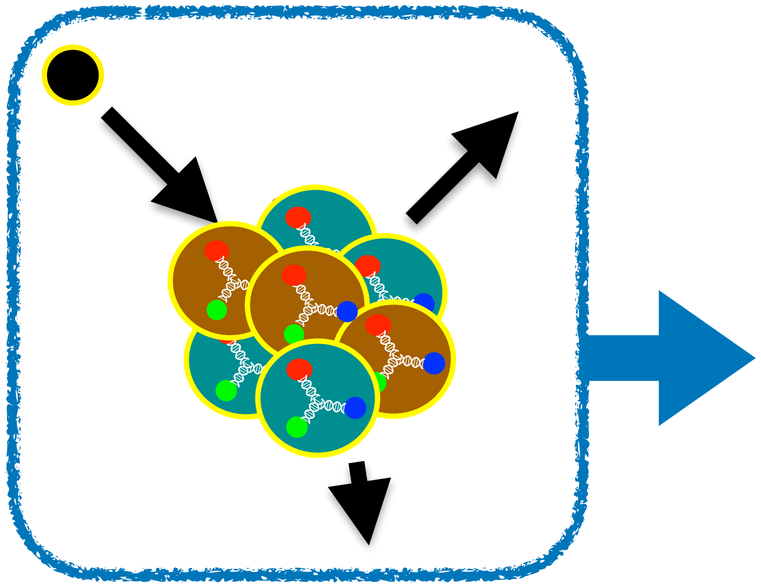
The NPLQCD Collaboration

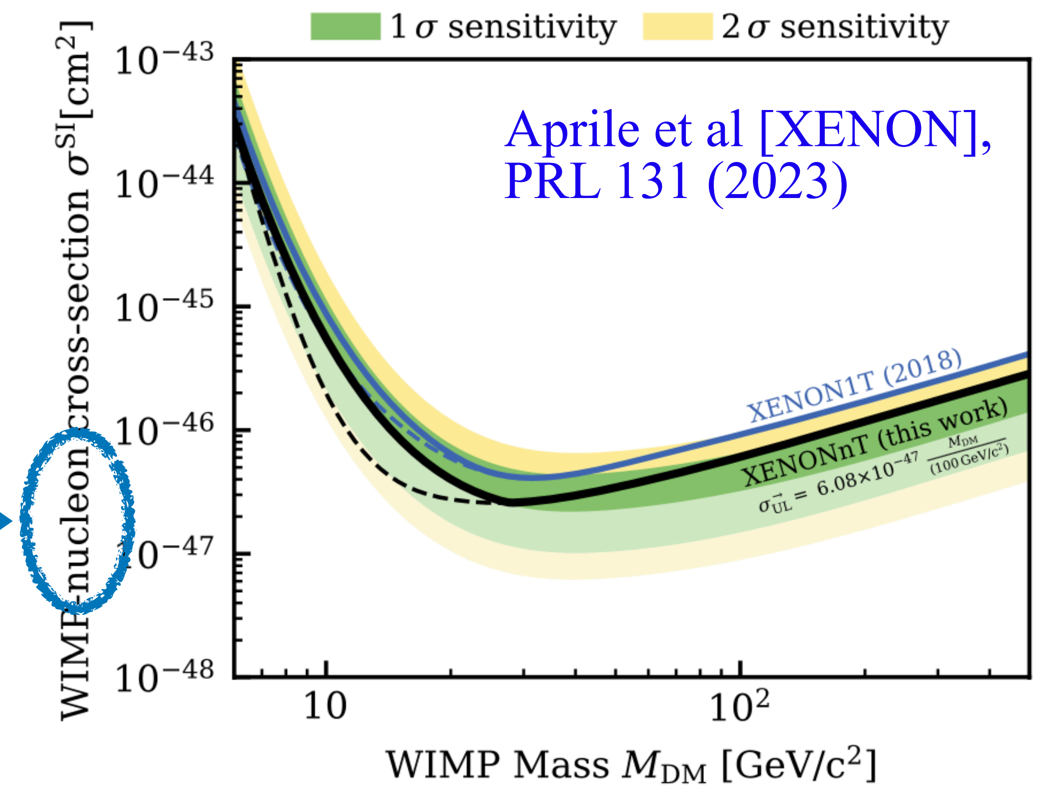
Physics is a team effort — I'm deeply grateful to have been a part of great teams

Nuclei and new physics

Nuclei are abundant and useful experimental targets

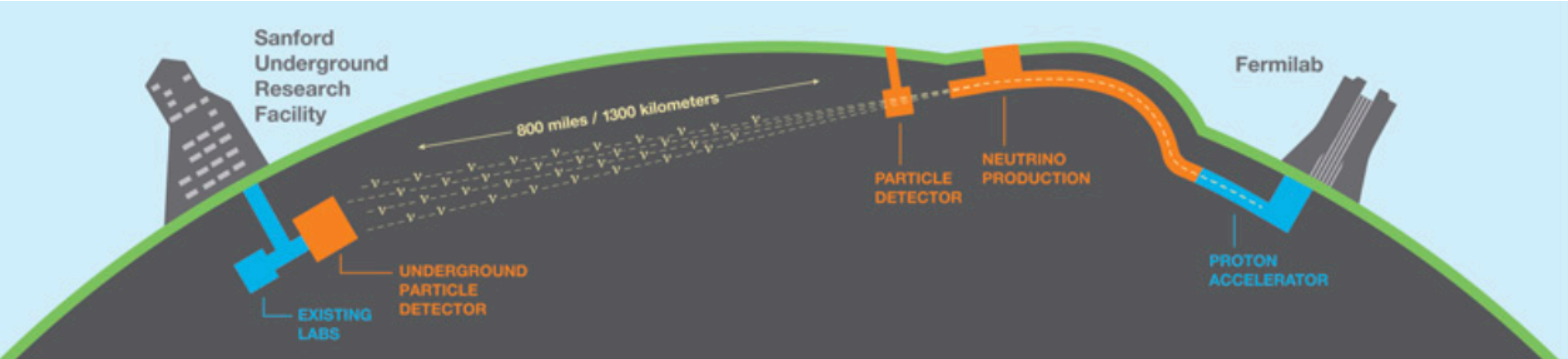
Relating new physics models to experimental data requires nuclear responses





- Dark matter direct detection (low-energy scalar)
- Neutrinoless double-beta decay (low-energy axial)
- Neutrino-nucleus scattering (low- and high-energy axial)

DUNE



High-energy scattering

High-energy cross sections factorize: *(perturbative coefficient) x (structure function)*

Deep inelastic scattering (DIS): $\sigma(Q^2) \sim \int dx\; H(Q^2, x, \mu)\, f_{q/A}(x, \mu)$

$$\ell + A \to \ell' + X$$

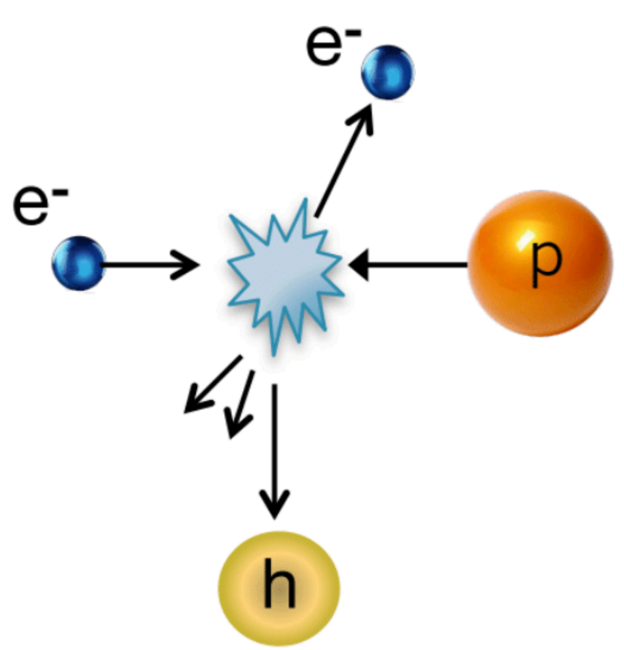
PDF ~ probability of parton q carrying momentum fraction x of hadron (or nucleus) A

Semi-inclusive DIS (SIDIS): $\sigma(Q^2, q_T) \sim \int dx\; H(Q^2, q_T, x, \mu)\, f^{\mathrm{TMD}}_{q/A}(q_T, x, \mu)\, D_{h/q}(q_T, x)$

$$\ell + A \to \ell' + h + X$$

Transverse Momentum Dependent PDF

Fragmentation function



TMDPDFs of nuclei needed for

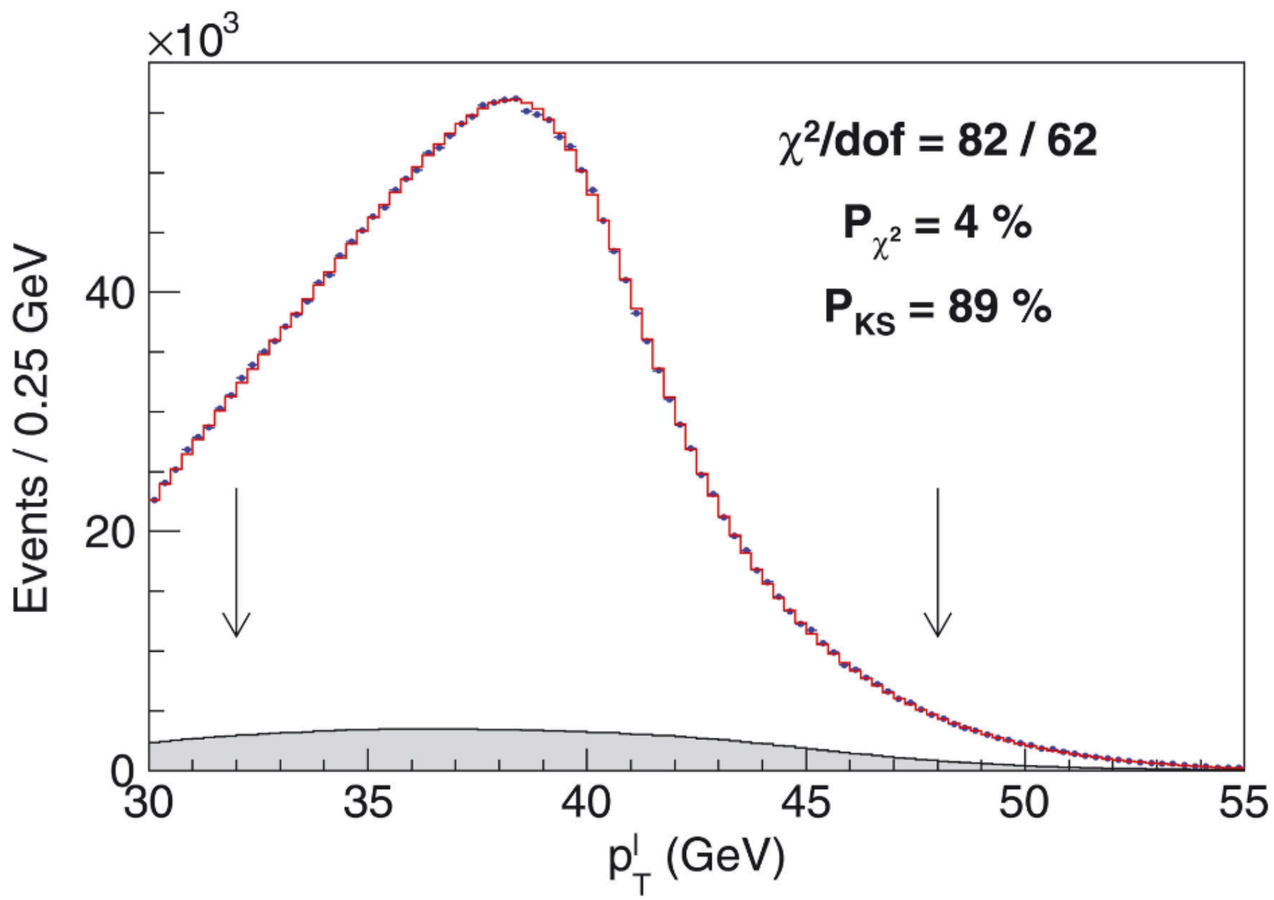
- Analyzing pion production at DUNE (CC1pi)
- Improving our understanding of QCD at the EIC

The W boson mass

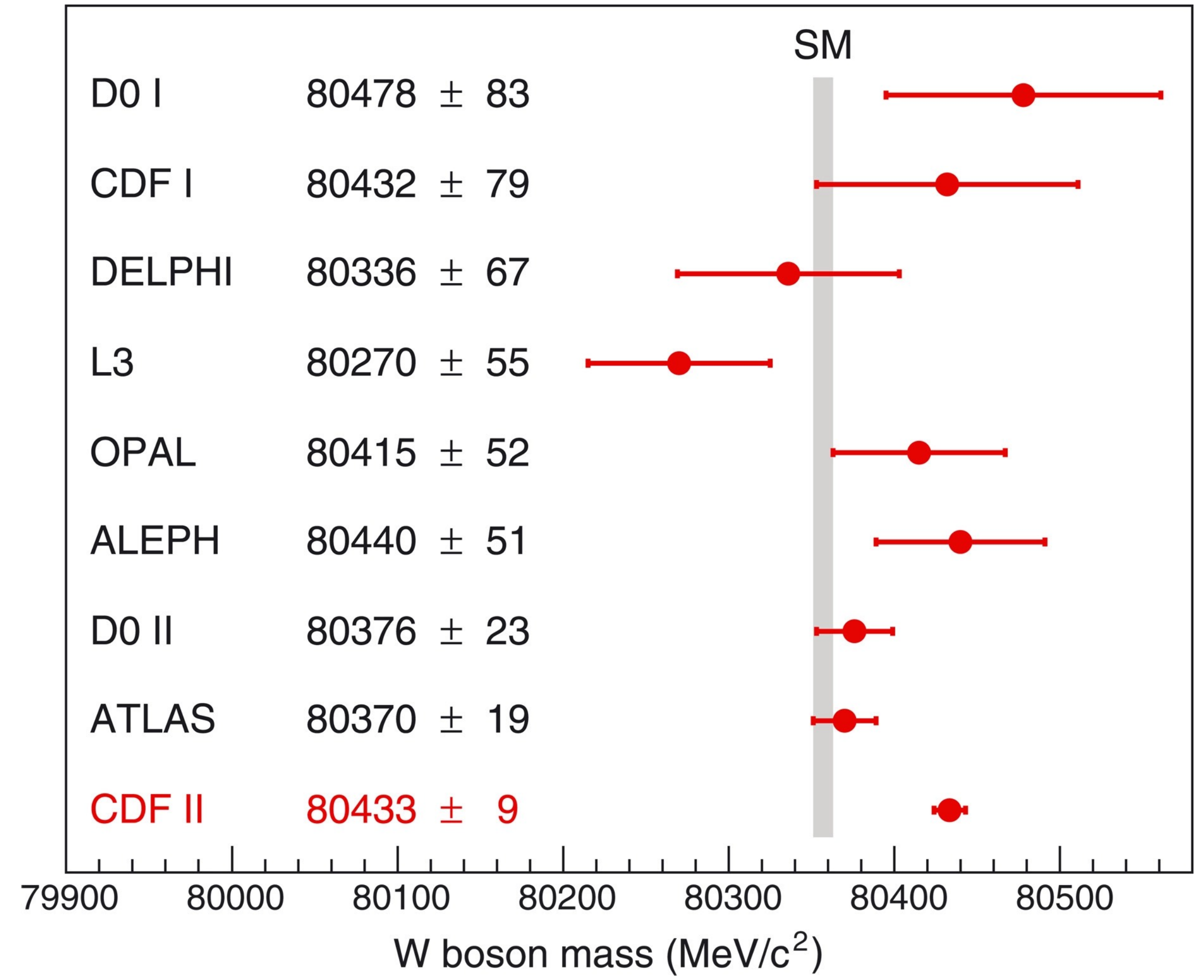
Precise measurement of M_W from CDF disagrees at 7 sigma with M_W obtained from electroweak precision fits

New physics?

Robust understanding of all QCD theory uncertainties essential



Aaltonen et al [CDF], Science 376 (2022)



Measurement made by fitting shapes of transverse momentum distributions to theory predictions including resumed and nonperturbative QCD effects

Distribution shapes are insensitive to many aspects of TMDPDFs but sensitive to flavor dependence and **"rapidity evolution"**

The Collins-Soper kernel

TMDPDFs depend on UV renormalization scale μ as well as a scale $\zeta \sim Q^2$ associated with the renormalization of rapidity divergences

$$f_{q/A}^{\mathrm{TMD}}(x, \vec{b}_T, \mu, \zeta) = f_{q/A}^{\mathrm{TMD}}(x, \vec{b}_T, \mu_0, \zeta_0)$$

$$\times \exp\left[\int_{\mu_0}^{\mu} \frac{d\mu'}{\mu'} \gamma_\mu^q(\mu', \zeta_0)\right] \exp\left[\frac{1}{2}\gamma_\zeta^q(\mu, b_T) \ln \frac{\zeta}{\zeta_0}\right]$$

UV anomalous dimension

Collins-Soper kernel

(rapidity anomalous dimension)

- Changing hard momentum scales requires evolving TMDPDFs in μ and ζ
- Evolution in μ is perturbative as long as μ is large, but evolution in ζ is always nonperturbative for $b_T \gtrsim \Lambda_{\mathrm{QCD}}^{-1}$
- Both anomalous dimensions are **independent of the hadron target**

CS kernel phenomenology

Fits to SIDIS and Drell-Yan data with multiple energy scales are sensitive to evolution effects and therefore the CS kernel

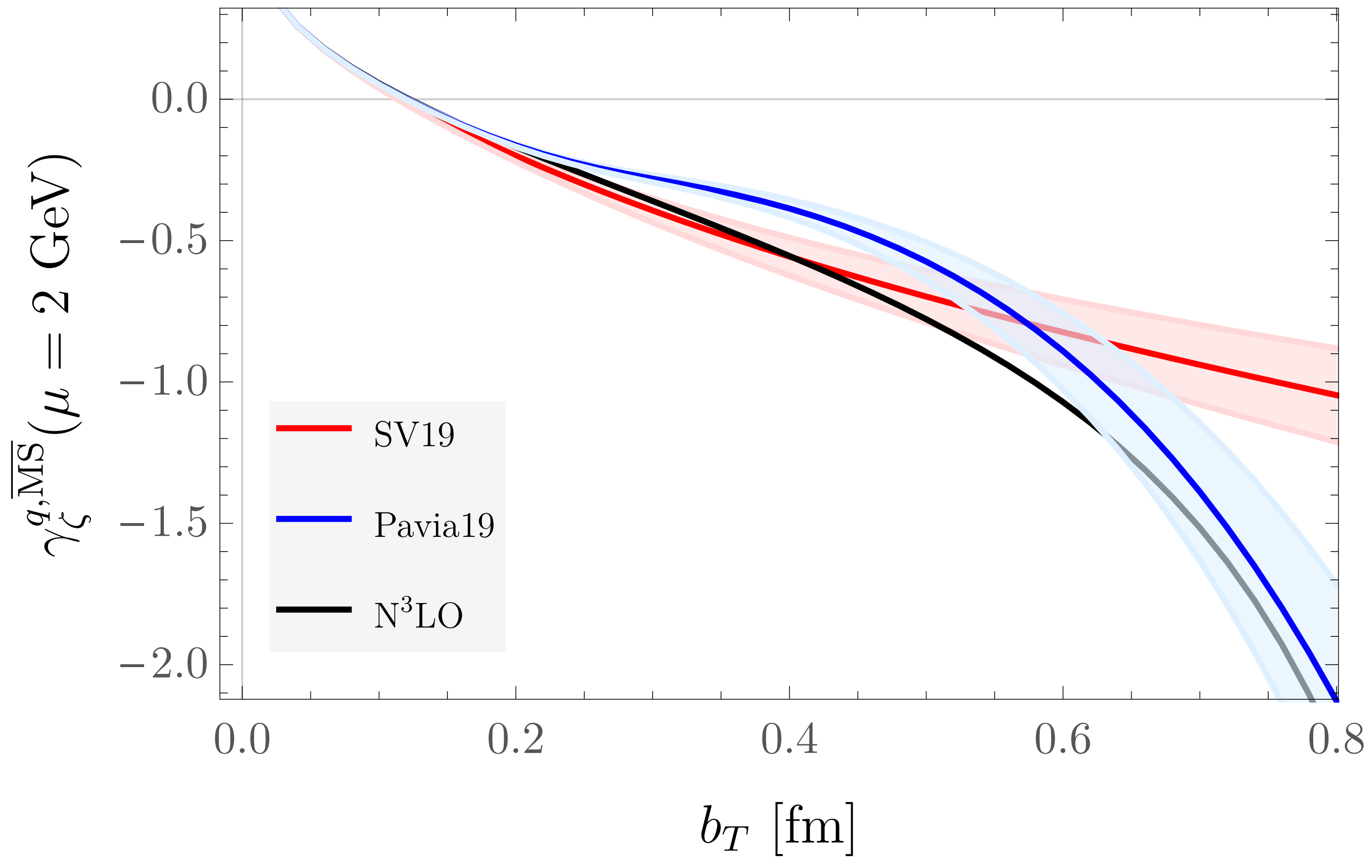
CS kernel can be extracted along with TMDPDF in global fits

SV19 - Scimemi and Vladimirov, JEHP 06 (2020)

(582 SIDIS + 457 DY data points)

Pavia19 - Bacchetta et al, JEHP 07 (2020)

(353 DY data points)



Modeling significant for

$$b_T \gtrsim 0.2\ \mathrm{fm}$$

(nonperturbative region)

Can we constrain the large b_T behavior of the CS kernel using lattice QCD?

My CS kernel collaborators

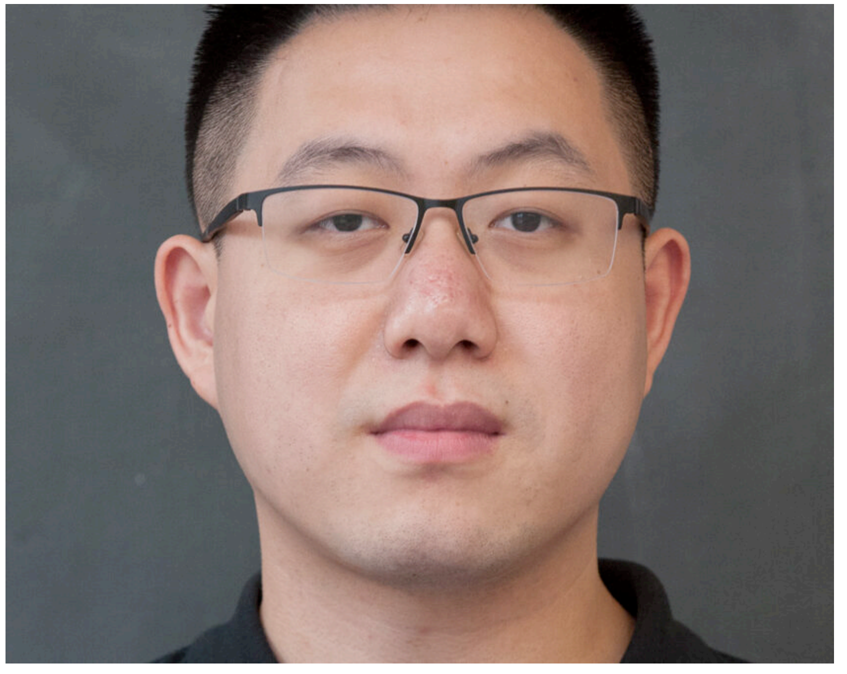
Phiala Shanahan

Yong Zhao

Shanahan, MW, Zhao: PRD 101 (2020), PRD 102 (2020), PRD 104 (2021)

Artur Avkhadiev

Yang Fu



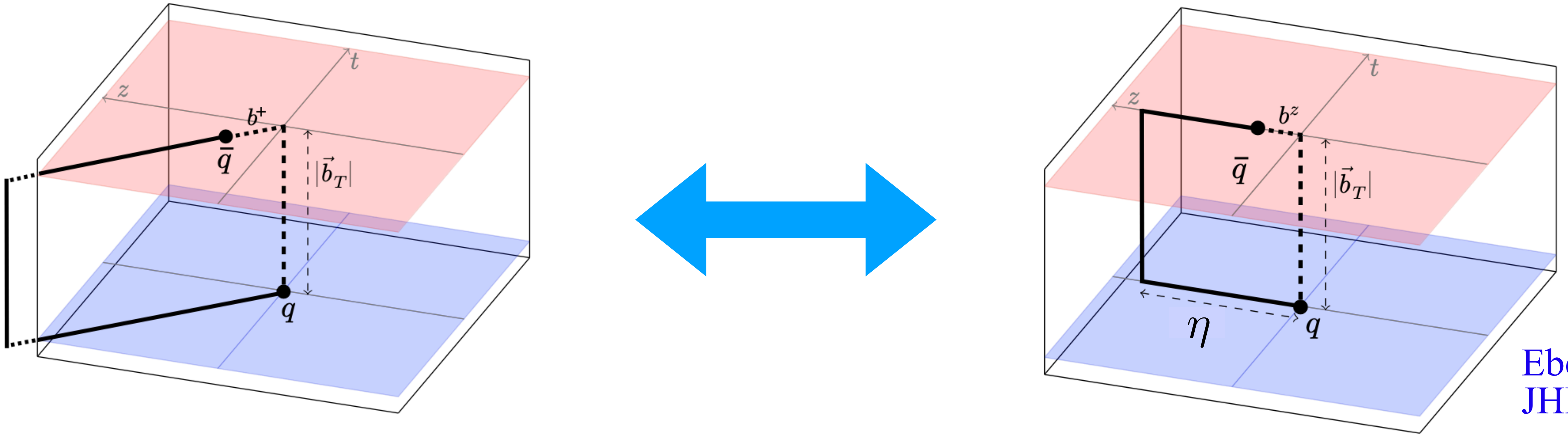
Avkhadiev, Shanahan, MW, Zhao: PRD 108 (2023), PRL 132 (2024)

Onward to gluons! See Yang's talk 3:05 Wed

The CS kernel from LQCD

Large momentum effective theory (LaMET) connects light-cone PDFs to Euclidean matrix elements that can be calculated using lattice QCD

Review: Ji et al, Rev. Mod. Phys. 93, 35005 (2021)



Ebert, Stewart, Zhao, JHEP 1909 (2019)

Quasi TMDPDFs are more complicated (soft factor), but quasi TMDPDF ratios are simply related to light-cone TMDPDF ratios

Musch et al, PRD 85 (2012)   Engelhardt et al, PRD 93 (2016)

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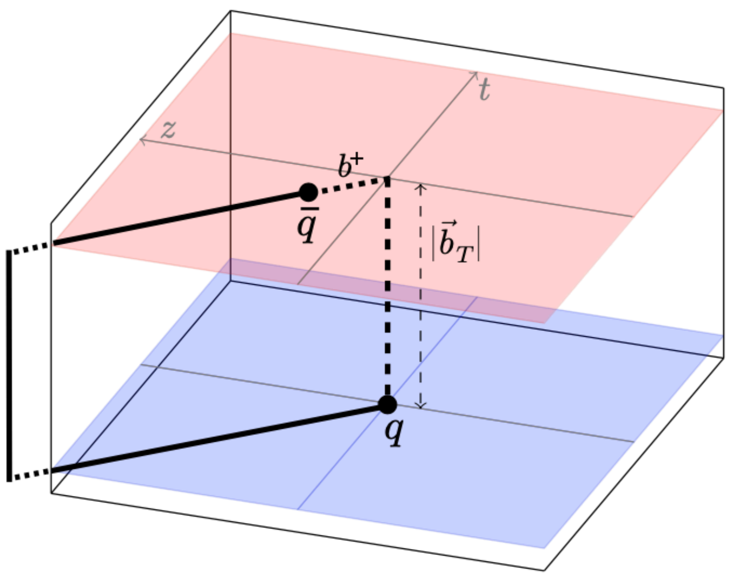

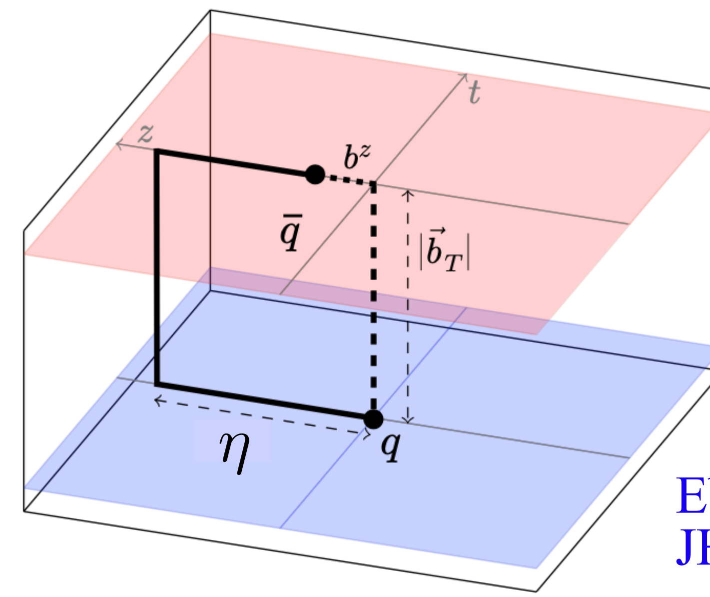

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Musch et al, PRD 85 (2012)   Engelhardt et al, PRD 93 (2016)

CS kernel related to quasi TMDPDF ratios

Euclidean quasi-beam function ratio

$$\gamma_\zeta^{q,\overline{\mathrm{MS}}}(b_T,\mu) = \frac{1}{\ln(P_1^z/P_2^z)} \ln \frac{C_{\mathrm{TMD}}^{\overline{\mathrm{MS}}}(\mu, xP_2^z) \int db^z e^{ib^z xP_1^z} \tilde{B}_{q/A}^{\overline{\mathrm{MS}}}(b^z, b_T, \eta, \mu, P_1^z)}{C_{\mathrm{TMD}}^{\overline{\mathrm{MS}}}(\mu, xP_1^z) \int db^z e^{ib^z xP_2^z} \tilde{B}_{q/A}^{\overline{\mathrm{MS}}}(b^z, b_T, \eta, \mu, P_2^z)}$$

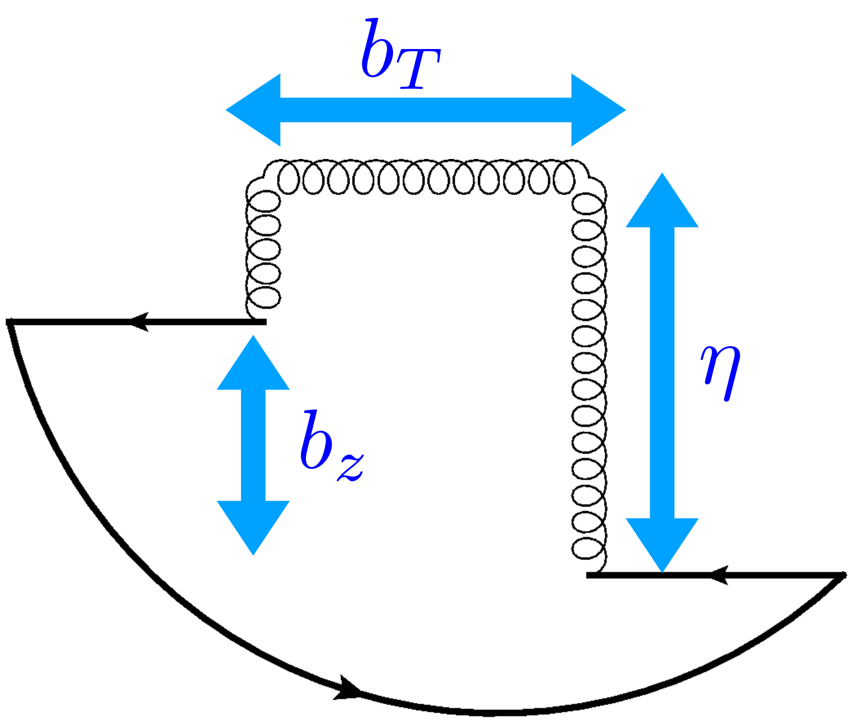
Perturbative matching factor known at NNLO

Ebert, Stewart, Zhao, PRD 99 (2019)

First LQCD exploration

CS kernel is a property of QCD vacuum, independent of hadronic state

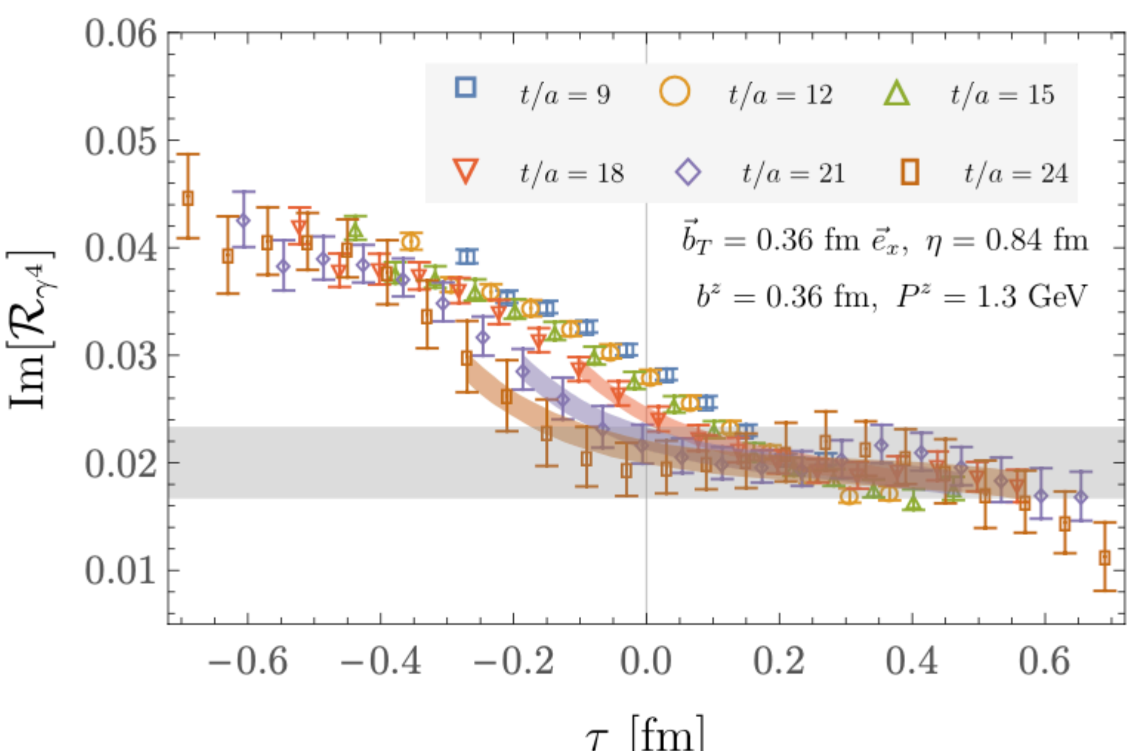
We can learn about nuclear structure using pion states!



In quenched ($N_f = 0$) QCD, exact results calculable using heavy quark probe

$$m_\pi \sim 1.2 \text{ GeV}$$

Allows high precision with only 400 quark propagator sources



Shanahan, MW, Zhao, PRD 102 (2020)

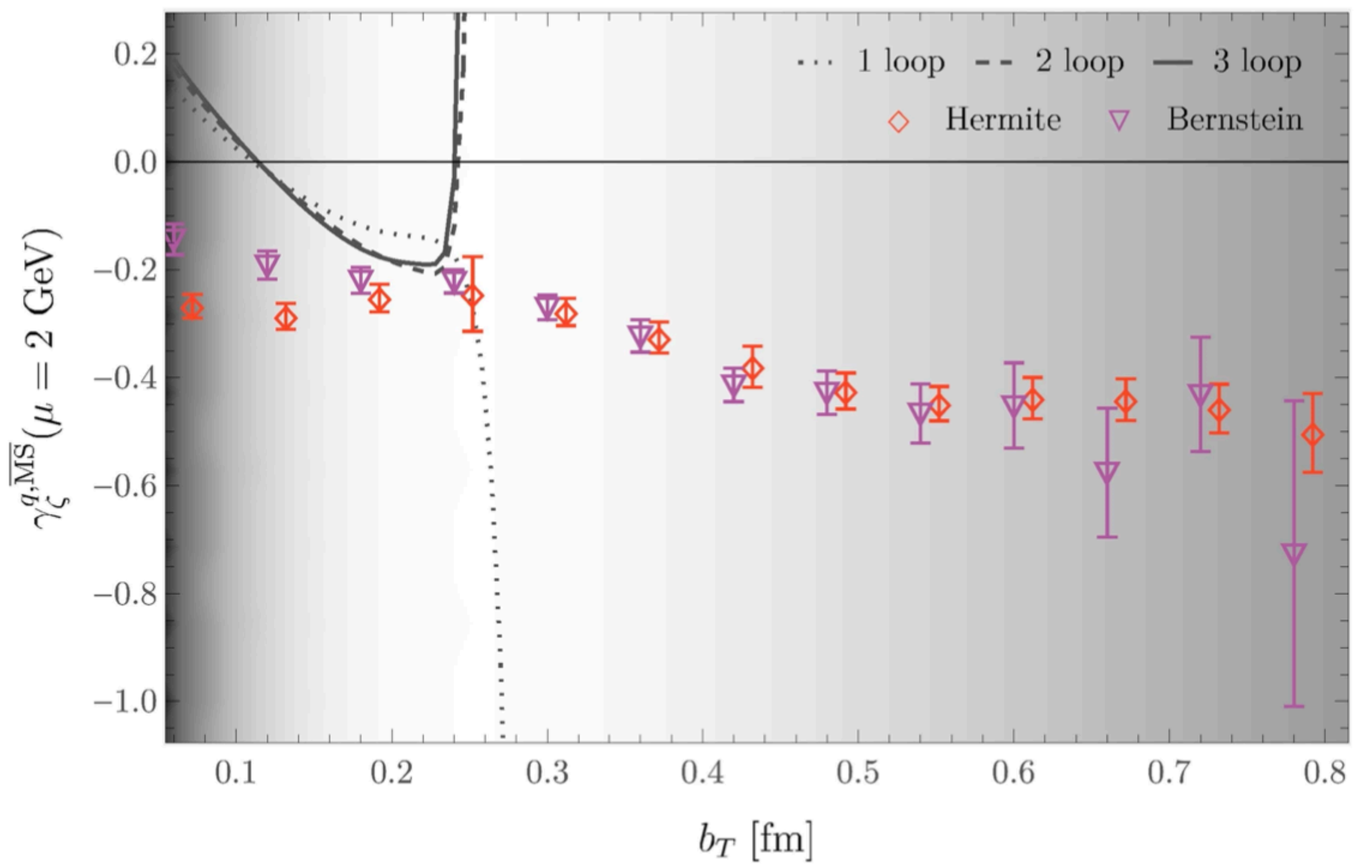
3 values of $\eta \in [0.6,\ 0.8]$ fm

3 values of $P^z \in [1.3,\ 2.6]$ GeV

All 16 Dirac structures and staple geometries b_T and b^z

35,660 bare matrix elements - robust automated fitting essential

Quenched LQCD results



Shanahan, MW, Zhao, PRD 102 (2020)

$m_\pi = 1.2$ GeV

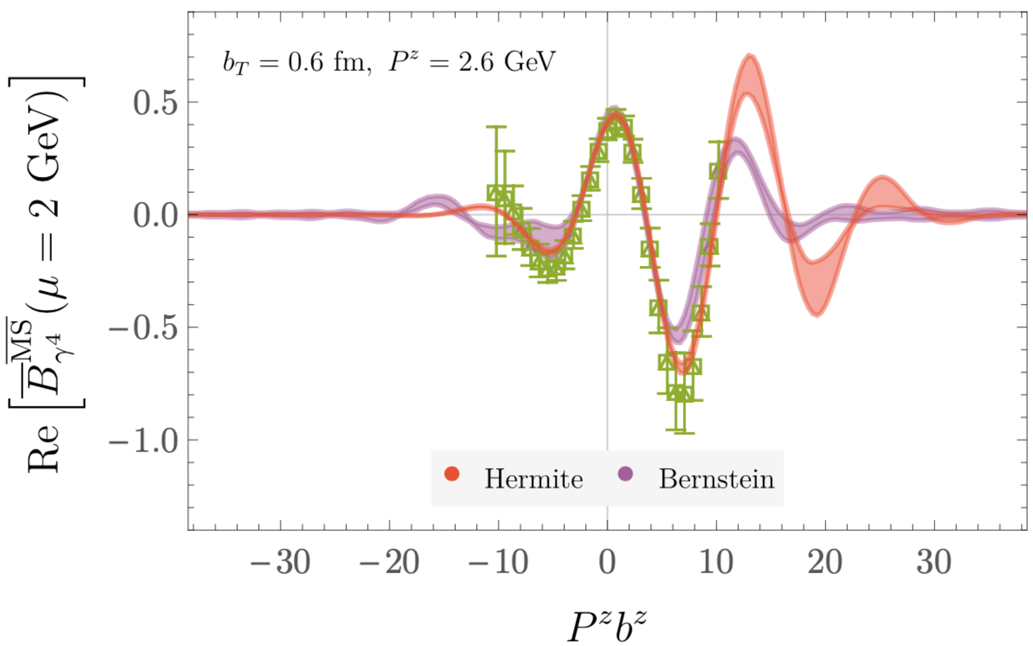
$L = 32a = 1.92$ fm

$P^z \in \{1.3,\ 1.9,\ 2.6\}$ GeV

$\eta \leq 0.8$ fm

CS kernel determined precisely for b_T extending into nonperturbative regime

Fourier transform truncation effects challenging to quantify, two different models used to extrapolate beam functions outside range of data



Dynamical LQCD exploration

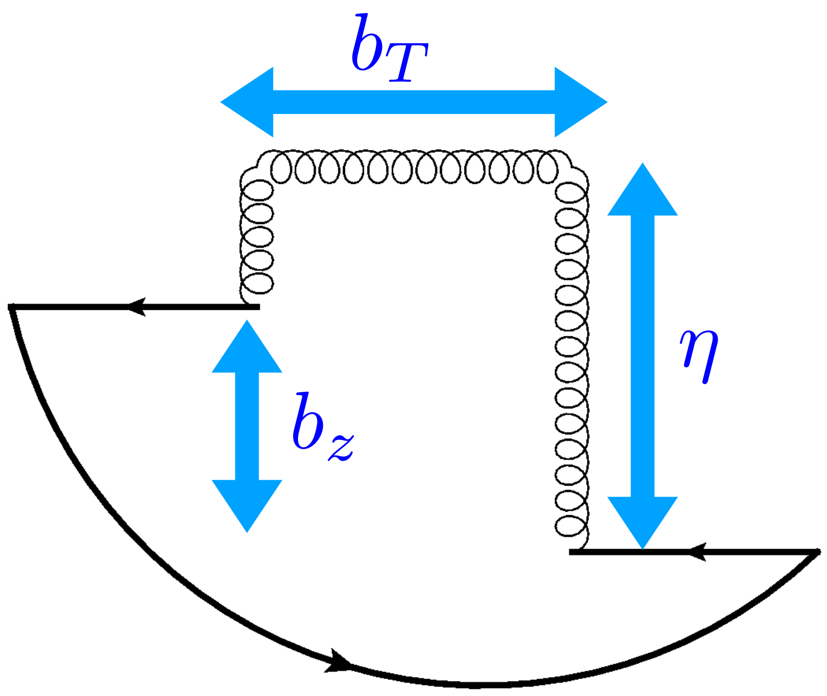
Mixed action: $N_f = 2 + 1 + 1$ MILC ensembles with ~physical quark masses

$a = 0.12\ \mathrm{fm} \qquad L = 48a = 5.6\ \mathrm{fm}$ Bazavov et al [MILC] PRD 87 (2013)

- Wilson valence quarks with tree-level clover improvement, $m_\pi = 538(1)\ \mathrm{MeV}$

- Wilson flow (fixed in lattice units) used as smearing in valence action to reduce statistical noise

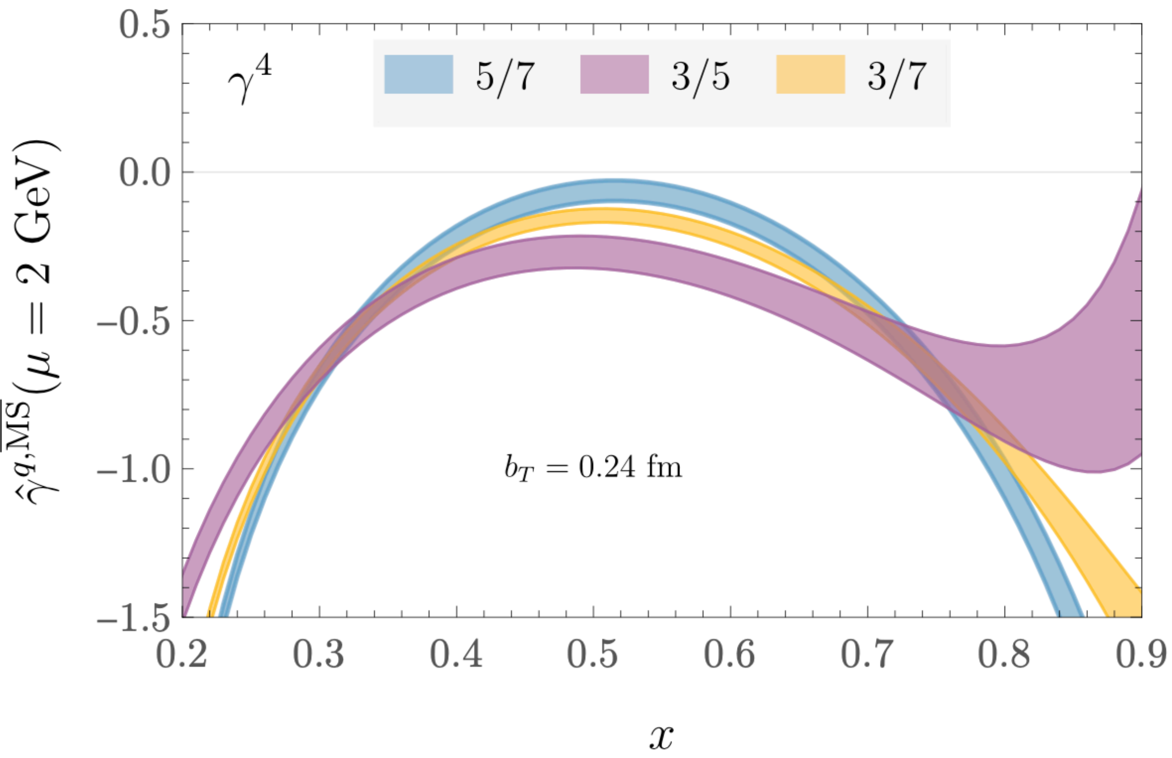
- Larger physical volume enable larger staple extents than in quenched calculation $\eta \leq 1.7\ \mathrm{fm}$



$(b^z P^z)_{\mathrm{max}} = 14.5$ vs quenched $(b^z P^z)_{\mathrm{max}} = 11$

Shanahan, MW, Zhao, PRD 104 (2021)

CS kernel systematics

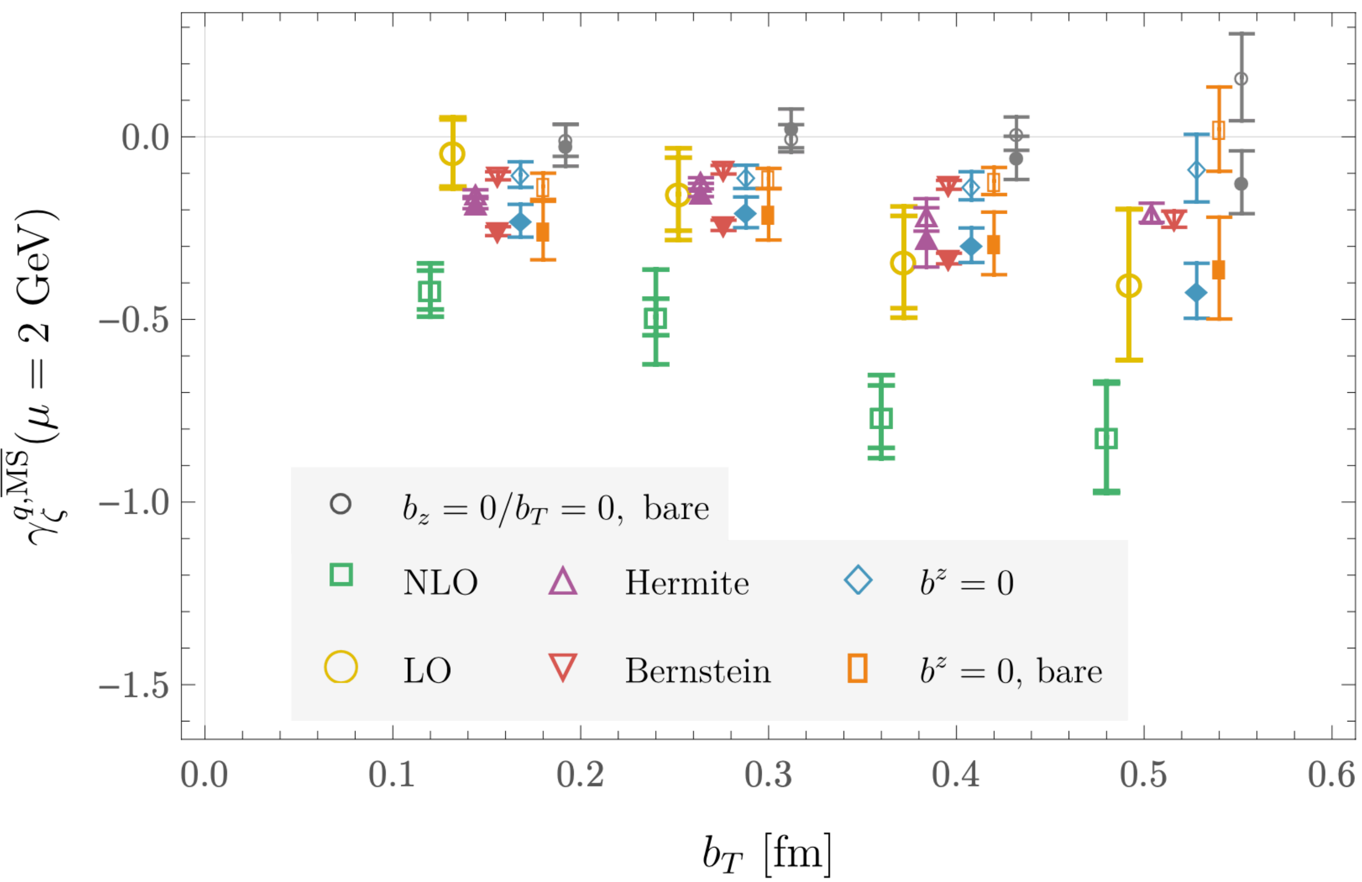


Still significant Fourier transform systematics

- x-dependence of CS kernel not successfully cancelled
- Differences between estimates with different momentum pairs visible

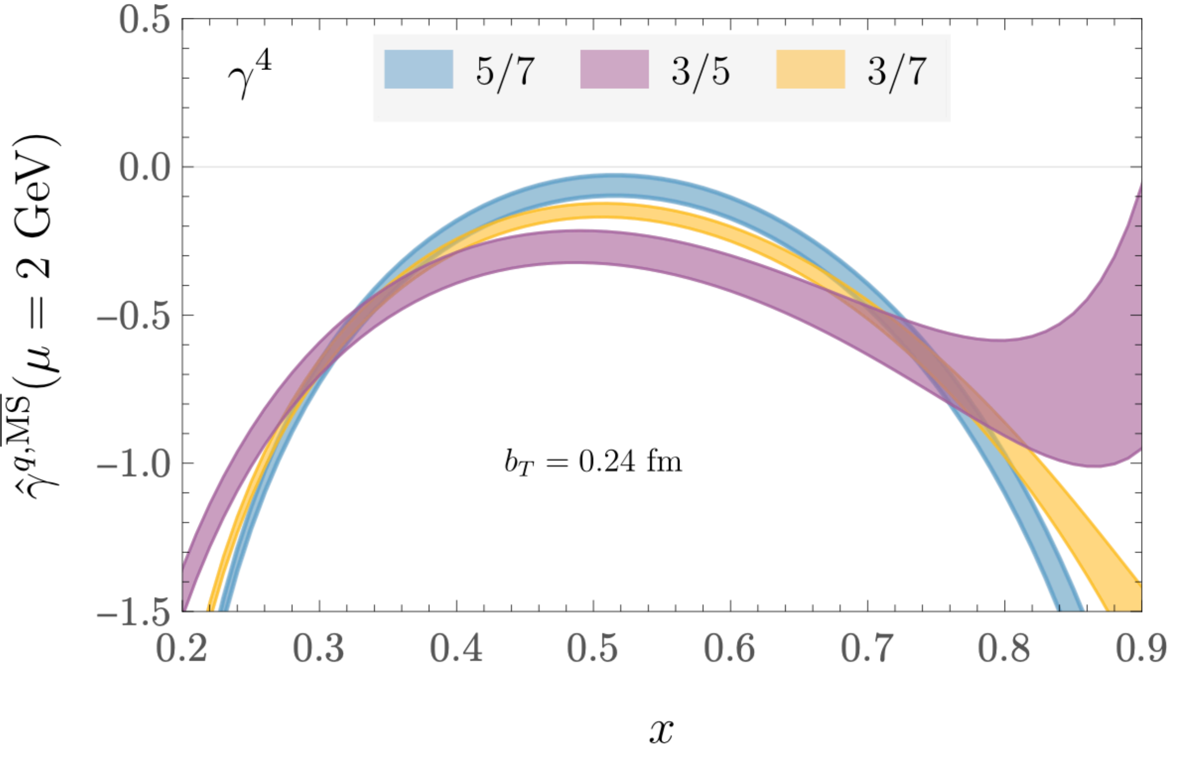
NLO quasi/light-cone matching effects significant

- Approximations valid only at LO used in previous calculations insufficient



Shanahan, MW, Zhao, PRD 104 (2021)

CS kernel systematics



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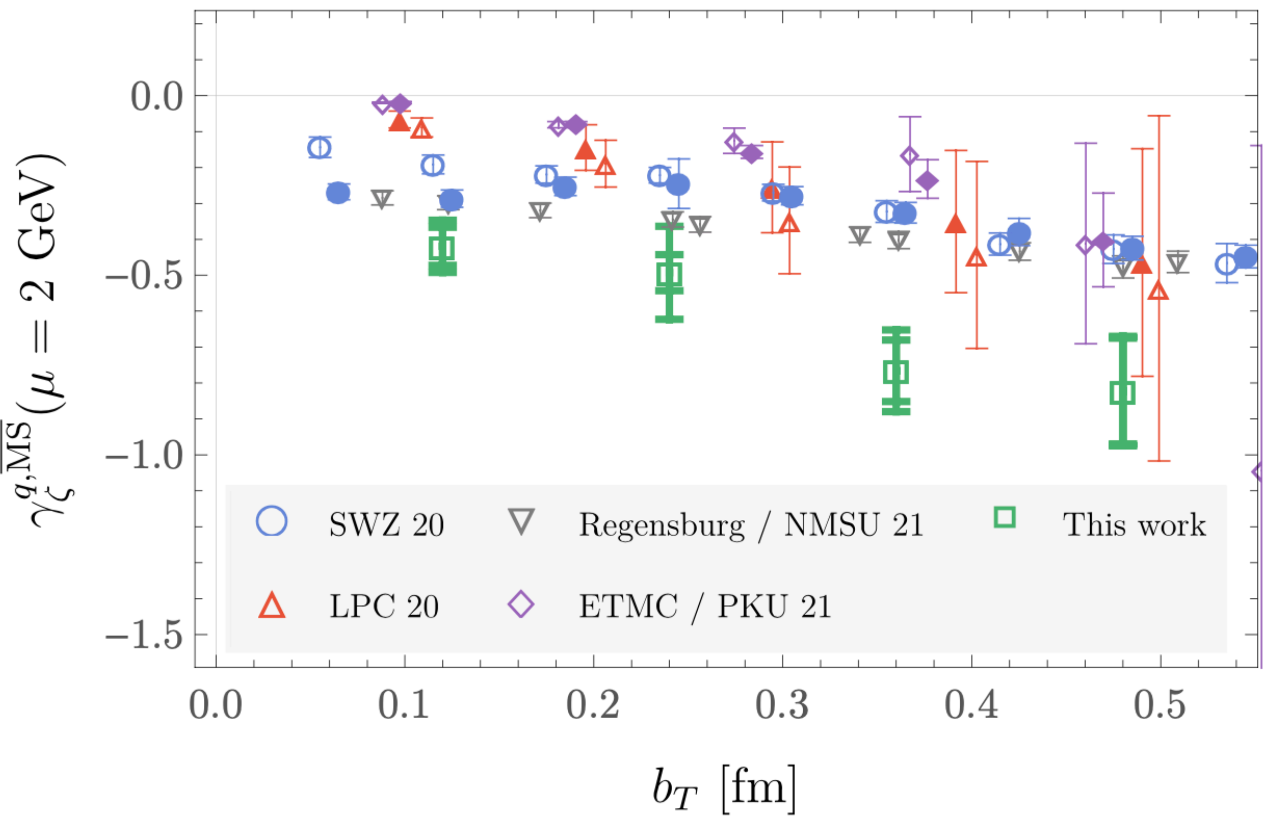


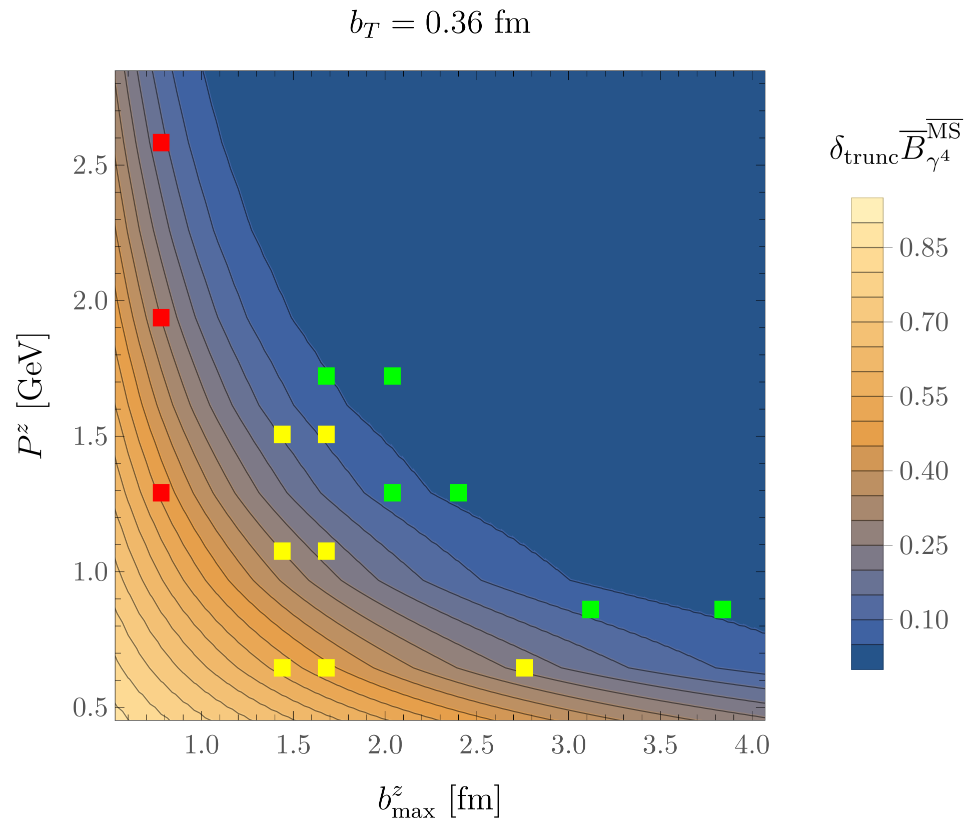
Shanahan, MW, Zhao, PRD 104 (2021)

Improved calculations

TMD wavefunctions reduce computational costs (requires 2pt instead of 3pt functions)

Chu et al [LPC], PRD 106 (2022)

- Larger boosts and staple extents reduce Fourier transform truncation effects



- Nearly physical quark masses

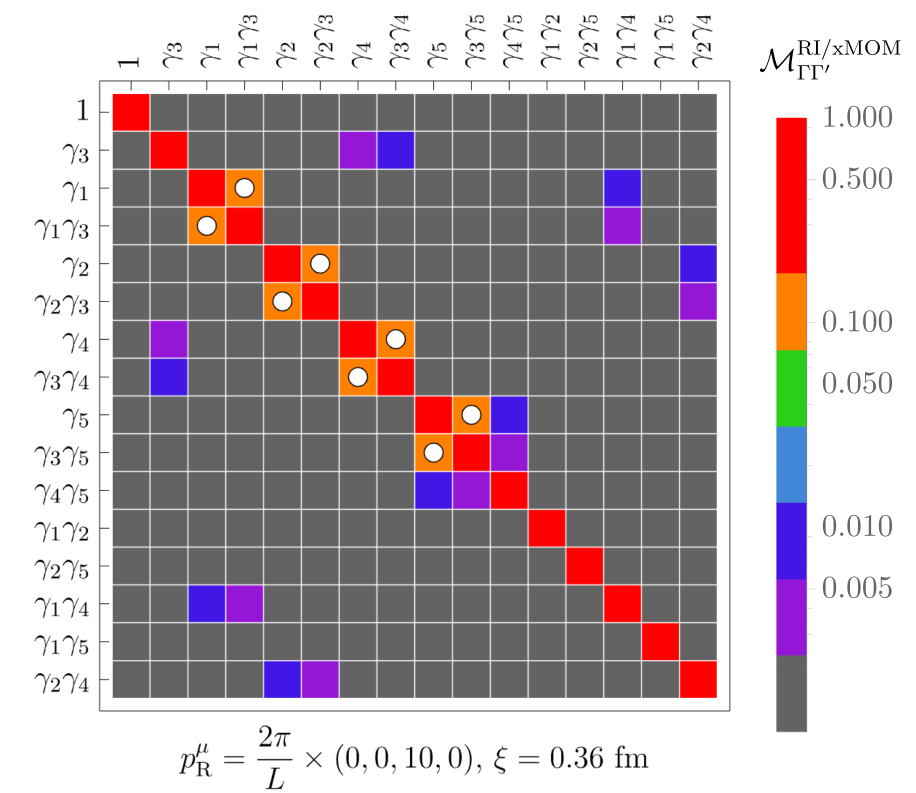
- Continuum limit from 3 MILC ensembles with different lattice spacings

- RI-xMOM scheme turns nonlocal operators into local operator products using auxiliary static quark fields

Ji, Zhang, and Zhao, PRL 120 (2018)

Green, Jansen, and Steffens, PRL 121 (2018)

Green, Jansen, and Steffens, PRD 101 (2020)

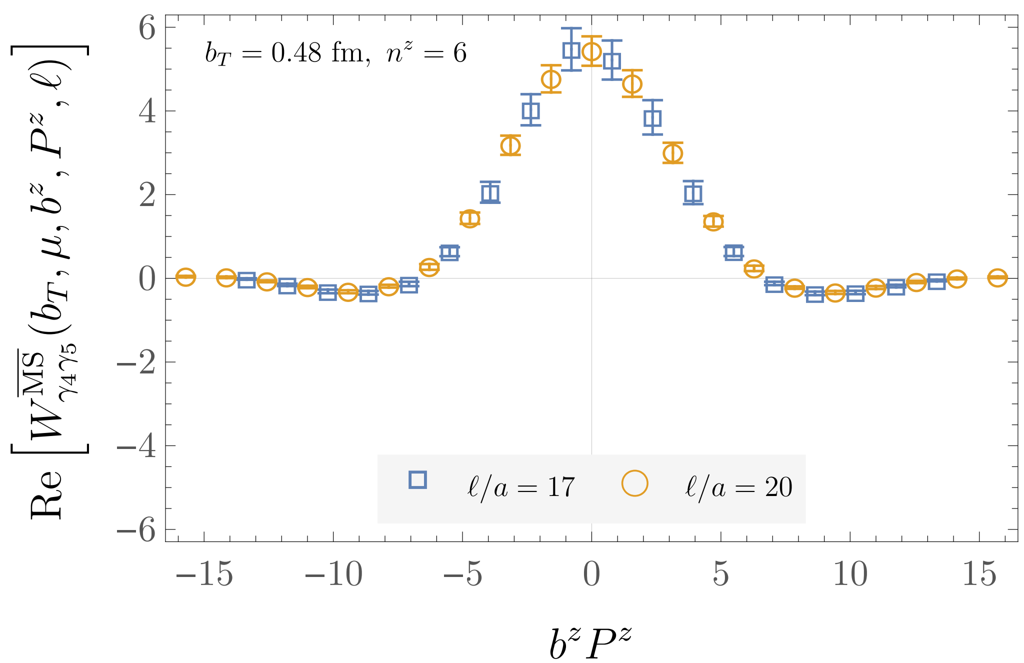


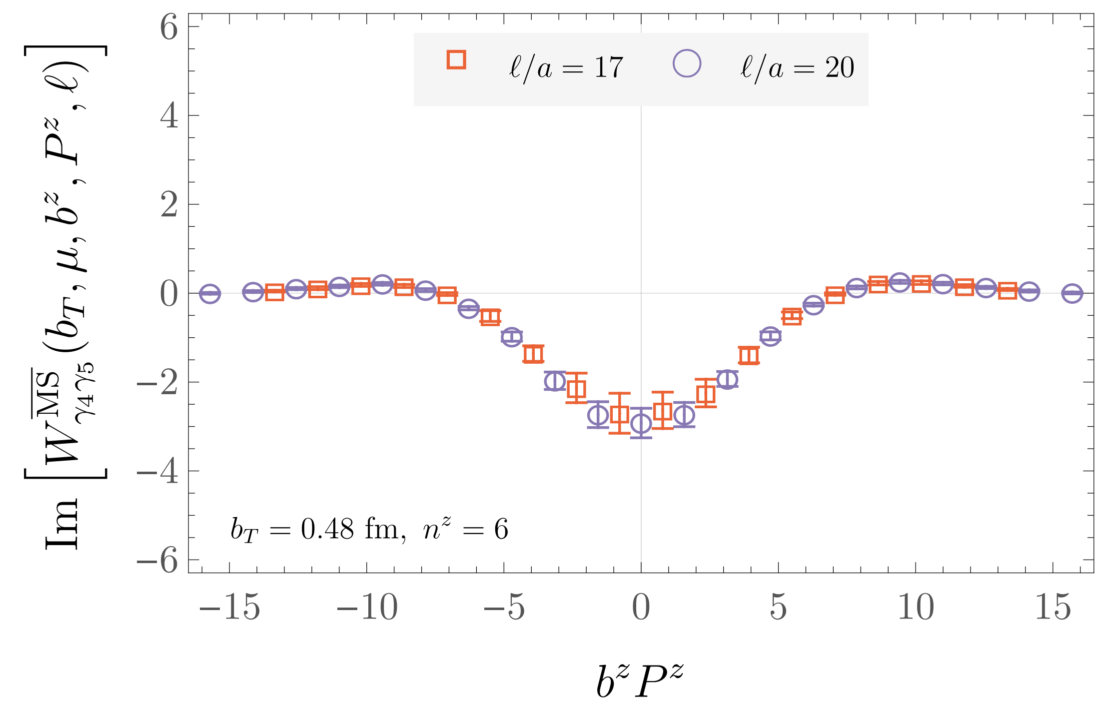
Avkhadiev, Shanahan, MW, Zhao, PRD 108 (2023)

Operator mixing patterns agree with perturbative expectations

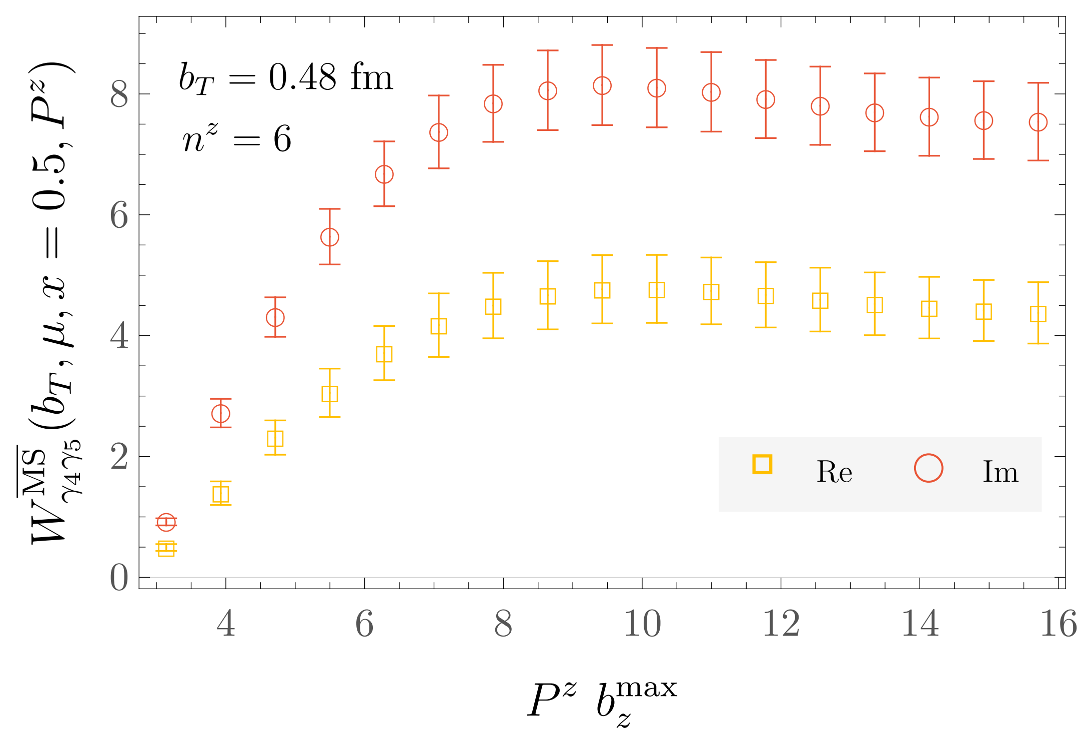
Fourier transform systematics

Precise TMD wavefunctions achieved, including large-$b^z P^z$ tails



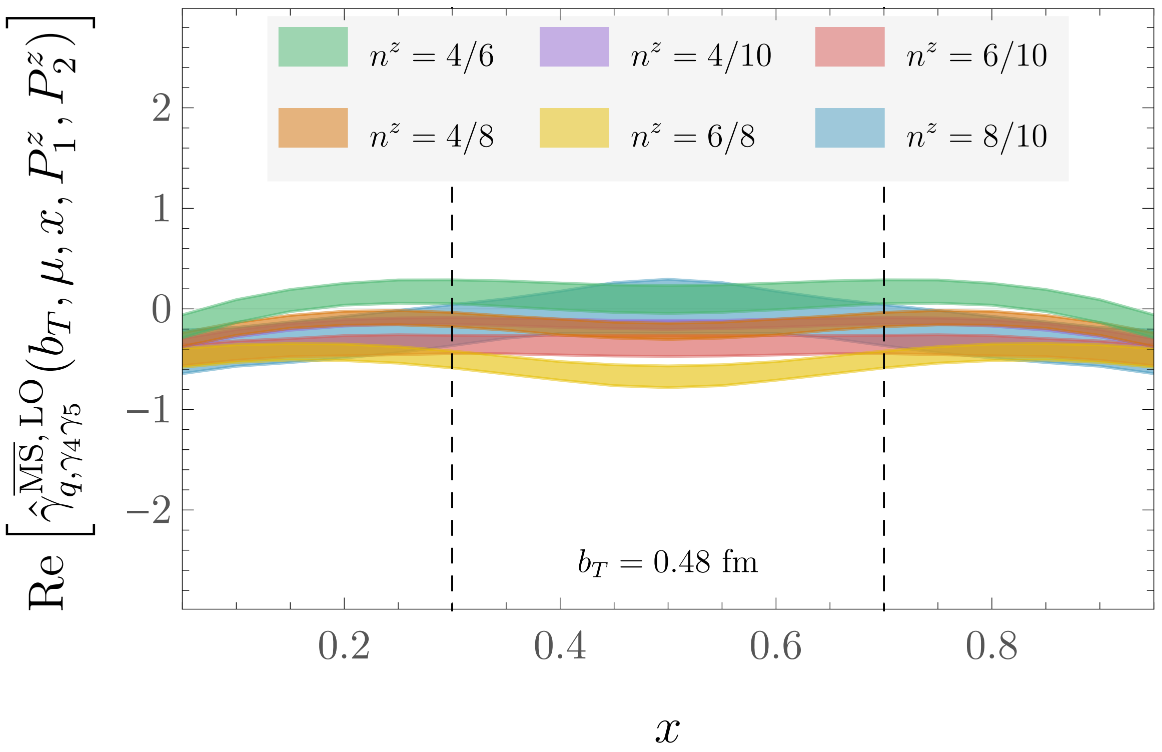


Large enough $b^z P^z$ achieved that simple DFTs show negligible truncation effects for all momenta studied



Avkhadiev, Shanahan, MW, Zhao, PRD 108 (2023)

Extracting the CS kernel

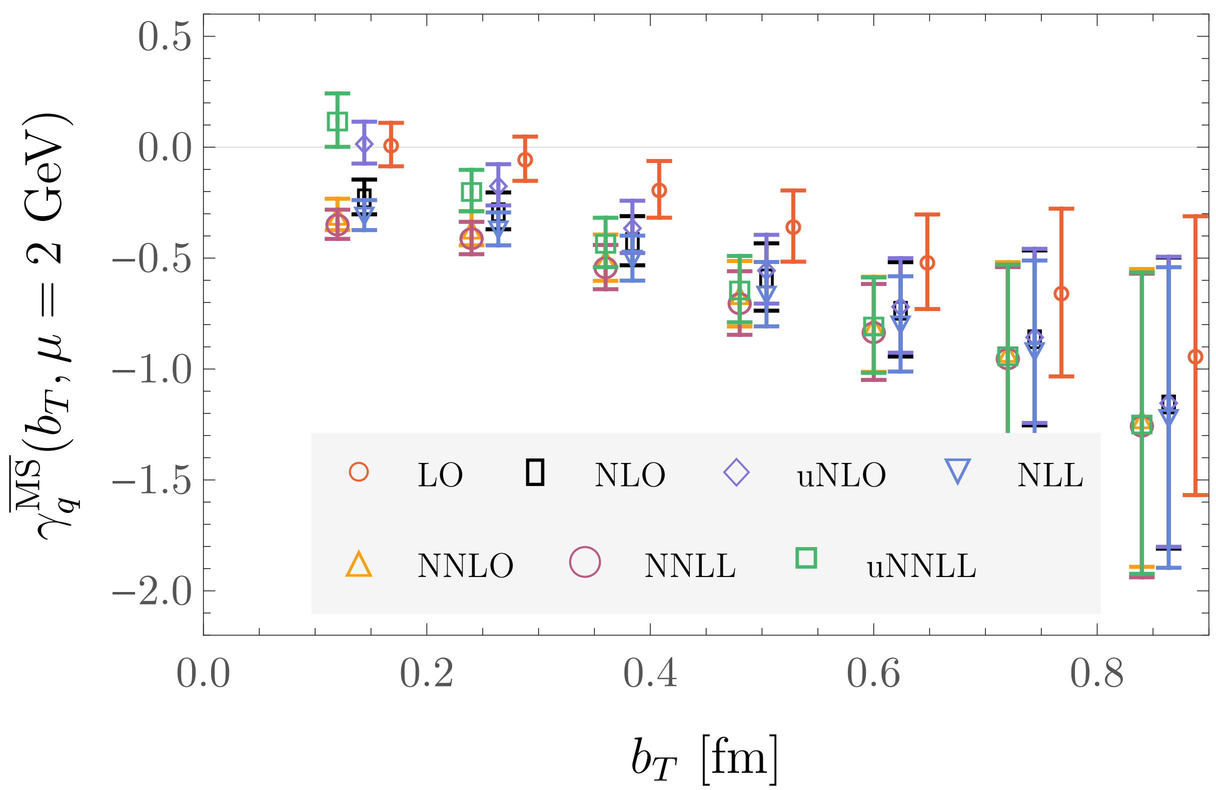


Ratios of TMD wavefunction DFTs show (asymptotically) expected x independence

CS kernel extracted from averaging over intermediate x and momentum pairs

LO, NLO, and NNLO perturbative matching shows clear convergence at large b_T

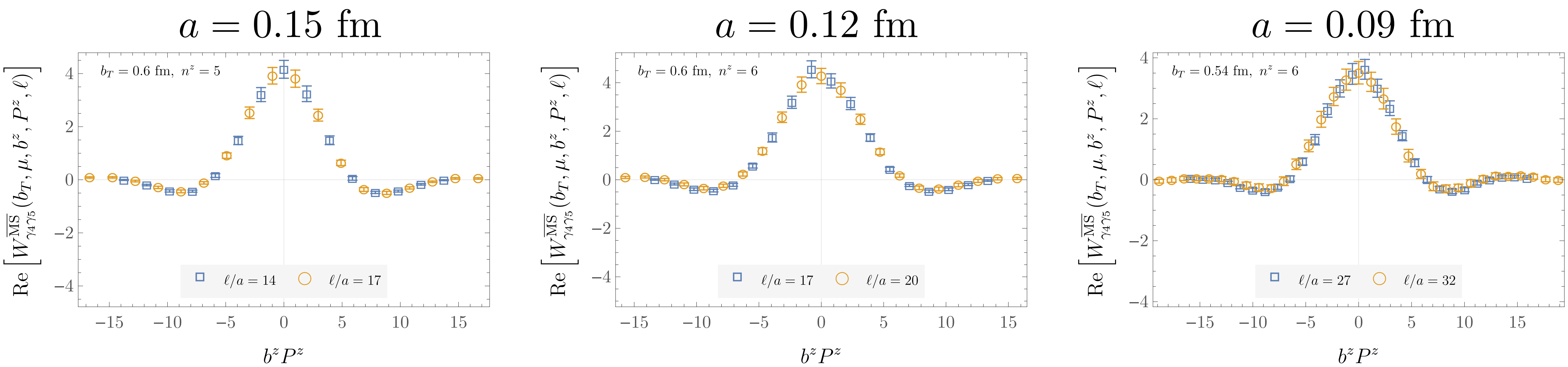
Resumed "unexpanded" matching improves small b_T convergence



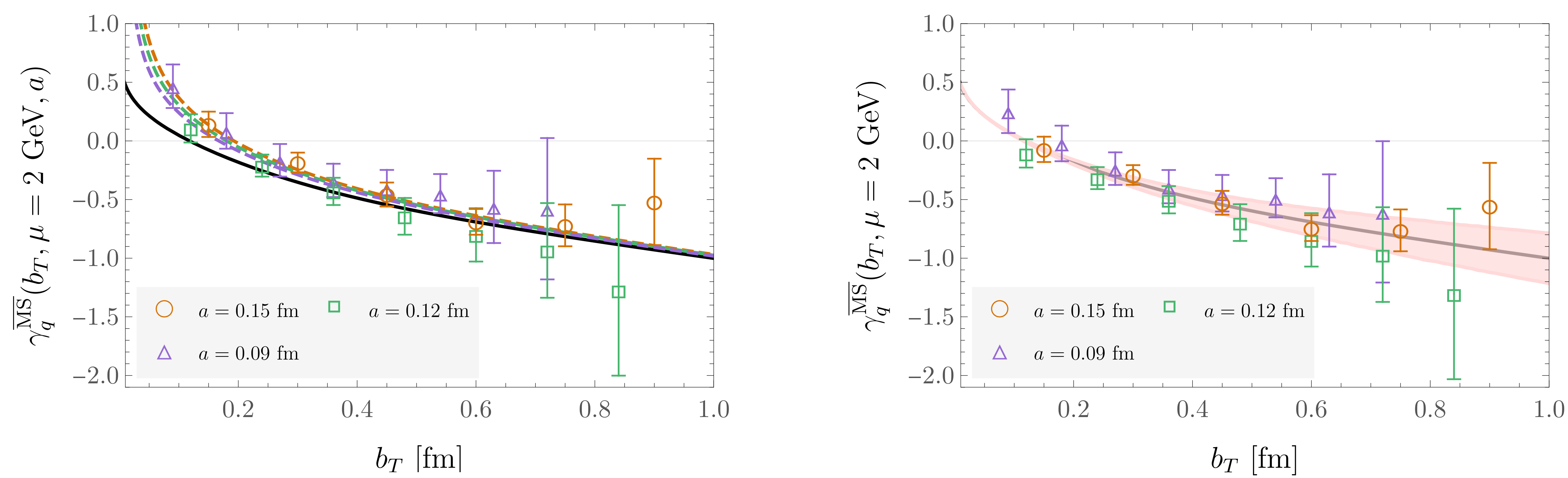
Avkhadiev, Shanahan, MW, Zhao, PRD 108 (2023)

Discretization effects

New calculations used two additional MILC ensembles with nearly physical (valence and sea) pion masses



Discretization effects subtracted by fitting to parameterization of continuum CS kernel + lattice artifacts



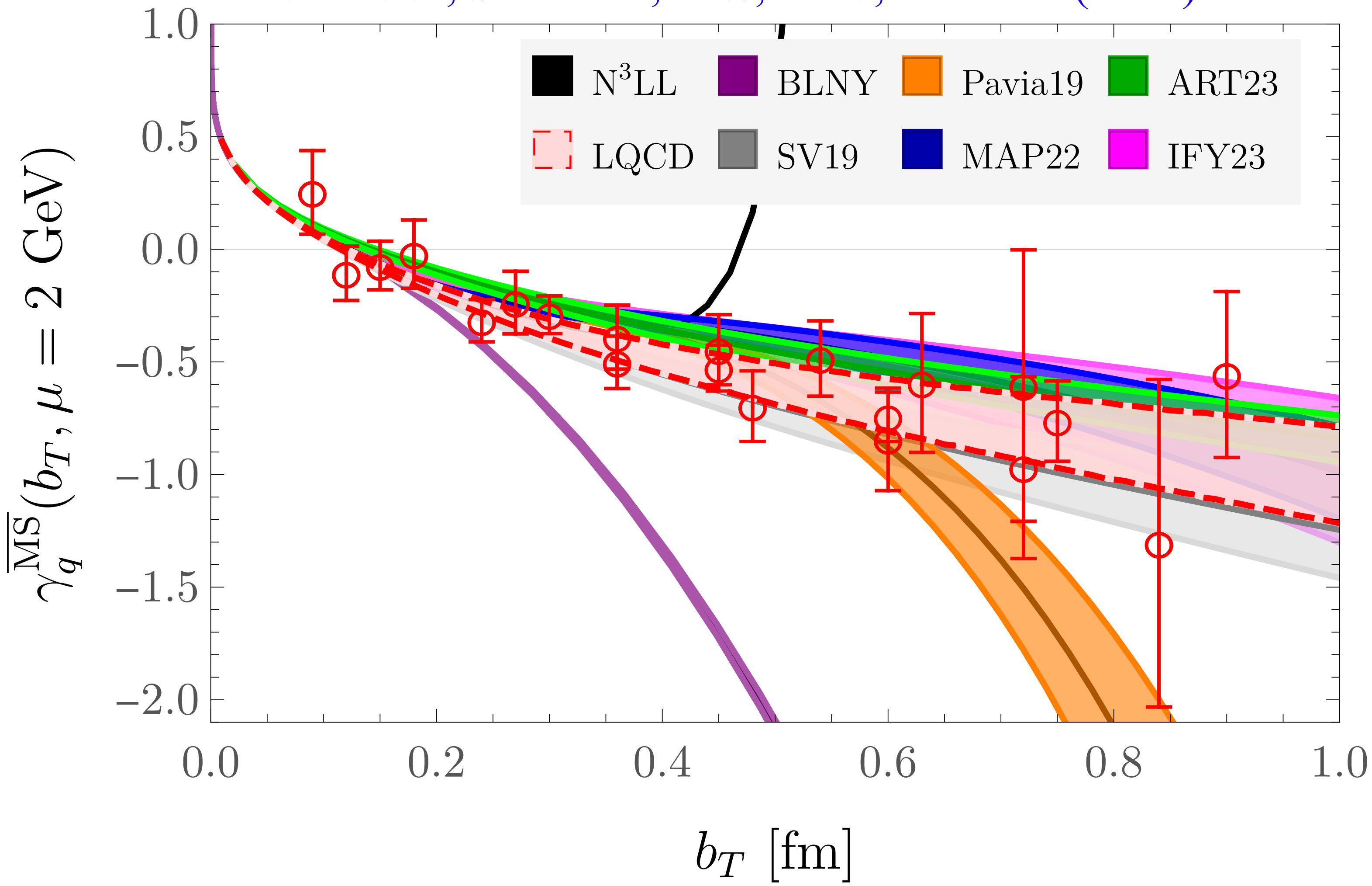
Avkhadiev, Shanahan, MW, Zhao, PRL 132 (2024)

The CS kernel from QCD

Continuum-limit LQCD results agree nicely with state-of-the-art phenomenological determinations of the CS kernel from global fits

LQCD precision is sufficient to exclude some models at large b_T

Avkhadiev, Shanahan, MW, Zhao, PRL 132 (2024)

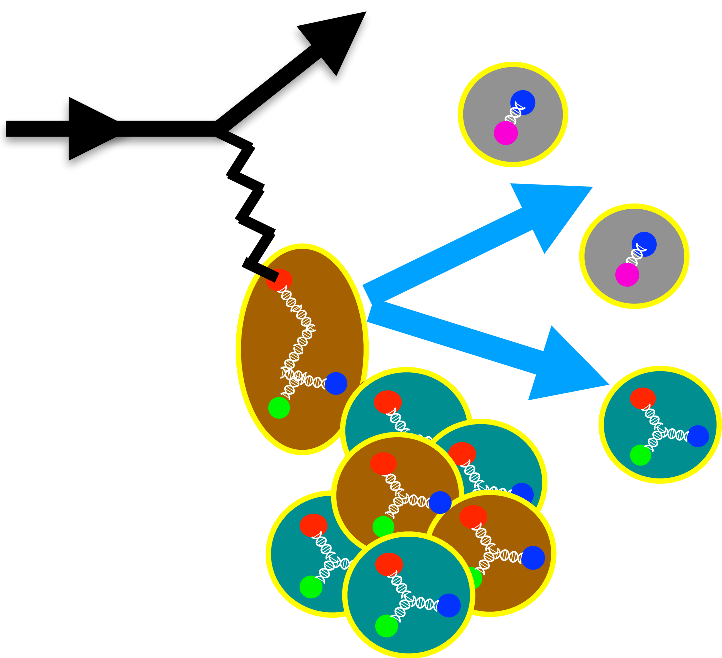


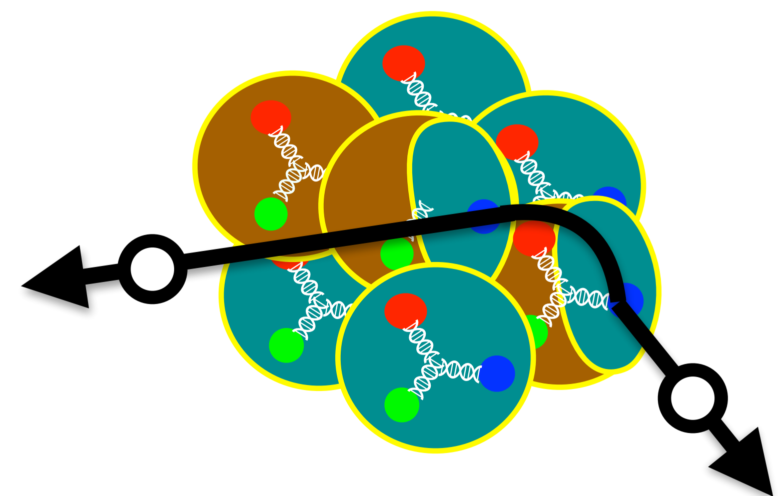
Continuum-limit LQCD results can be directly included in future global fits

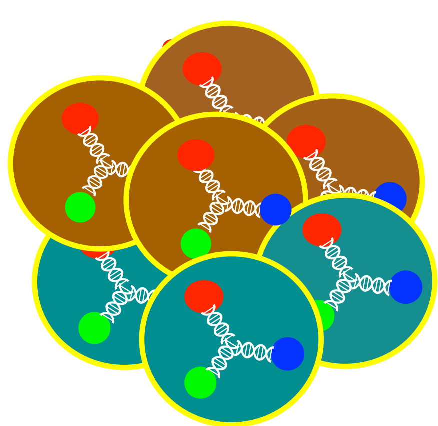
Nonperturbative effects can summarized by one parameter: $c_0 = 0.32(12)$

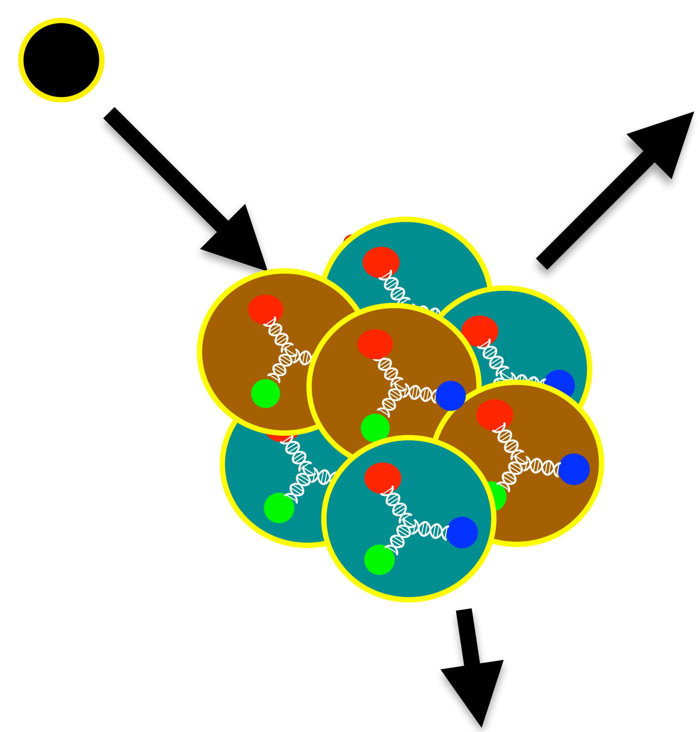
Nuclear physics from LQCD

Lattice QCD is a many-body method — just simulate a few 100 quarks







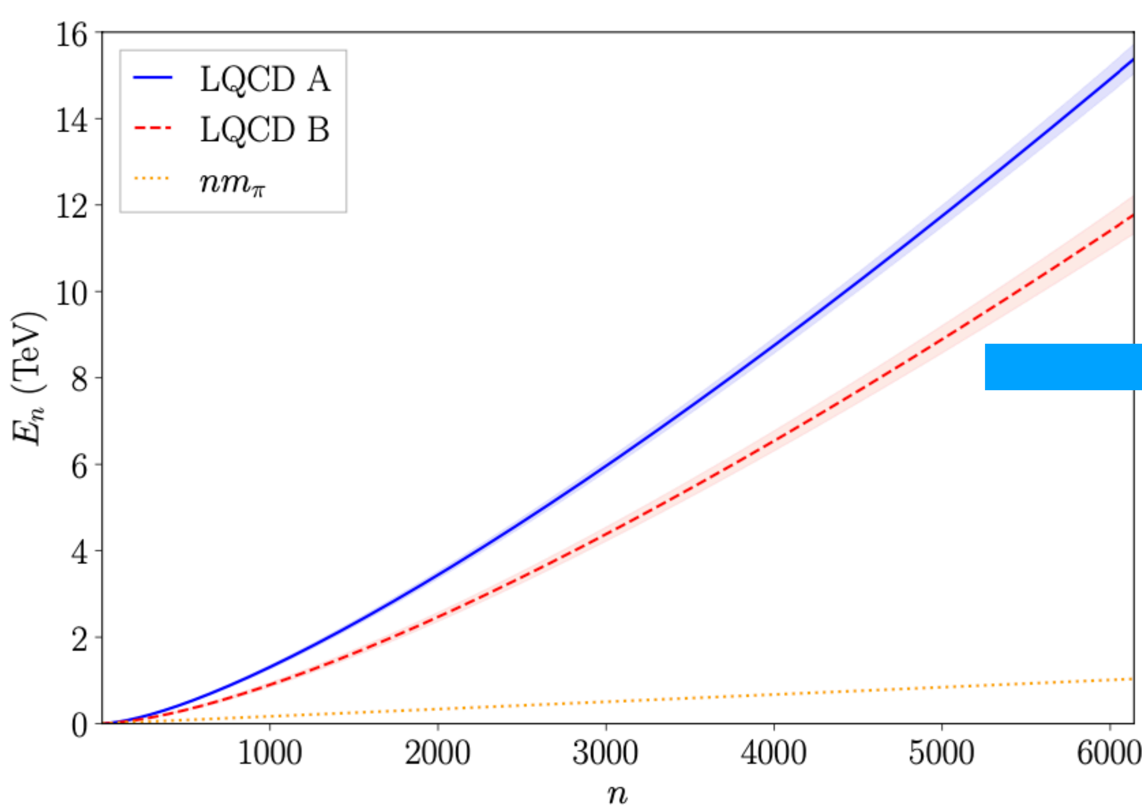


Nuclear physics from LQCD

Lattice QCD is a many-body method — just simulate a few 100 quarks

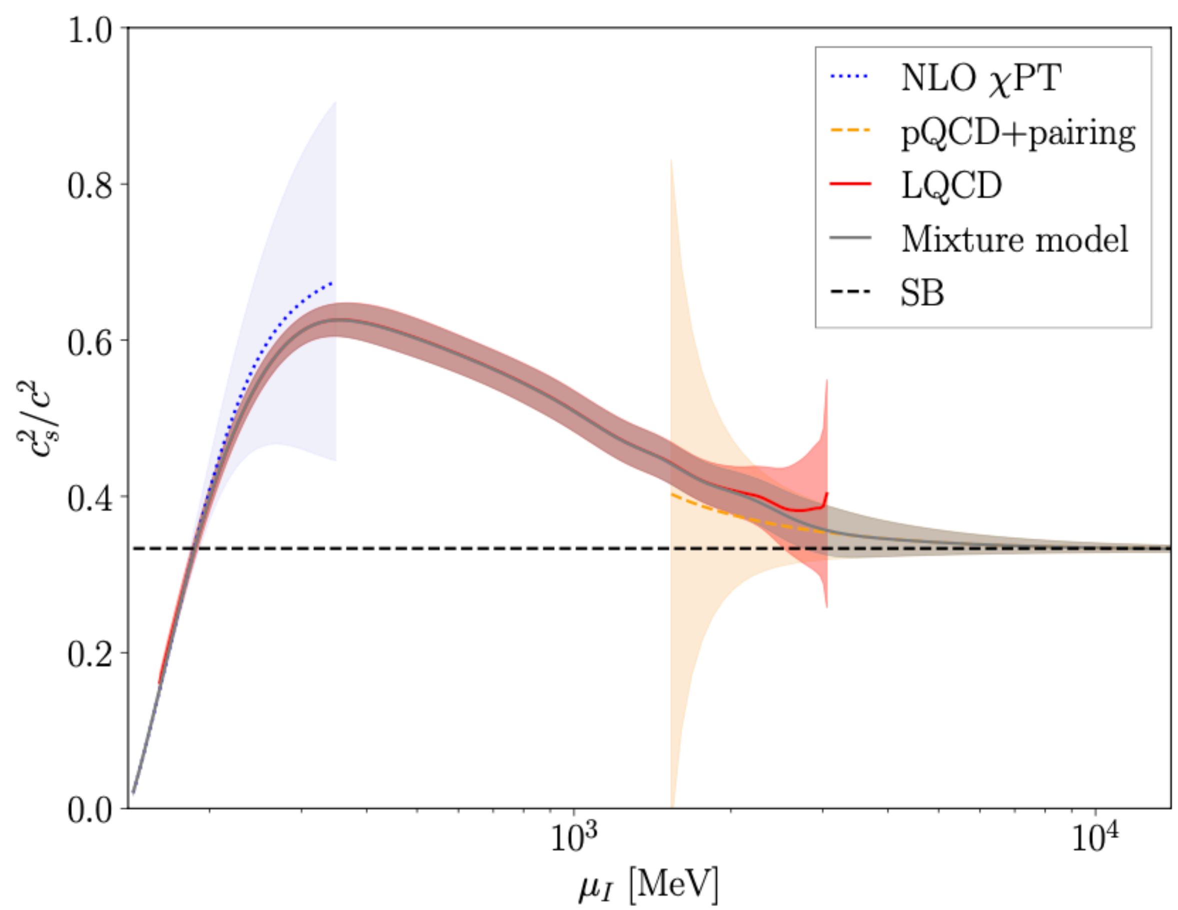
See Will Detmold's talk Thursday at 10am

Energy spectrum of up to 6000 pions in a box:



Abbot, Detmold, Romero-Lopez, MW et al [NPLQCD], PRD 108 (2023)

Speed of sound at large isospin density



Abbot, Detmold, Romero-Lopez, MW et al [NPLQCD], arXiv:2406.09273

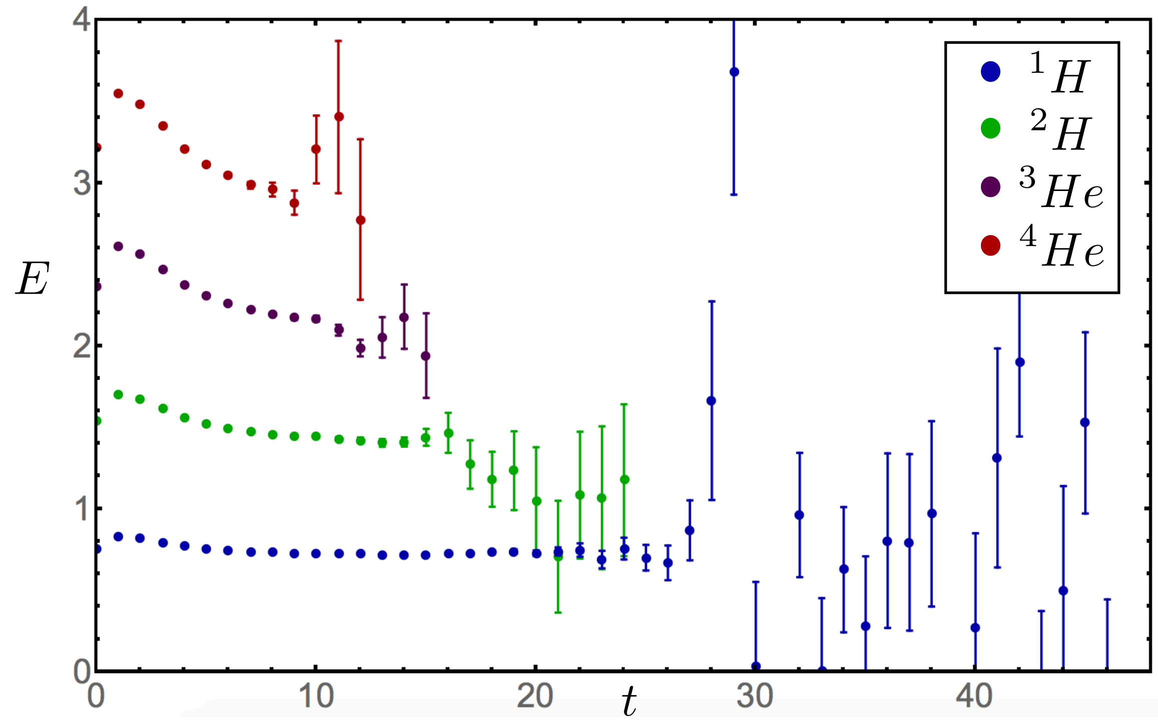
What's so hard about nuclei?

Lattice QCD is a many-body method — just simulate a few 100 quarks

1) Too many Wick contractions

2) Small energy gaps to excited states

3) Exponential signal-to-noise degradation



$$aE(t) = -\ln \frac{C(t+a)}{C(t)} = aE_0 + \ldots$$

What's so hard about nuclei?

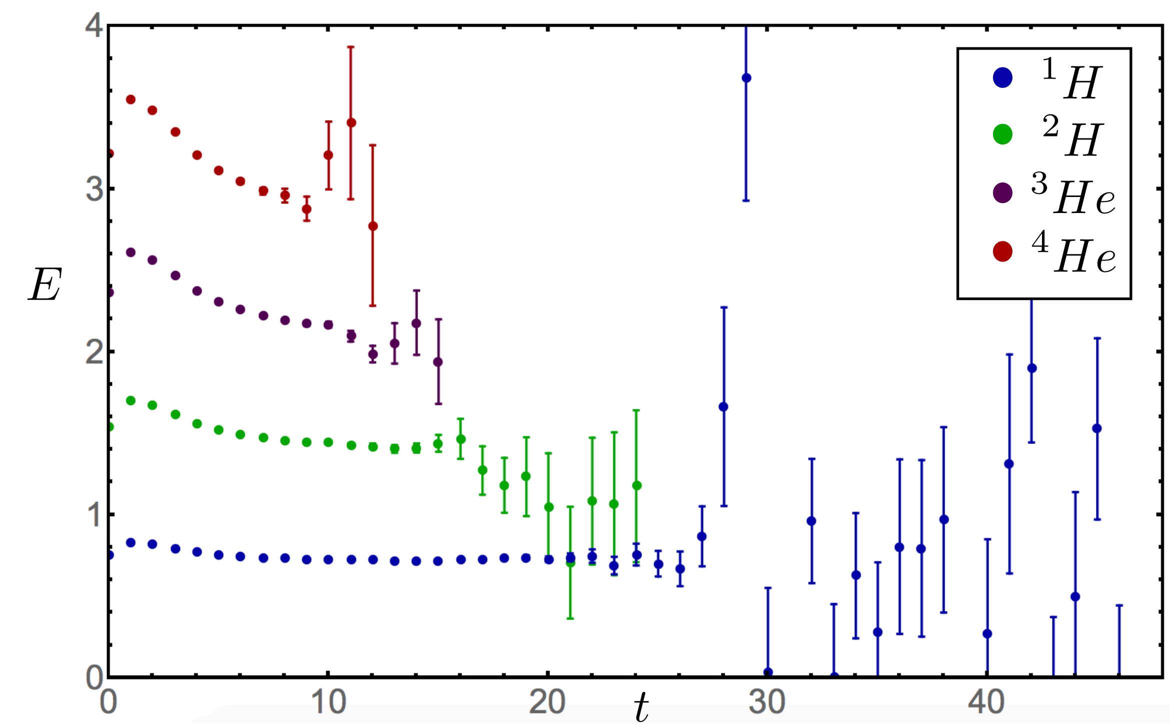
Lattice QCD is a many-body method — just simulate a few 100 quarks

~~**1) Too many Wick contractions**~~

Detmold and Orginos, PRD 87 (2013)

2) Small energy gaps to excited states

3) Exponential signal-to-noise degradation



$$aE(t) = -\ln \frac{C(t+a)}{C(t)} = aE_0 + \dots$$

What's so hard about nuclei?

Lattice QCD is a many-body method — just simulate a few 100 quarks

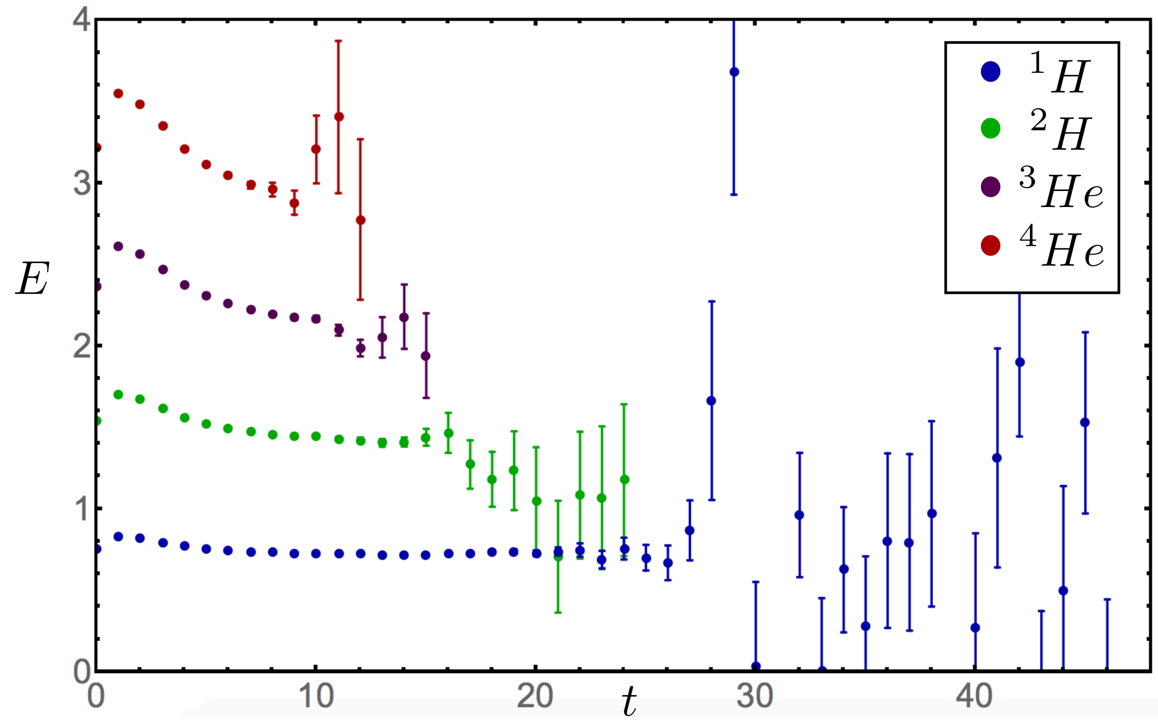
~~1) Too many Wick contractions~~

Detmold and Orginos, PRD 87 (2013)

2) Small energy gaps to excited states

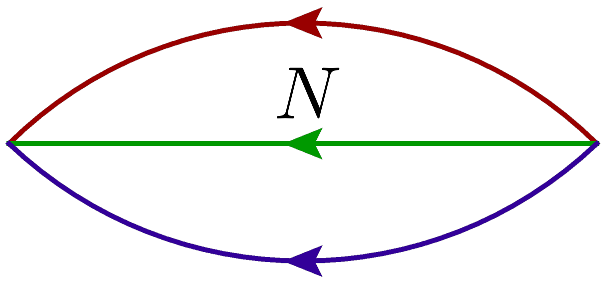
$\delta \approx 4\pi^2/(M_N L^2)$ or $\delta \approx B_A$

3) Exponential signal-to-noise degradation



$$aE(t) = -\ln \frac{C(t+a)}{C(t)} = aE_0 + \ldots$$

The signal-to-noise problem



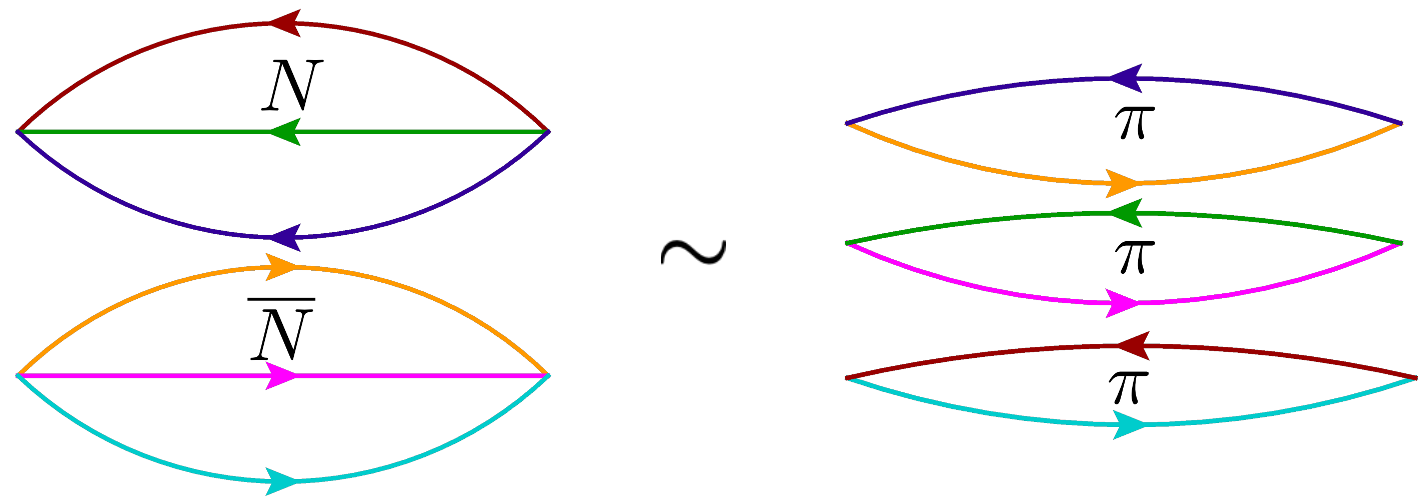
Nucleon ground state dominates correlation function for large t

$$C_N(t) \sim e^{-M_N t}$$

Variance of nucleon correlation function is itself a correlation function with quantum numbers of $N\overline{N}$

The lightest allowed state is 3π

$$\mathrm{Var}[C_N(t)] \sim e^{-3m_\pi t}$$



Implies signal-to-noise ratios scale as

$$\mathrm{StN}[C_N(t)] = \frac{\langle C_N(t)\rangle}{\sqrt{\mathrm{Var}[C_N(t)]}} \sim e^{-(M_N - \frac{3}{2}m_\pi)t}$$

Parisi, Phys.Rept. 103 (1984)

Lepage, TASI (1989)

Same analysis for a system of *A* nucleons:

$$\mathrm{StN}[C_A(t)] = \frac{\langle C_A(t)\rangle}{\sqrt{\mathrm{Var}[C_A(t)]}} \sim e^{-A(M_N - \frac{3}{2}m_\pi)t}$$

The sign/al-to-noise problem

Nucleon correlation functions are complex in generic gauge field backgrounds

Complex phases of correlation functions give path integrals “sign problems”

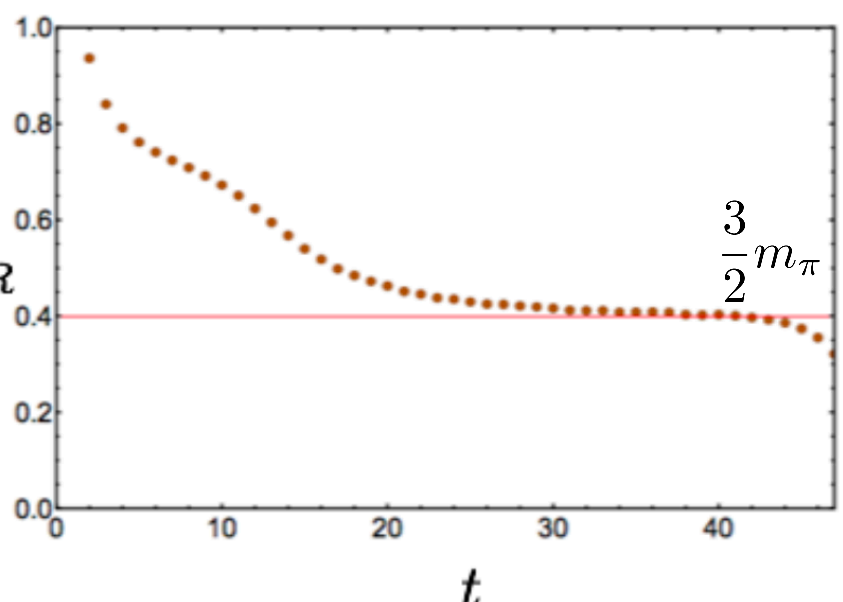
$$C_N(t) = \frac{1}{Z}\int \mathcal{D}U\ e^{-S(U)}\ \left|C_N(t)\right| e^{i\theta_N(t)}$$

Integral can’t be interpreted as a probability

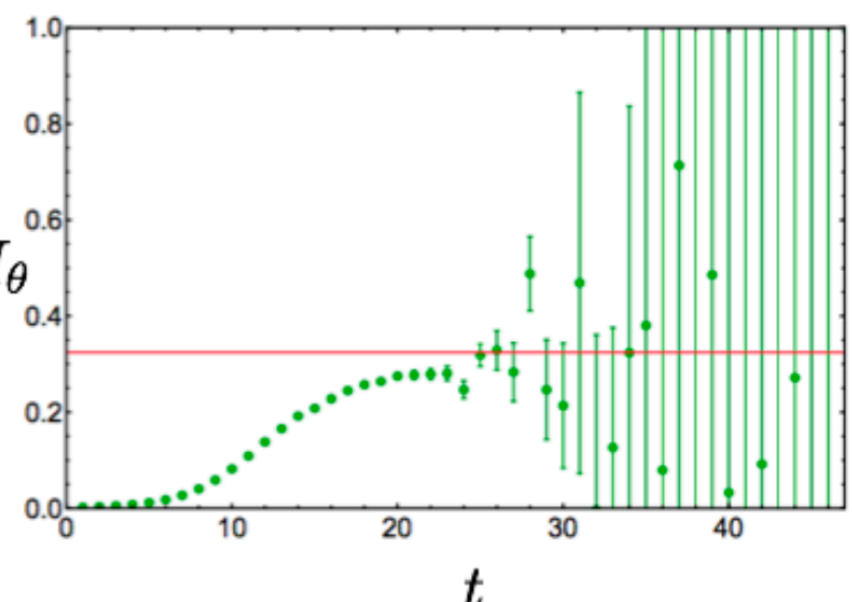
The same phase fluctuations are responsible for the full severity of the signal-to-noise problem for the nucleon and nuclei

M_R

Neglects $e^{i\theta_N}$



M_θ



$M_N - \frac{3}{2}m_\pi$

Neglects $|C_N|$

MW, Savage PRD 96 (2017)

What's so hard about nuclei?

Lattice QCD is a many-body method — just simulate a few 100 quarks

~~**1) Too many Wick contractions**~~

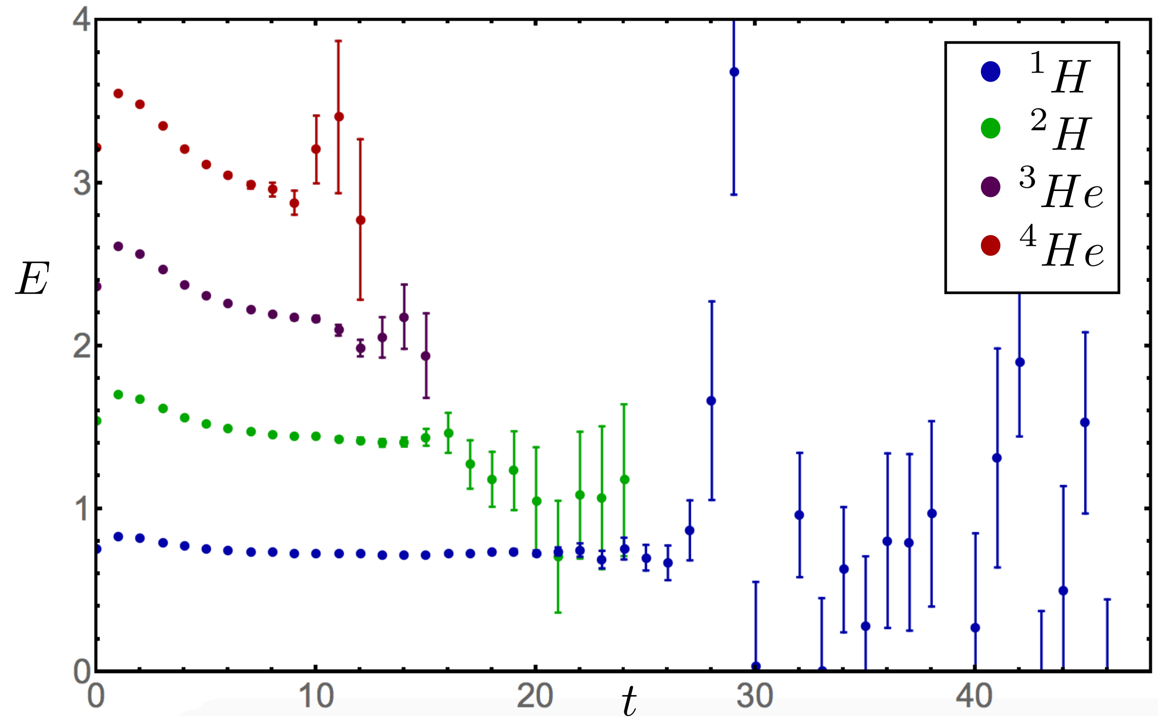
Detmold and Orginos, PRD 87 (2013)

2) Small energy gaps to excited states

$\delta \approx 4\pi^2/(M_N L^2)$ or $\delta \approx B_A$

3) Exponential signal-to-noise degradation

$\mathrm{StN} \sim e^{-A(M_N - \frac{3}{2}m_\pi)t}$



$$aE(t) = -\ln \frac{C(t+a)}{C(t)} = aE_0 + \ldots$$

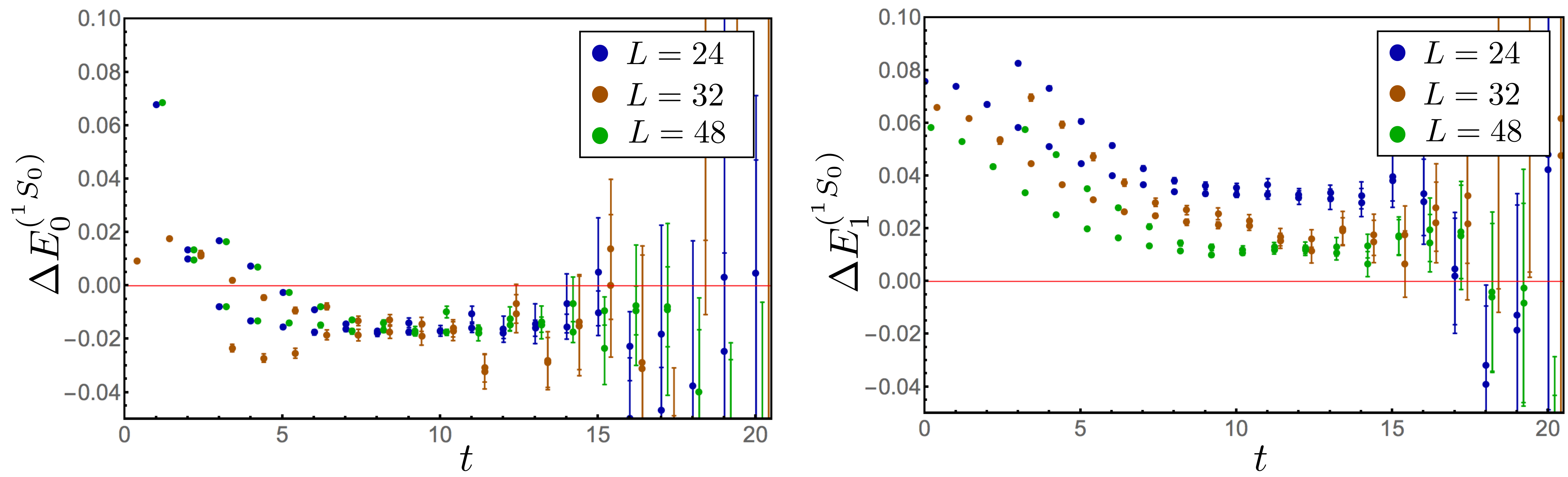
Getting large enough imaginary times to suppress excited-state effects can be challenging or impossible for multi-nucleon systems

Nuclei from LQCD

First calculations of 2-5 baryon (asymmetric) correlation functions

Beane et al [NPLQCD], PRD 87 (2013)	$L = 2.9 \text{ fm} \to 5.8 \text{ fm}$	$a = 0.145 \text{ fm}$	$m_\pi \sim 806 \text{ MeV}$
Yamazaki et al, PRD 86 (2012)	$L = 3.5 \text{ fm} \to 7.0 \text{ fm}$	$a = 0.09 \text{ fm}$	$m_\pi \sim 510 \text{ MeV}$

- Ground state energy appears approximately volume independent
- First excited state shows volume dependence consistent with unbound
- Operators with two different smearings give consistent results



Data from Beane et al [NPLQCD], PRD 87 (2013)

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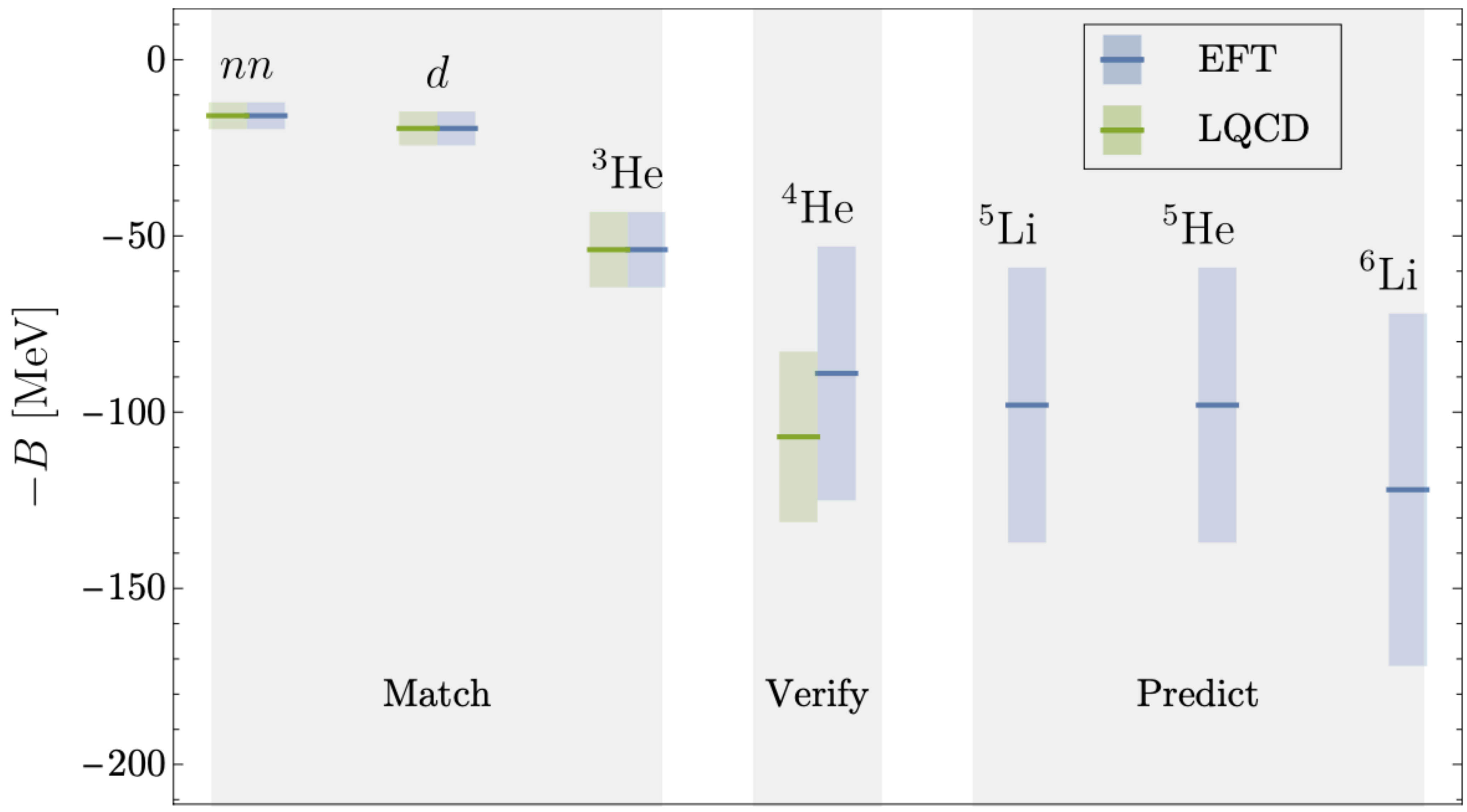


EFT: Barnea et al, PRL 114 (2015)

My NPLQCD Collaborators

Beane

Chang

Davoudi

Detmold

Grebe

Illa

Jay

Murphy

Orginos

Parreño

Perry

Savage

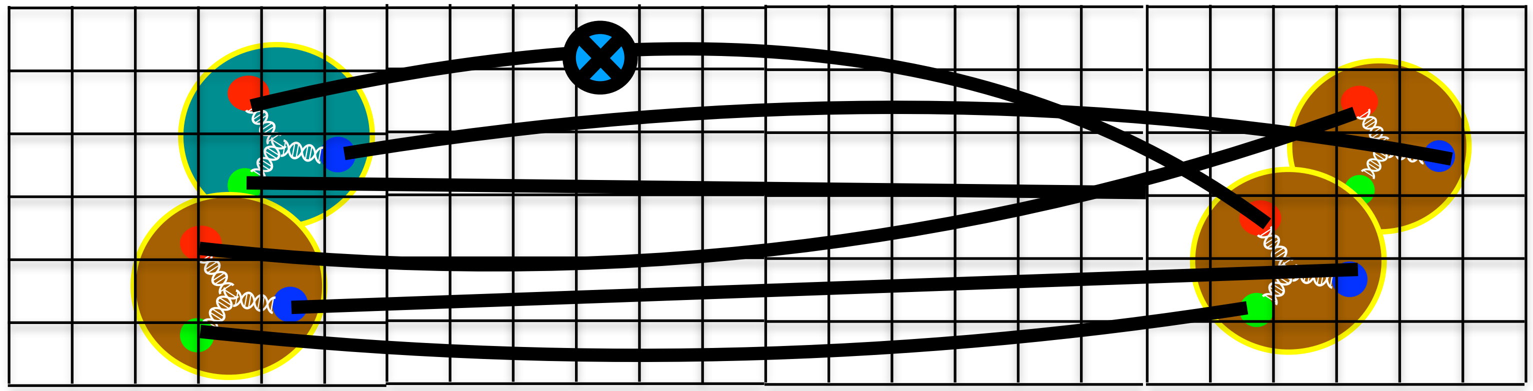
Shanahan

Tiburzi

Winter

Two-body axial currents

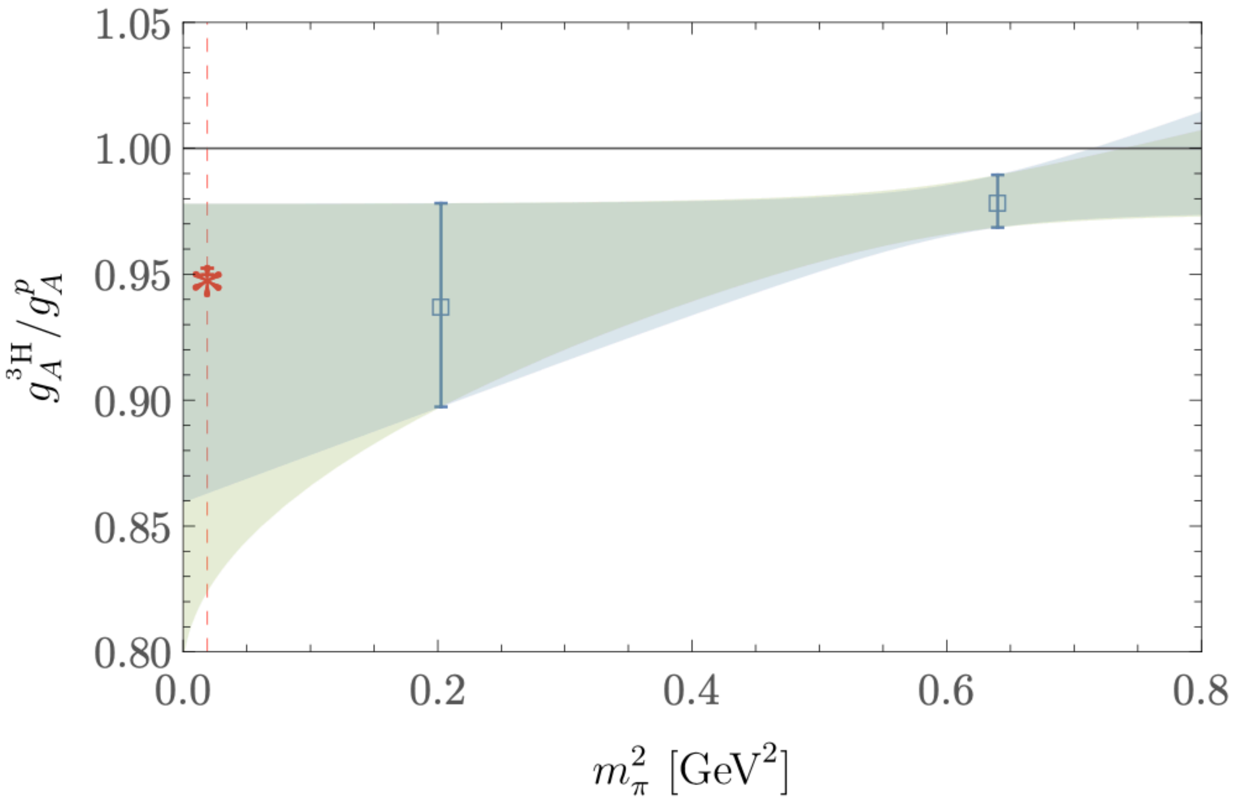
Two-nucleon axial matrix elements relevant for proton-proton fusion computed, used to constrain two-body currents in pionless EFT for $m_\pi = 806 \text{ MeV}$



Savage, MW et al [NPLQCD], PRL 119 (2017)

See talk by Zi-Yu Wang, Wed 12:35

Axial current matrix element calculations with $m_\pi = 450 \text{ MeV}$ permit preliminary extrapolations to physical quark masses



Parreño, MW et al [NPLQCD] PRD 103 (2021)

Matrix elements of two axial currents constrain $2\nu\beta\beta$ in poinless EFT

Shanahan, MW et al [NPLQCD], PRL 119 (2017)

Tiburzi, MW et al [NPLQCD], PRD 96 (2017)

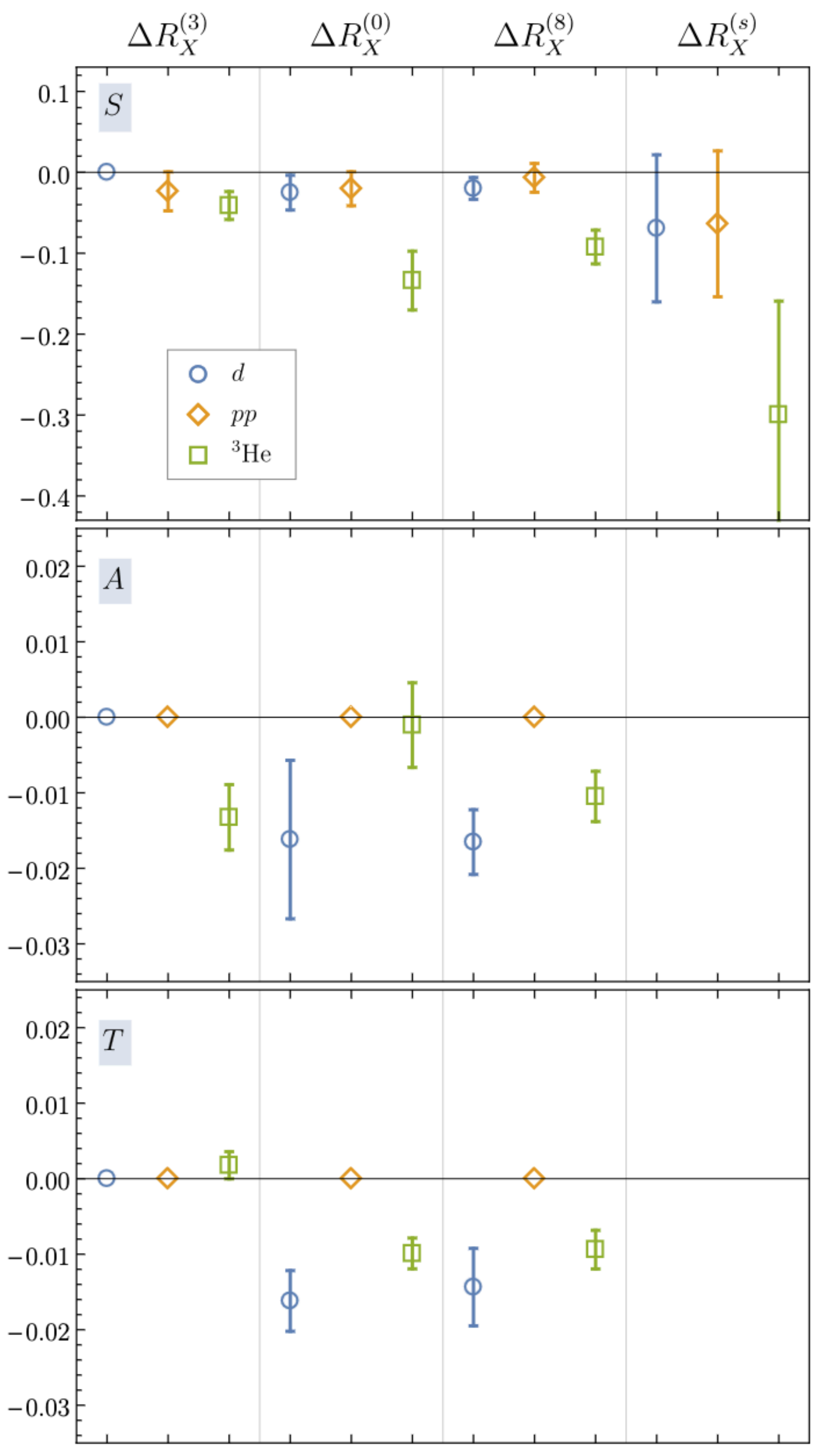
More complicated two-body currents important for $0\nu\beta\beta$, first study:

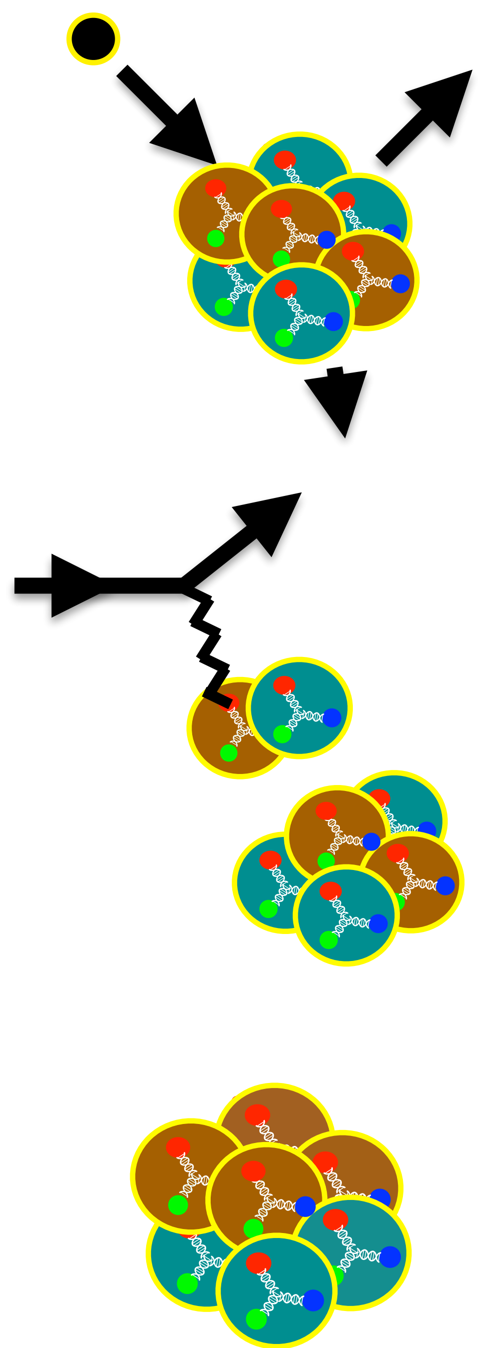
Davoudi, Grebe, MW et al, arXiv:2402.09362

See plenary talk by Anthony Grebe on Saturday

Scalar, axial, and tensor charges

Flavor decompositions of scalar, axial, and tensor charges for 1-3 nucleons, $m_\pi = 806\ \mathrm{MeV}$





Nuclear effects on these charges are relevant for

Scalar

- Dark matter direct detection

Axial

- Single- and double-beta decay, neutrino-nucleus scattering

Tensor

- CP violating nuclear EDMs

Chang, MW et al [NPLQCD], PRL 120 (2018)

Nuclear momentum fractions

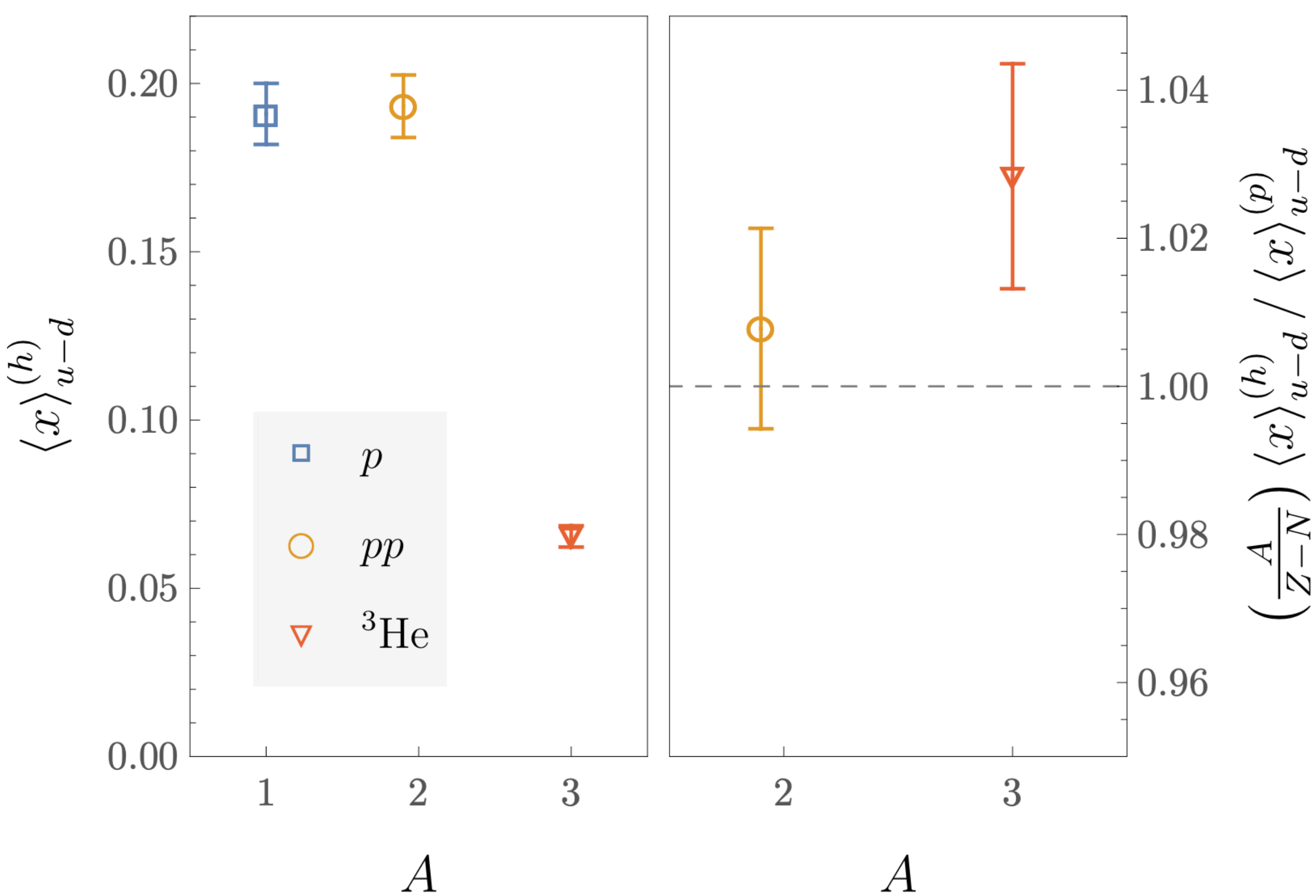
First calculations of gluon and isovector quark momentum fractions of light nuclei

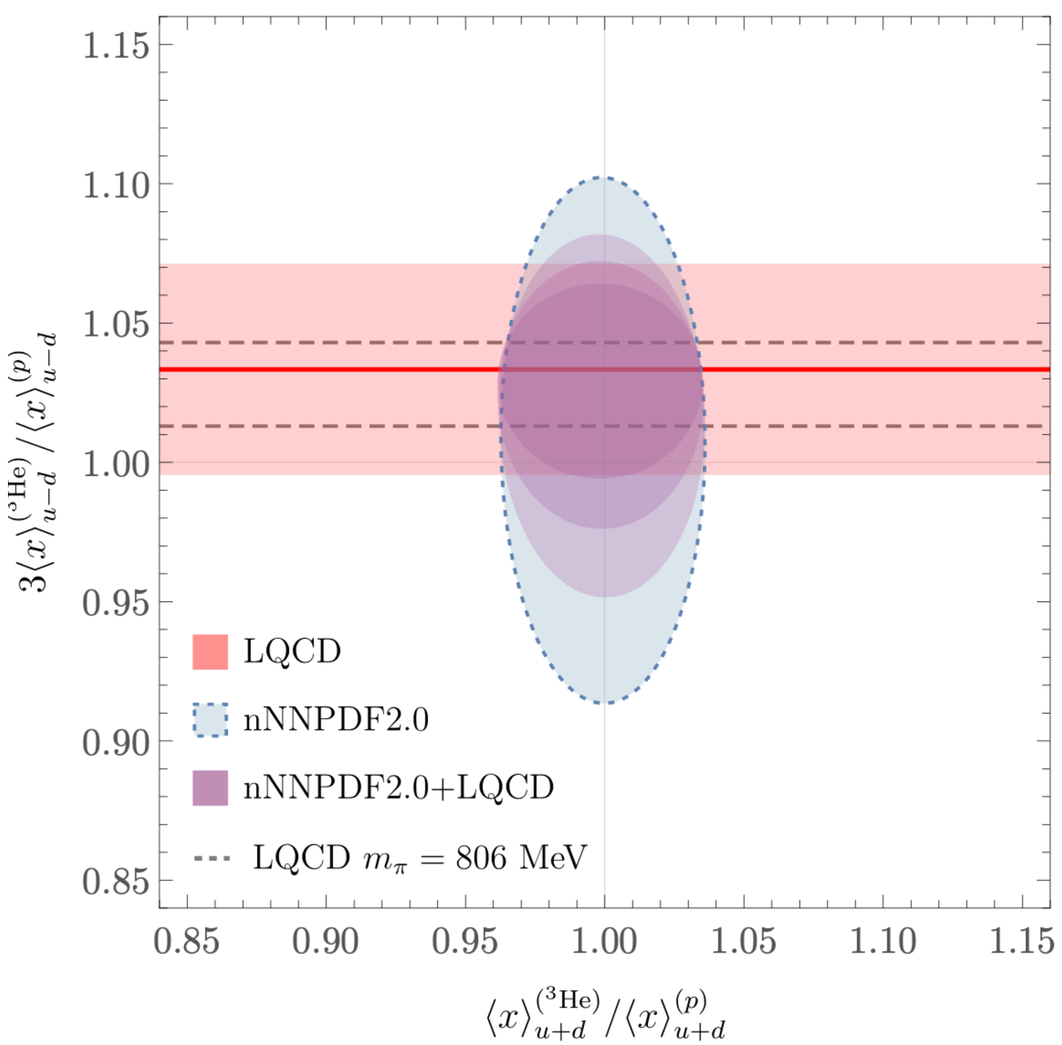
Winter, MW et al [NPLQCD], PRD 96 (2017)

Detmold, MW et al [NPLQCD] PRL 126 (2021)

Results matched to pionless EFT to determine two-body current operator relevant for isovector EMC effects

Demonstrates potential for LQCD to usefully constrain nuclear PDFs, although systematic uncertainties are not fully controlled





Systematic uncertainties

Present-day LQCD studies of nuclei still have several systematic uncertainties that need to be studied in detail

- Heavier than physical quark masses only
- One lattice spacing
- Excited-state effects

Systematic uncertainties

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- Heavier than physical quark masses only
- One lattice spacing
- Excited-state effects

Gap between ground and two-nucleon finite-volume “scattering” states becomes small for large volumes, ground-state dominance relies on overlap factors

$$Z_0 e^{-E_0 t}\left(1 + \frac{Z_1}{Z_0} e^{-\delta t} + \ldots\right) \qquad \delta \sim \frac{4\pi^2}{ML^2}$$

For non-positive-definite correlation functions, cancellations between the ground and excited-state could in principle conspire to form a “false plateau”

See e.g. Iritani et al, JHEP 10 (2016)

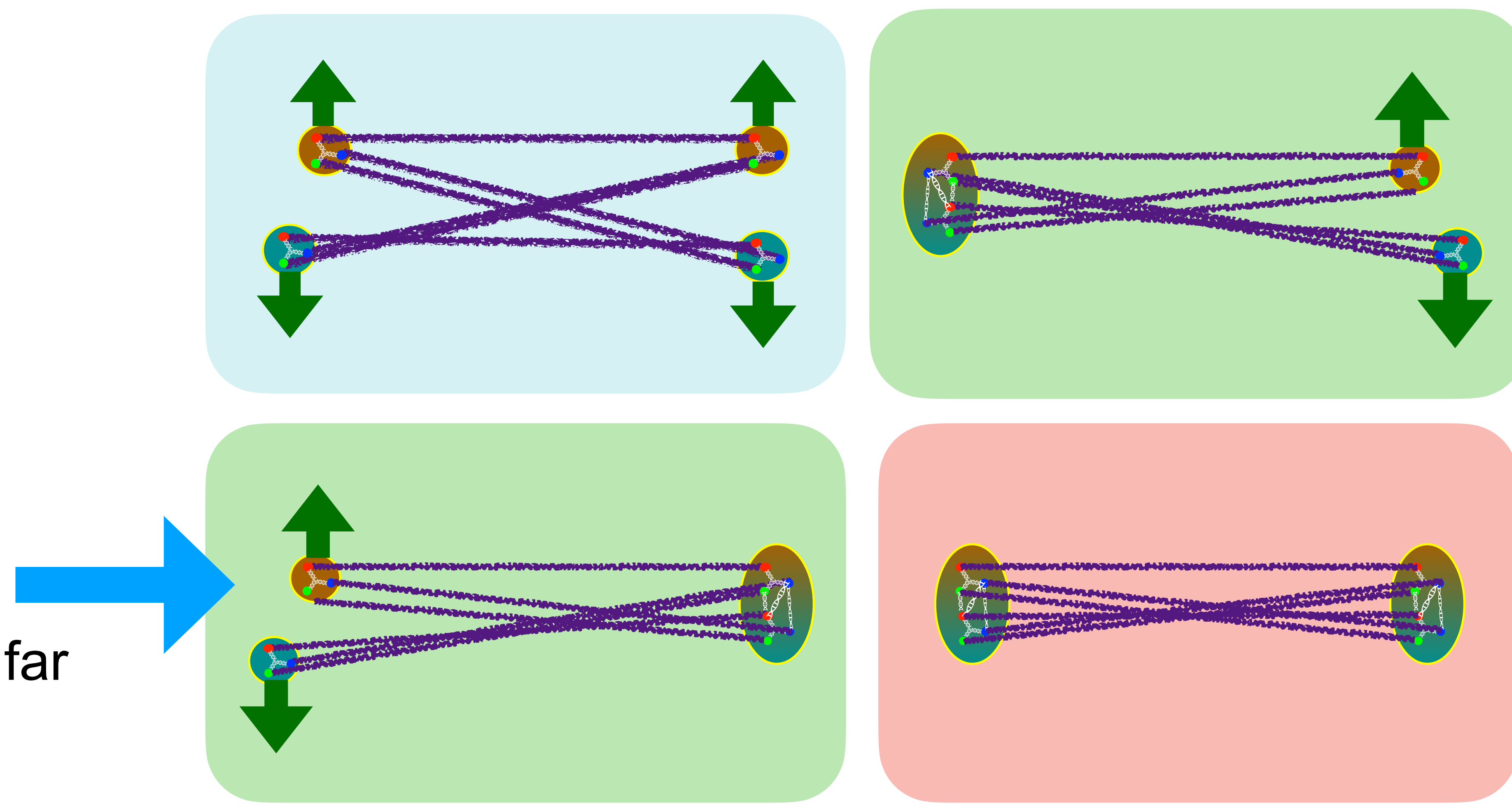
All Z factors in spectral representation guaranteed to be positive for symmetric correlation functions

$$\left\langle \mathcal{O}\,\overline{\mathcal{O}} \right\rangle = \sum_n |Z_n|^2 e^{-E_n T}$$

Variational methods

Robust upper bounds on energy spectrum can be obtained by diagonalizing symmetric matrices of correlation functions

All LQCD nuclear matrix element calculations so far



Although application of variational methods to multi-nucleon systems has long been advocated, it has only recently become computationally feasible

Distillation:

Peardon et al PRD 80 (2009)

Morningstar et al PRD 83 (2011)

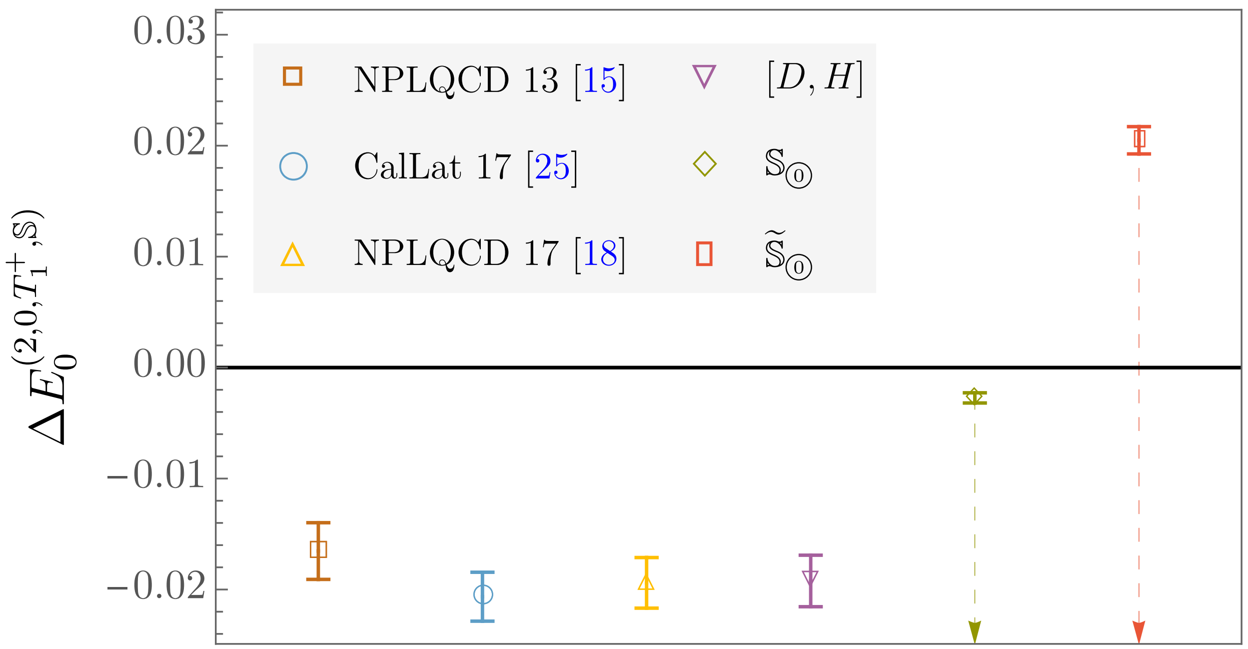
Sparsening:

Detmold, MW et al, PRD 104 (2021)

Li et al, PRD 103 (2021)

Two-nucleon variational bounds

Variational upper bounds obtained using different interpolating operator sets are consistent

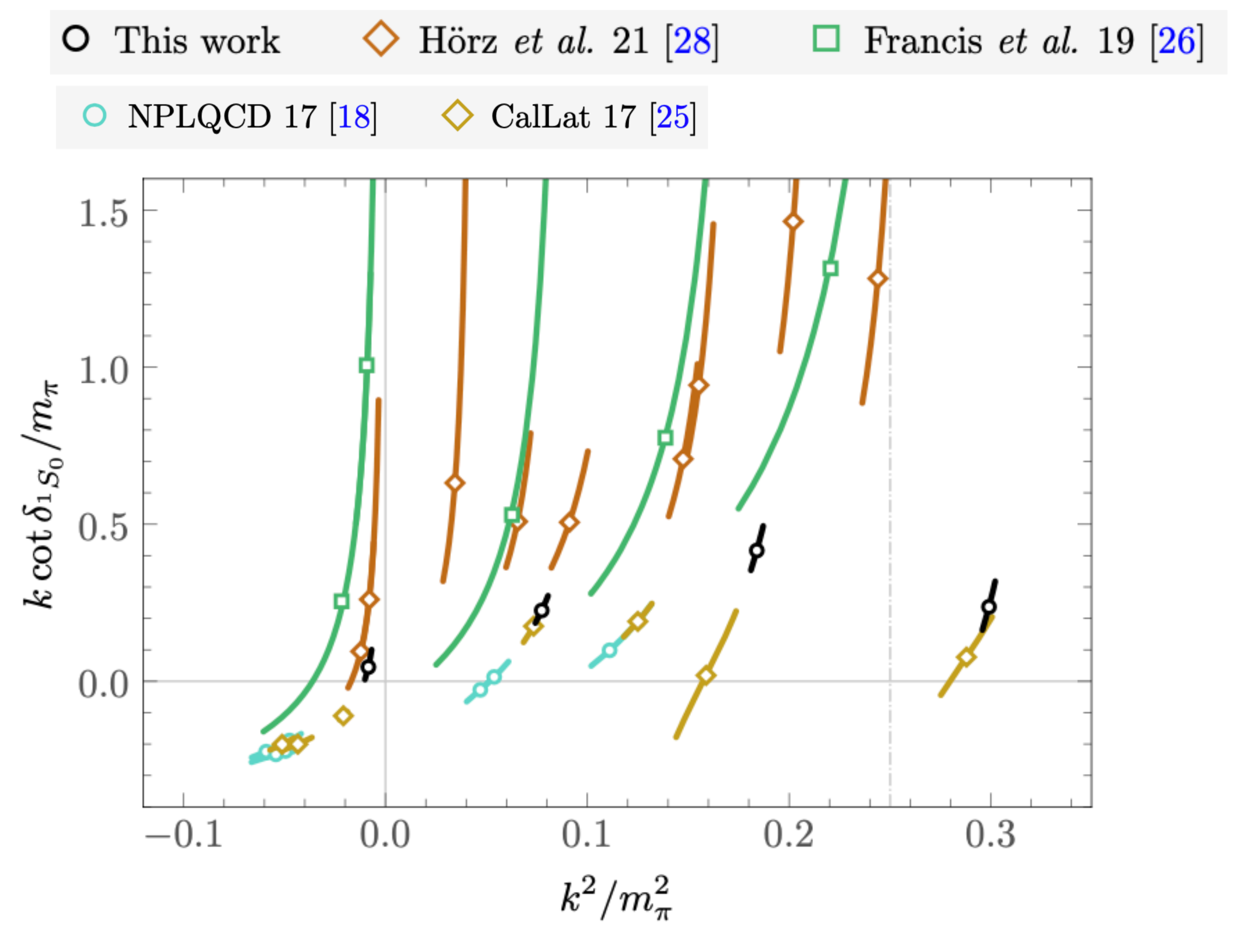


Ground-state energy **estimates** using different interpolating-operator sets show large discrepancies

See talk by Robert Perry, Wed 11:35

Phase shifts obtained using asymmetric vs variational energy estimates suggest qualitatively different physics (bound vs unbound)

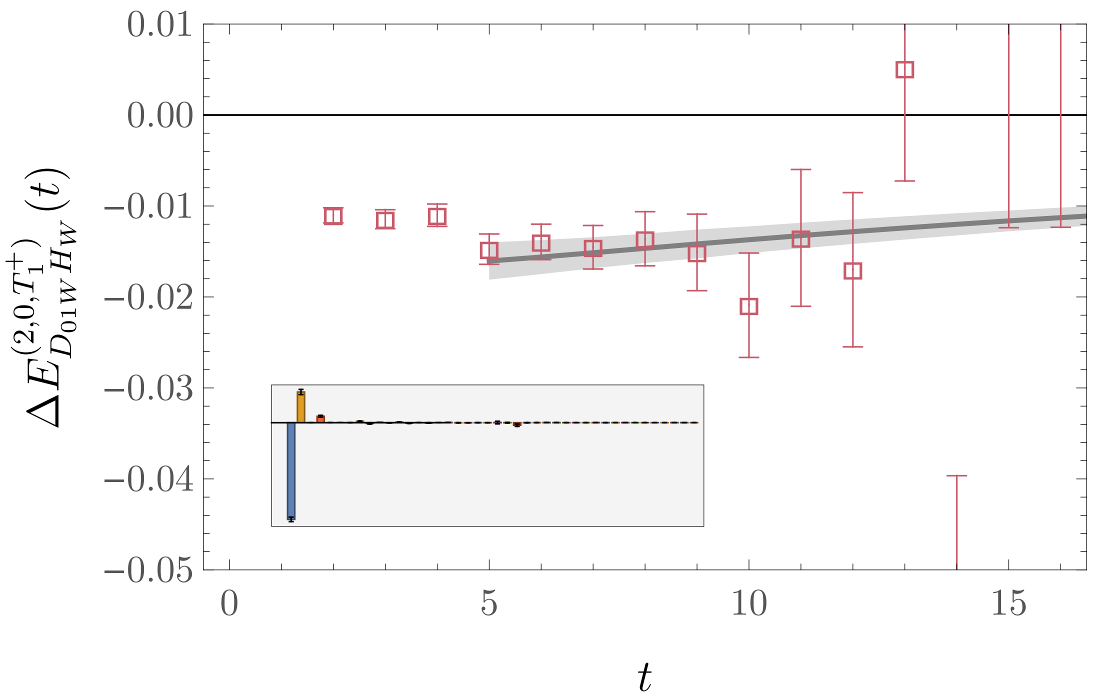
Amarasinghe, MW et al [NPLQCD], PRD 107 (2023)



Results by different groups using similar interpolating operators show good consistency

Excited states or overlap problem?

Apparent plateau of hexaquark-dibaryon correlation function can be reproduced by a linear combination of ground- and excited-state GEVP energy levels



GEVP predicts slow approach from below for much larger

$$t \gg 40a \sim 6\ \mathrm{fm}$$

Toy model: 2 operators, 3 states

$$Z_{\mathrm{n}}^{(A)} = (\epsilon, \sqrt{1-\epsilon^2}, 0)$$
$$Z_{\mathrm{n}}^{(B)} = (\epsilon, 0, \sqrt{1-\epsilon^2})$$

- Both operators have small overlap ϵ with ground state
- Operators are approximately orthogonal

GEVP eigenvalues controlled by first and second excited state (**not** ground state) for $\epsilon^2 \ll e^{t(E_1-E_0)}$

$$\lambda_0^{(AB)} = e^{-(t-t_0)E_1} + O(\epsilon^2)$$
$$\lambda_1^{(AB)} = e^{-(t-t_0)E_2} + O(\epsilon^2)$$

Off-diagonal correlator conversely has perfect ground-state overlap

Lanczos, the transfer matrix, and the signal-to-noise problem

MW, arXiv:2406.20009

Hackett, MW, arXiv:2407.21777

Cornelius Lanczos

Daniel Hackett

Spectroscopy = finding eigenvalues

Lattice theories do not have continuous time translation symmetry defining Hamiltonian

$$\mathcal{O}(t) = e^{-Ht}\mathcal{O}e^{Ht}$$ ✗

Discrete time translation symmetry enables definition of transfer matrix T

$$\mathcal{O}(ka) = T^k\mathcal{O}(T^{-1})^k$$ ✓

Energy spectrum = - ln (spectrum of eigenvalues of T)

$$T\big|n\big\rangle = \big|n\big\rangle\lambda_n \qquad E_n = -\ln\lambda_n$$

Correlation functions are matrix elements of powers of T

$$C(t) \equiv \langle\psi(t)\psi^\dagger(0)\rangle = \Big\langle\psi\Big|T^{t/a}\Big|\psi\Big\rangle + \ldots$$

Lanczos and the transfer matrix

- Standard effective mass = "power-iteration algorithm" for finding eigenvalues

$$|b_k\rangle \propto T^{k-1}|\psi\rangle \quad \Rightarrow \quad \frac{\langle b_k|T|b_k\rangle}{\langle b_k|b_k\rangle} = \frac{C((k+1)a)}{C(ka)} = E(ka)$$

von Mises and Pollaczek-Geiringer, Zeitschrift Angewandte Mathematik und Mechanik 9, 58 (1929)

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von Mises and Pollaczek-Geiringer, Zeitschrift Angewandte Mathematik und Mechanik 9, 58 (1929)

- Modern computational linear algebra uses more sophisticated methods, e.g.

Lanczos algorithm

Lanczos, J. Res. Natl. Bur. Stand. B 45, 255 (1950)

Applied to LQCD since at least Barbour et al (1984)

$$|v_j\rangle \propto [T - T^{(m)}]|v_{j-1}\rangle$$

$$T^{(m)}_{ij} = \langle v_i|T|v_j\rangle \quad \Rightarrow \quad E^{(m)}_k = -\ln \lambda^{(m)}_k$$

- Exponentially faster convergence for systems with small gaps $\delta = a(E_1 - E_0)$

Kaniel, Mathematics of Computation 20, 369 (1966)

Paige, PhD thesis 1971

Saad, SIAM 17 (1980)

$$|E_0 - E^{(m)}_0| \propto e^{-4m\sqrt{\delta}} \ll |E_0 - E(ka)| \propto e^{-2m\delta}$$

The residual bound

- Lanczos approximation error after finite number of iterations directly computable:

$$\min_{\lambda \in \{\lambda_n\}} |\lambda_k^{(m)} - \lambda| \leq |\beta_{m+1}\, s_{mk}^{(m)}|$$

Eigenvectors of $T^{(m)}$

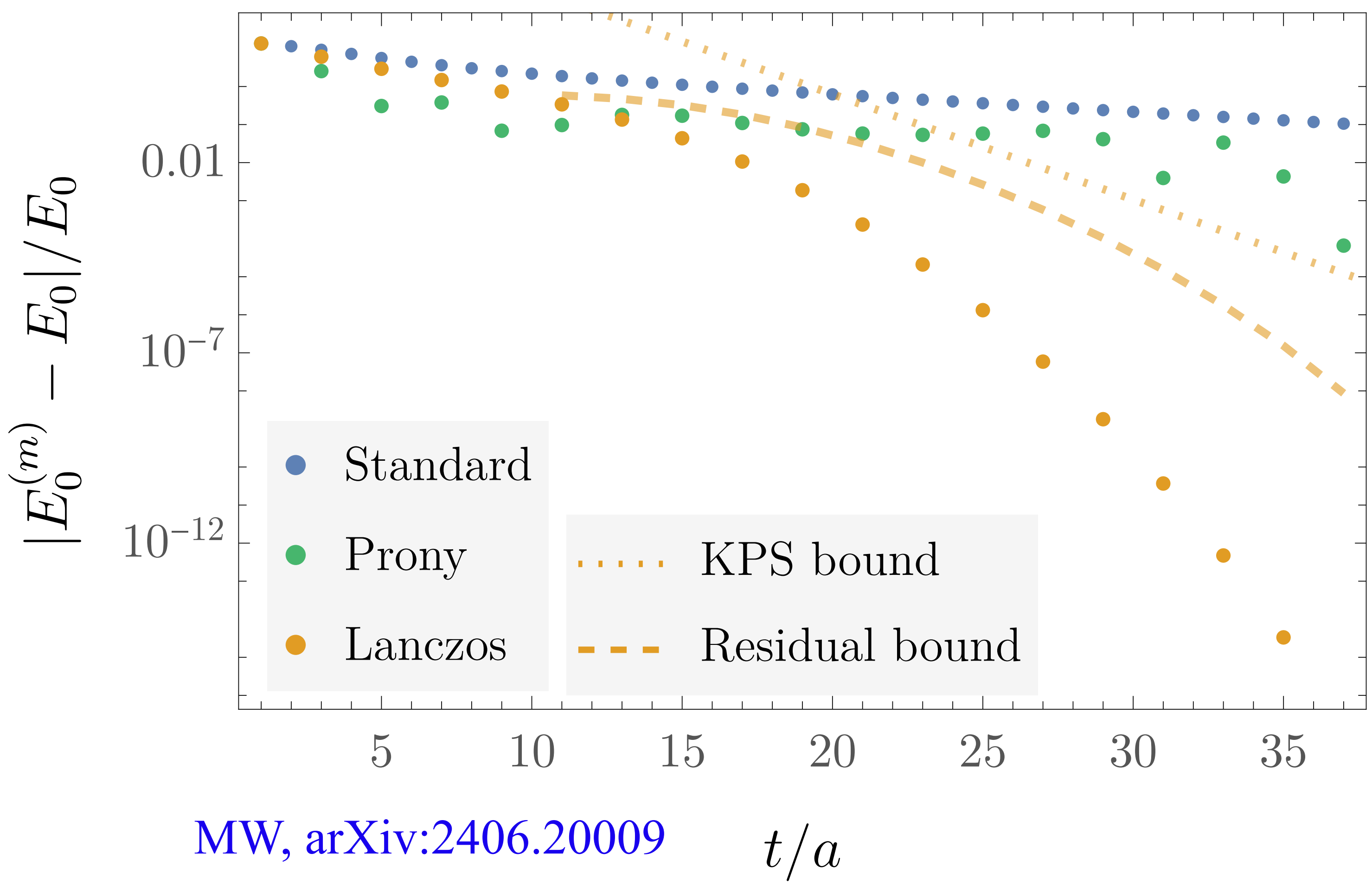
Matrix element $T^{(m)}_{m(m+1)}$

Paige, PhD thesis 1971

Rigorous quantification of excited-state effects!

But the LQCD transfer matrix is infinite-dimensional….

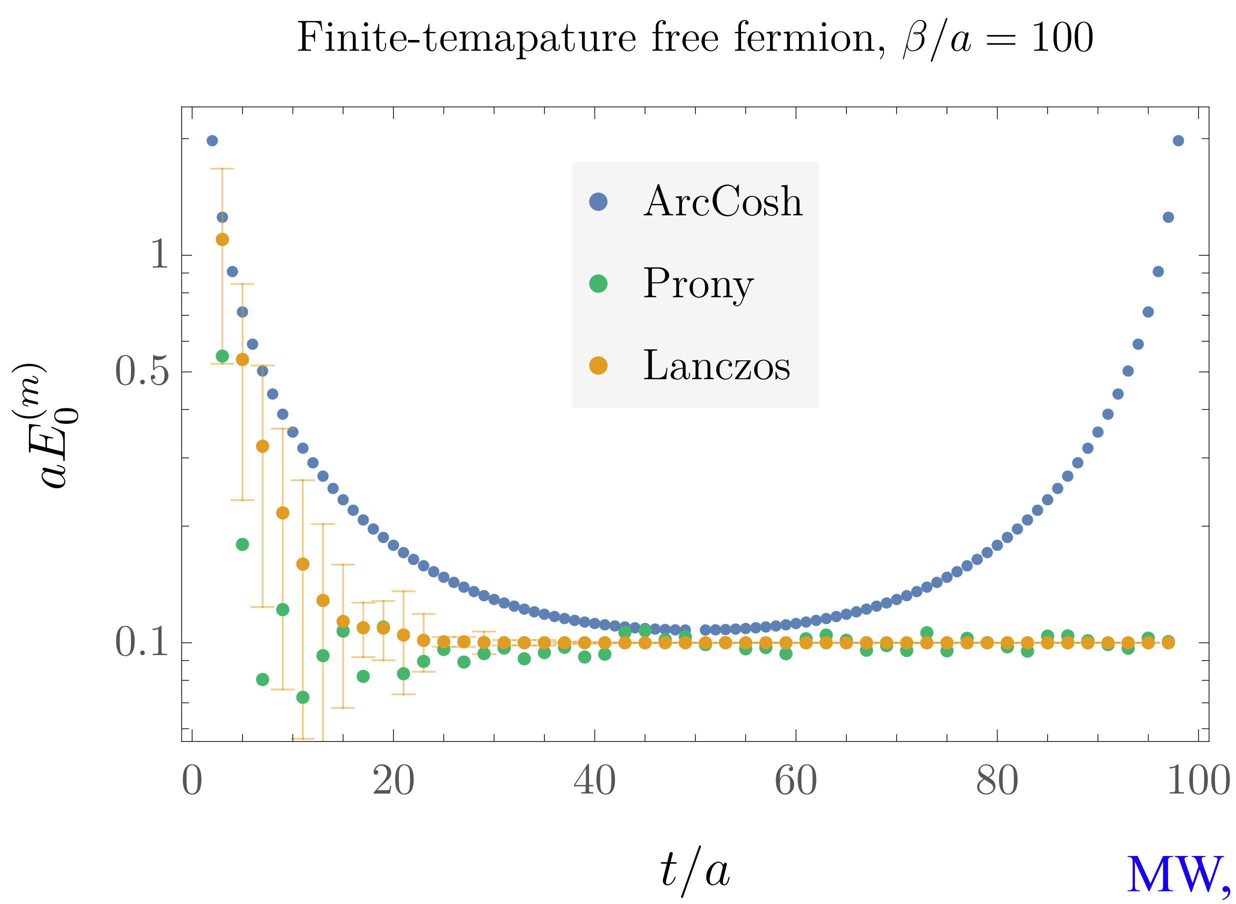
- Applying Lanczos feasible by computing matrix elements $T_{ij}^{(m)}$ recursively
- Faster convergence evident in studies of toy data

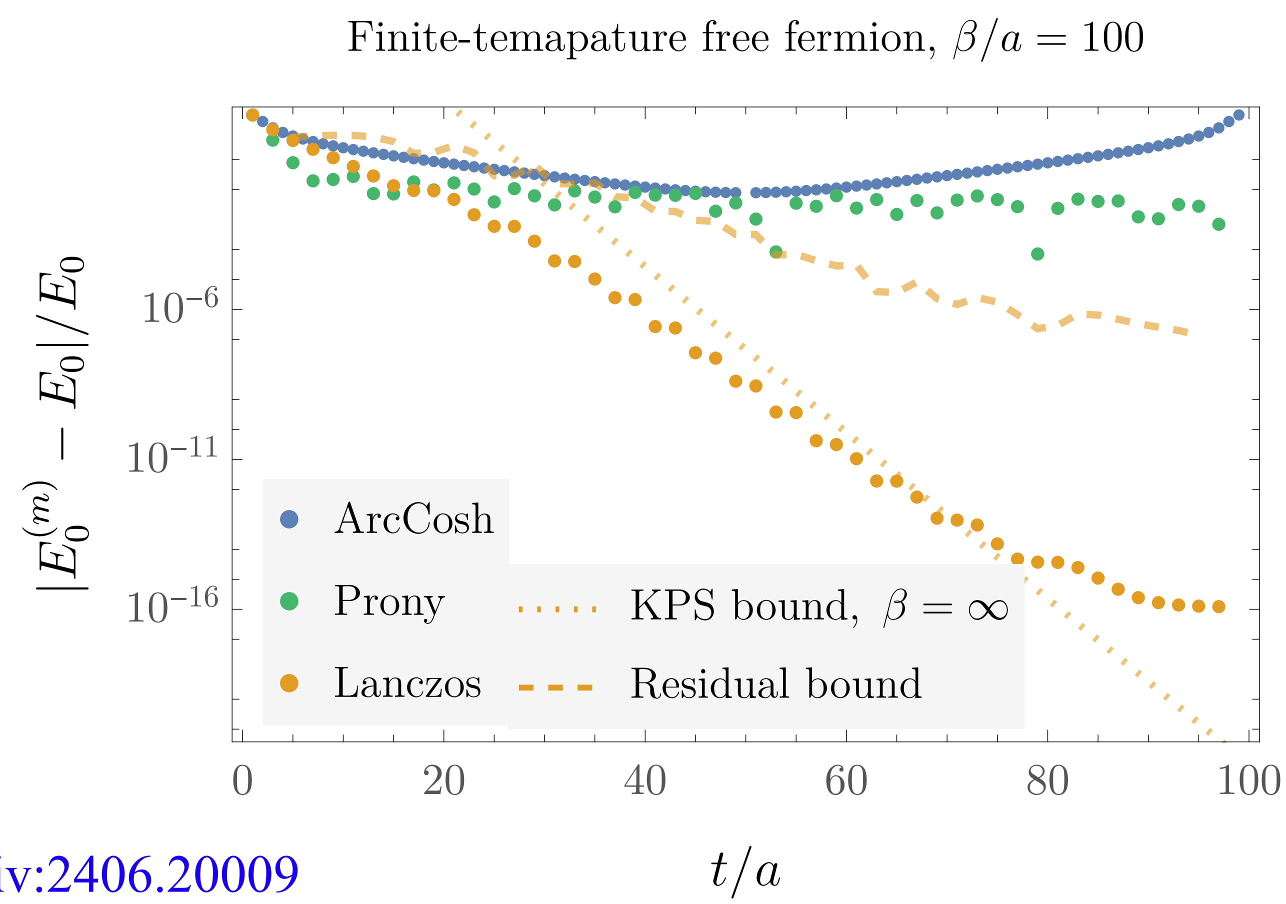


MW, arXiv:2406.20009

Heating things up

- Lanczos works at finite inverse temperature (temporal lattice extent)
- Eigenvalues converge and residual bound is accurate even past the midpoint of the lattice





MW, arXiv:2406.20009

- Arbitrary-precision arithmetic required to achieve high convergence
- Lanczos is known to be numerically unstable with fixed-precision arithmetic … what about statistical noise?

Will noise destroy Lanczos?

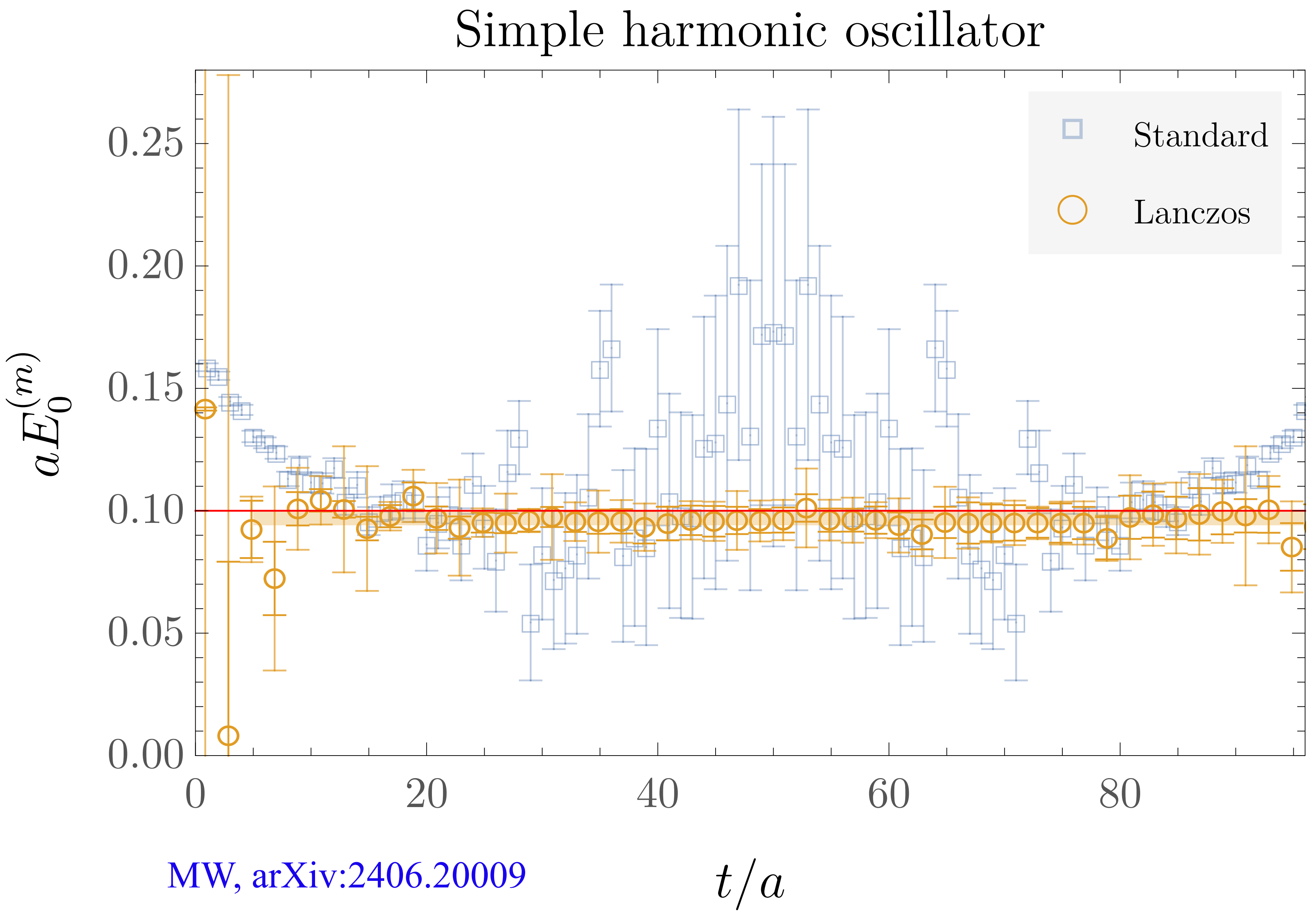
Will noise destroy Lanczos?

- No

Will noise destroy Lanczos?

- No

- Lanczos is surprisingly robust to large-time correlation function noise



MW, arXiv:2406.20009

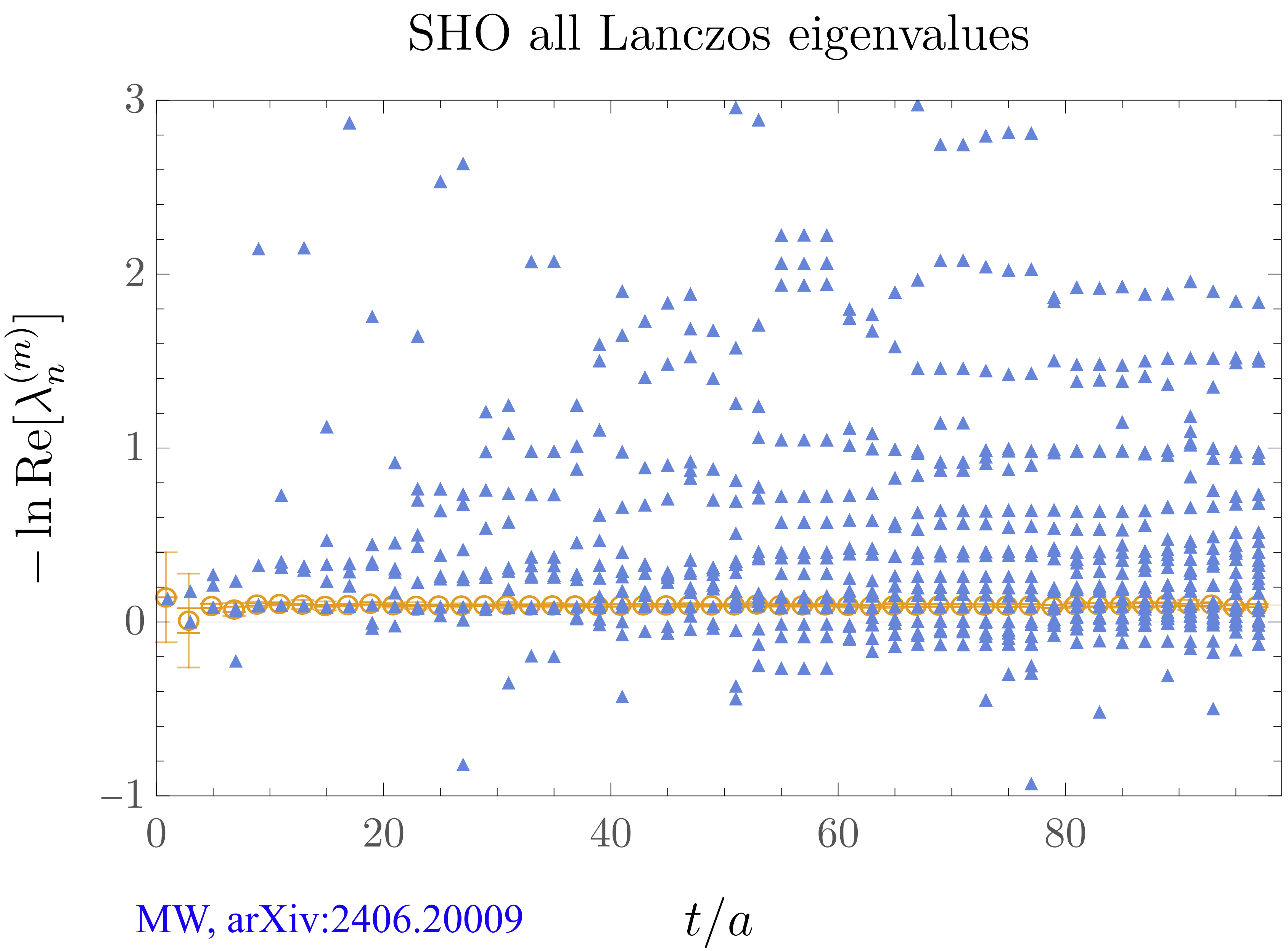
Is it really that easy?

Is it really that easy?

- No

Is it really that easy?

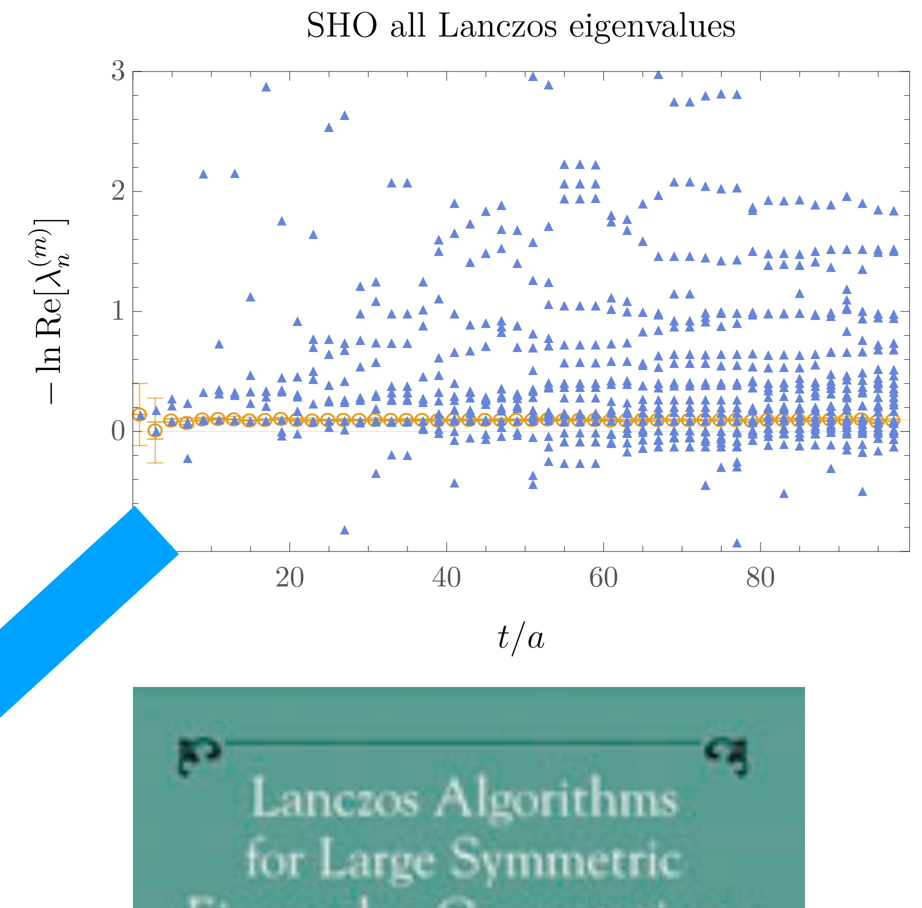
- No
- Lanczos produces an increasingly dense forest of “spurious eigenvalues”

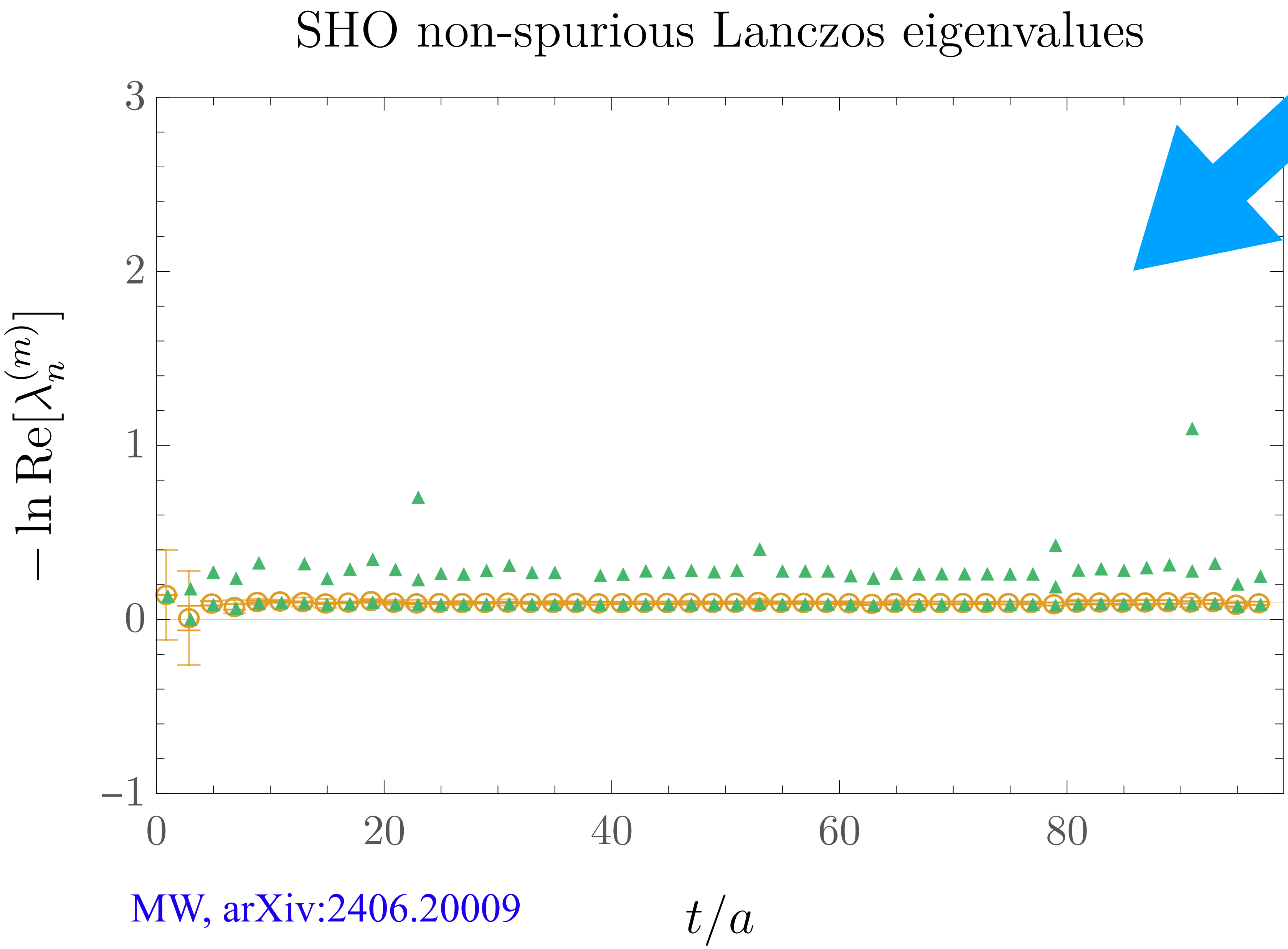


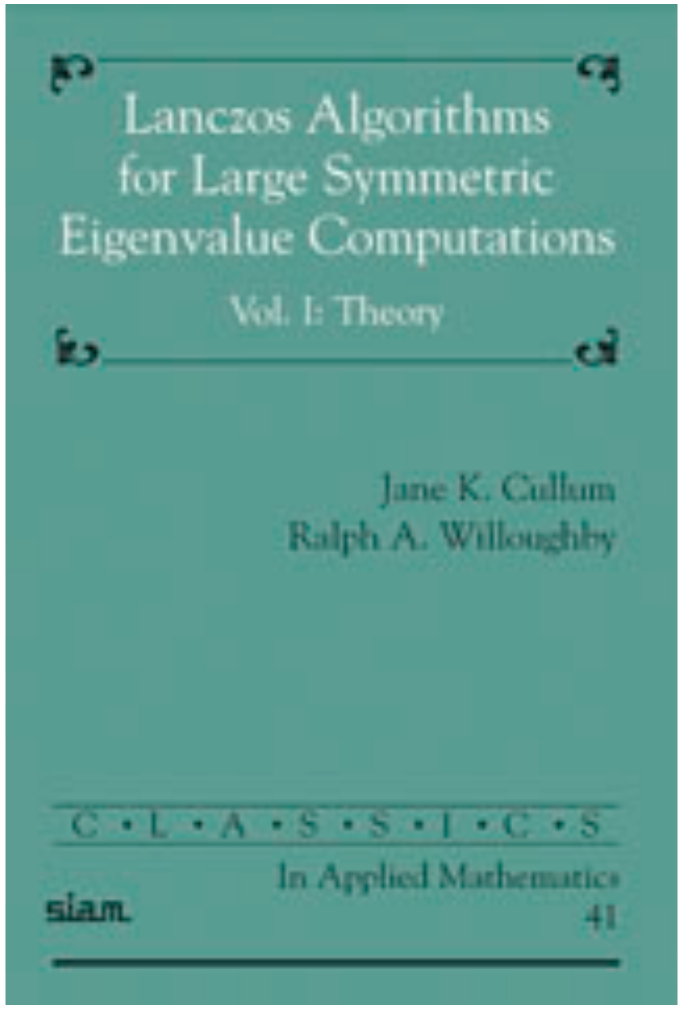
MW, arXiv:2406.20009

Spurious eigenvalues

- We need a way to automatically detect which eigenvalues are spurious and get rid of them







MW, arXiv:2406.20009

Cullum-Willoughby

- Jane Cullum and Ralph Willoughby developed a useful criterion for identifying spurious eigenvalues in 1981

Cullum and Willoughby, Journal of Computational Physics 44, 329 (1981)

DEFINITION 1. Spurious ≡ Outwardly similar or corresponding to something without having its genuine qualities.

$$T^{(m)} = \begin{pmatrix} \alpha_1 & \beta_2 & & & & 0 \\ \gamma_2 & \alpha_2 & \beta_3 & & & \\ & \gamma_3 & \alpha_3 & \ddots & & \\ & & \ddots & \ddots & \beta_{m-1} & \\ & & & \gamma_{m-1} & \alpha_{m-1} & \beta_m \\ 0 & & & & \gamma_m & \alpha_m \end{pmatrix}$$

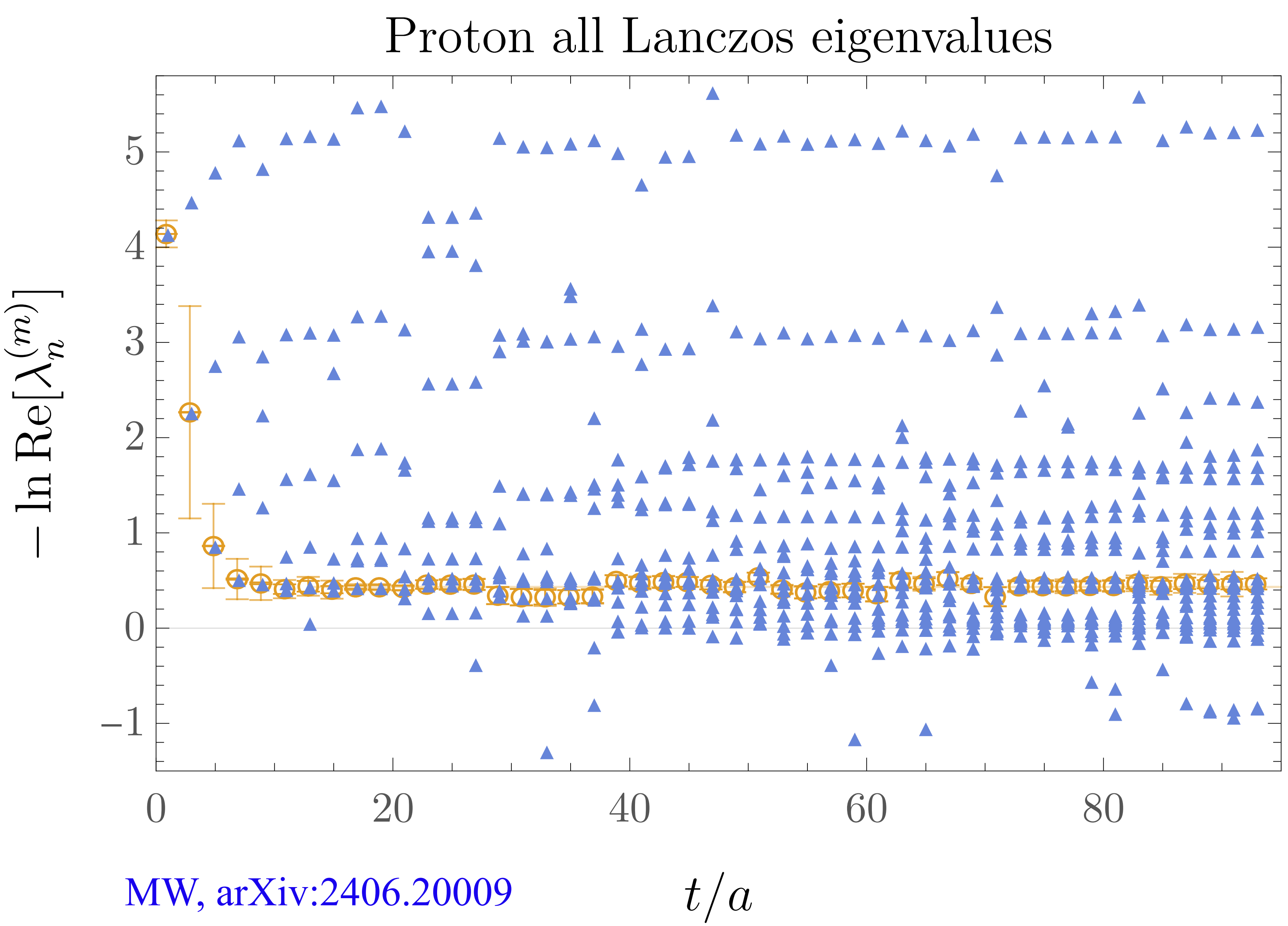
$$T_2^{(m)} = \begin{pmatrix} \cancel{\alpha_1} & \cancel{\beta_2} & & & & 0 \\ \cancel{\gamma_2} & \alpha_2 & \beta_3 & & & \\ & \gamma_3 & \alpha_3 & \ddots & & \\ & & \ddots & \ddots & \beta_{m-1} & \\ & & & \gamma_{m-1} & \alpha_{m-1} & \beta_m \\ 0 & & & & \gamma_m & \alpha_m \end{pmatrix}$$

DEFINITION 2. Any simple eigenvalue of T_m that is pathologically close to an eigenvalue of $\hat{T}_2$ will be called "spurious."

Think positive

- Since transfer matrix is positive-definite by assumption, any eigenvalues with non-zero imaginary parts can be discarded as spurious
- “Non-zero” can be kept exact even in the presence of noise by adopting oblique Lanczos formalism

  Saad, SIAM 19 (1982)



MW, arXiv:2406.20009

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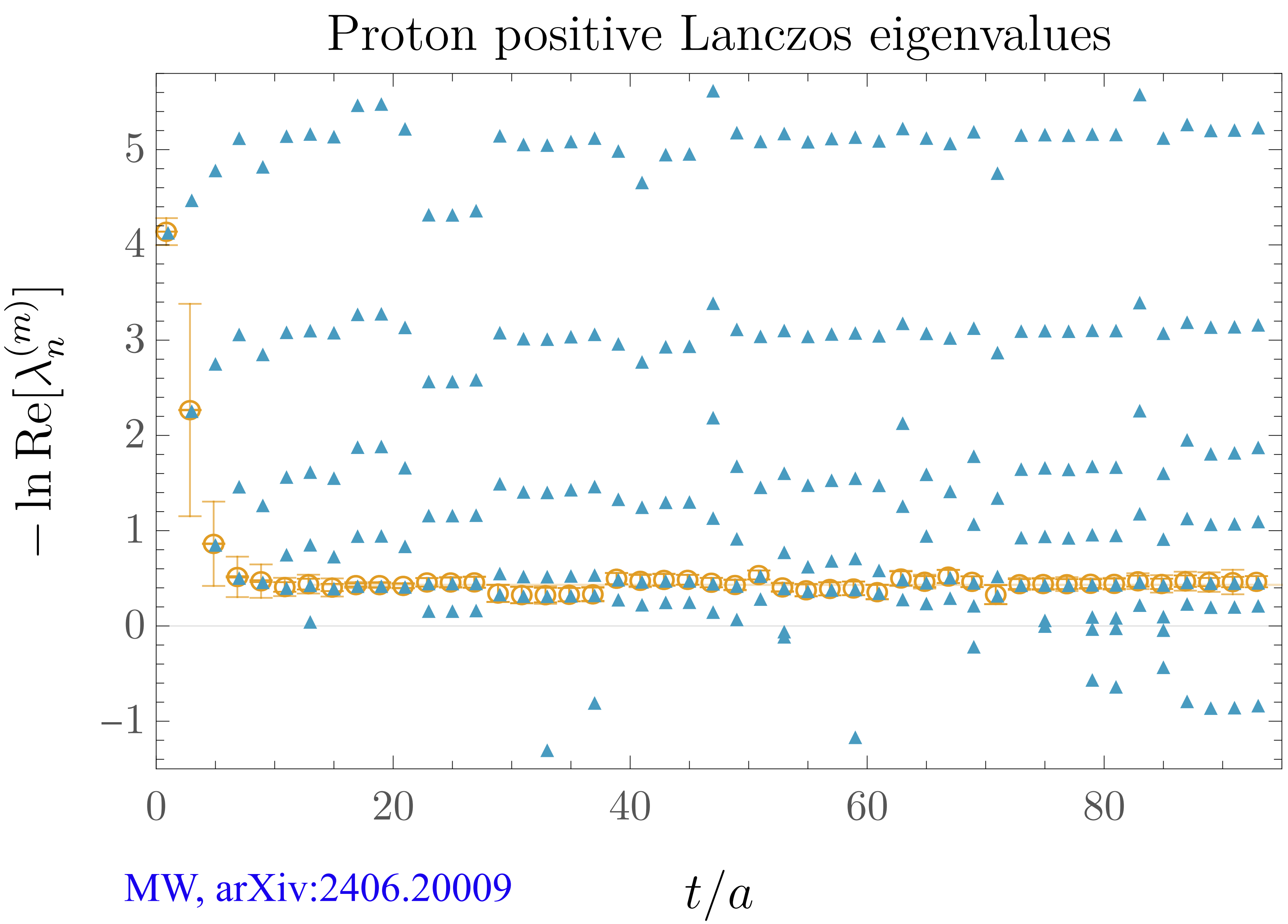


- This gets rid of many spurious eigenvalues but still leaves some that must be wrong because they correspond to $M_N < m_\pi$

MW, arXiv:2406.20009

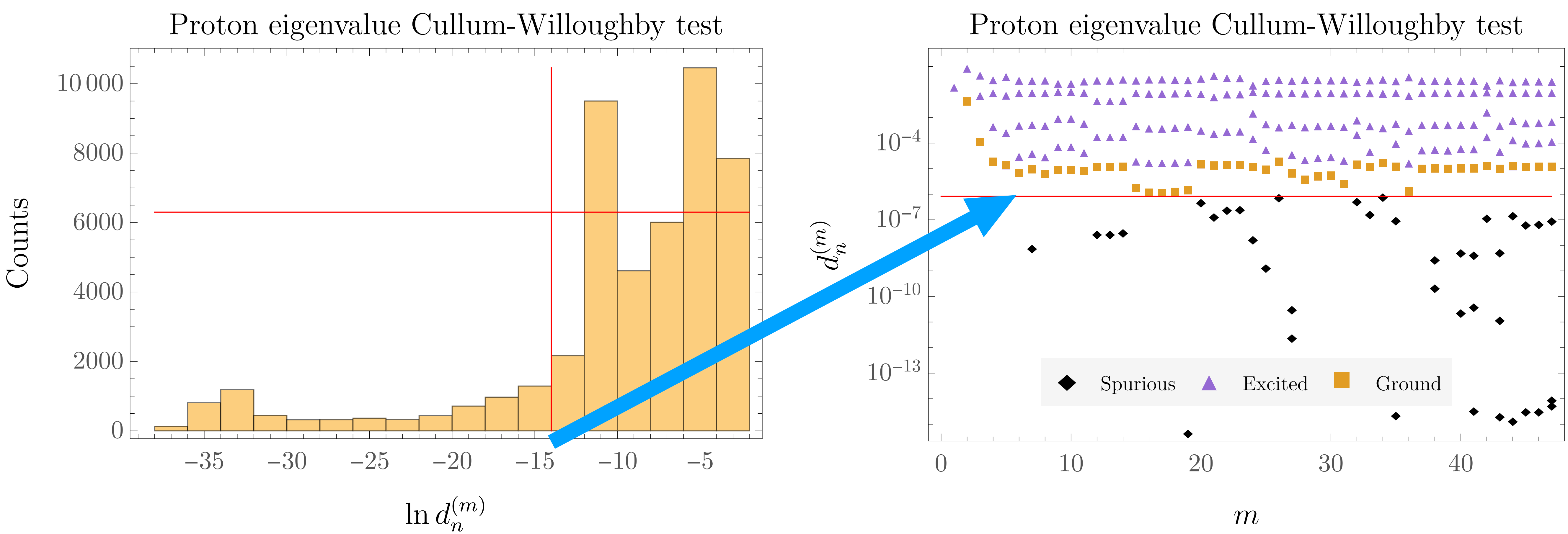
Bootstrapping Cullum-Willoughby

- Defining “pathologically close” is easy for finite matrices with floating-point roundoff error, harder for Monte Carlo simulations of infinite-dimensional matrices

Definition 1. Spurious ≡ Outwardly similar or corresponding to something without having its genuine qualities.

- Distances between $T^{(m)}$ and $T_2^{(m)}$ fluctuate due to noise much more for spurious than non-spurious eigenvalues

- Use bootstrap histograms to define cutoff

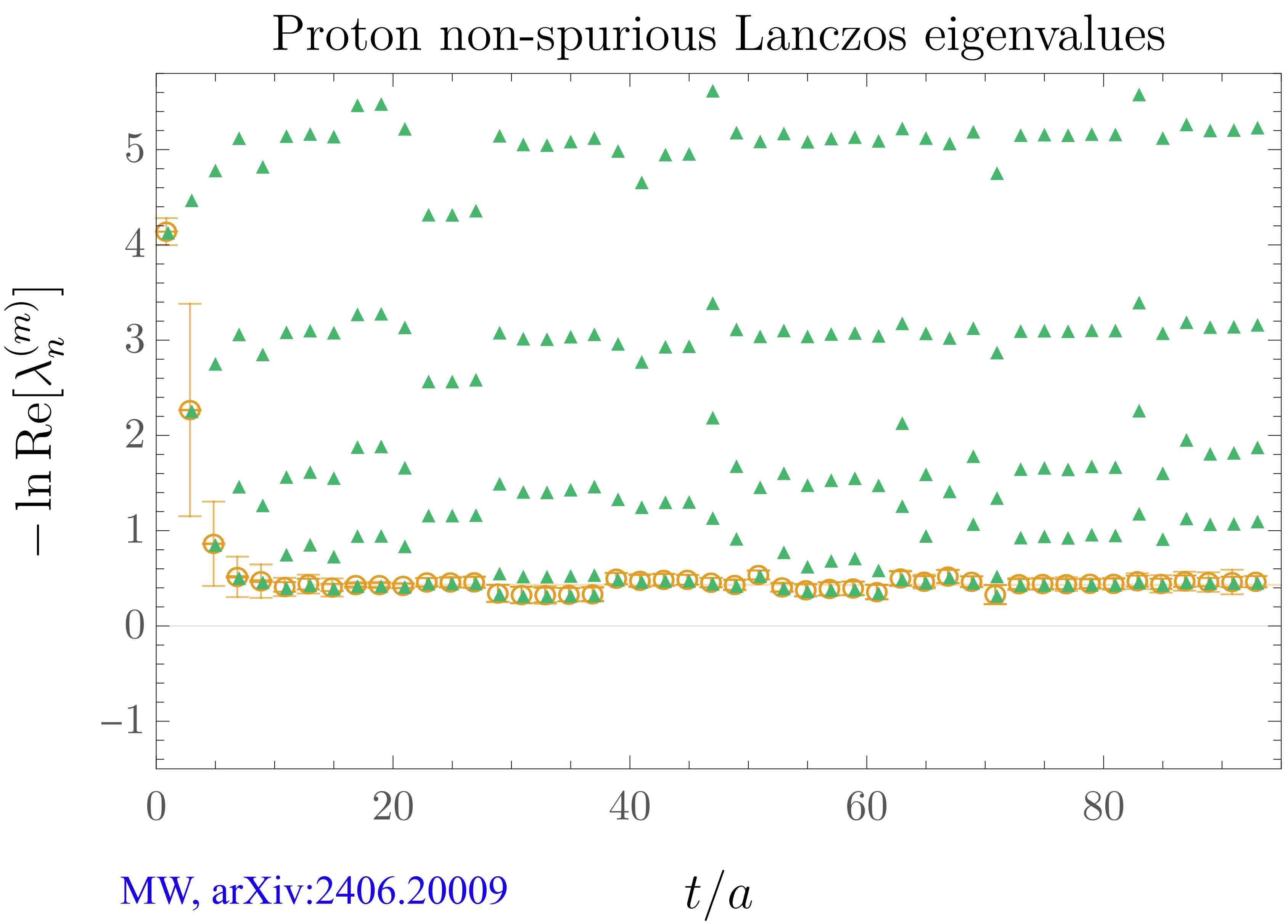


Non-spurious proton energies

- Largest eigenvalue not removed as spurious defines ground-state energy

$$E_0 = -\ln \lambda_0^{(m)}$$

- Excited-state energies also accessible

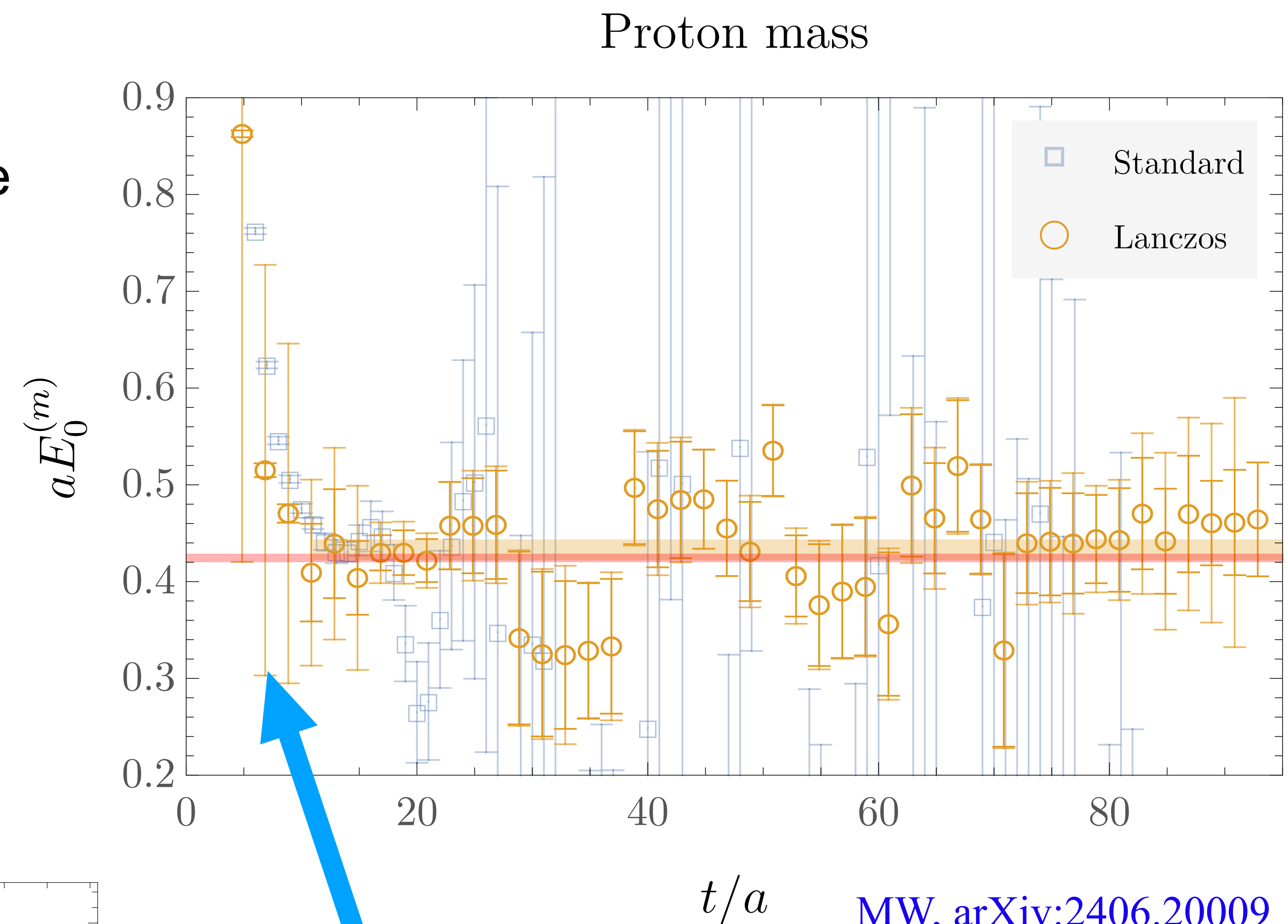


MW, arXiv:2406.20009

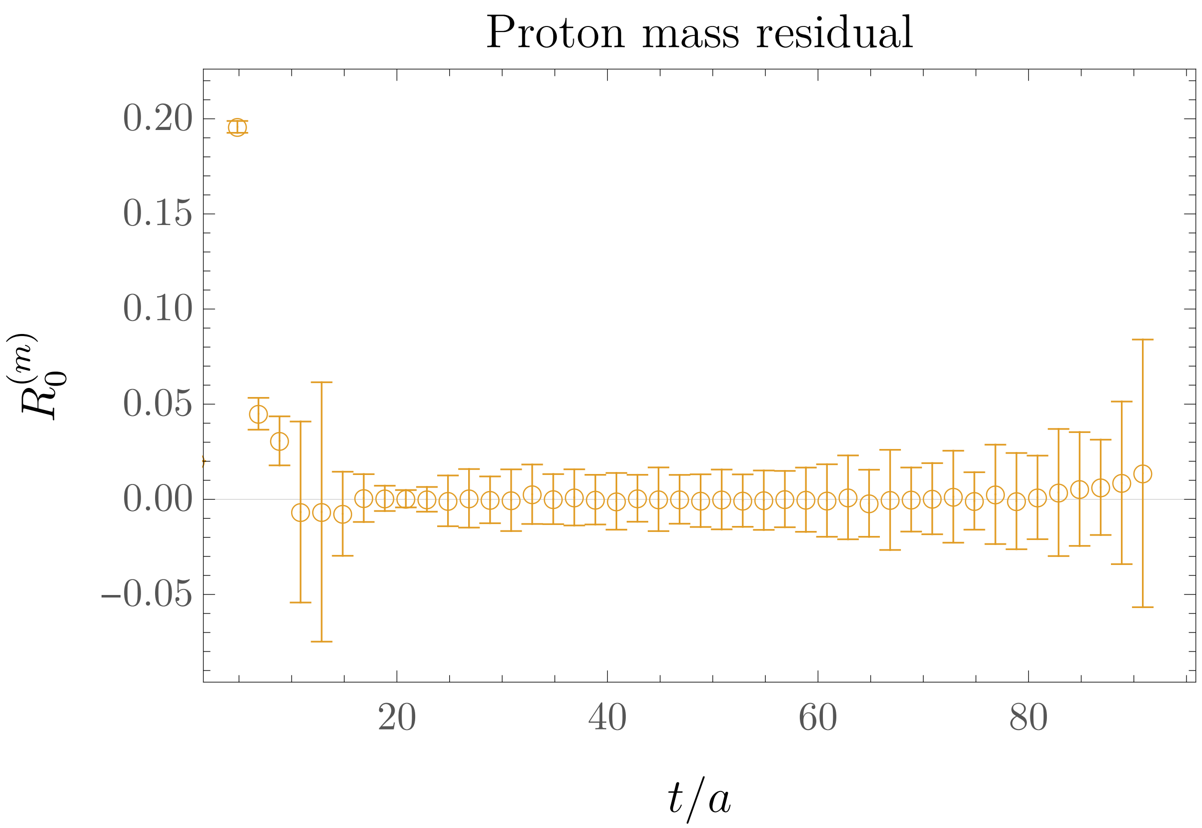
Lanczos proton mass results

- Bootstrap uncertainties complicated by outliers due to spurious eigenvalue misidentification within bootstrap samples

- Robust estimators e.g. based on confidence intervals critical



MW, arXiv:2406.20009

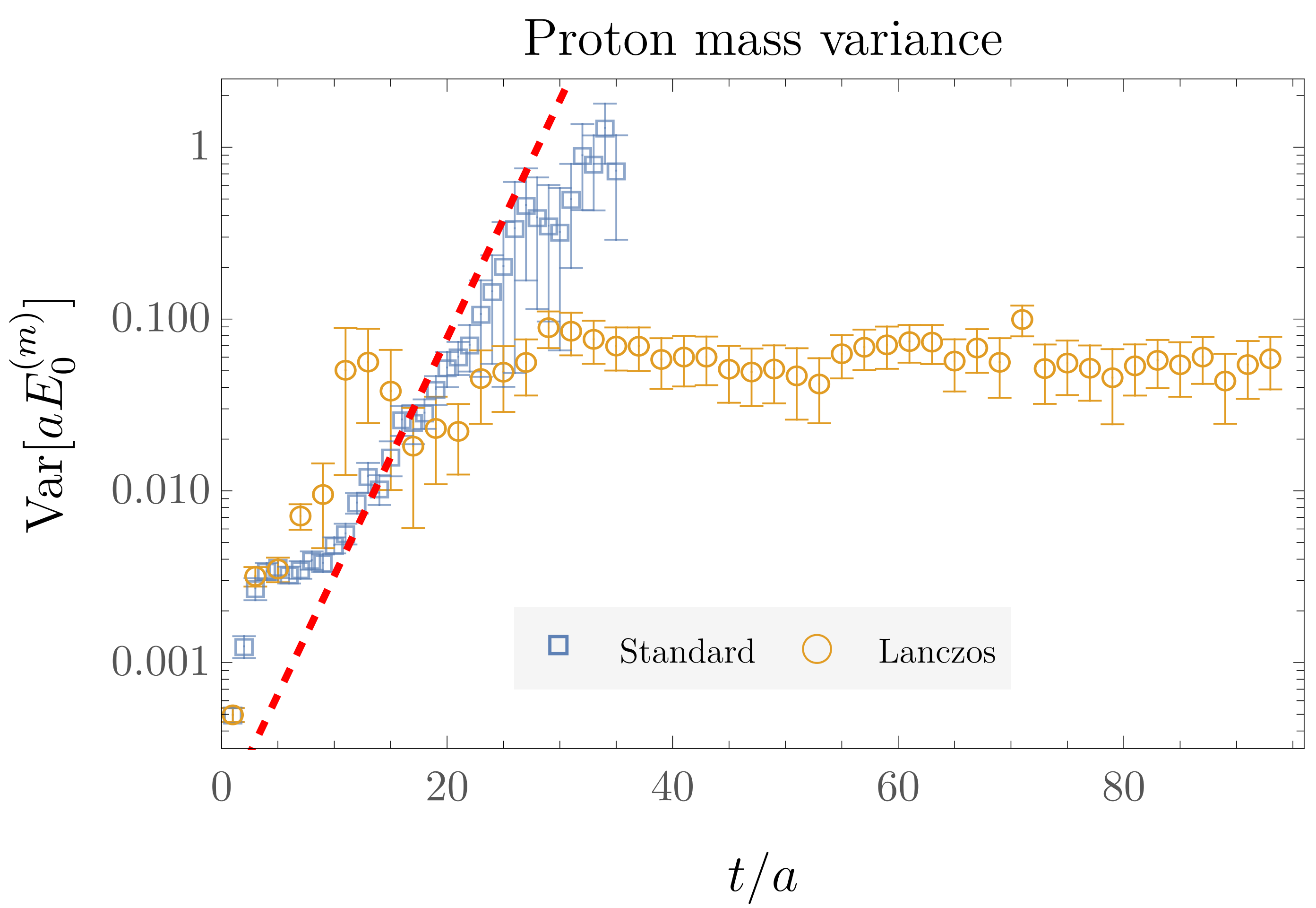


- Residual bound can be used to identify when Lanczos results have converged, provides bound on finite-t approximation errors

Projecting out the noise

- Signal-to-noise of Lanczos results does not degrade exponentially for large t

Why?



- Projection operator solution to signal-to-noise problem:

Della Morte and Giusti, Comp. Phys. Communications 180 (2009)

$$\langle \mathcal{O}(t)\overline{\mathcal{O}}(0)\rangle \longrightarrow \langle \mathcal{O}(t)P\overline{\mathcal{O}}(0)\rangle$$

removes states from variance without quantum numbers of "signal squared," e.g. three-pion states in nucleon variance

- Building such projectors is hard — but Lanczos provides Krylov-space approximations

Saad, SIAM 17 (1980)   Saad, SIAM 19 (1982)

$$P_n^{(m)} \equiv |y_n^{(m)}\rangle\langle y_n^{(m)}| \approx |n\rangle\langle n|$$

Lanczos LQCD spectroscopy

- Lanczos enables rapid convergence even with small energy gaps
- Two-sided error bounds allow excited-state effects to be fully quantified
- Lanczos results do not show exponential signal-to-noise degradation

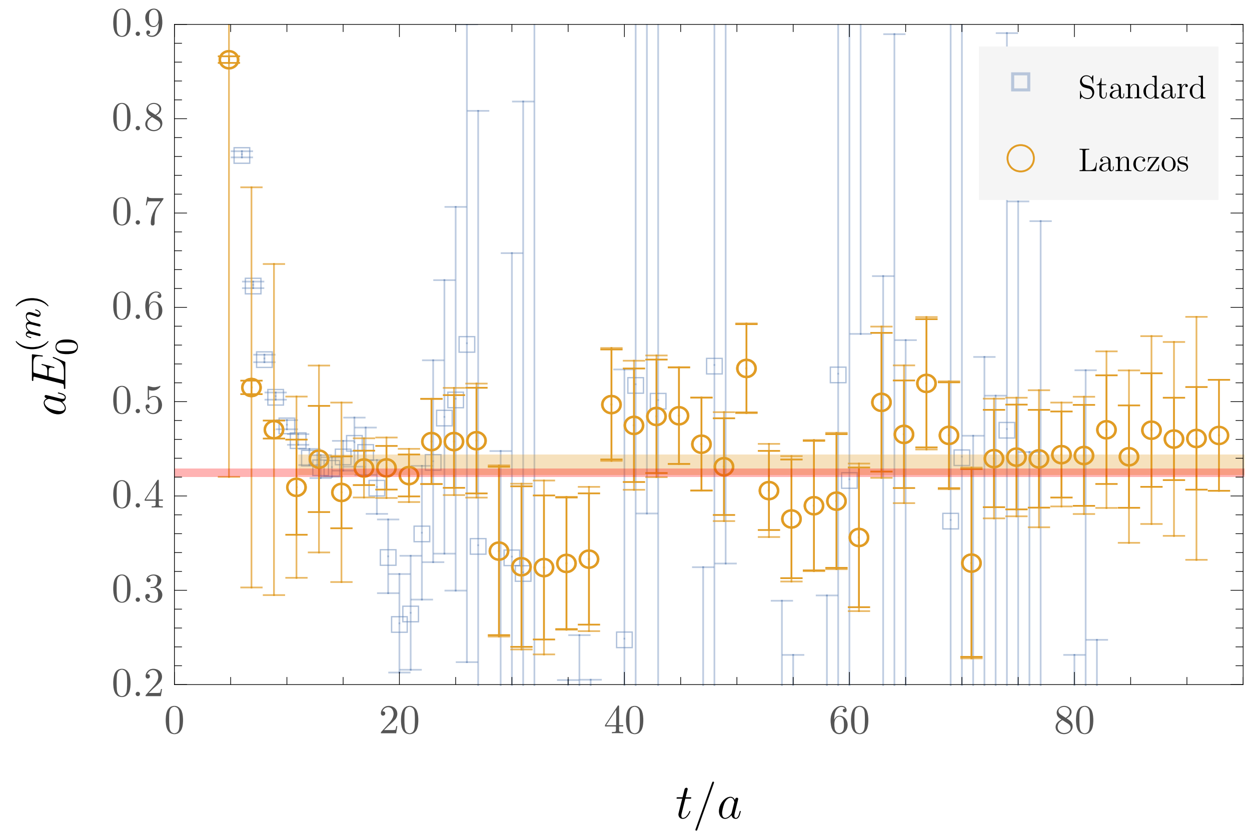
~~1) Too many Wick contractions~~

Detmold and Orginos, PRD 87 (2013)

2) Small energy gaps to excited states

3) Exponential signal-to-noise degradation

Proton mass



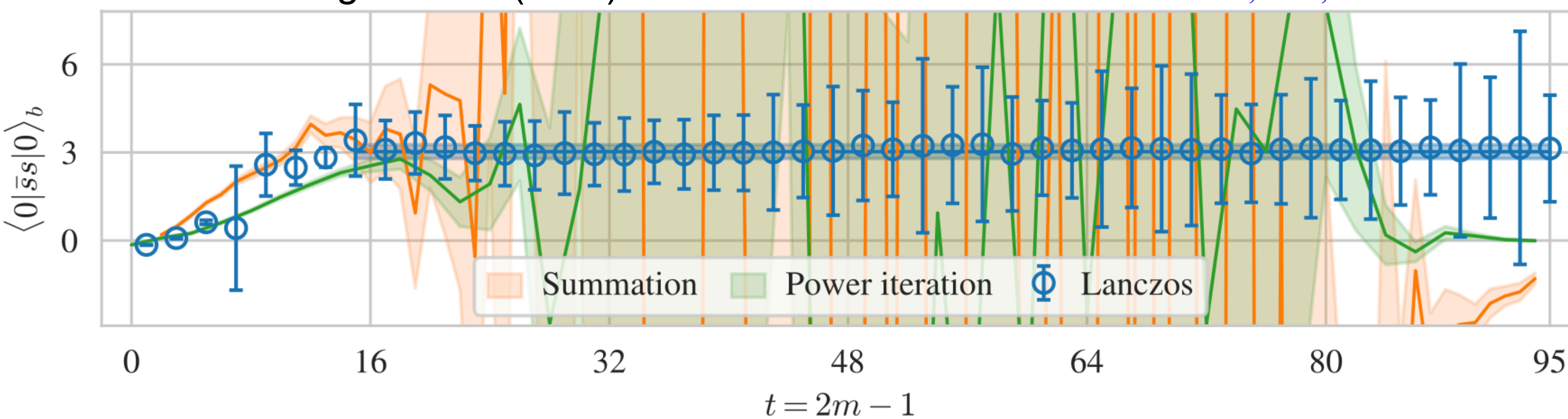
- Spurious eigenvalues lead to challenges: Cullum-Willoughby + bootstrap sufficient?

Lanczos shows promise for LQCD studies of nucleons and nuclei where isolating ground states is challenging; further study needed!

Lanczos for matrix elements

Nucleon strange scalar (bare) matrix element

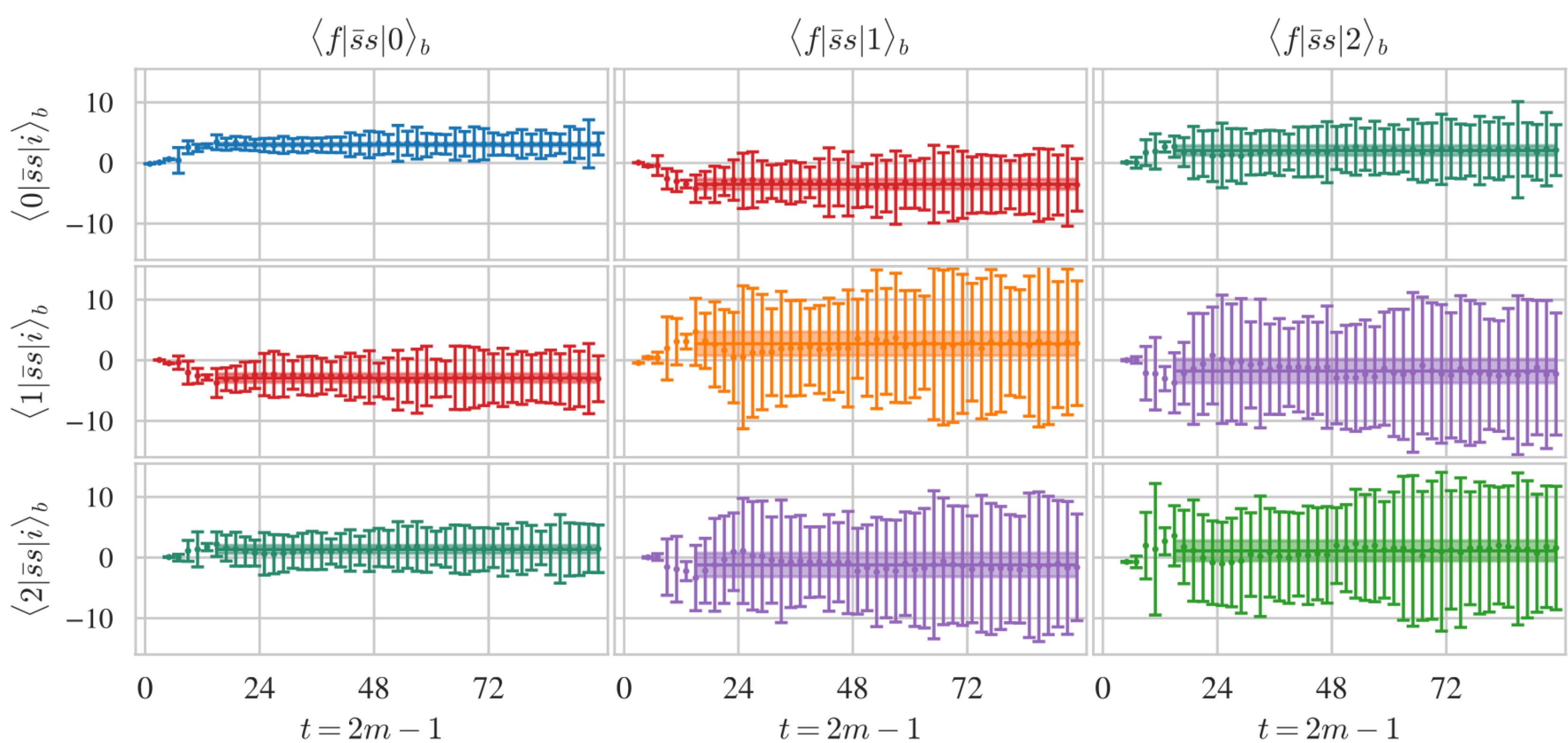
Hackett, MW, arXiv:2407.21777

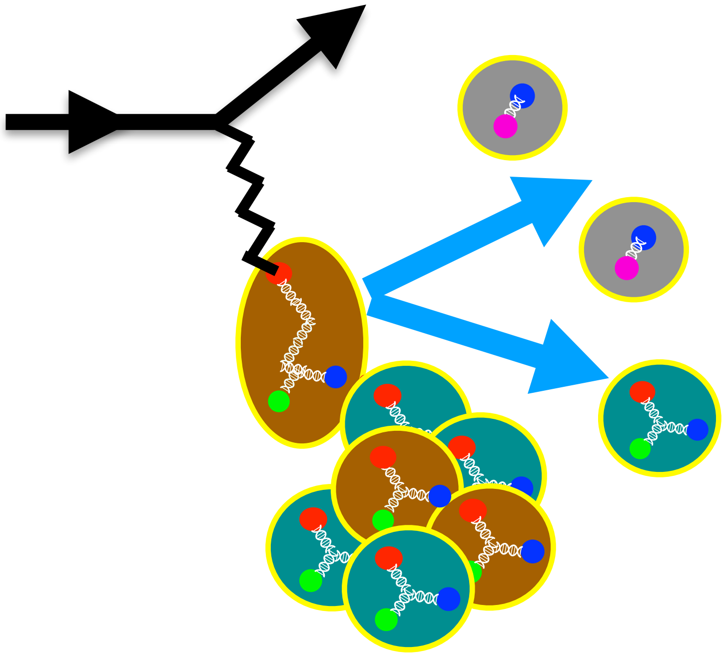


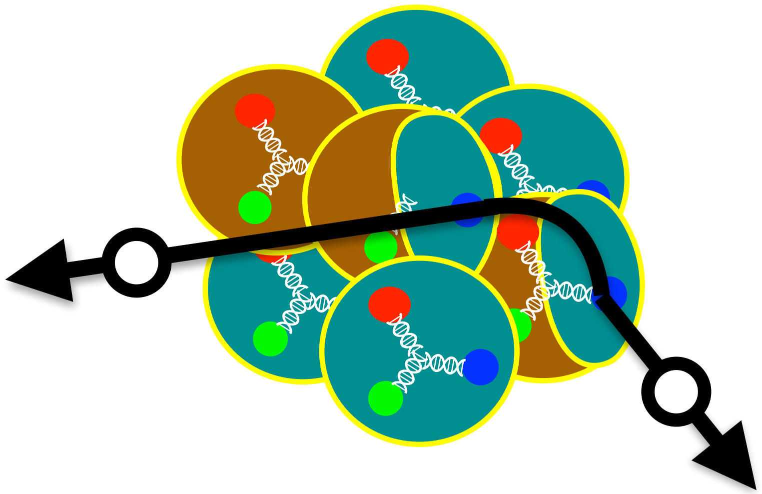
Lanczos eigenvectors provide change of basis allowing matrix elements to be extracted from 3pt functions with simple matrix multiplication

- Excited / transition matrix elements accessible

See Dan Hackett's talk at 12:35 Friday







Thank you!