Fermilab U.S. DEPARTMENT OF ENERGY Office of Science

Uncertainties in lattice QCD spectroscopy

Michael Wagman

MITP Topical Workshop: Uncertainty quantification in nuclear physics

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Lattice QCD

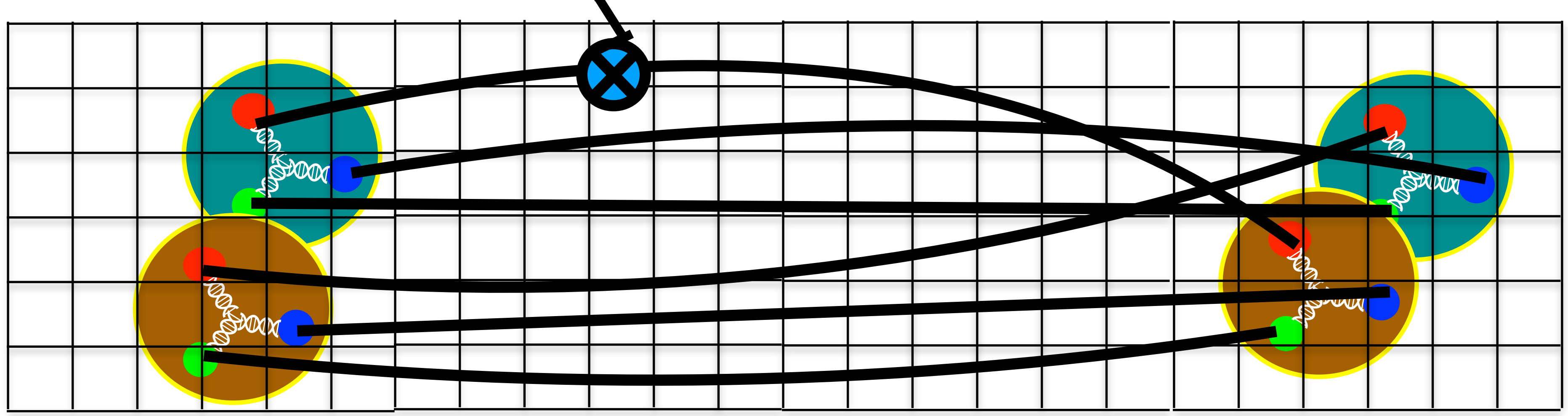
Lattice QCD enables nonperturabtive calculations of QCD path integrals numerically

$$\langle \mathcal{O} \rangle = \int \mathcal{D}U \mathcal{D}\overline{q} \mathcal{D}q \; e^{-S_{QCD}(U,q,\overline{q})} \; \mathcal{O}(U,q,\overline{q}) \approx \frac{1}{N_{\text{cfg}}} \sum_{i=1}^{N_{\text{cfg}}} \mathcal{O}(U_i)$$

Quark fields integrated out analytically, propagators obtained with matrix inversion

(Dirac matrix size ~ $10^9 \times 10^9$)

Monte Carlo sample gluon fields with probability $\propto e^{-S}$



$$\langle f | J | i \rangle \propto \langle 0 | \quad f \quad\quad J \quad\quad i^\dagger \quad | 0 \rangle$$

Finite volume + non-zero lattice spacing:

→ finite number of integrals to compute

$$\mathcal{D}q \equiv \prod_{\mu=1}^{4} \prod_{x_\mu=0}^{(L/a)-1} dq(x)$$

Nuclear physics from LQCD

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

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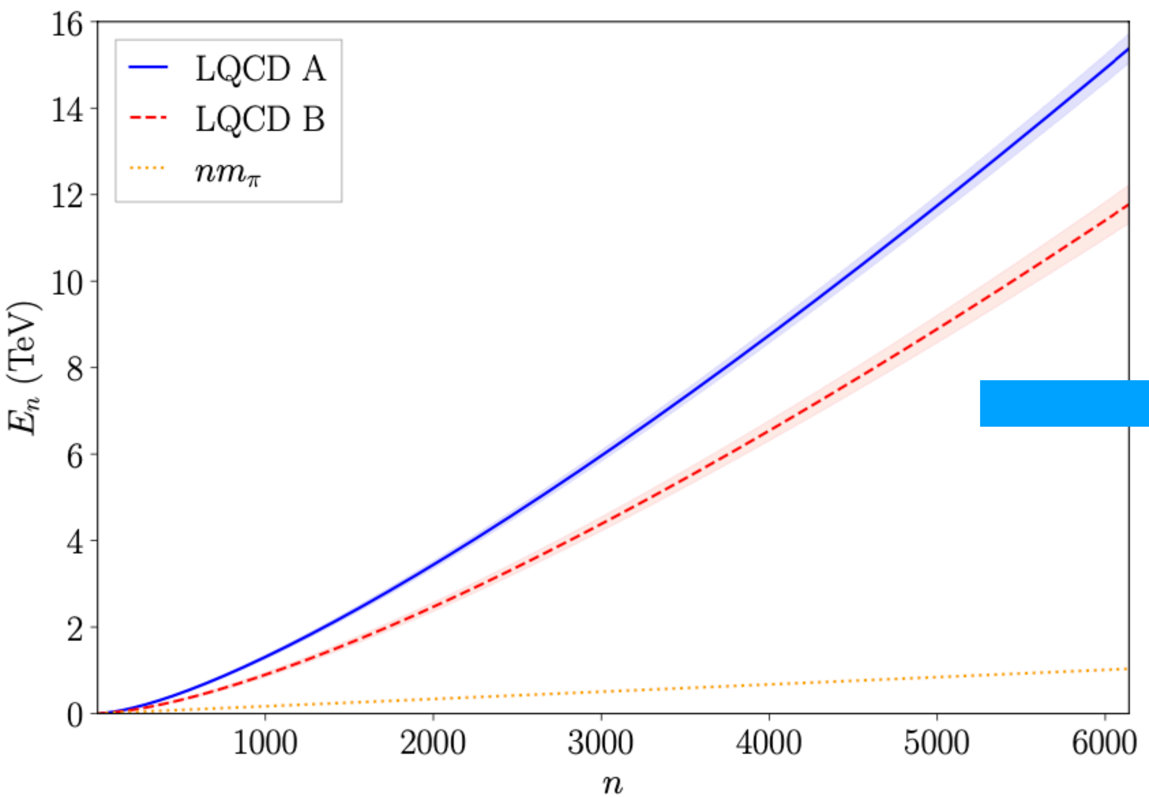
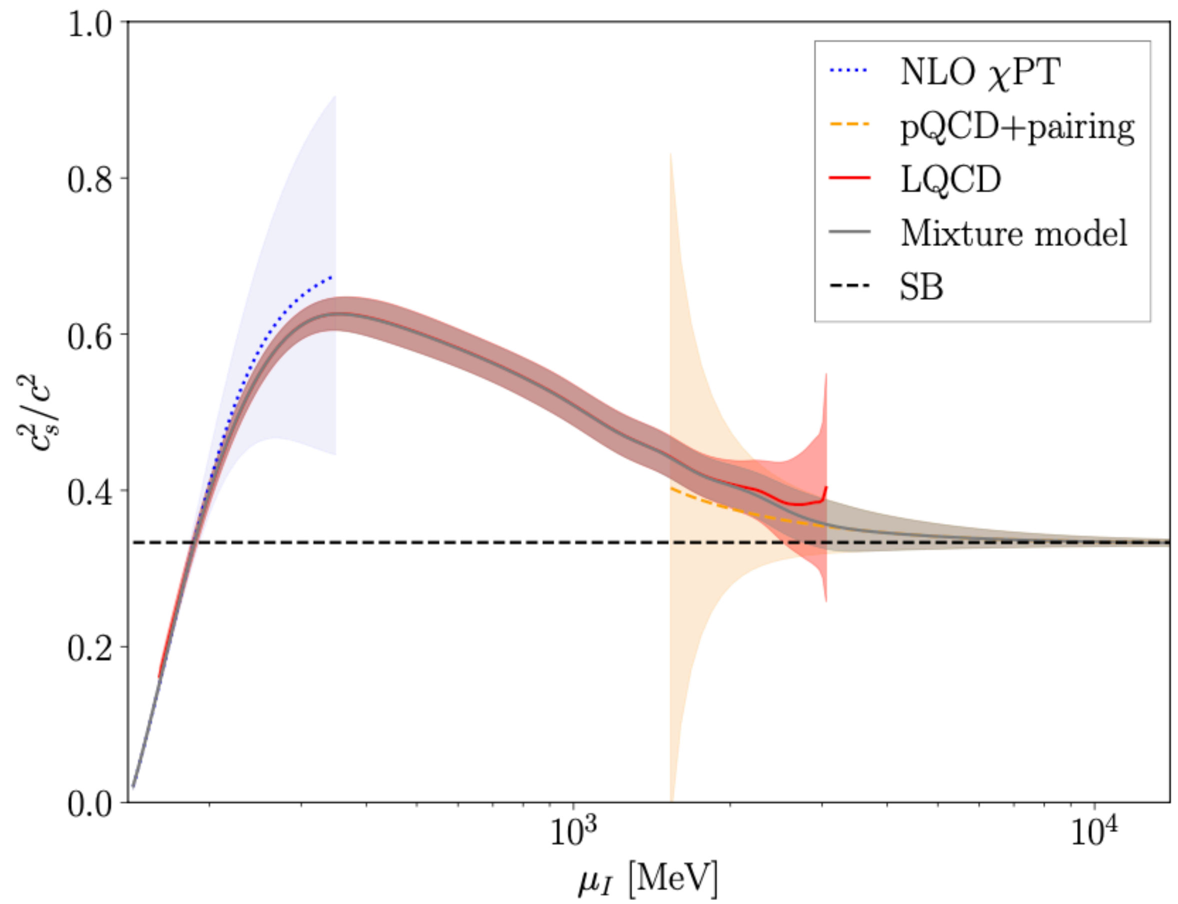
Energy spectrum of up to 6000 pions in a box:



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

Previous world record: 72 pions

Detmold, Orginos, and Shi, PRD 86 (20212)

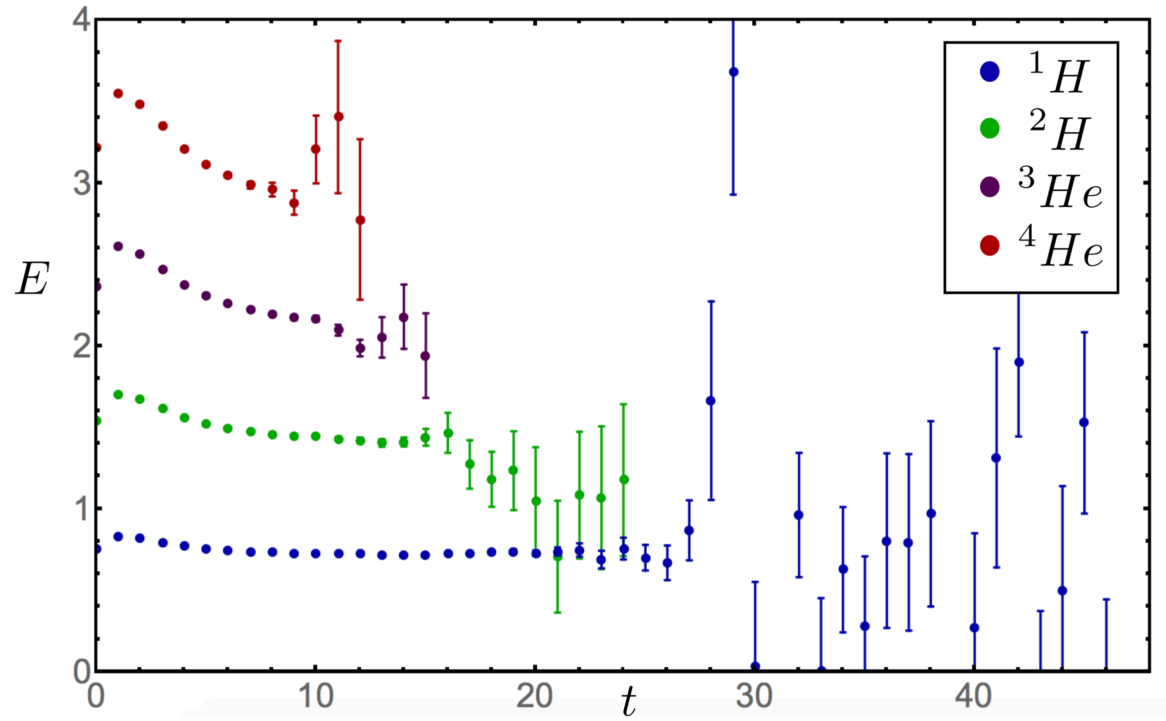
What's so hard about nuclei?

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



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

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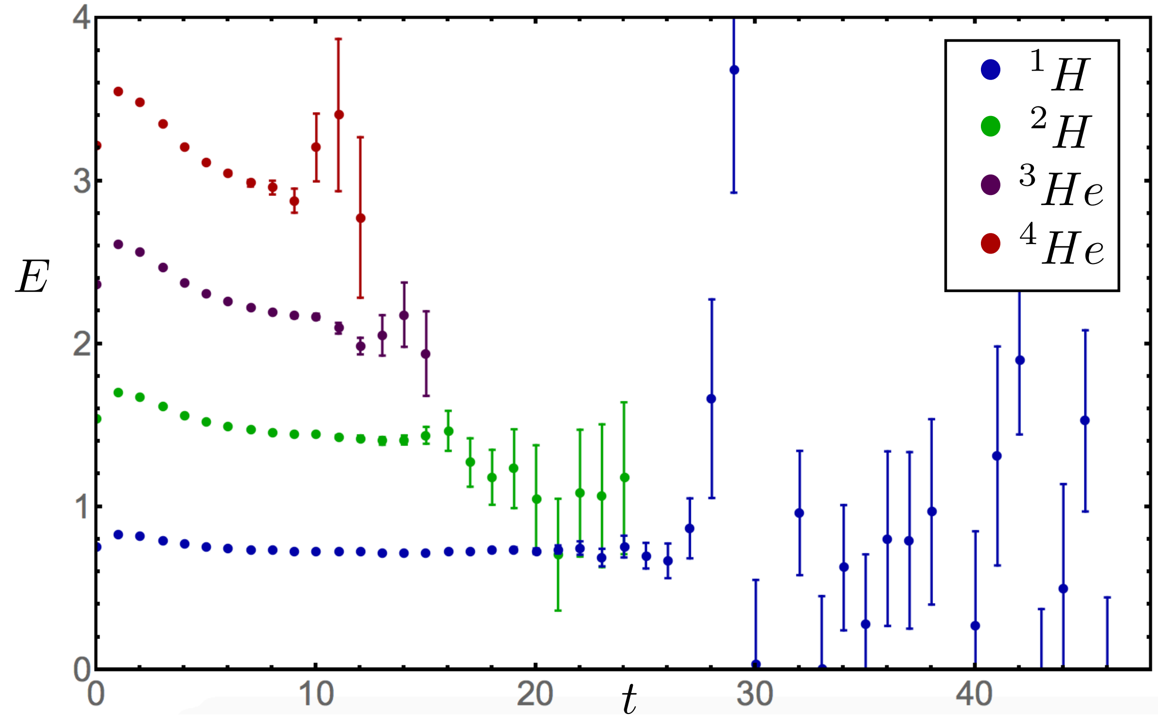
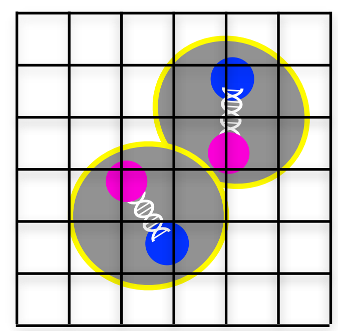


$$aE(t) = -\ln \frac{C(t+a)}{C(t)} = aE_0 + \ldots$$

Bound vs scattering states

Working in finite volume is not only necessary for LQCD, it can be helpful

- Excitation gaps vanish in infinite-volume for unbound systems
- Volume dependence of energy spectra can distinguish bound vs scattering states

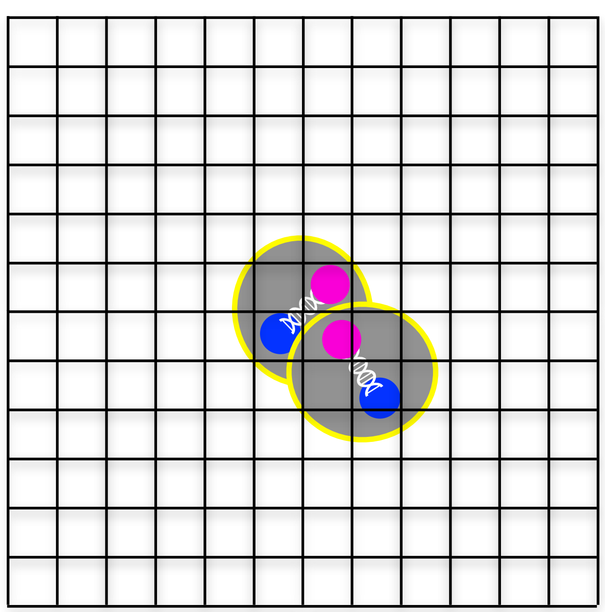


Infinite-volume bound state

$$[E(L) - E(\infty)] \propto \frac{e^{-\gamma L}}{\gamma L}$$

Infinite-volume scattering state

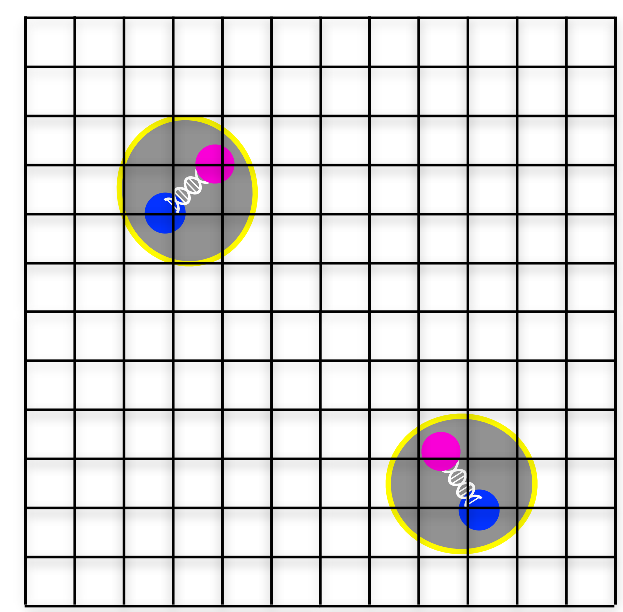
$$[E(L) - E(\infty)] \propto \frac{a}{ML^3}$$



Quantization condition proven for generic relativistic QFT

Lüscher, Commun. Math. Phys. 105 (1986)

Review: Briceño, Dudek, Young, Rev. Mod. Phys. 90 (2018)



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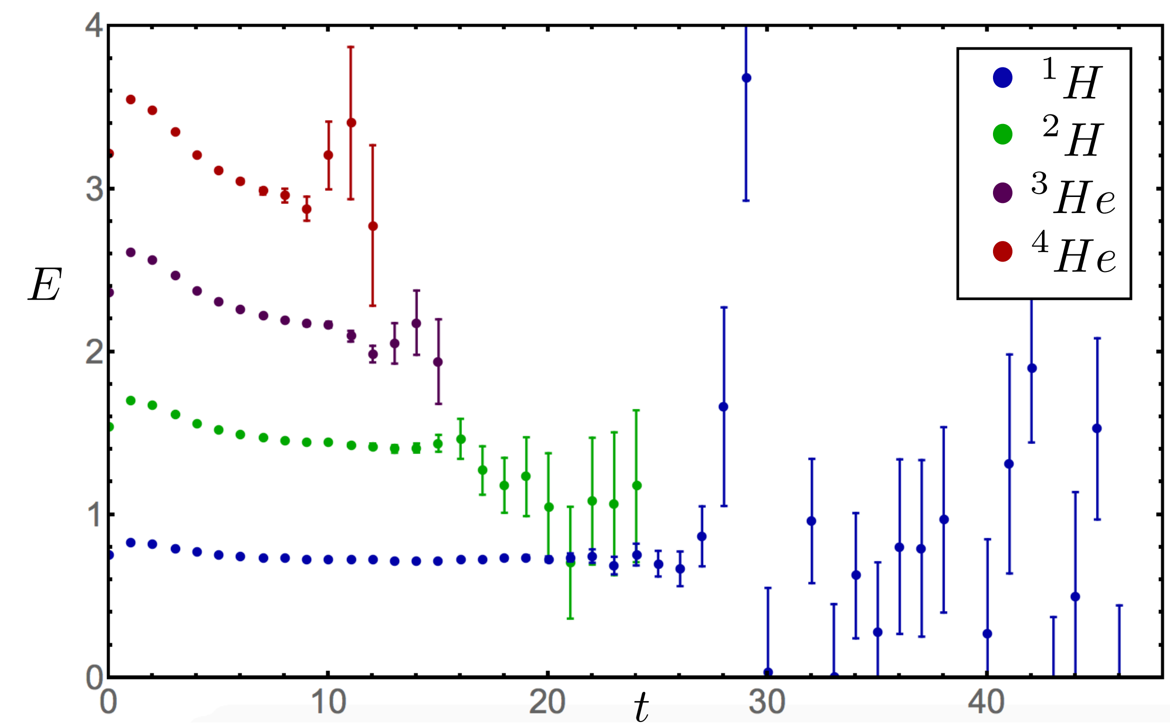


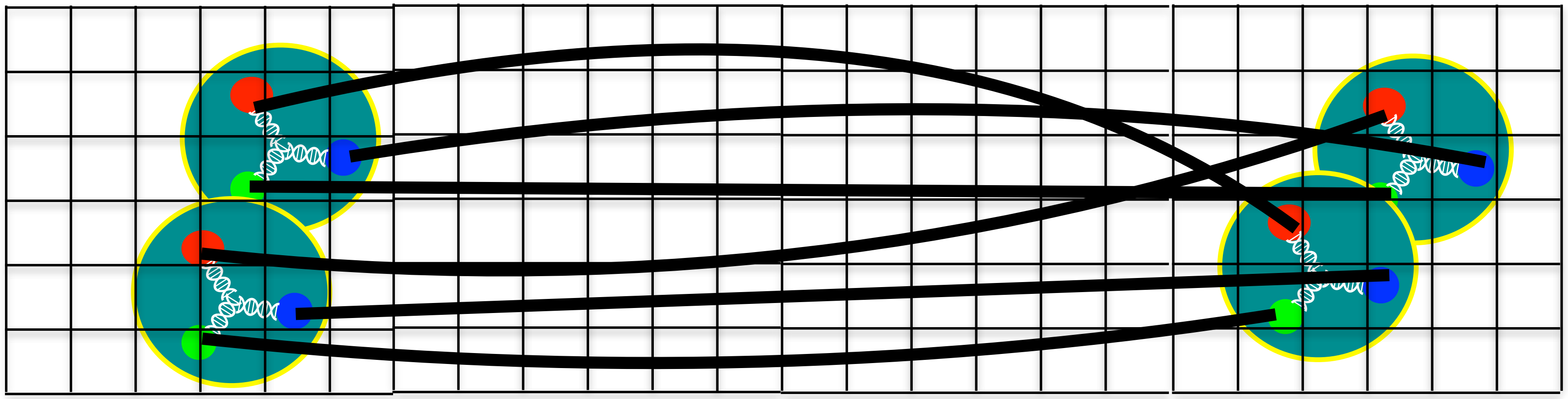
$$aE(t) = -\ln \frac{C(t+a)}{C(t)} = aE_0 + \dots$$

Correlation functions

We don't know the wave functions of QCD energy eigenstates *a priori*

- Start with "interpolating operators" that have the right quantum numbers
- Large (imaginary) *t* behavior of correlation functions governed by E_0

2-point function:



$$C_A(t) = \langle 0|A(t)A^\dagger(0)|0\rangle = \sum_n \langle 0|A(0)e^{-Ht}|n\rangle \langle n|A^\dagger(0)|0\rangle + \dots$$

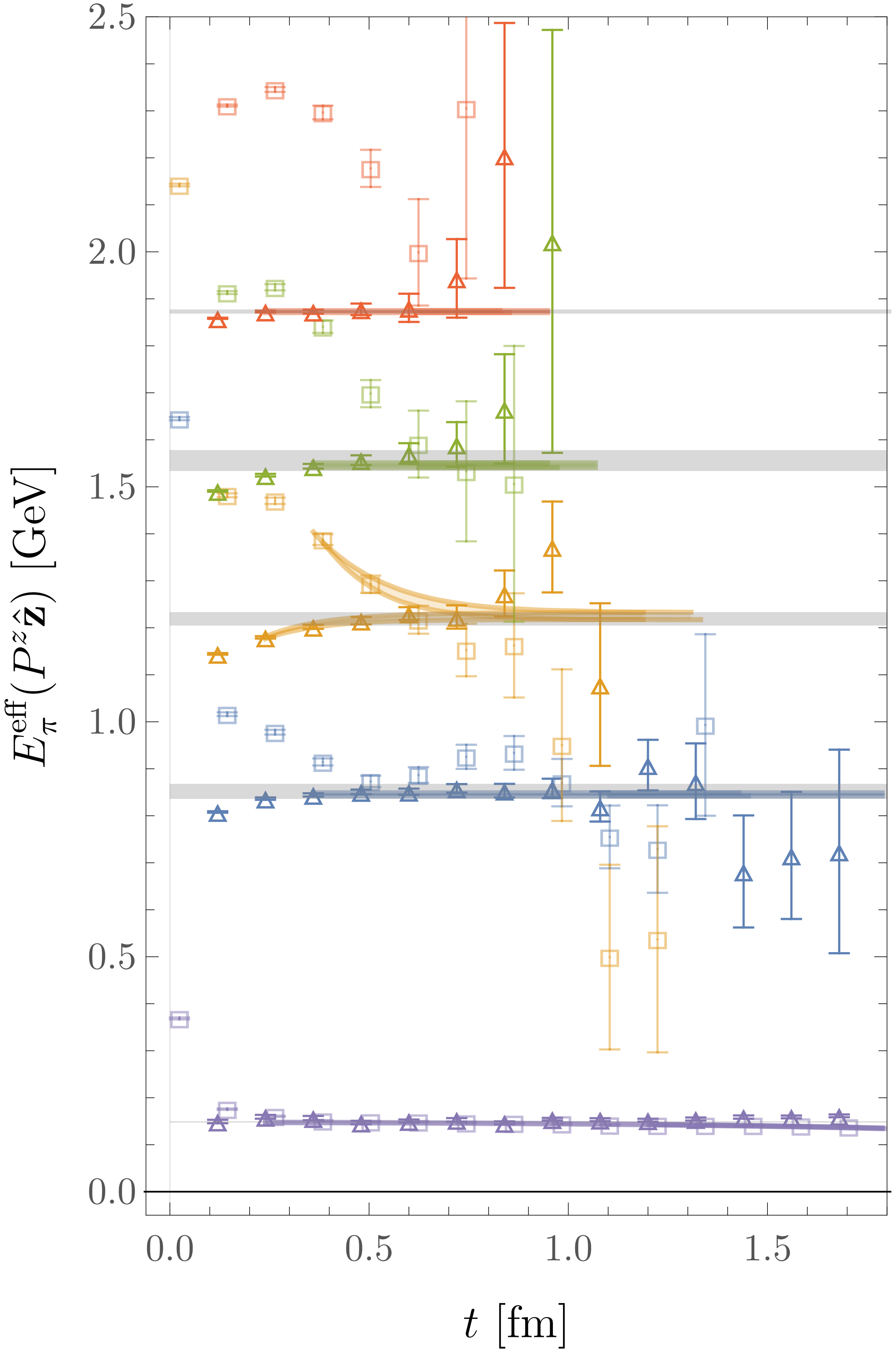
$$= \sum_n |Z_n|^2 e^{-E_n t}$$

Imaginary time evolution $e^{-iHt_{\text{real}}} = e^{-H(it_{\text{real}})}$

Lowest-energy state with same quantum numbers dominates **for sufficiently large *t***

$$C_A(t) \propto e^{-E_0 t} + \dots$$

Effective masses

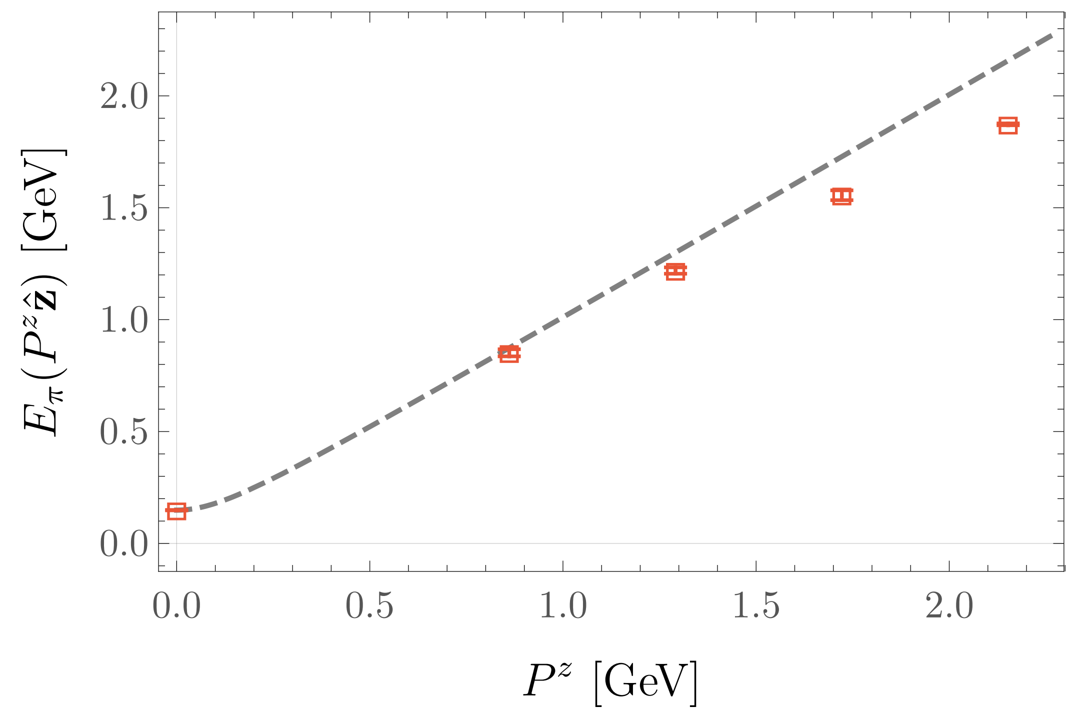


$$E^{\text{eff}}(t) = \frac{1}{a}\ln\left[\frac{C_A(t+a)}{C_A(t)}\right] = E_0 + \mathcal{O}(e^{-(E_1-E_0)t})$$

Effective mass "plateau" signals ground state dominates correlation function at finite t

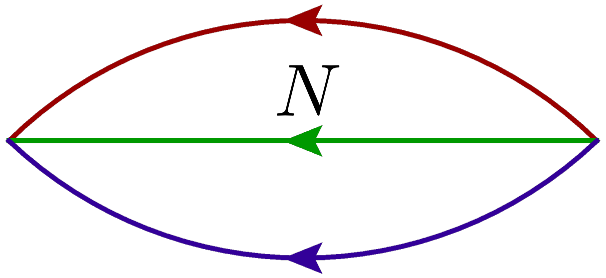
For simple states, e.g. low-momentum pion, simple interpolating operators and t ~ 1 fm appear sufficient

Fitted dispersion relations agree with continuum expectations + discretization effects



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

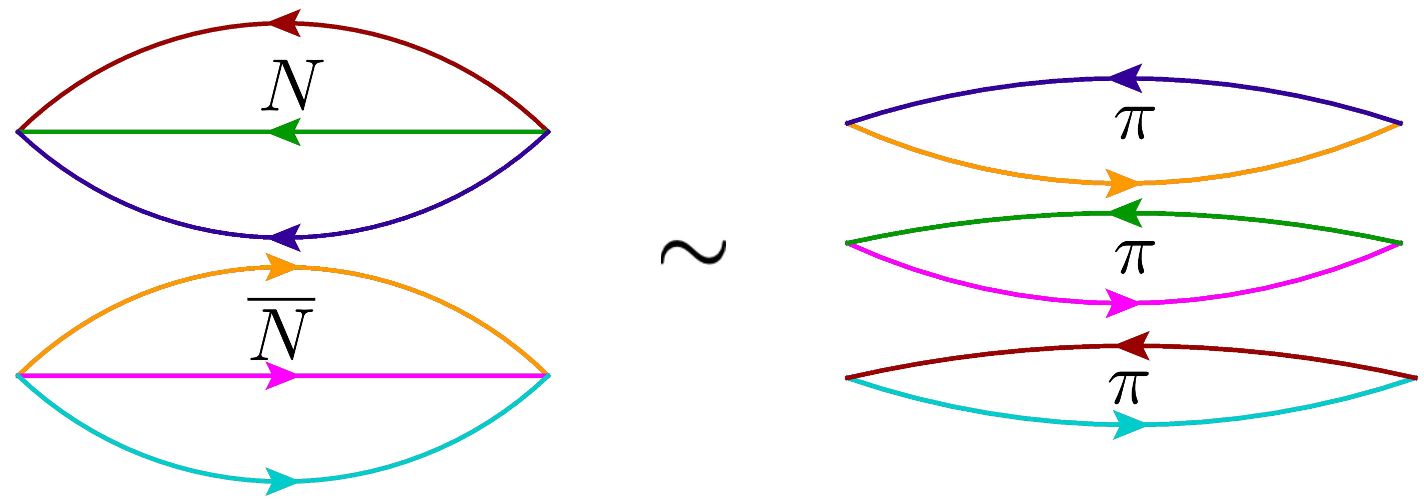
The signal-to-noise problem



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:

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

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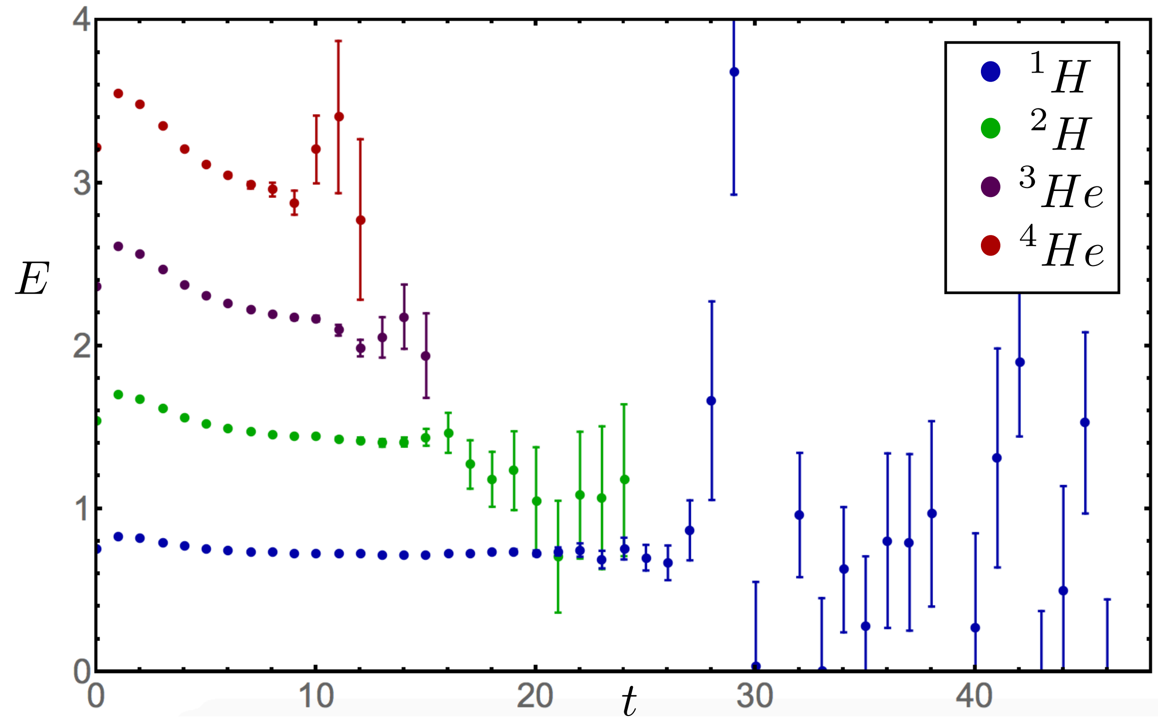
$\mathrm{StN} \sim e^{-A(M_N - \frac{3}{2}m_\pi)t}$



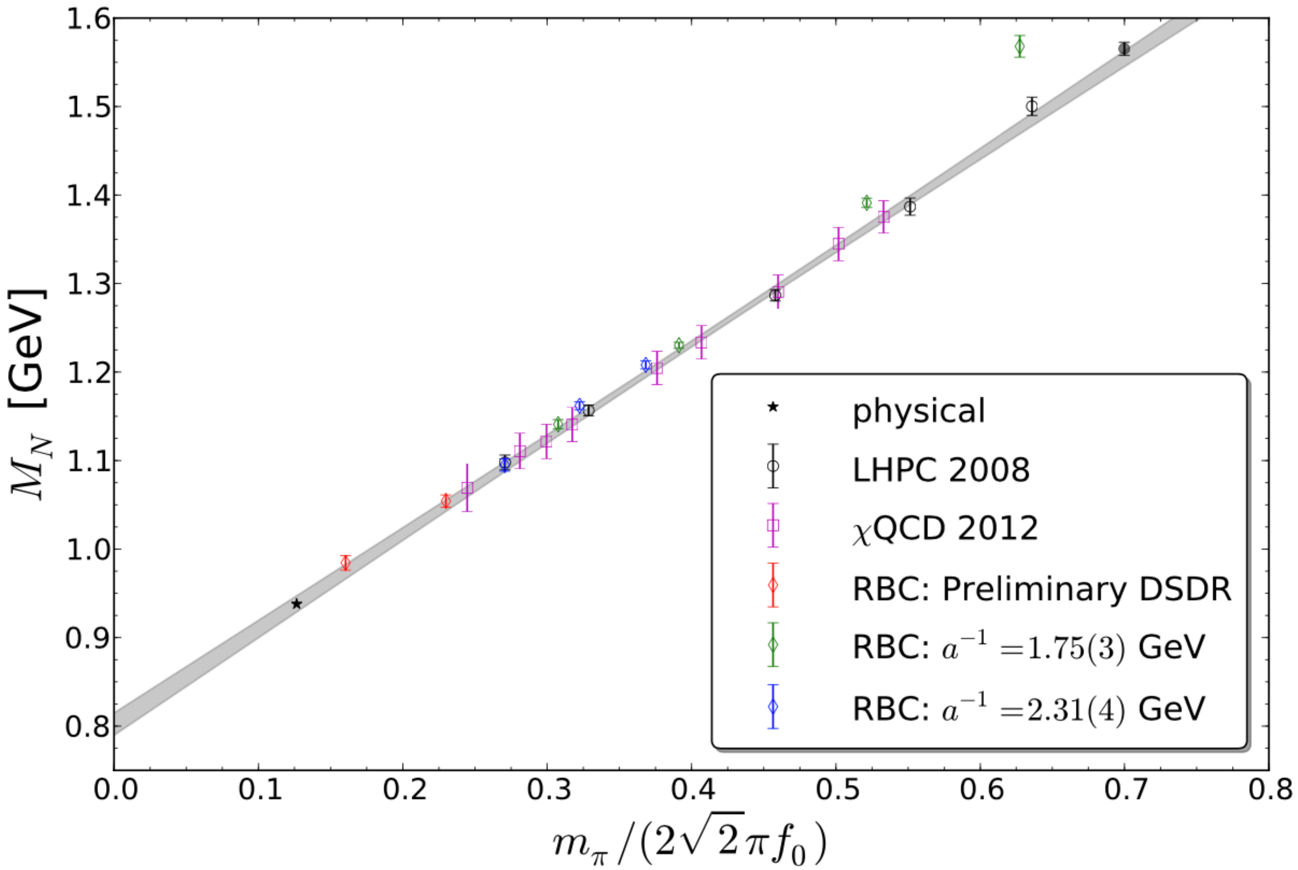
$$aE(t) = -\ln \frac{C(t+a)}{C(t)} = aE_0 + \ldots$$

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

Signal-to-noise and quark mass

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

Exponential signal-to-noise degradation becomes less severe at large quark masses



Walker-Loud, PoS LATTICE2013 (2014)

Empirical formula for $m_\pi \gtrsim m_\pi^{\mathrm{phys}}$

$$M_N \approx 800\ \mathrm{MeV} + m_\pi$$

(note this is the **wrong** scaling near the chiral limit)

$$M_N - \frac{3}{2}m_\pi \approx 800\ \mathrm{MeV} - \frac{1}{2}m_\pi$$

Exponent halved for $m_\pi \sim 800\ \mathrm{MeV}$, many proof-of-principle calculations of multi-nucleon systems performed for quark masses in this regime

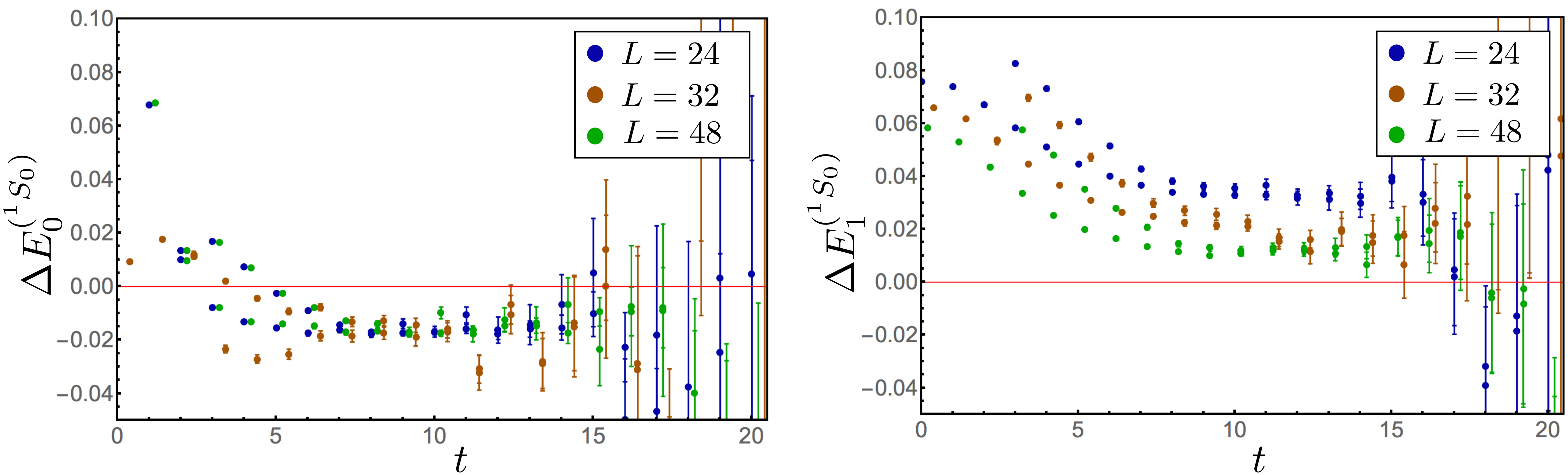
Nuclei from LQCD

Calculations of 2-5 baryon correlation functions using asymmetric correlation functions

Beane et al [NPLQCD], PRD 87 (2013) $L = 2.9 \text{ fm} \rightarrow 5.8 \text{ fm}$ $a = 0.145 \text{ fm}$ $m_\pi \sim 806 \text{ MeV}$

Yamazaki et al, PRD 86 (2012) $L = 3.5 \text{ fm} \rightarrow 7.0 \text{ fm}$ $a = 0.09 \text{ fm}$ $m_\pi \sim 510 \text{ MeV}$

- 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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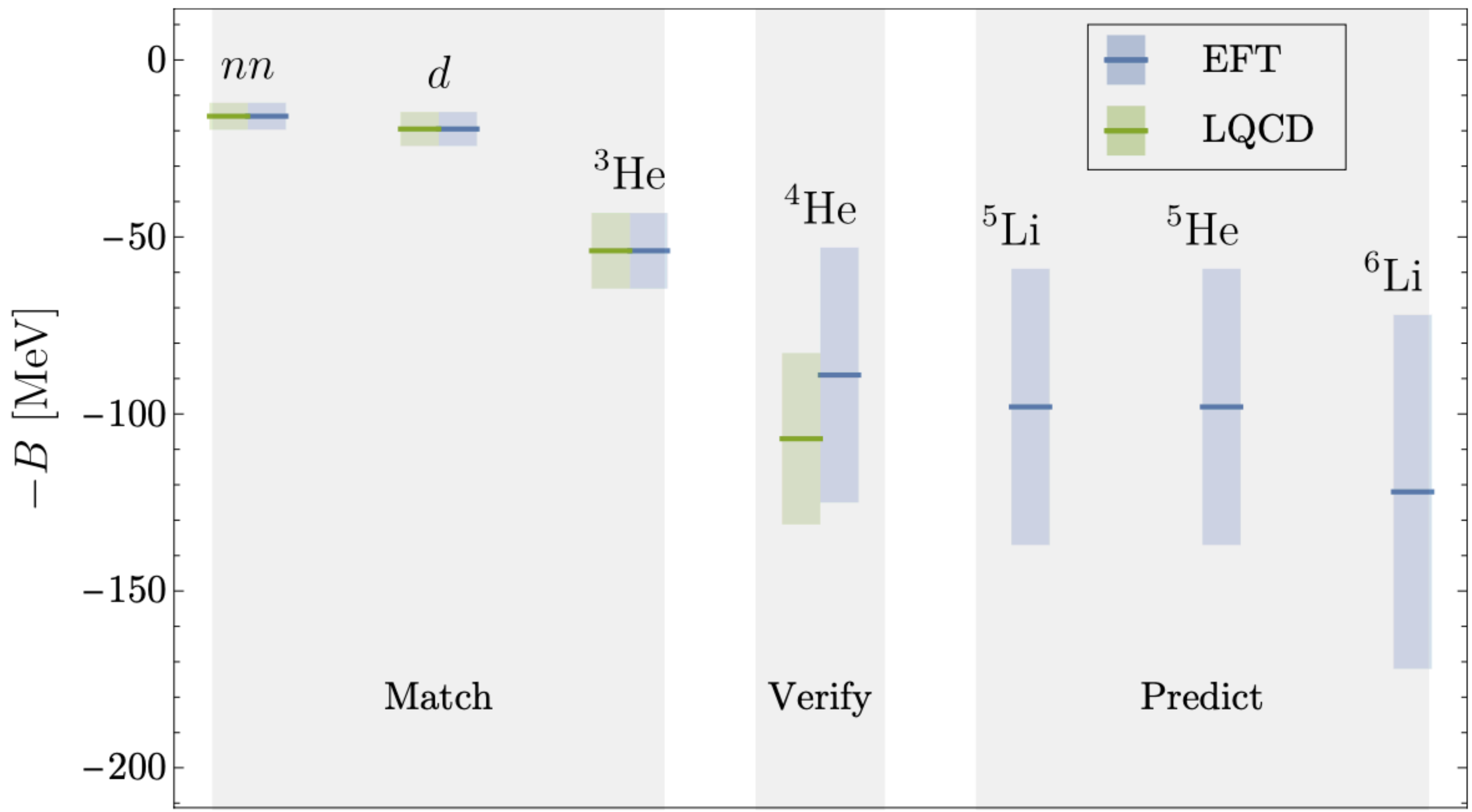
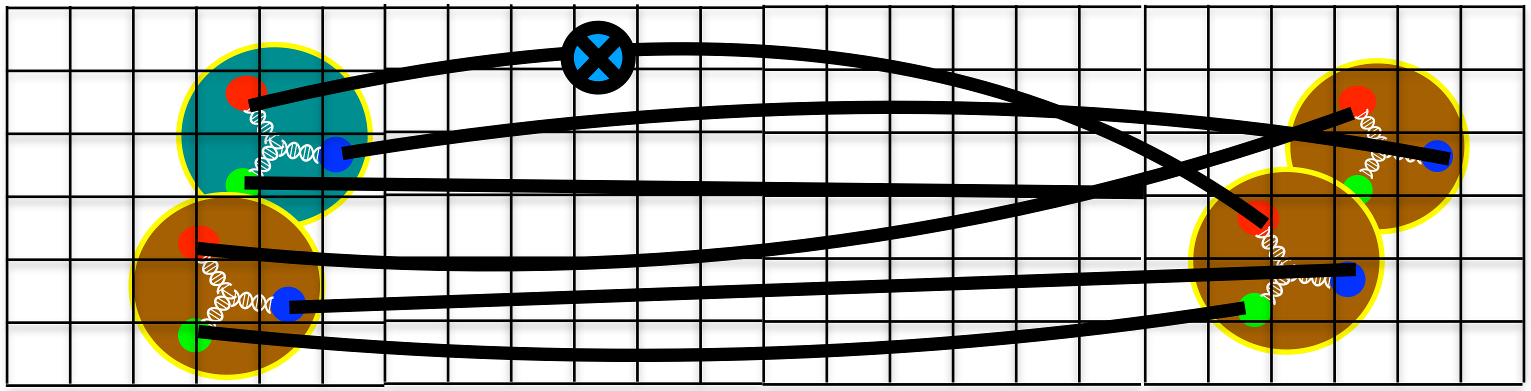


EFT: Barnea et al, PRL 114 (2015)

Two-body currents in LQCD

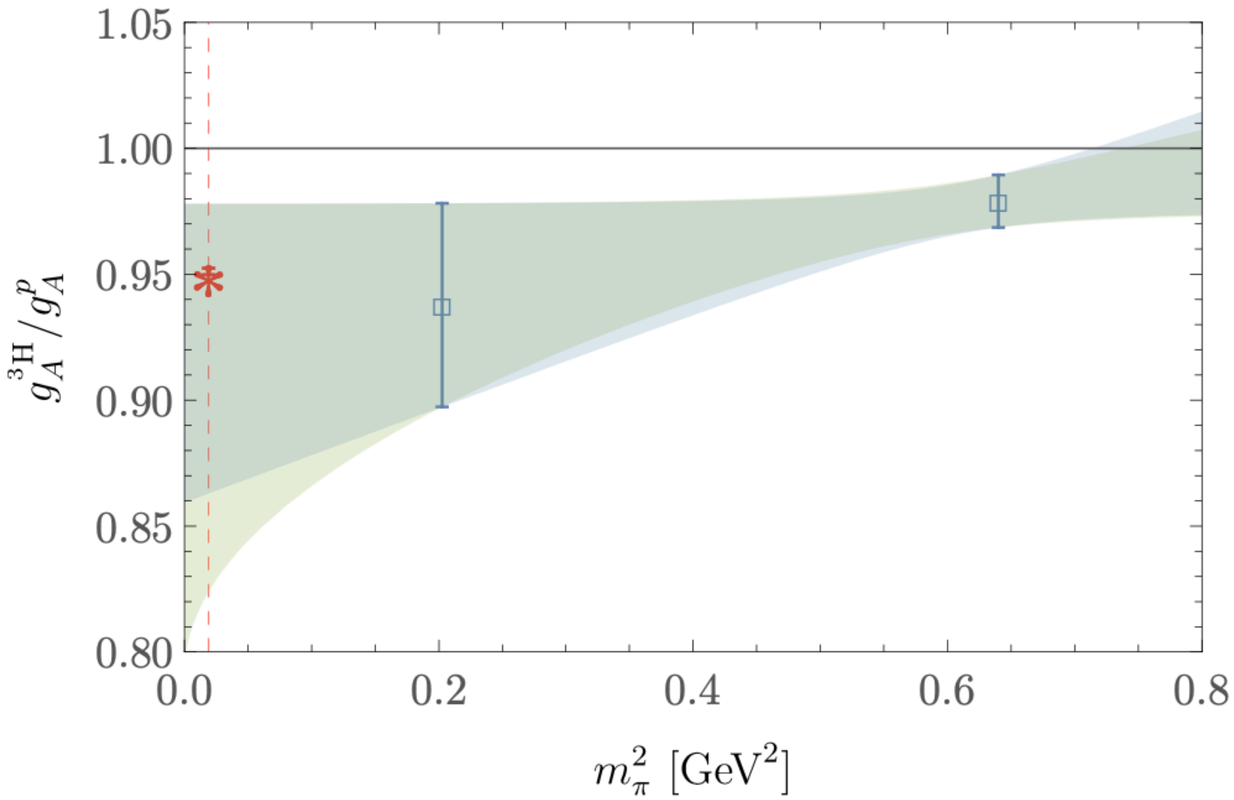
Two-nucleon axial matrix elements relevant for proton-proton fusion computed, used to constrain two-body currents



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

Flavor decomposition of axial matrix elements of two and three nucleon systems computed with $m_\pi = 806\ \mathrm{MeV}$

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



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

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

Analogous two-body currents important for double-beta decay, first study:

Davoudi, Grebe, MW et al, arXiv:2402.09362

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

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

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

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

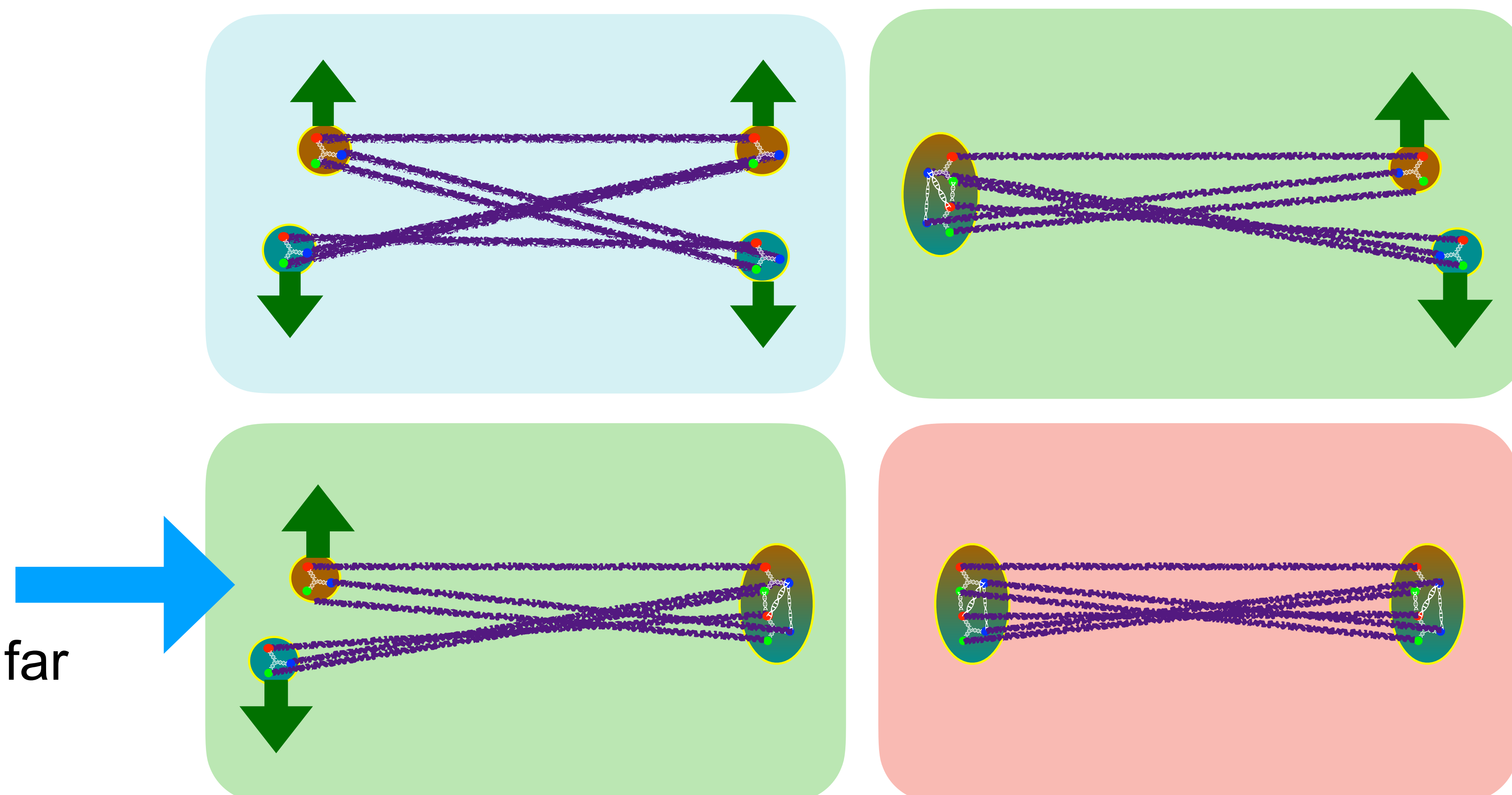
See e.g. Iritani et al, JHEP 10 (2016)

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

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

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:

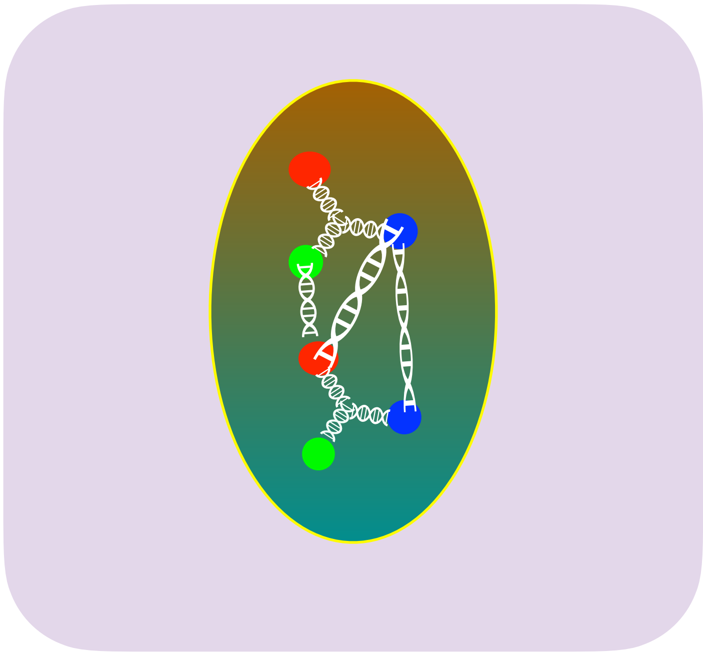
Detmold, MW et al, PRD 104 (2021)

Li et al, PRD 103 (2021)

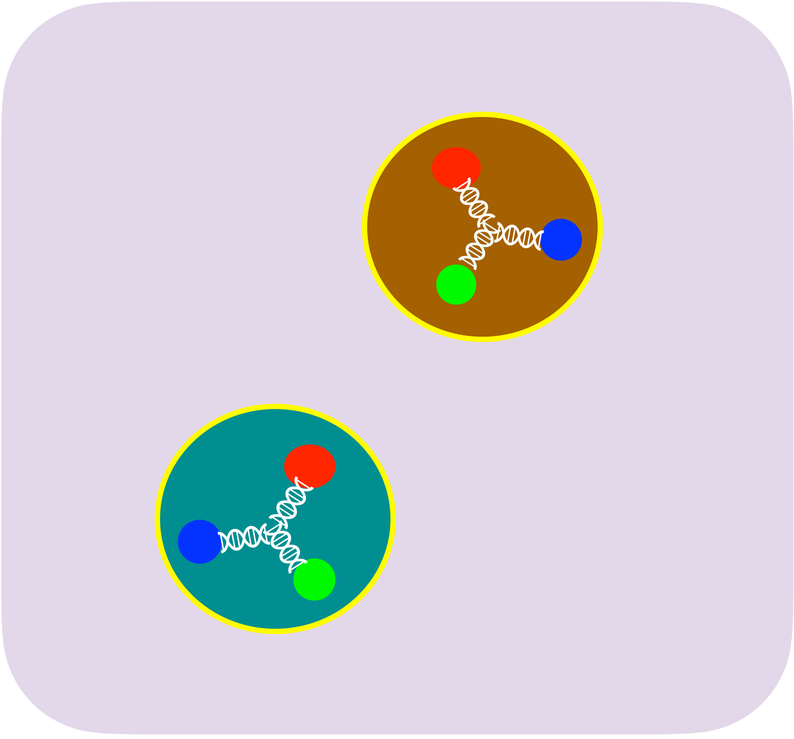
Six-quark operator catalog

Many six-quark operators have the right quantum numbers to describe a deuteron at rest

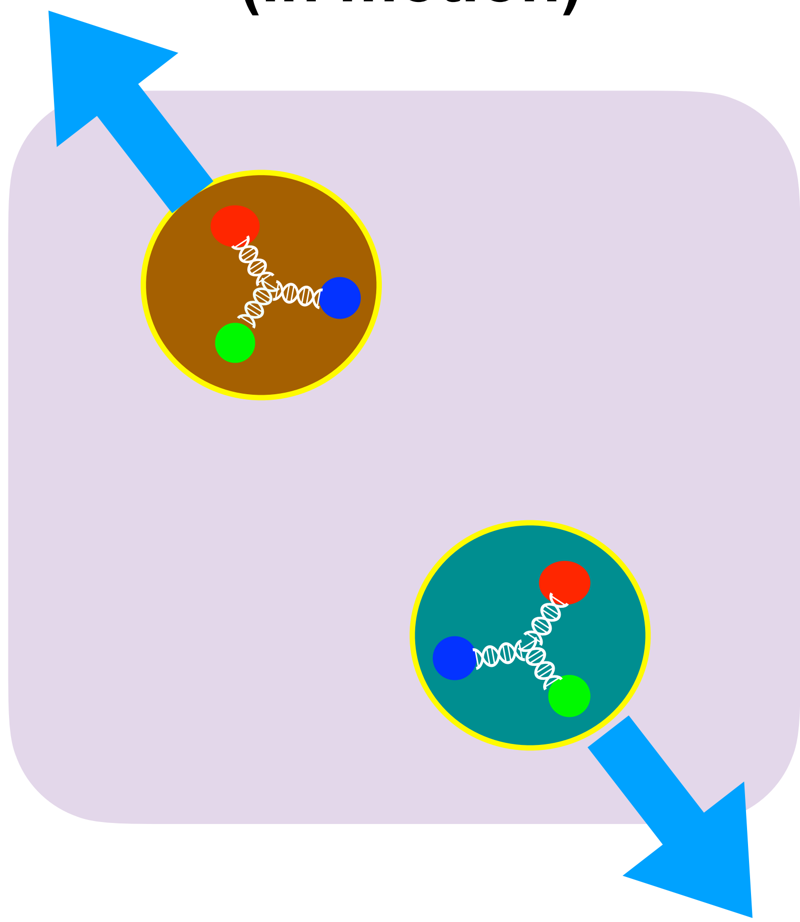
Hexaquark



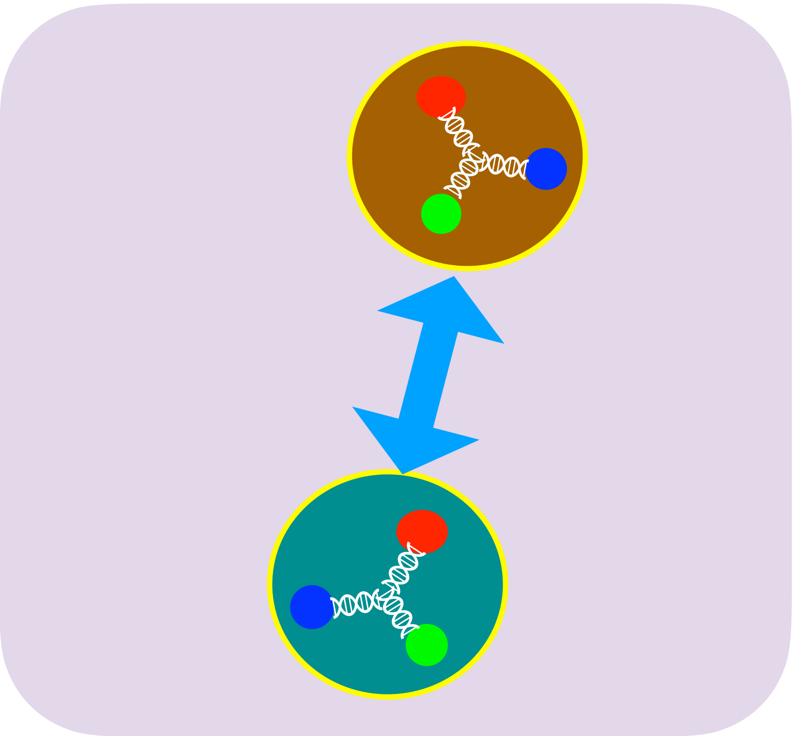
Two nucleons (at rest)



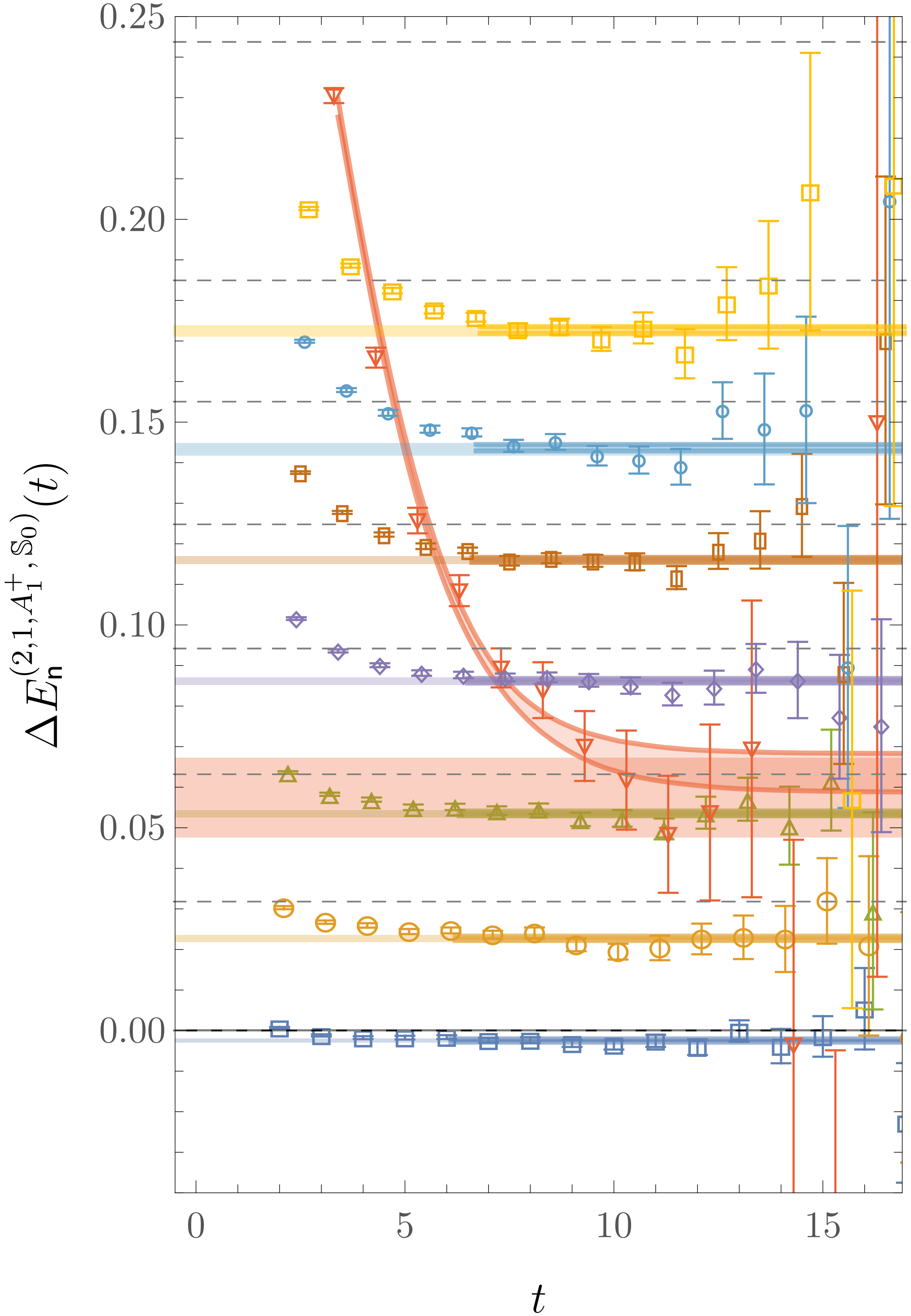
Two nucleons (in motion)



Two correlated nucleons

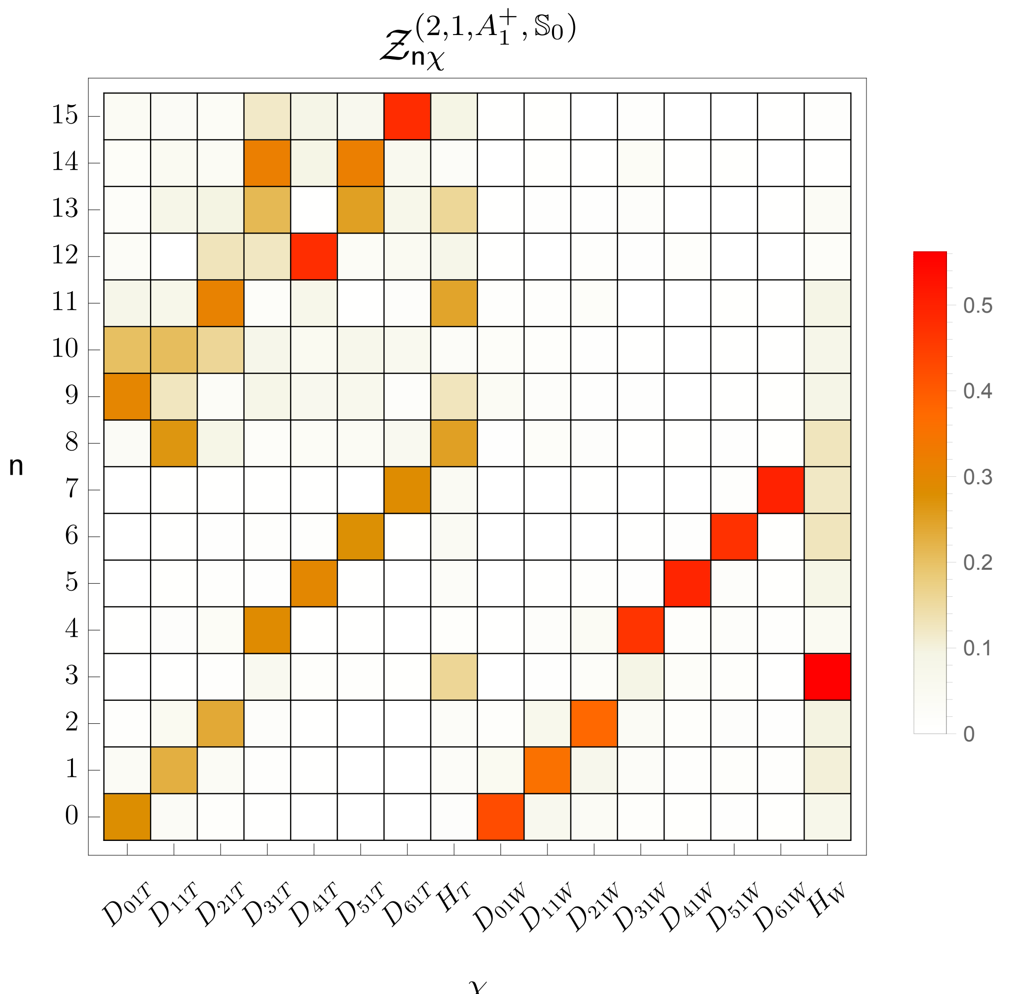


Two neutrons in a box



Diagonalization of correlation-function matrices can be used to remove excited-state contamination from states strongly overlapping with other operators

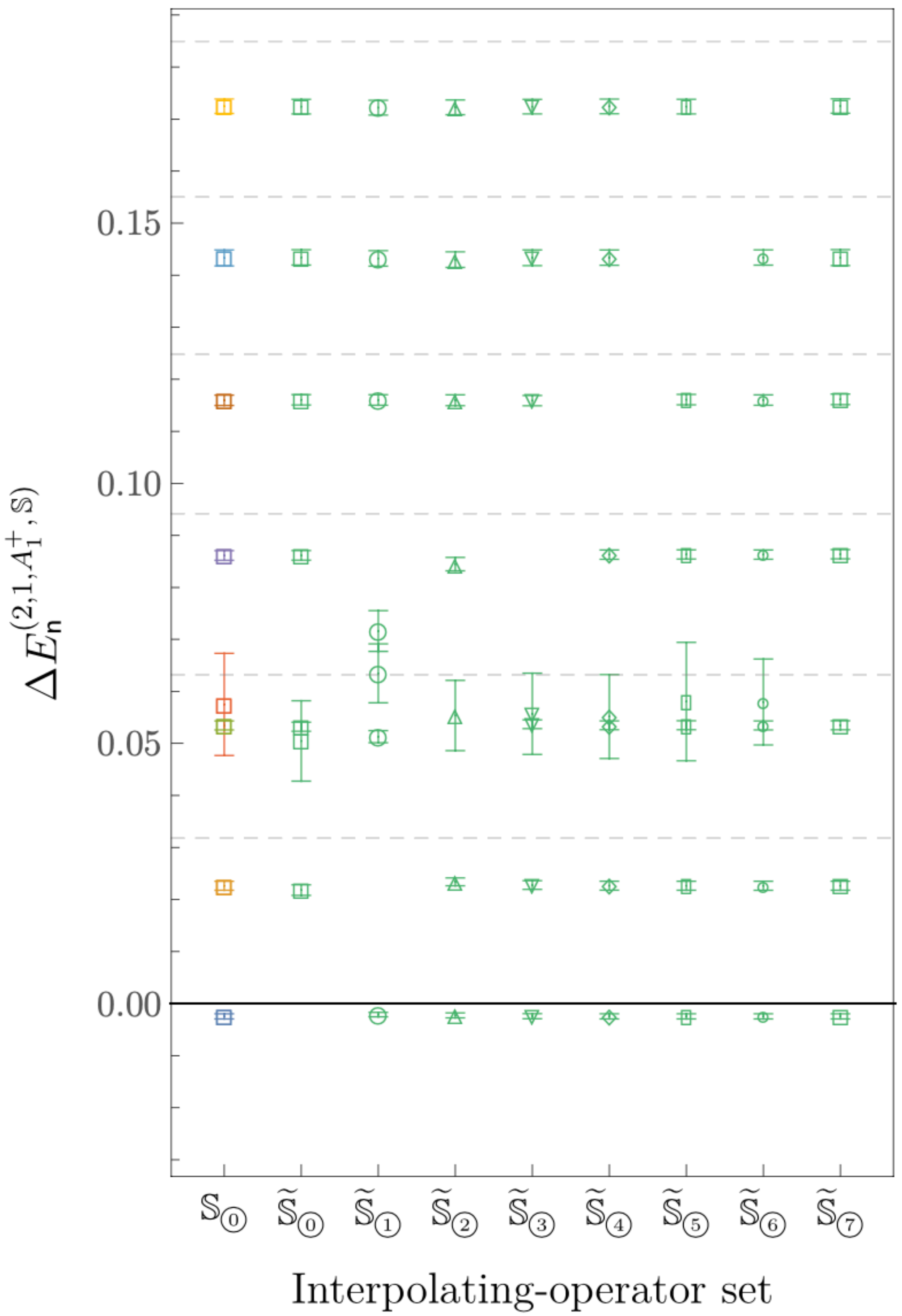
Each energy level dominantly overlaps with one operator structure, sub-dominant operators collectively 30%



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

Interpolating operator dependence

Removing interpolating operators leads to "missing energy levels" for states dominantly overlapping with omitted operators



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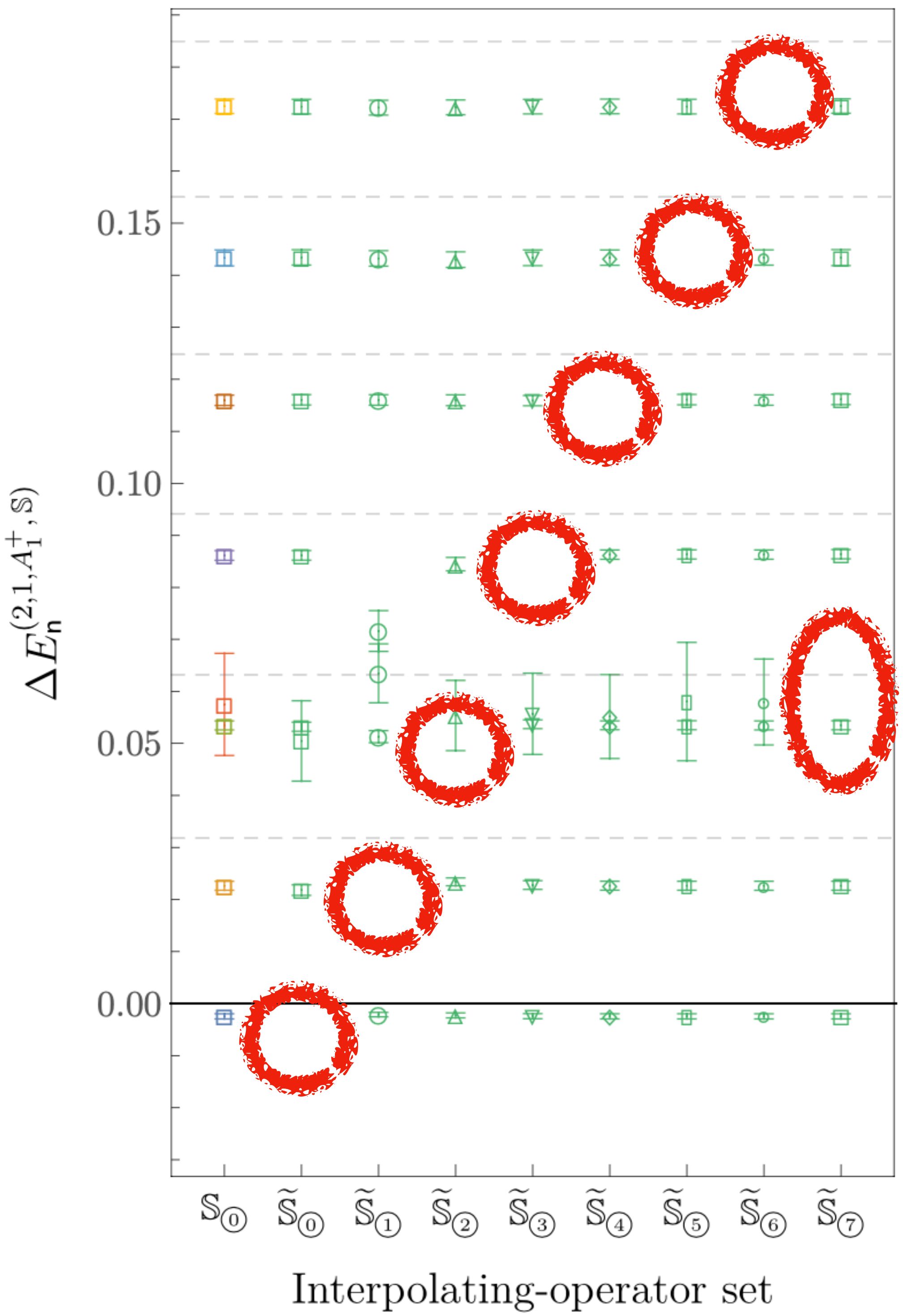
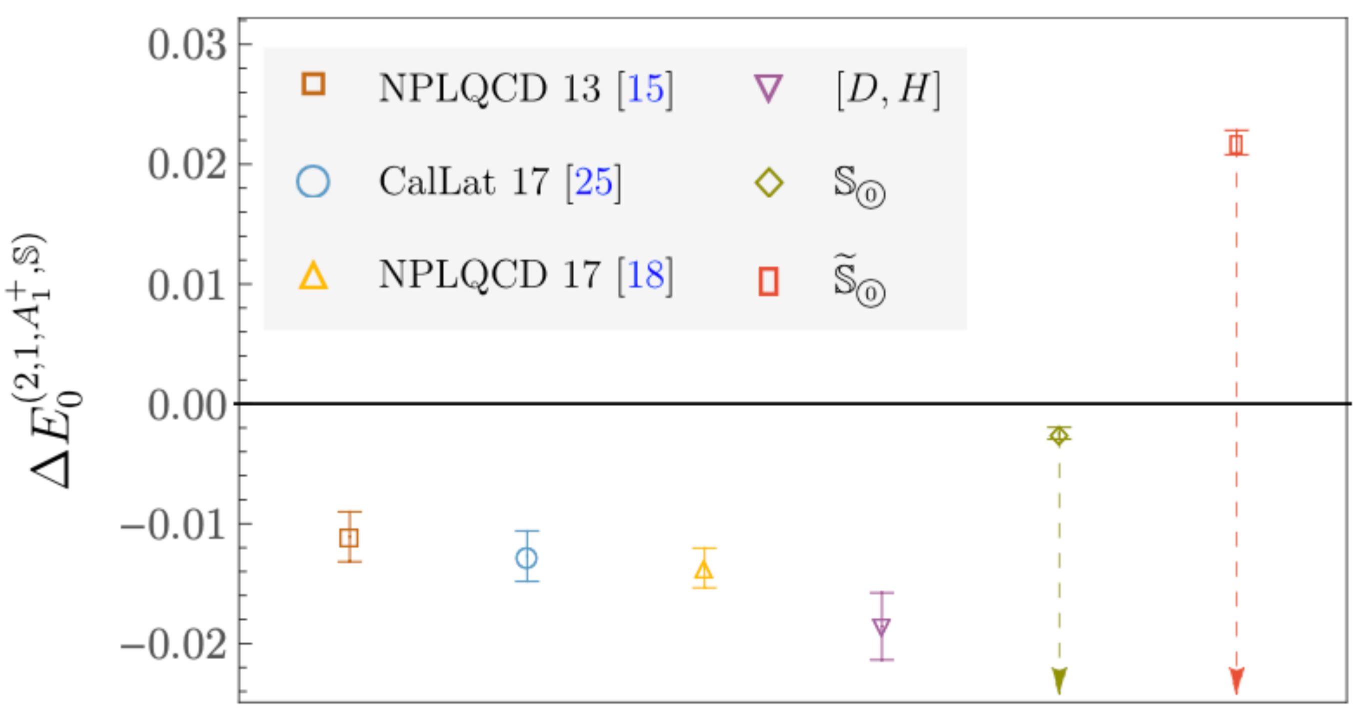


✔ **Variational upper bounds** obtained using different interpolating operator sets are consistent



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

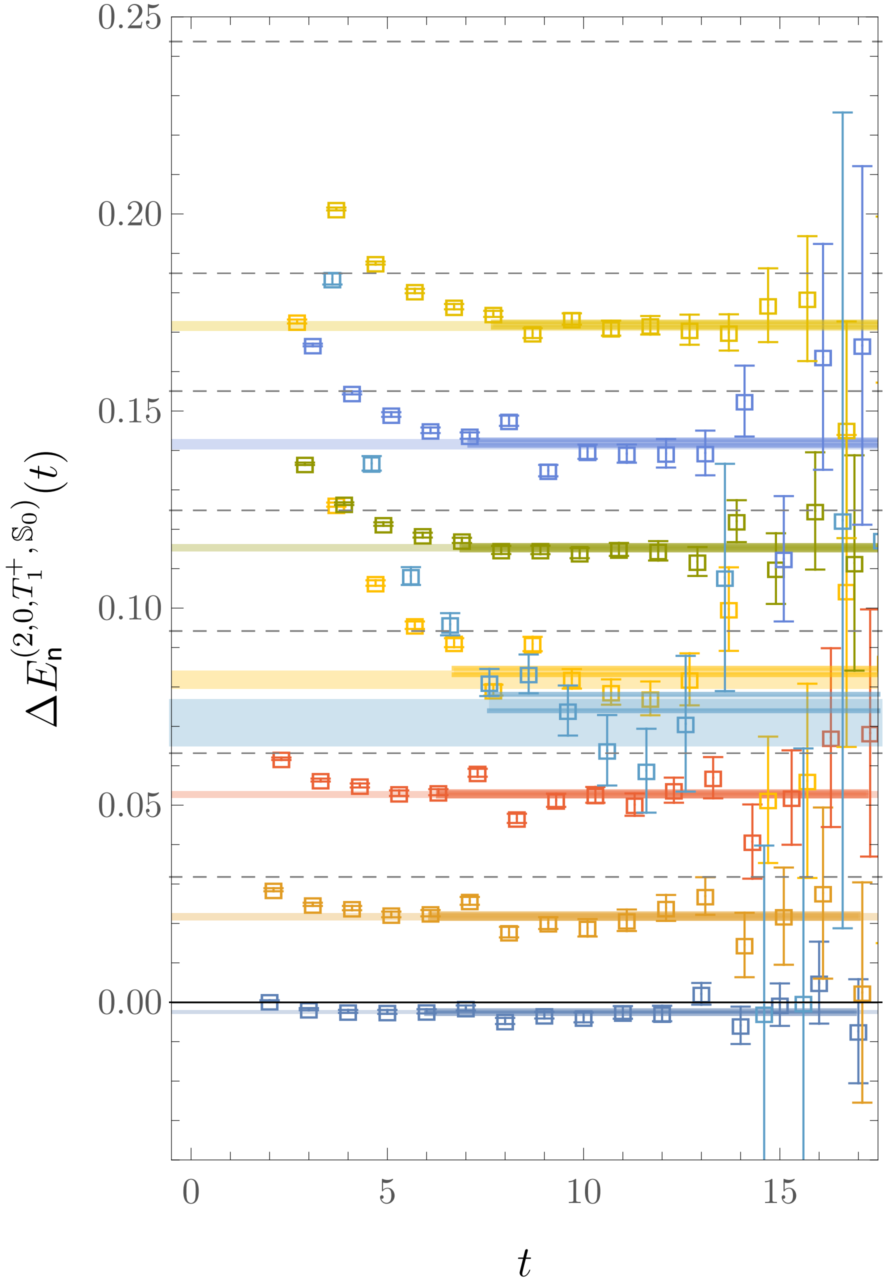
Amarasinghe, MW et al [NPLQCD], PRD 107 (2023)

The deuteron channel

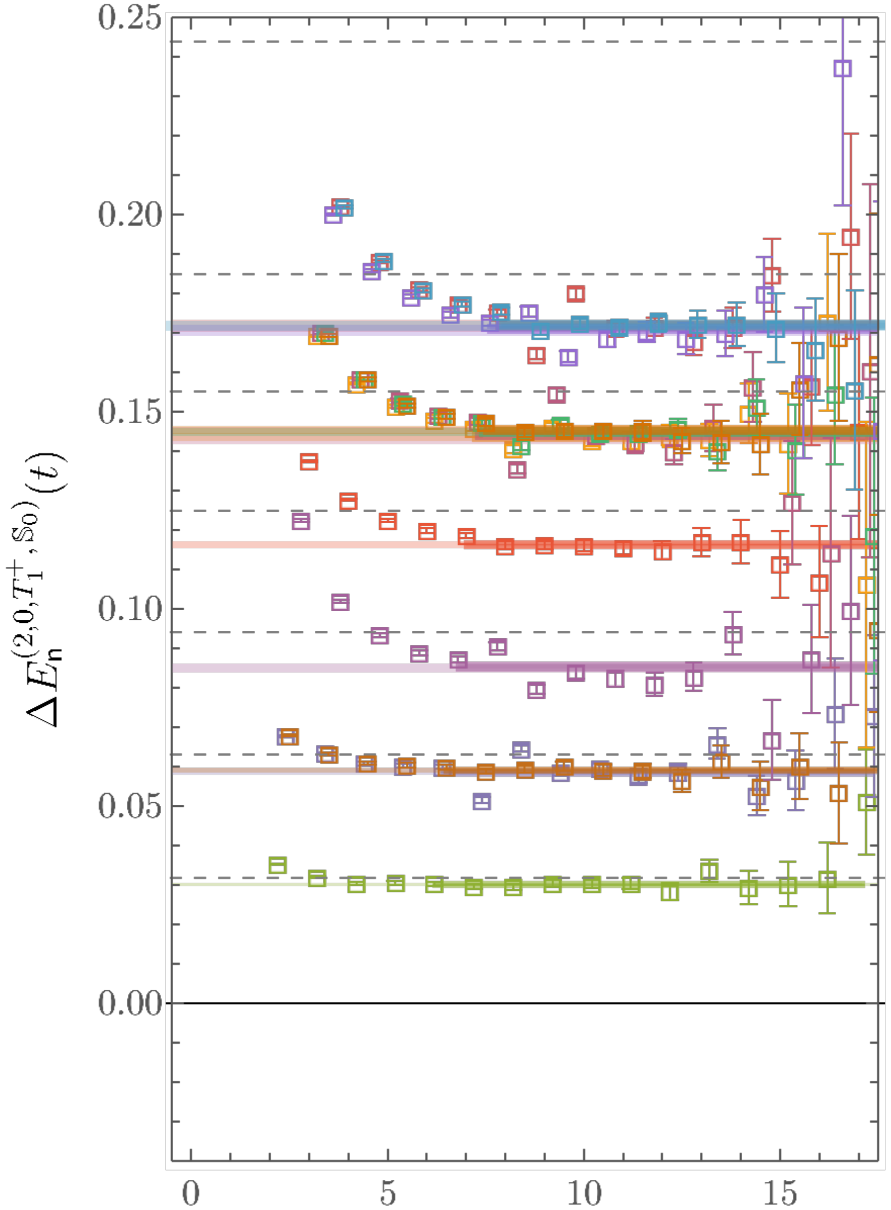
Spin-orbit coupling complicates the deuteron channel

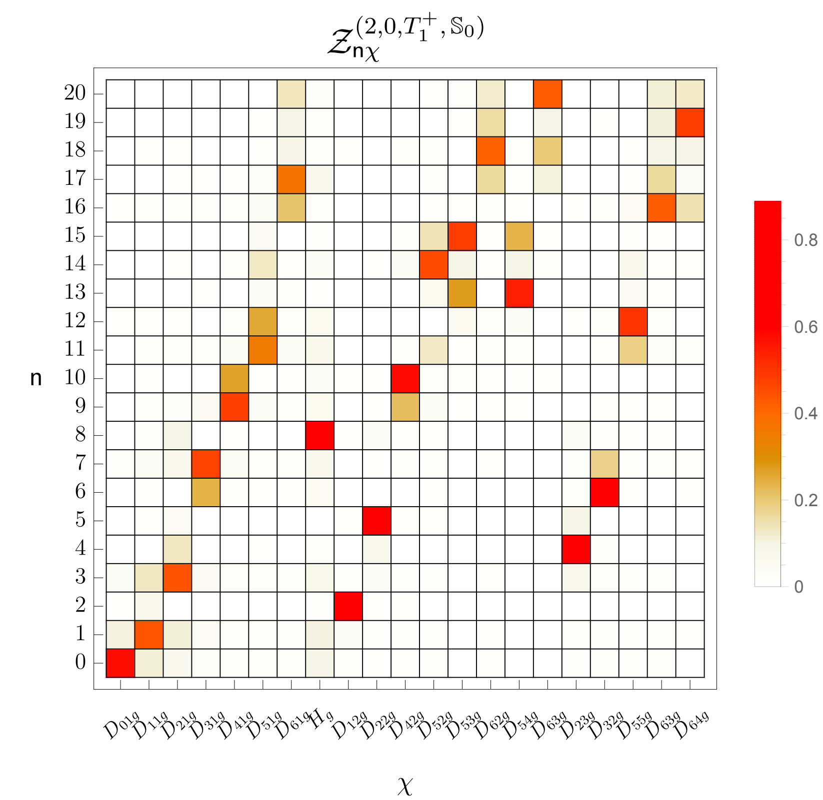
Finite-volume analogs of *S*-wave and *D*-wave operators included to provide a complete set of dibaryon operators with sufficiently low relative momentum

Dominantly *S*-wave



Dominantly *D*-, *G*-, or *I*-wave



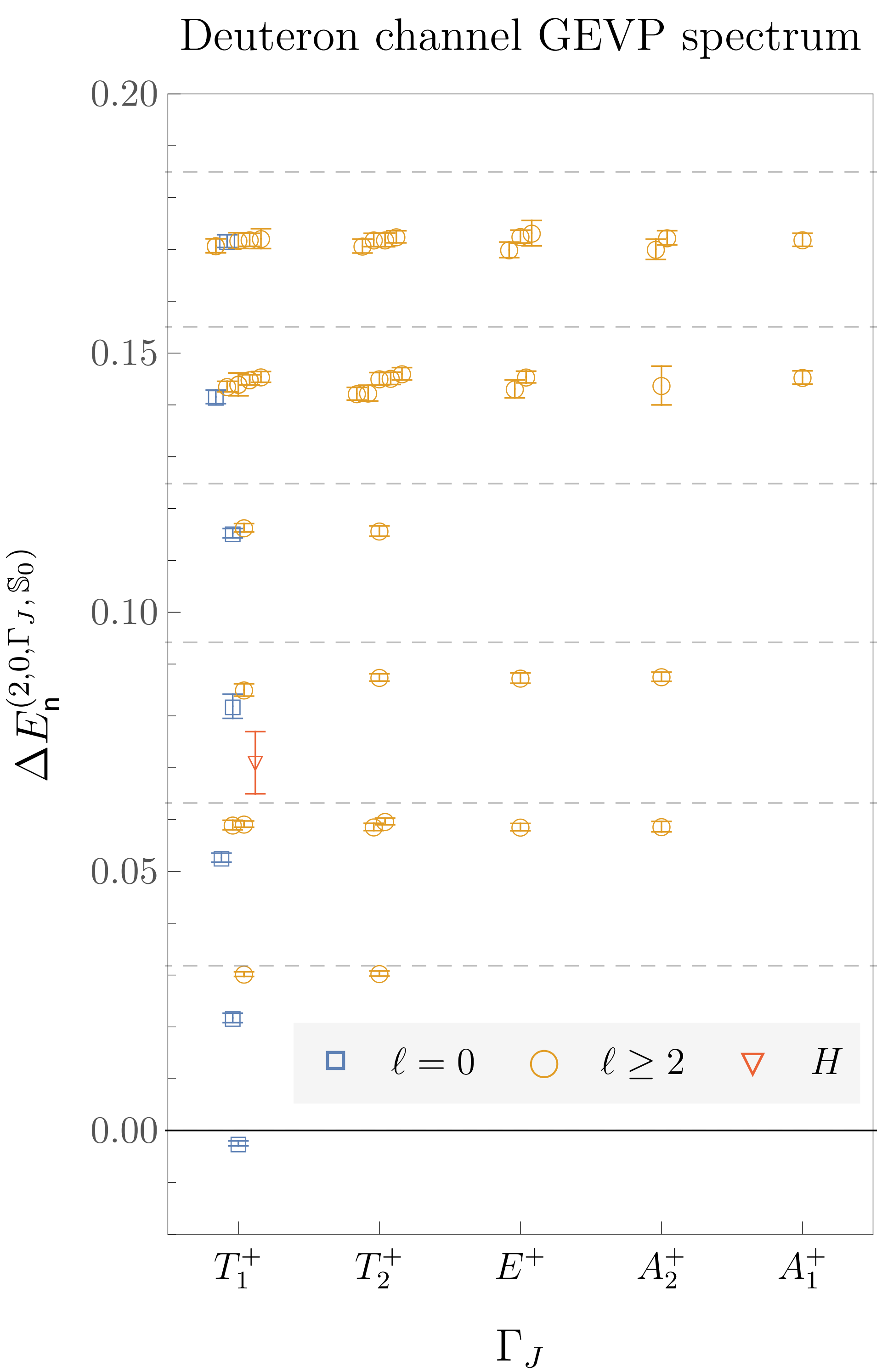


Low-energy states again have majority overlap with 1 operator structure

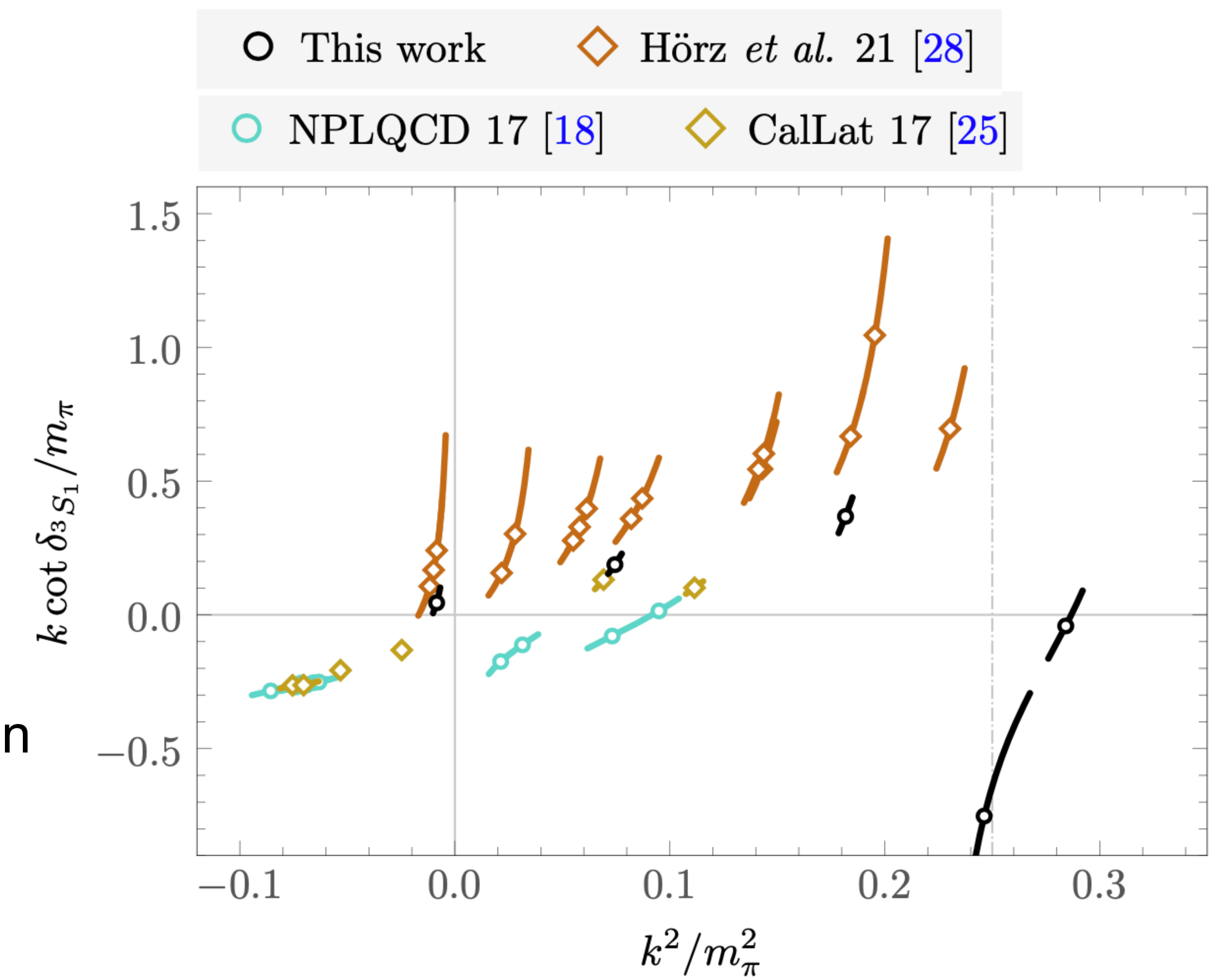
Amarasinghe, MW et al [NPLQCD], PRD 107 (2023)

Towards *NN* scattering from LQCD

Variational calculations including a wide range of two-nucleon operators lead to precise determinations of *NN* energy spectra, constraints on *NN* phase shifts



Lüscher quantization condition

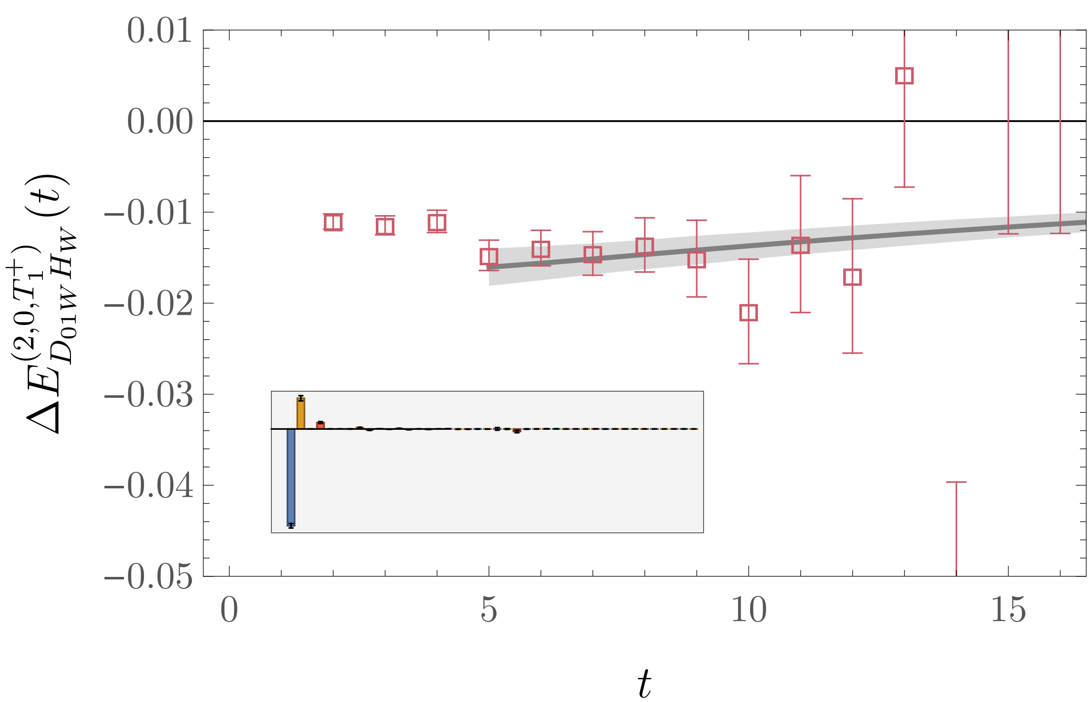


- Consistency among studies with similar interpolating operators
- Significant tensions between calculations with different operators

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

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

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

Toy model: 2 operators, 3 states

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

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

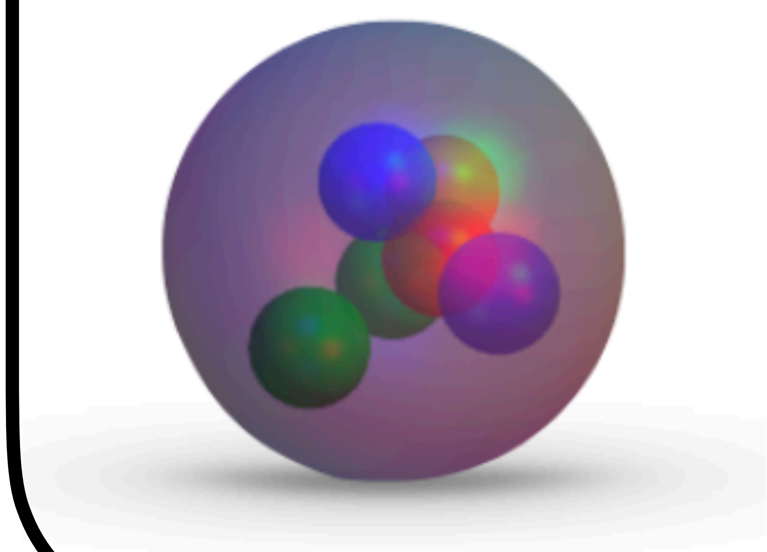
GEVP eigenvalues controlled by first and second excited state (**not** ground state) for $\epsilon \ll e^{t(E_1-E_0)}$

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

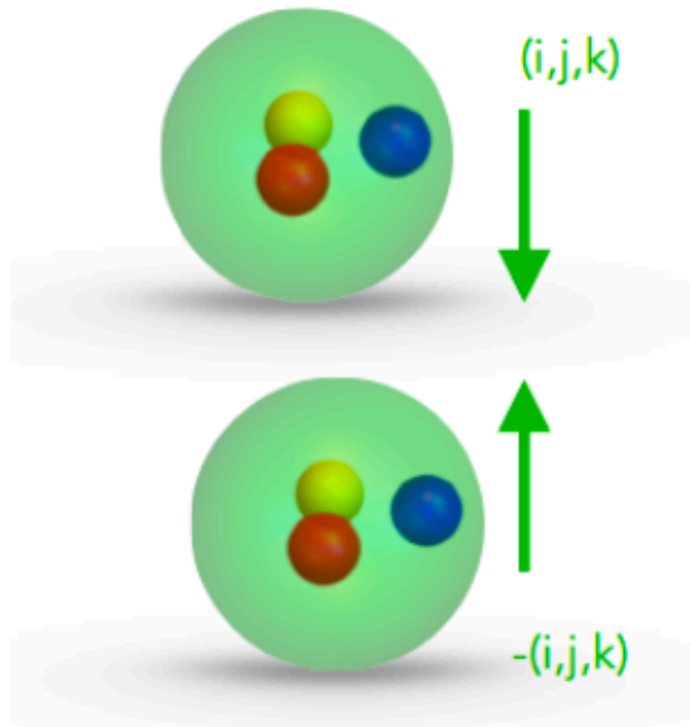
Off-diagonal correlator conversely has perfect ground-state overlap

Broadening the operator catalog

- Complete bases of local hexaquark operators with deuteron and dineutron quantum numbers

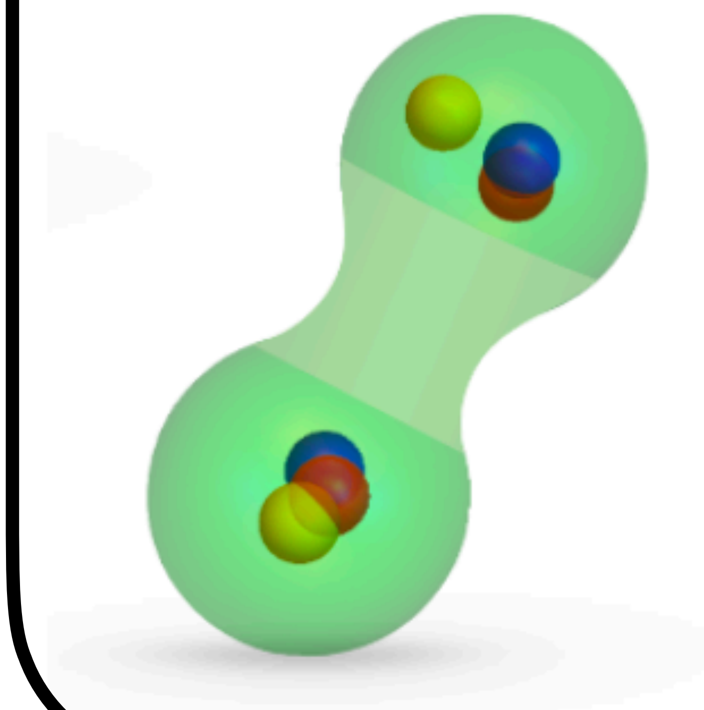


Detmold, Perry, MW et al [NPLQCD], arXiv:2404.12039



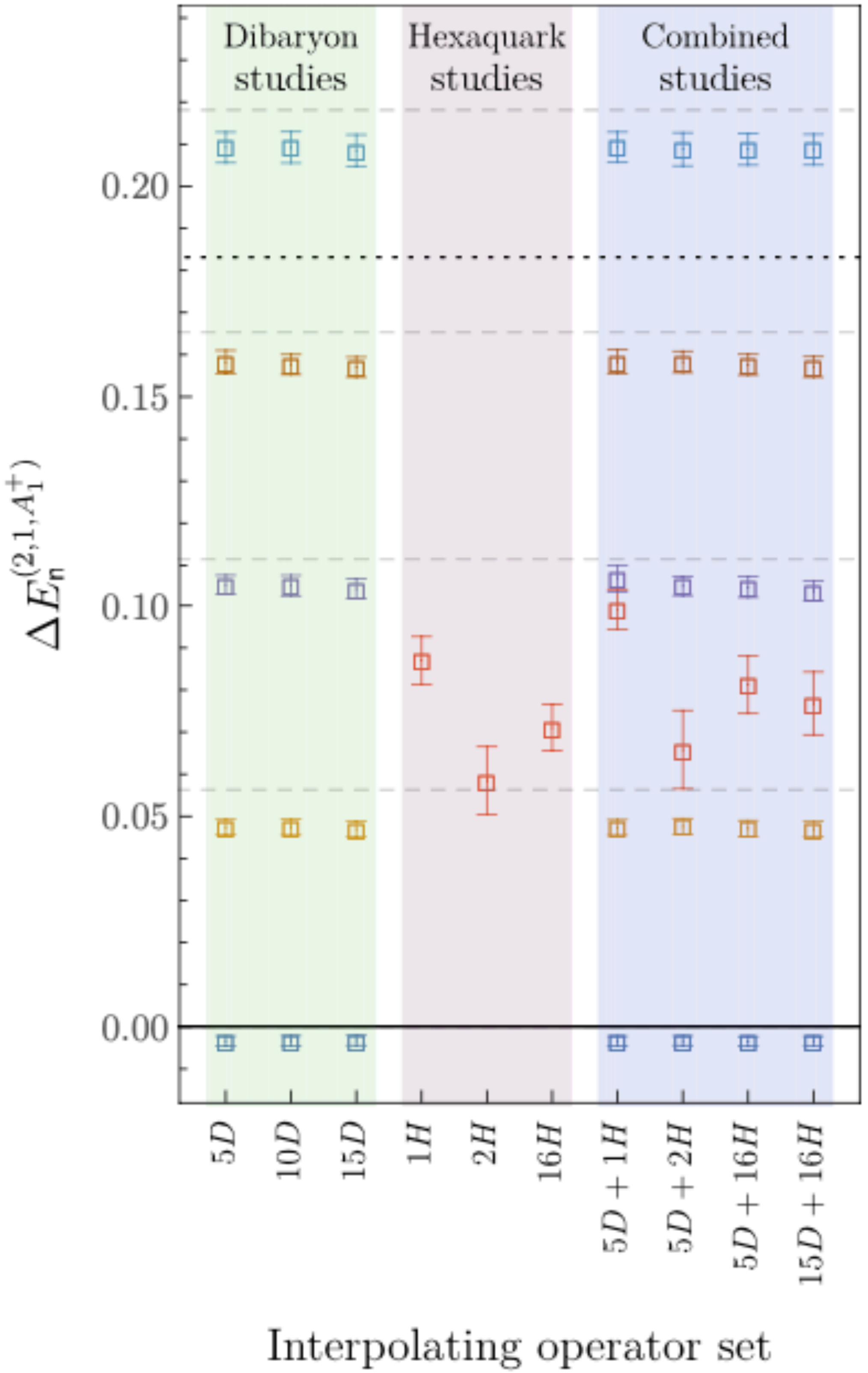
- Plane-wave dibaryon operators including all spinor components*

- Exponentially correlated quasi-local operators including all spinor components*



*previous study used only the Dirac basis upper components arising in nonrelativistic quark models

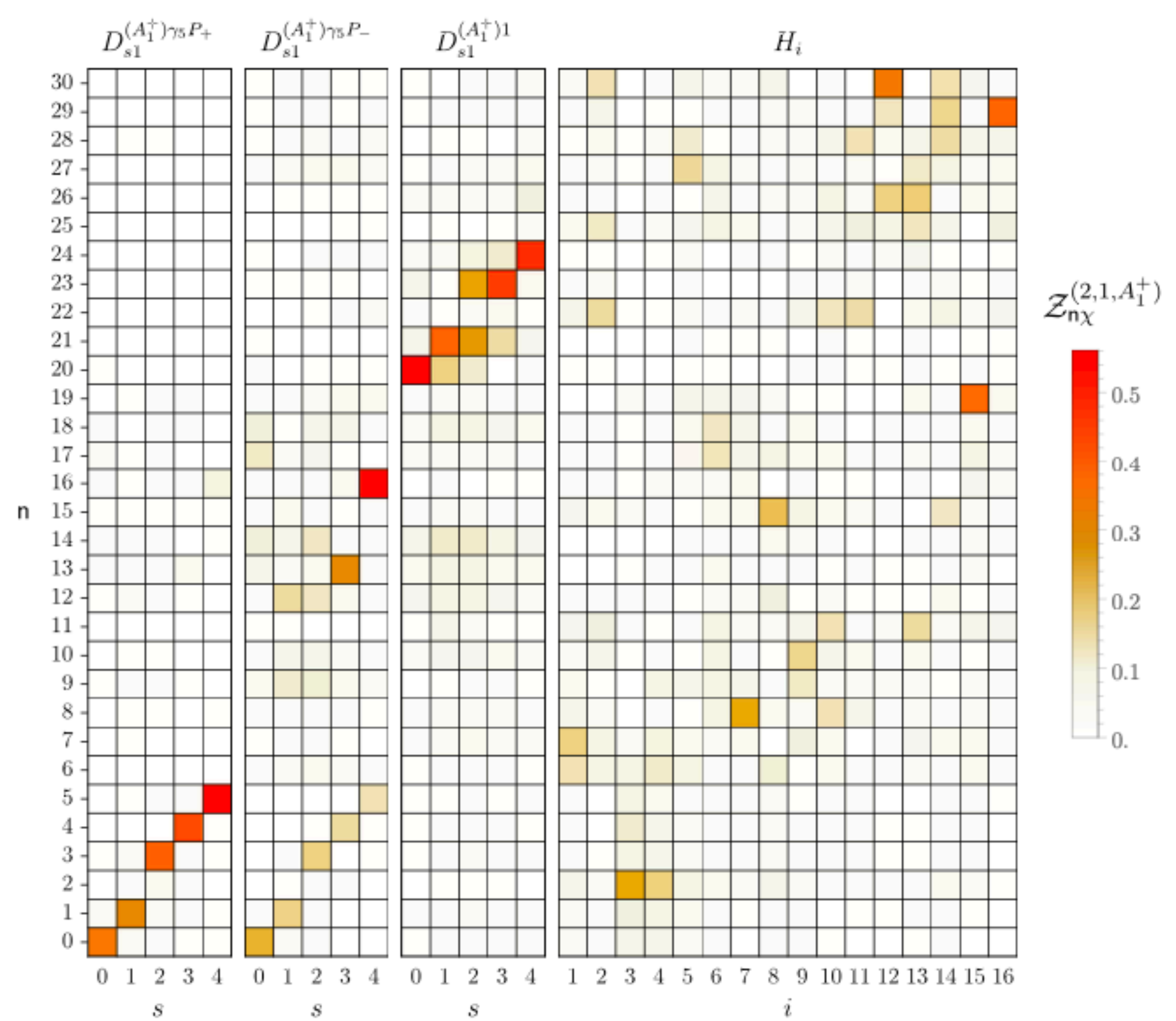
New operator results



Detmold, Perry, MW et al [NPLQCD], arXiv:2404.12039

Hidden-color hexaquark and lower-spin-component dibaryon operators do not significantly affect low-energy spectrum

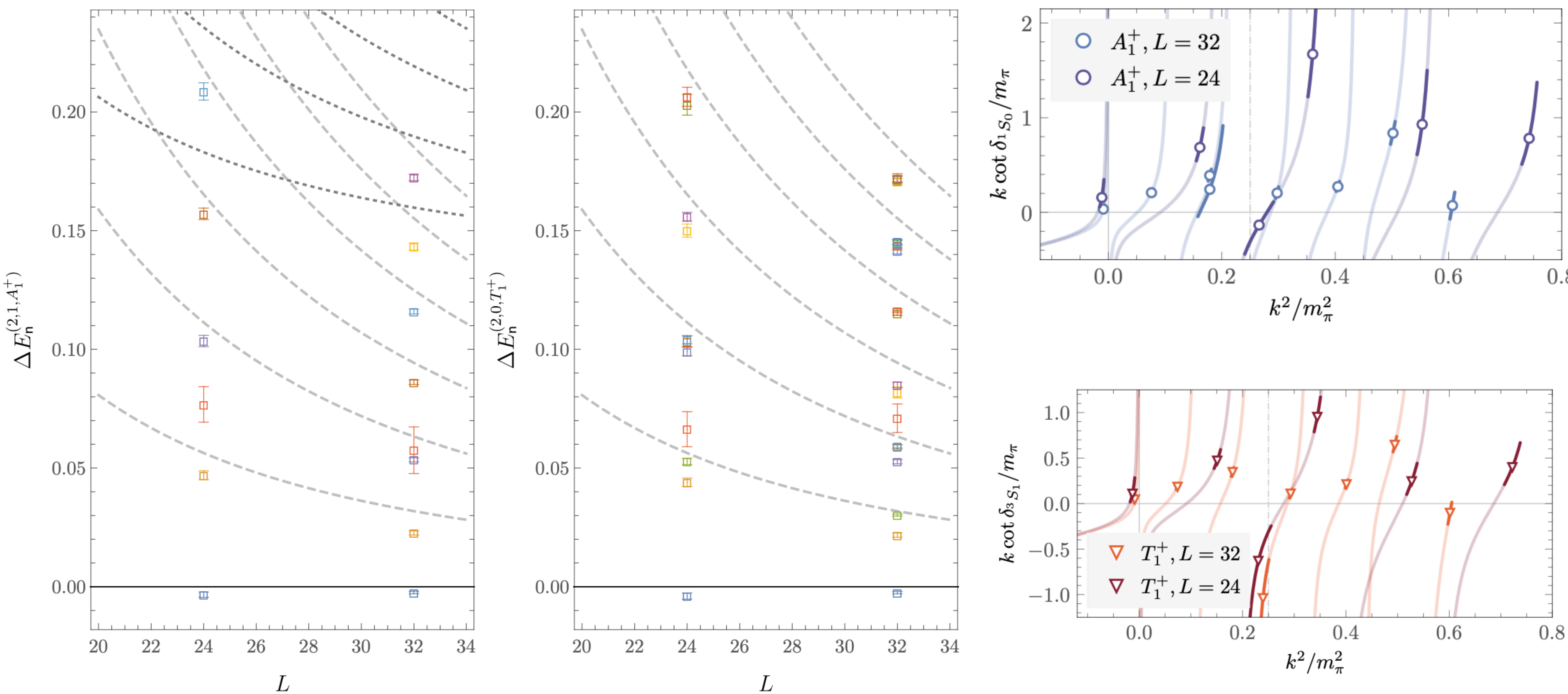
- Hidden-color hexaquarks overlap predominantly with particular excited states that may have novel structure



Two-nucleon variational bounds

Variational bounds: robust evidence that there is an "extra" energy level in both deuteron and dineutron spectra beyond those arising for non-interacting nucleons

Variational bounds: if saturated, then ground state is unbound and there is some sort of resonant feature in *I*=1 and *I*=0 nucleon-nucleon scattering (at this quark mass)



Detmold, Perry, MW et al [NPLQCD], arXiv:2404.12039

Another way to look at LQCD spectroscopy

MW, arXiv:2406.XXYY

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

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

MW, arXiv:2406.XXYY

Lanczos and the transfer matrix

- Standard effective mass = “power-iteration algorithm” for finding eigenvalues

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

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

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

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

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

- 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 $T^{(m)}$

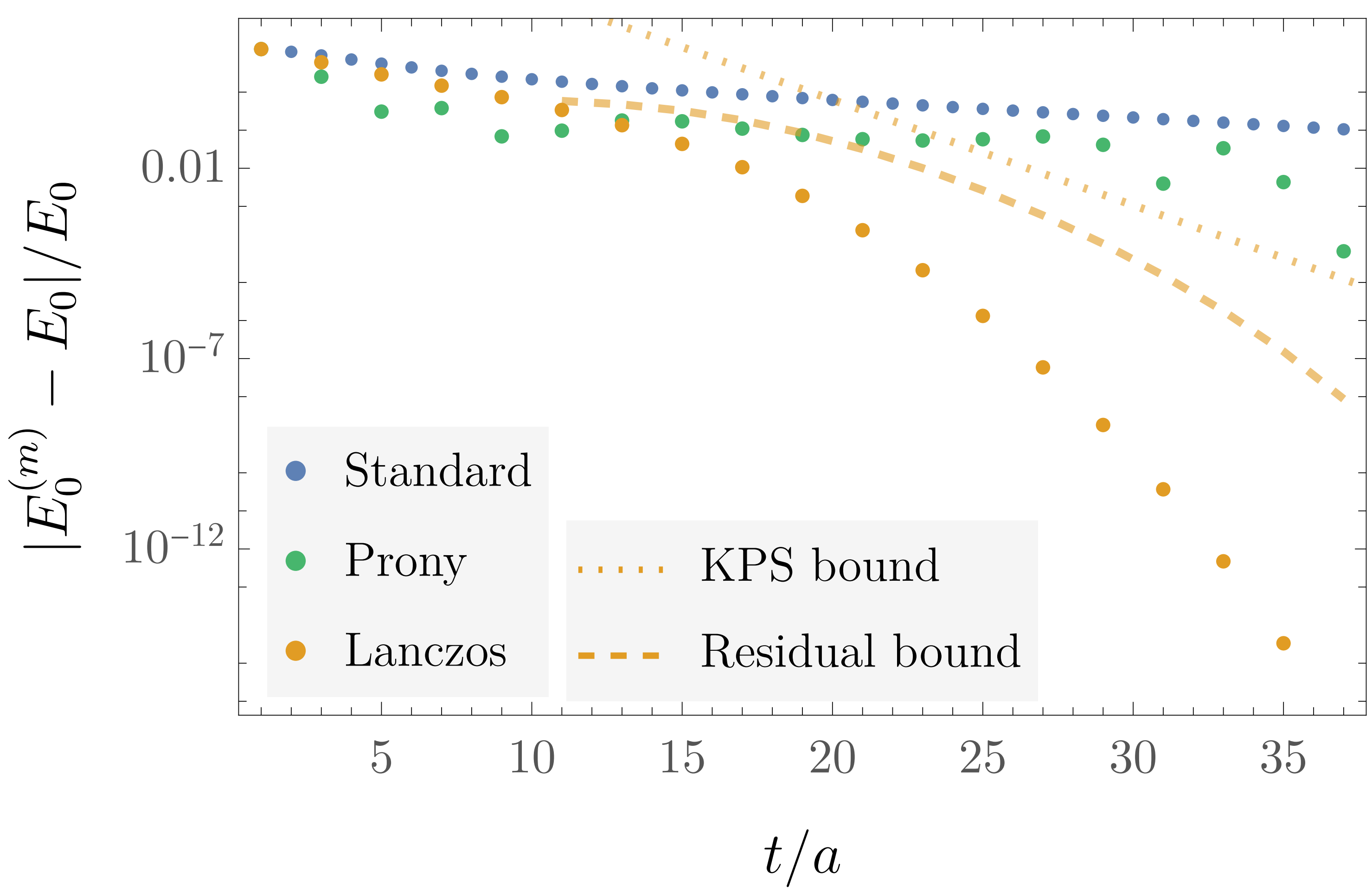
Matrix element $T^{(m)}_{m(m+1)}$

Paige, PhD thesis 1971

Rigorous quantification of excited-state effects!

But the LQCD transfer matrix is infinite-dimensional….

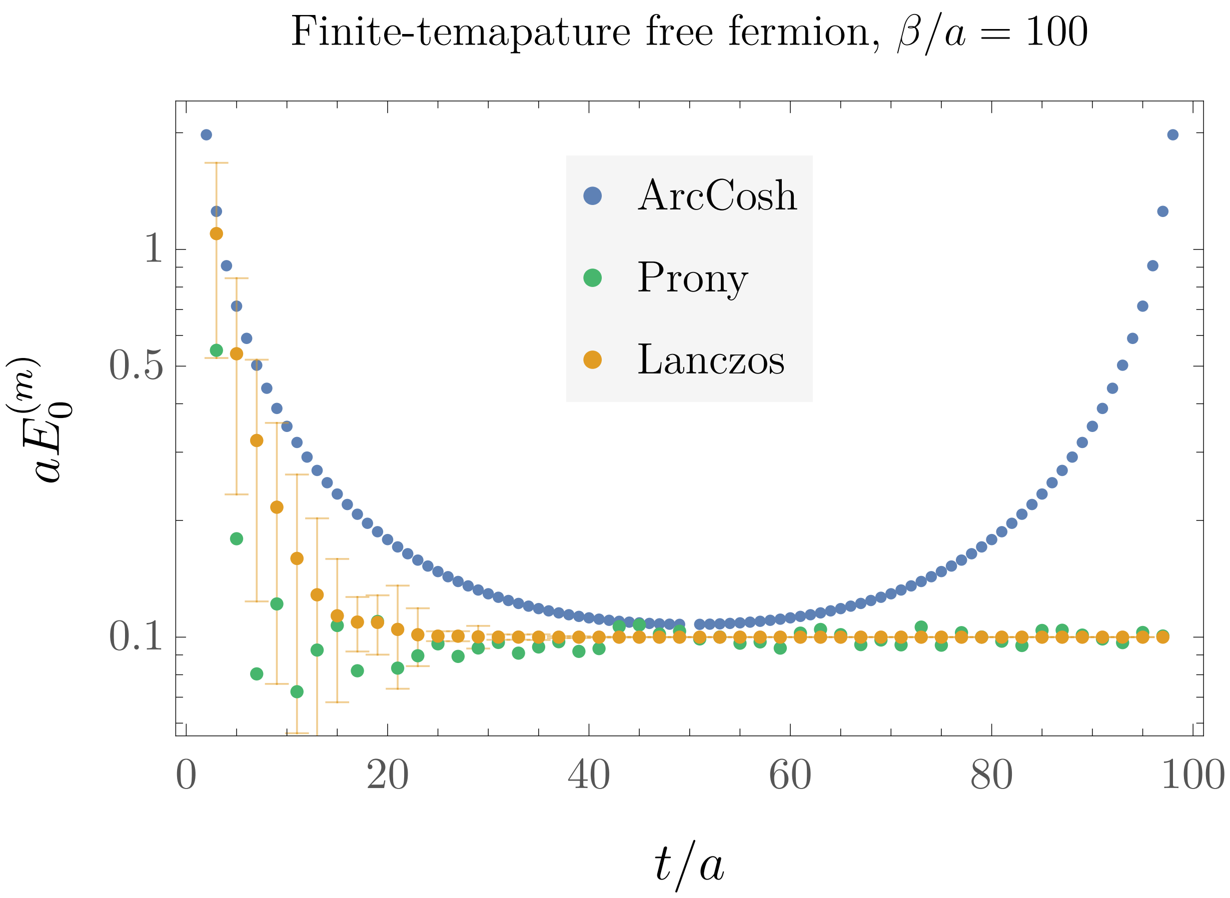
- Applying Lanczos feasible by computing matrix elements $T_{ij}^{(m)}$ recursively
- Faster convergence evident in studies of toy data

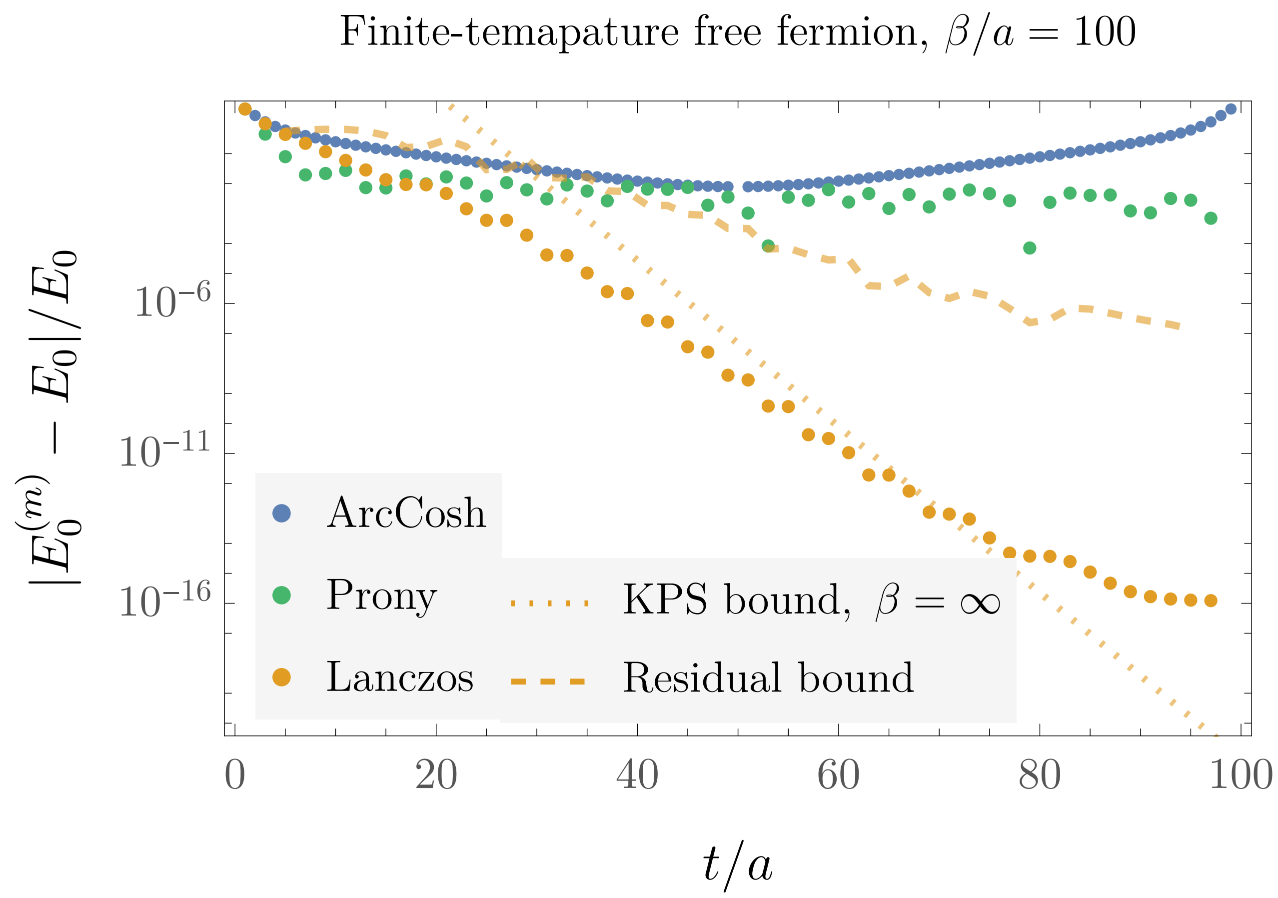


MW, arXiv:2406.XXYY

Heating things up

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





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

MW, arXiv:2406.XXYY

Will noise destroy Lanczos?

MW, arXiv:2406.XXYY

Will noise destroy Lanczos?

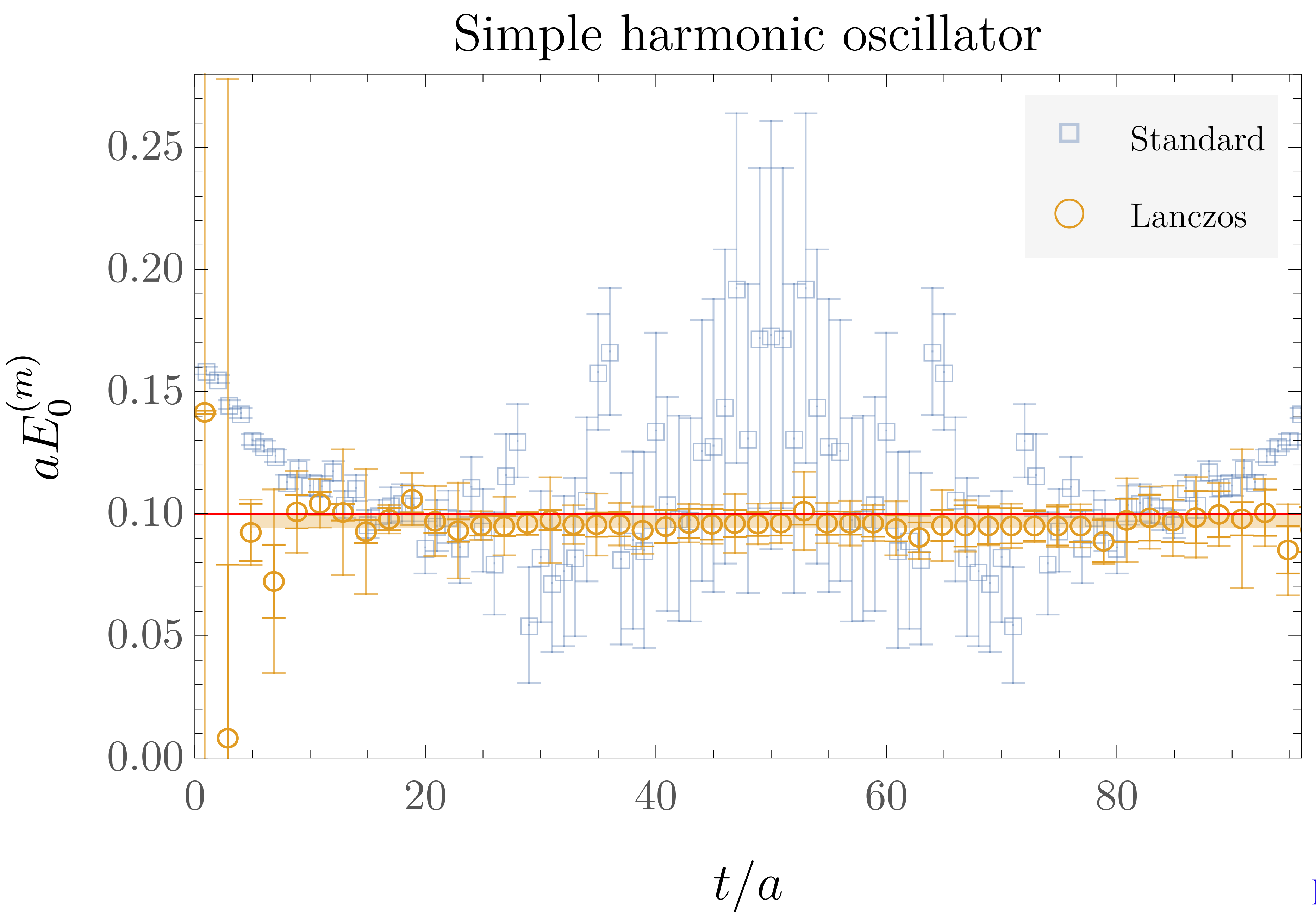
- No

MW, arXiv:2406.XXYY

Will noise destroy Lanczos?

- No

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



MW, arXiv:2406.XXYY

Is it really that easy?

MW, arXiv:2406.XXYY

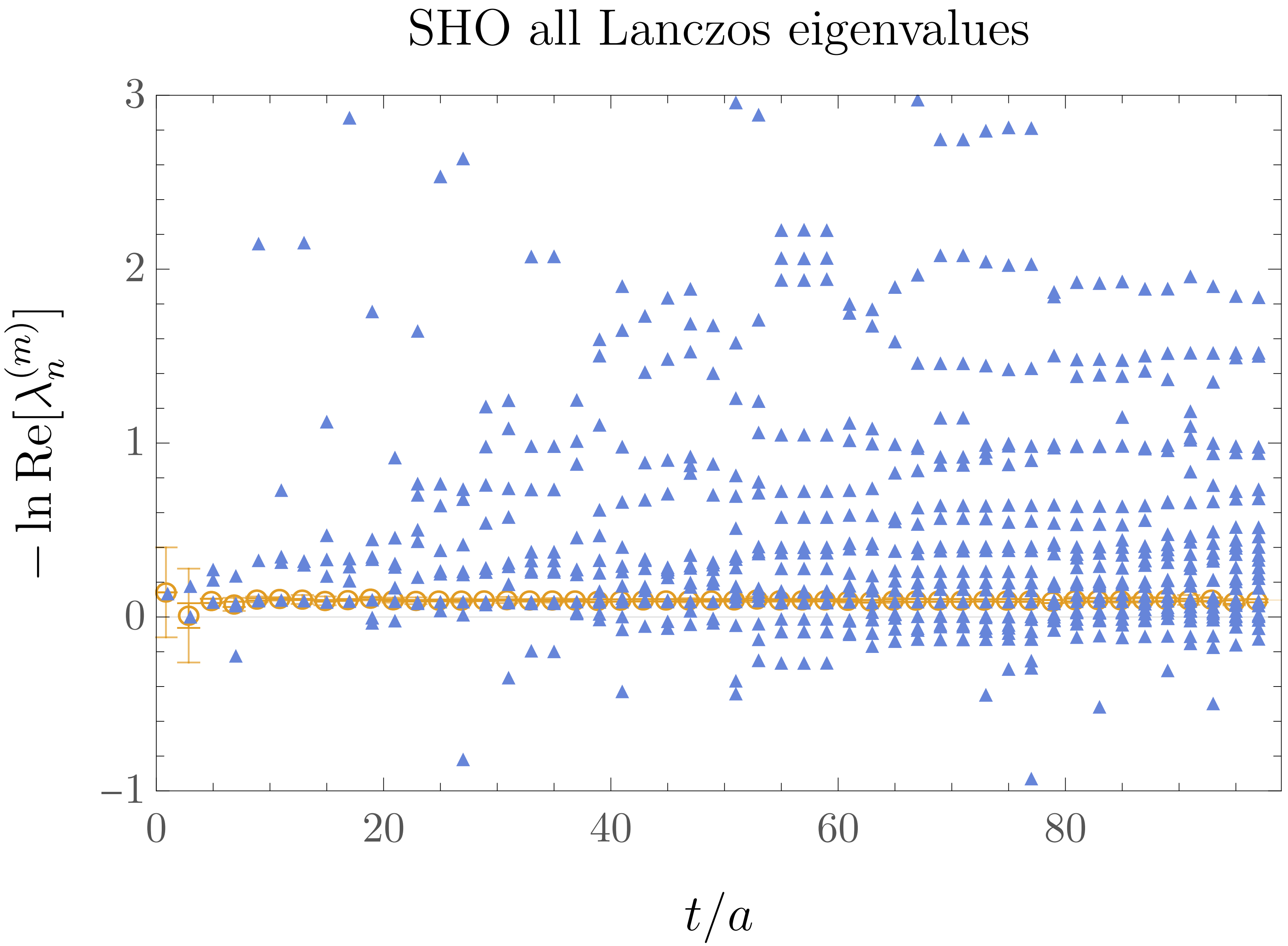
Is it really that easy?

- No

Is it really that easy?

- No

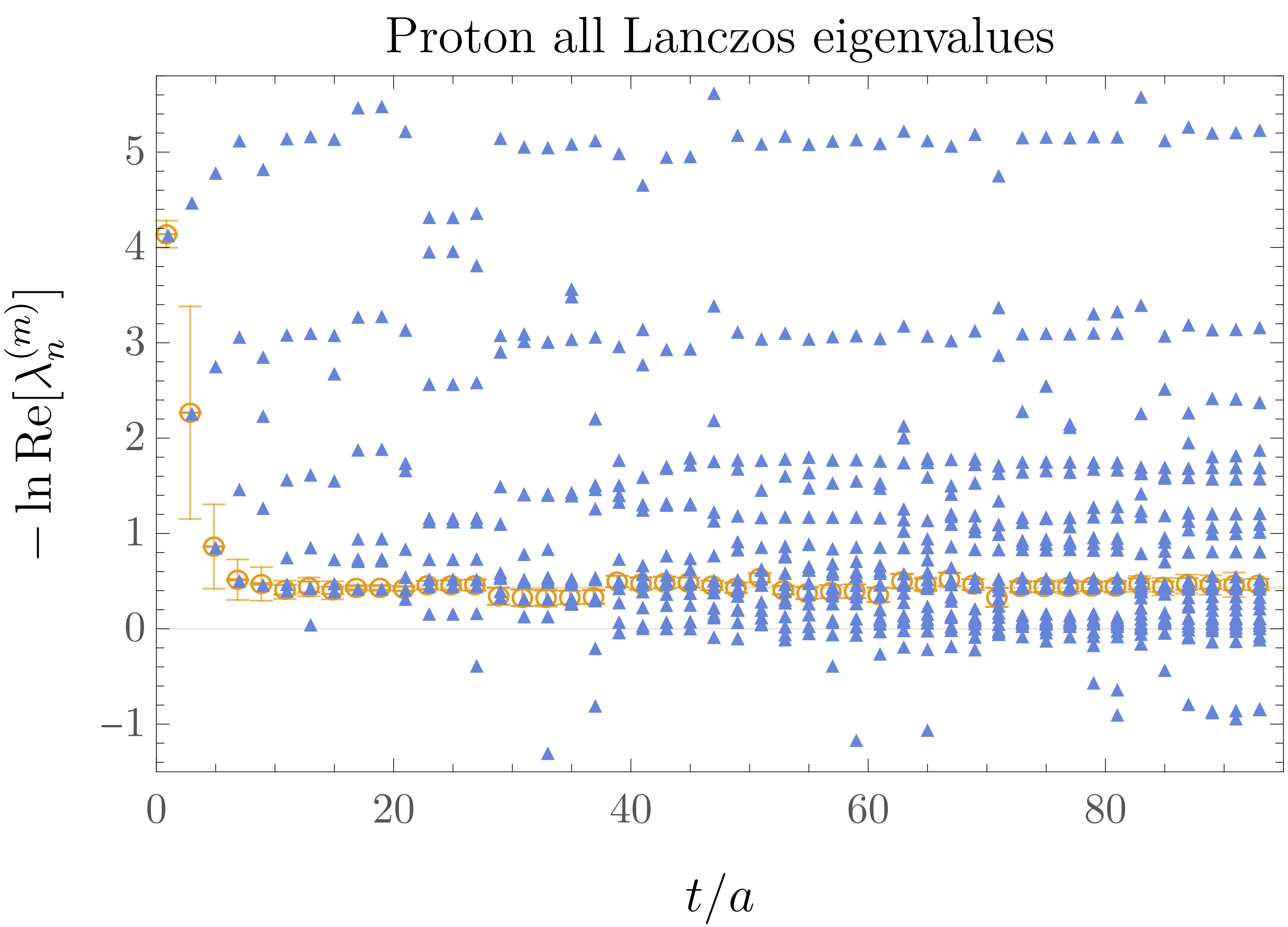
- Lanczos produces an increasingly dense forest of “spurious eigenvalues”



MW, arXiv:2406.XXYY

Conservation of evil

- Lanczos can be applied to LQCD correlation functions just as easily
- Lots of eigenvalues values come out

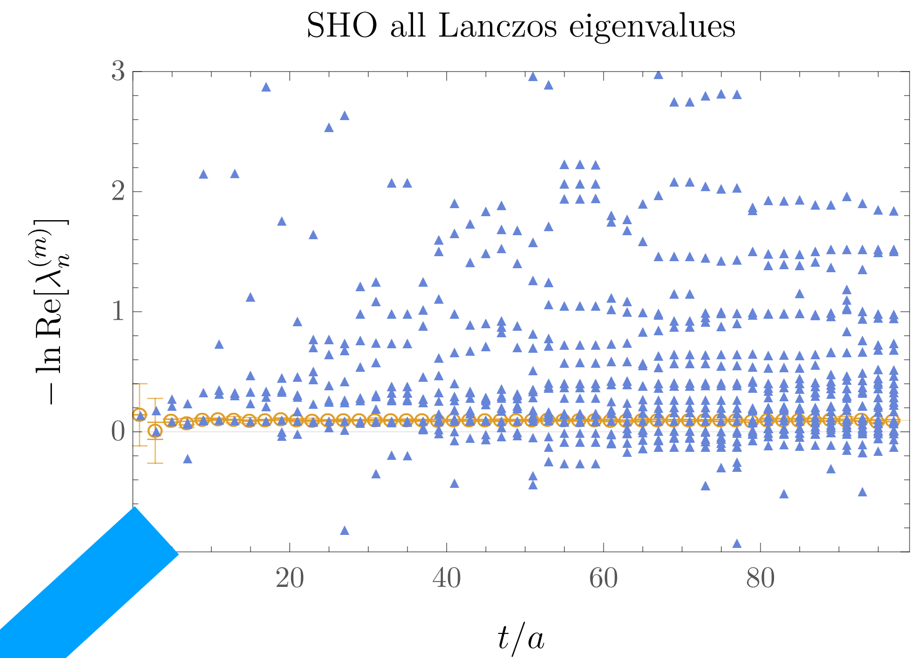


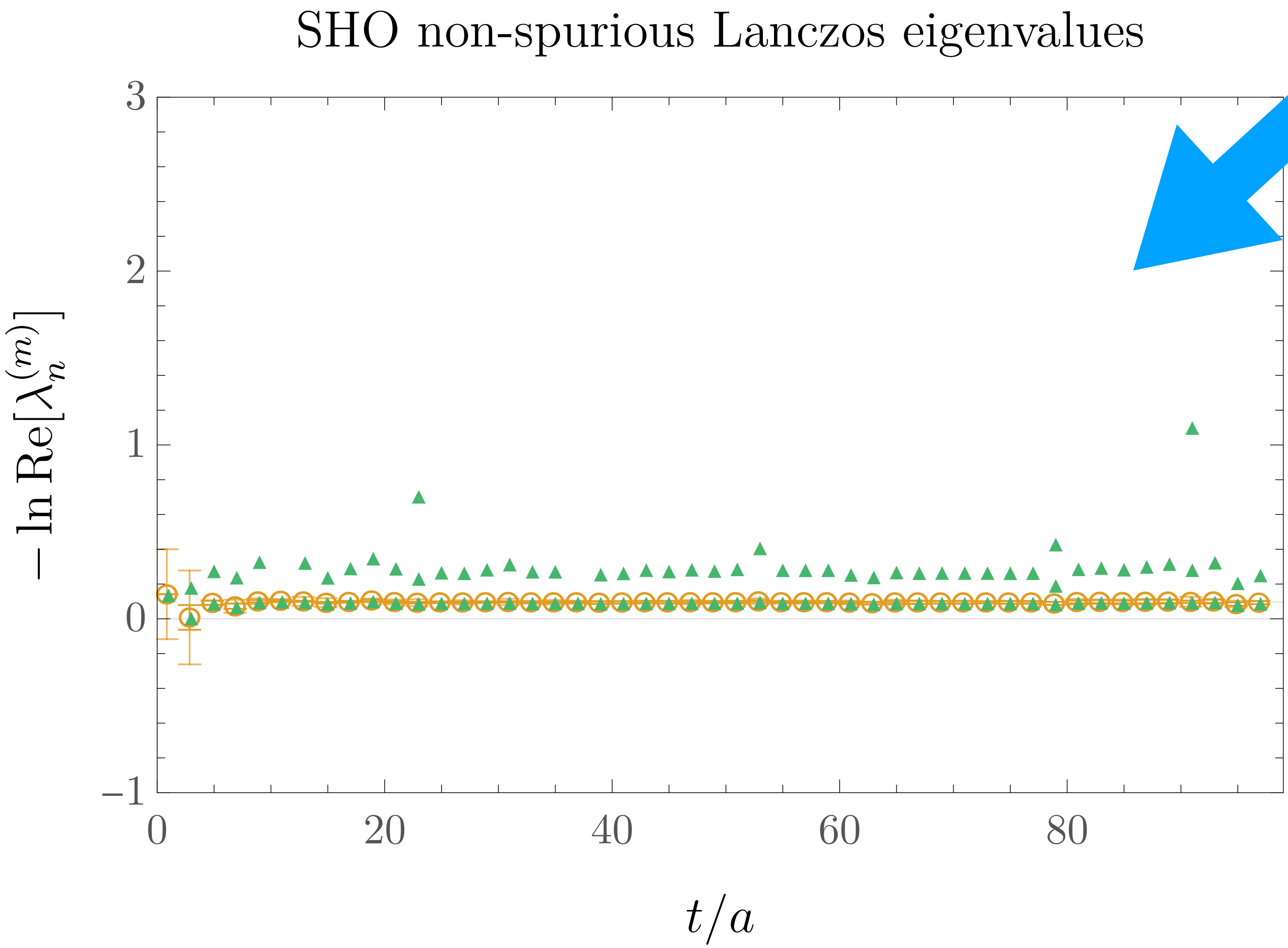
- Known from linear algebra applications that some converge to desired eigenvalues but others are “spurious”

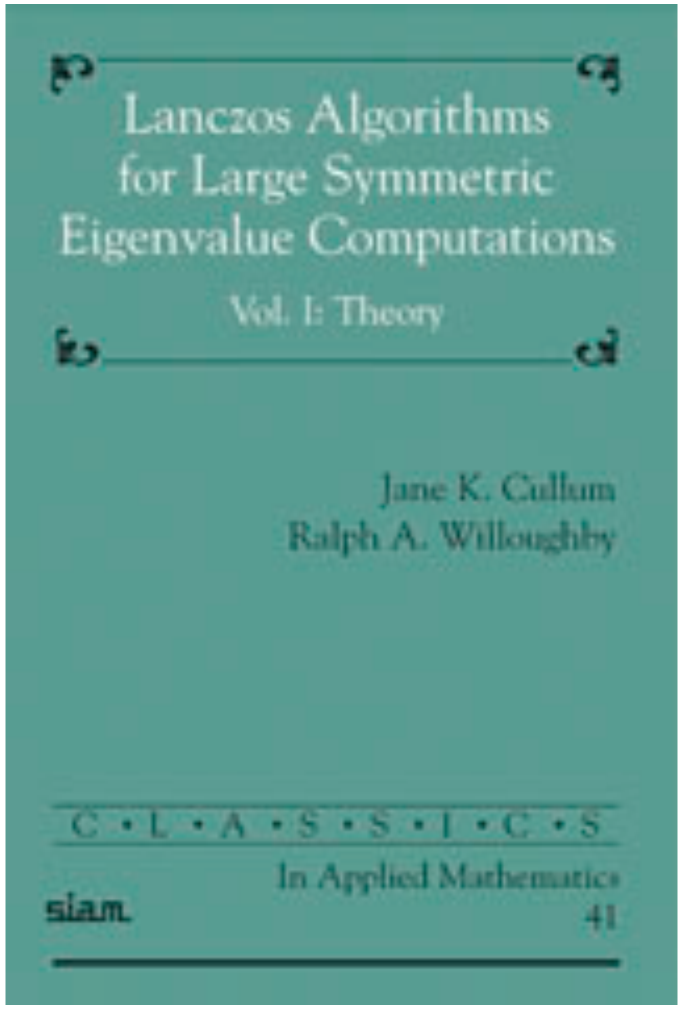
MW, arXiv:2406.XXYY

Spurious eigenvalues

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







MW, arXiv:2406.XXYY

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.

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

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

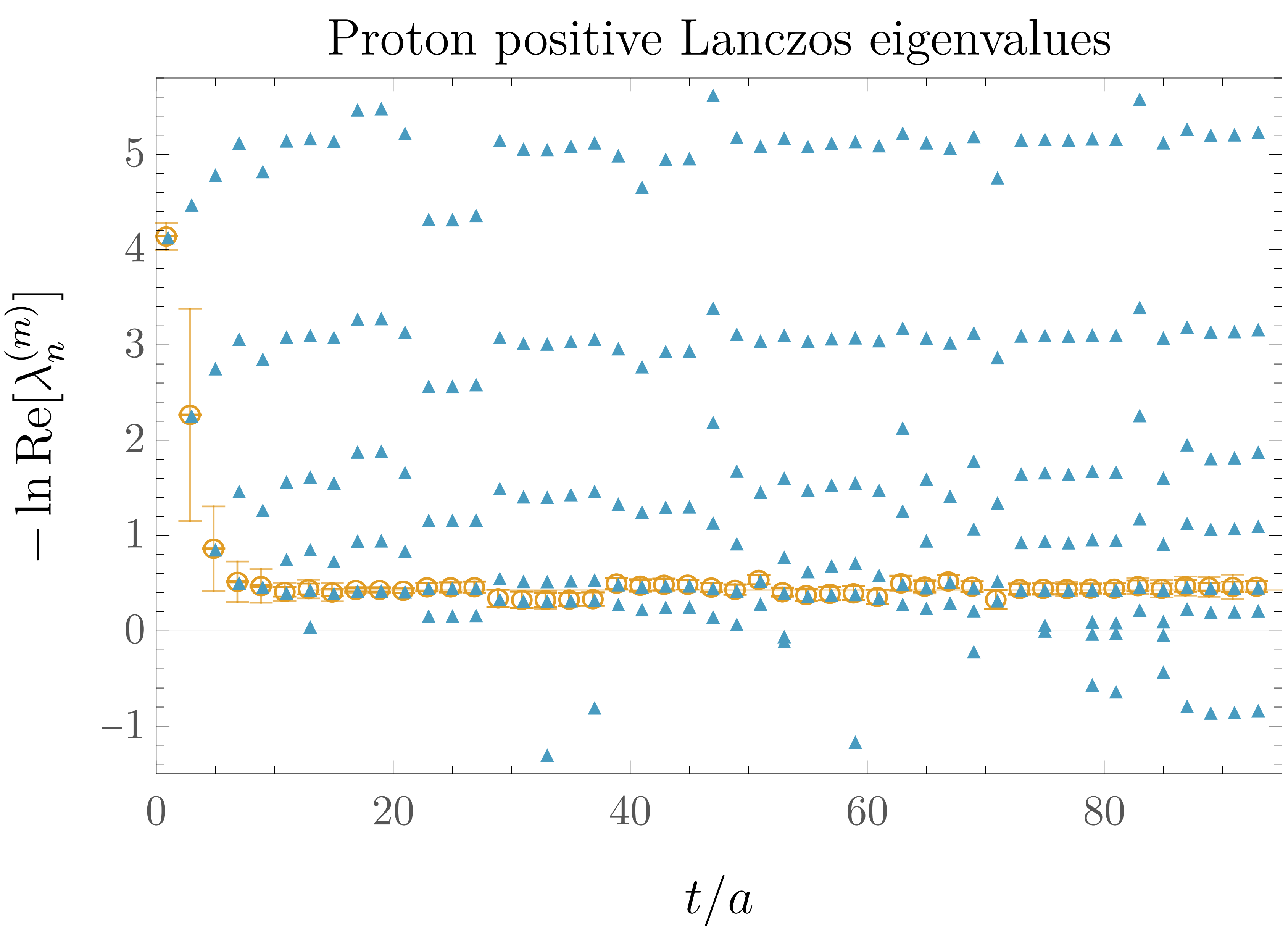
Definition 2. Any simple eigenvalue of T_m that is pathologically close to an eigenvalue of $\hat{T}_2$ will be called "spurious."

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)



- 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.XXYY

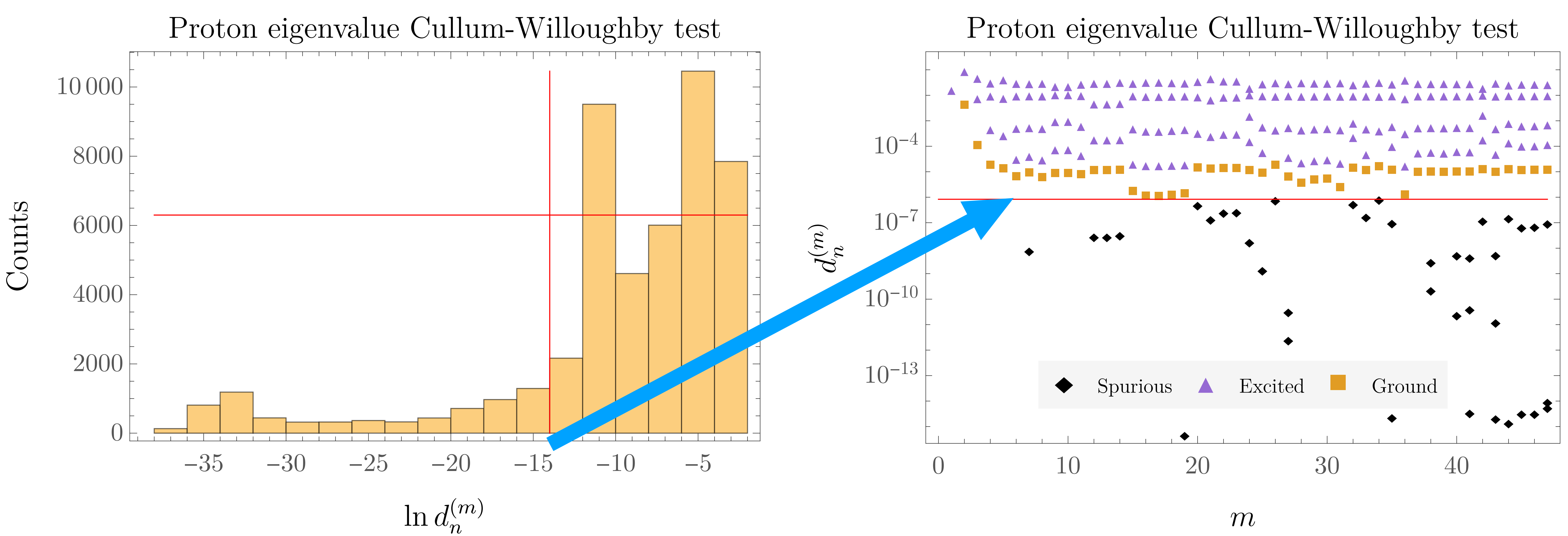
Bootstrapping Cullum-Willoughby

- 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

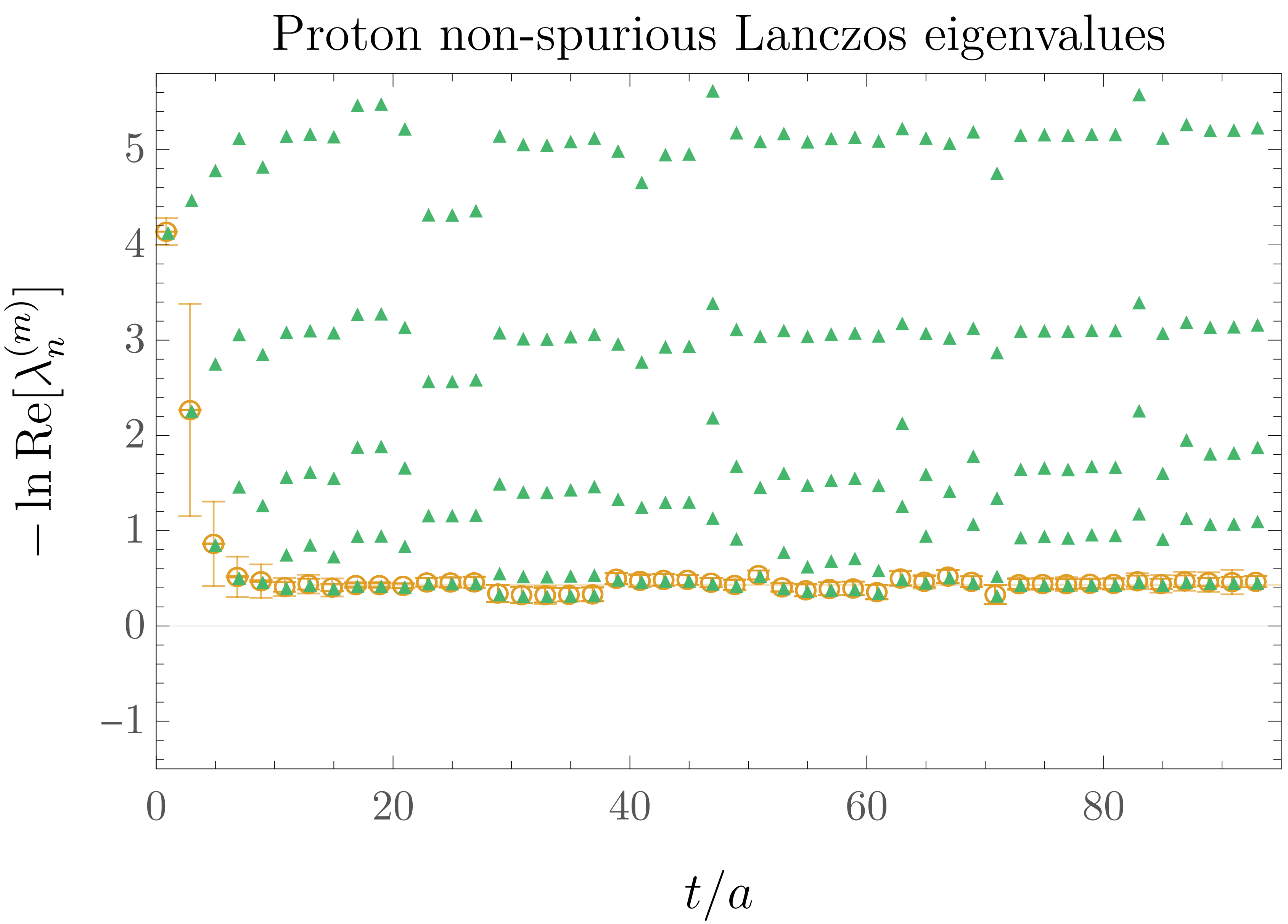


Non-spurious proton energies

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

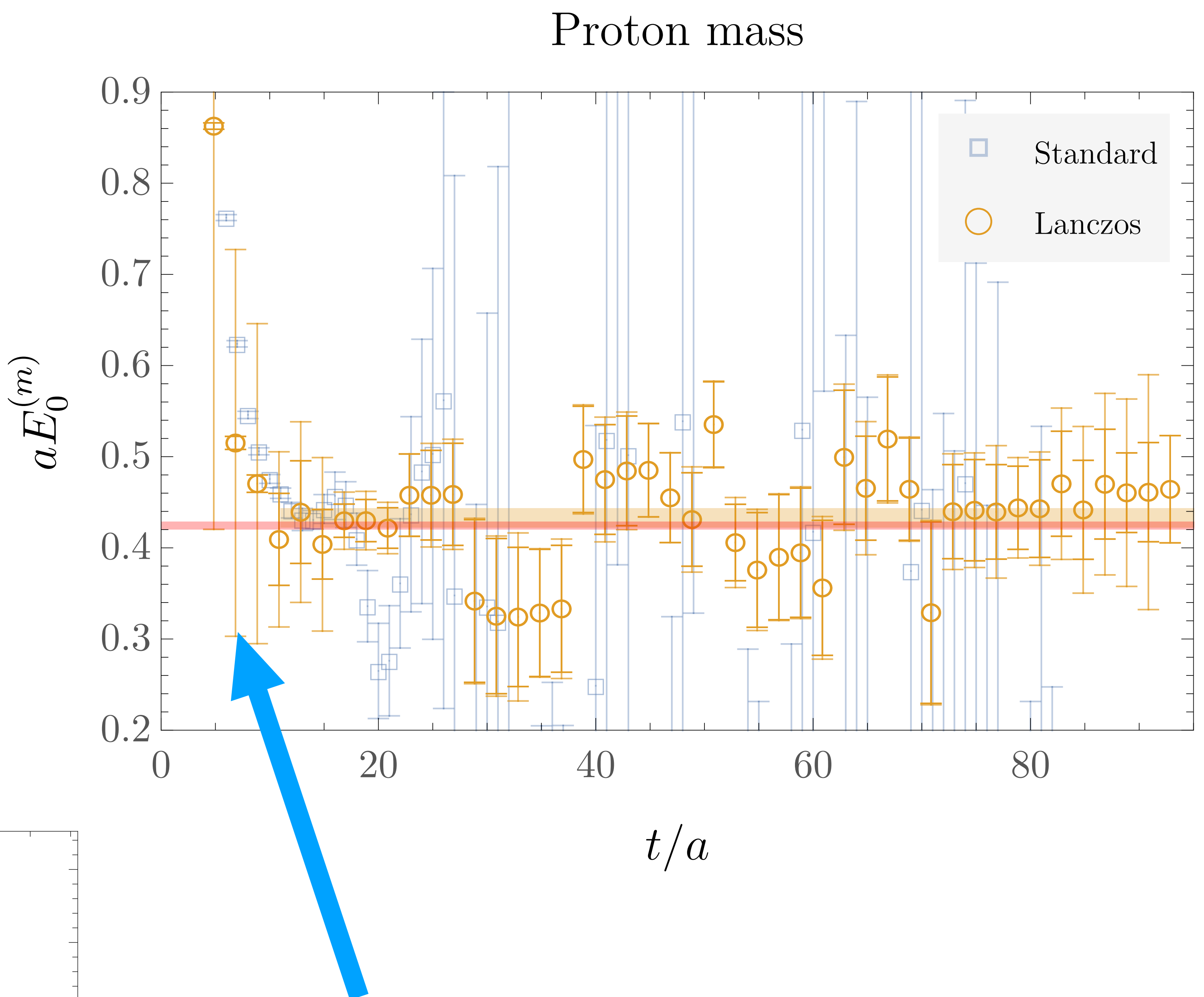
$$E_0 = -\ln \lambda_0^{(m)}$$

- Excited-state energies also accessible



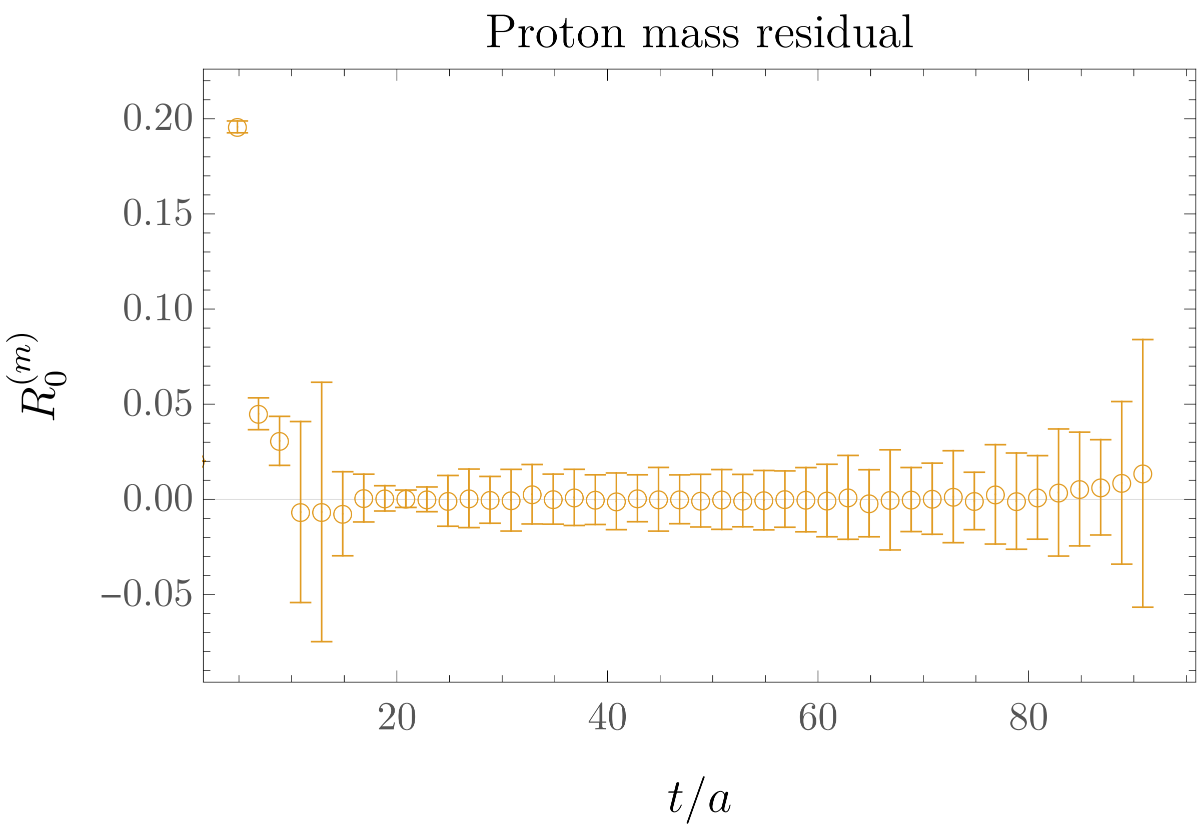
MW, arXiv:2406.XXYY

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

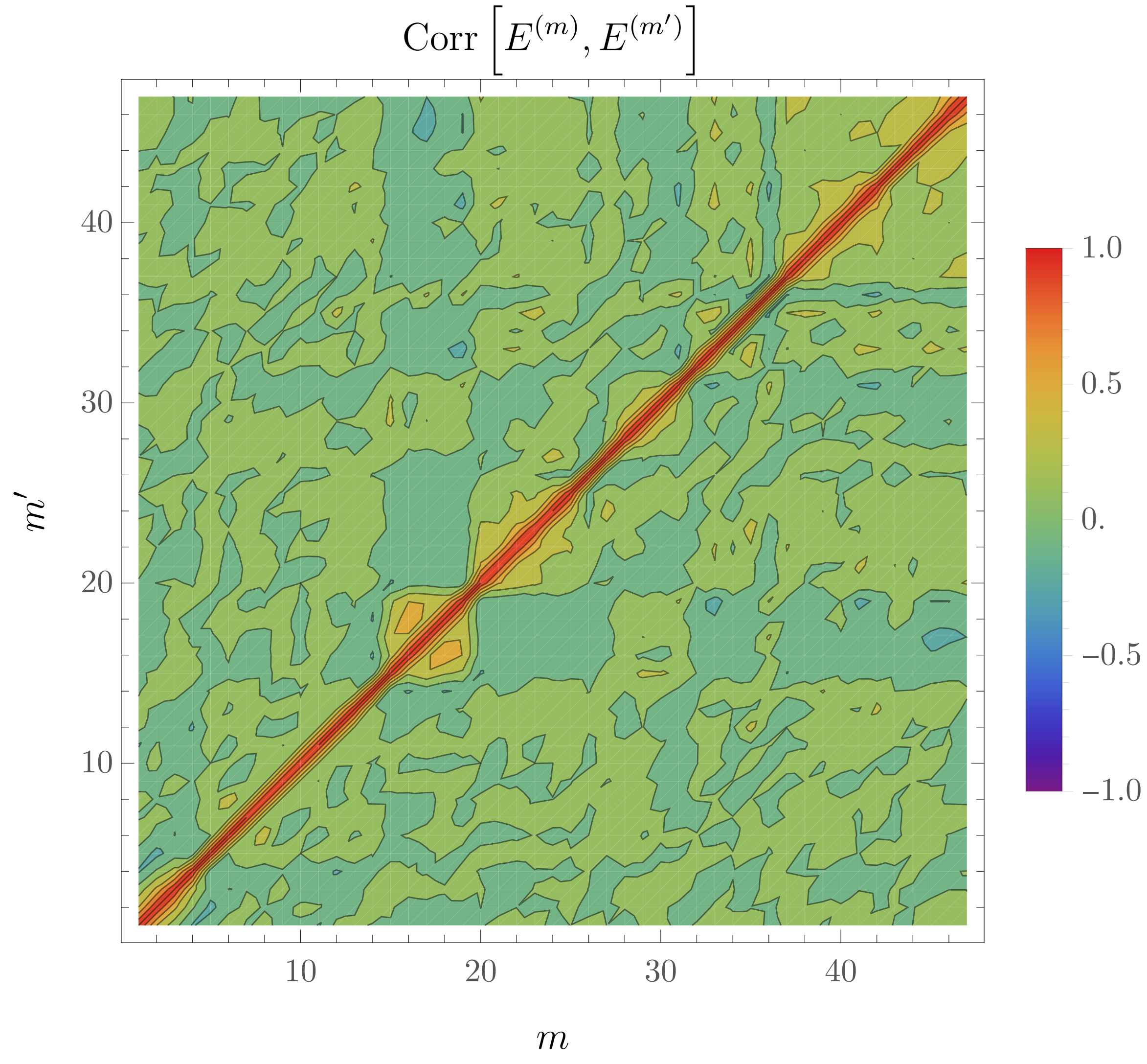


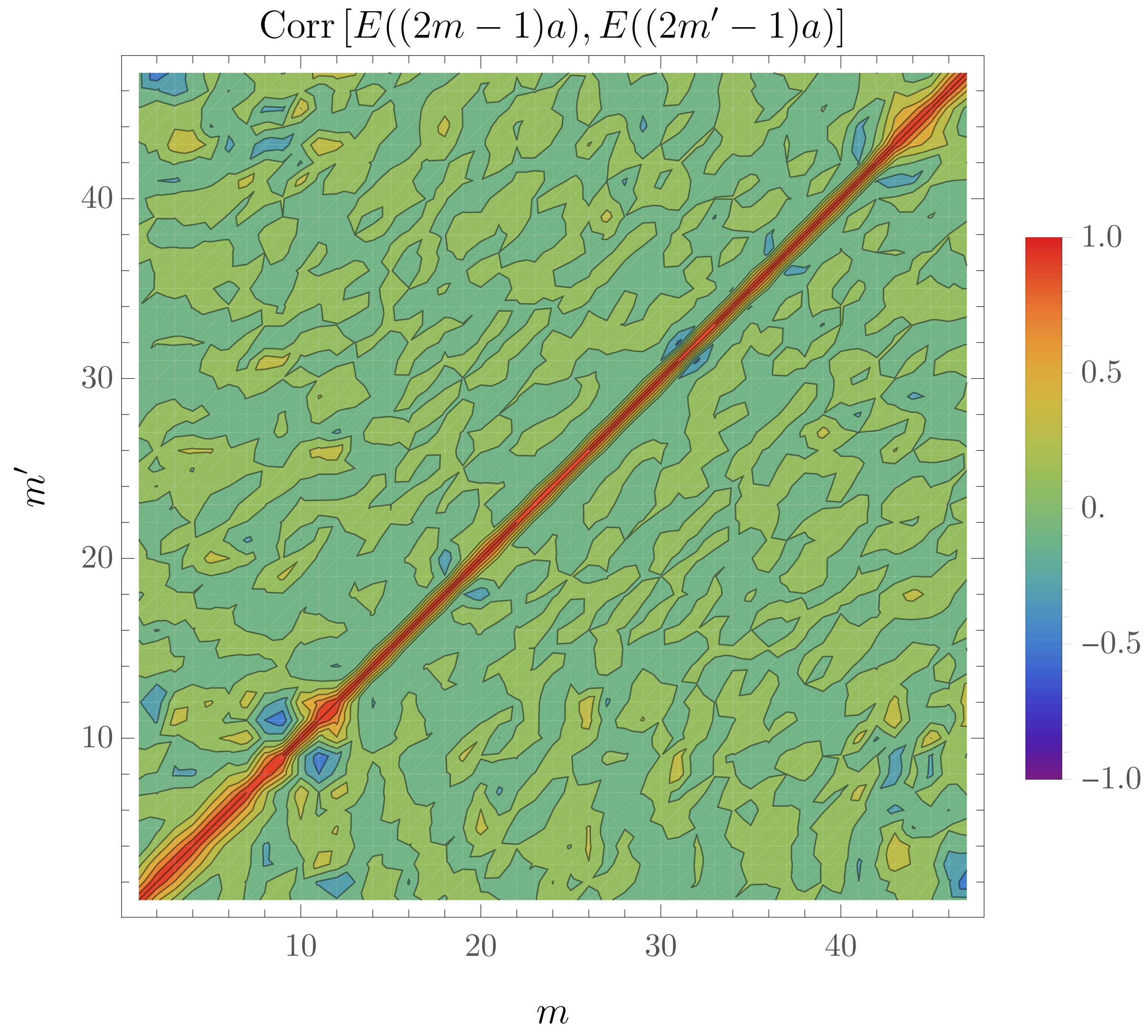
- Residual bound can be used to identify when Lanczos results have converged, provides estimate of finite-t approximation errors

MW, arXiv:2406.XXYY

Correlations

- Correlations between Lanczos results at different imaginary times fall off rapidly with similar scale to correlations between standard effective mass results



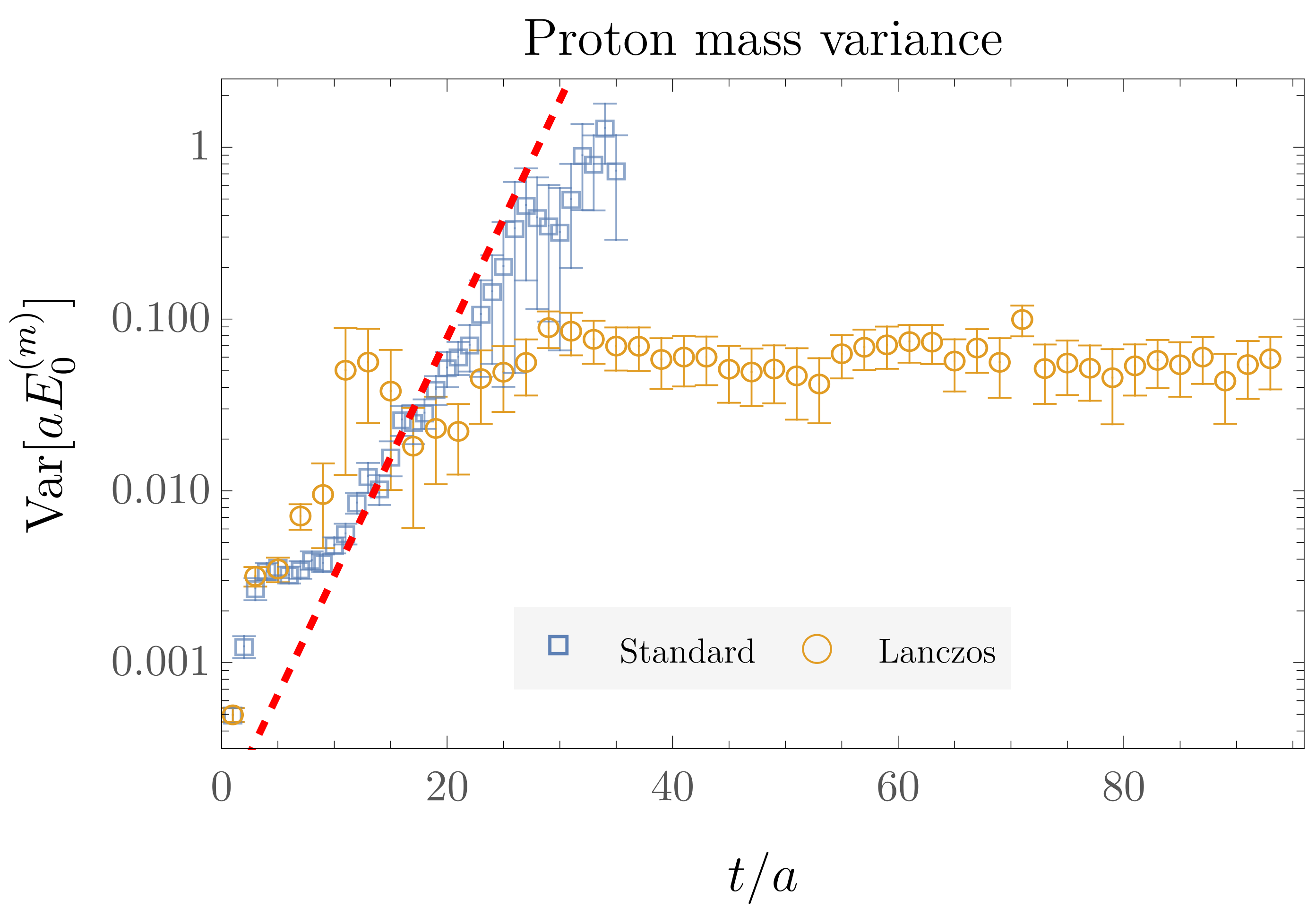


MW, arXiv:2406.XXYY

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

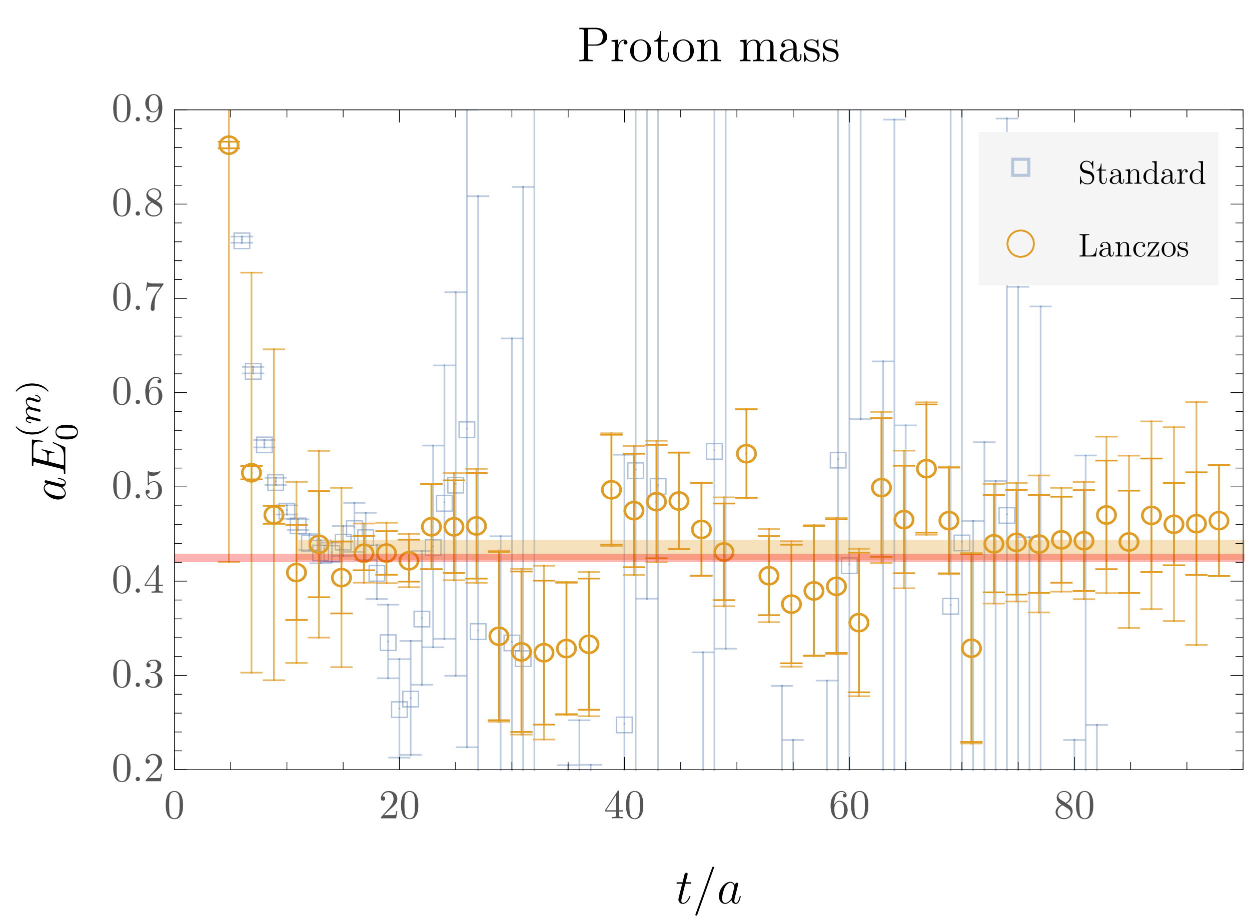
- Building such projectors is hard — but Lanczos provides Krylov-space approximations

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

- 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!

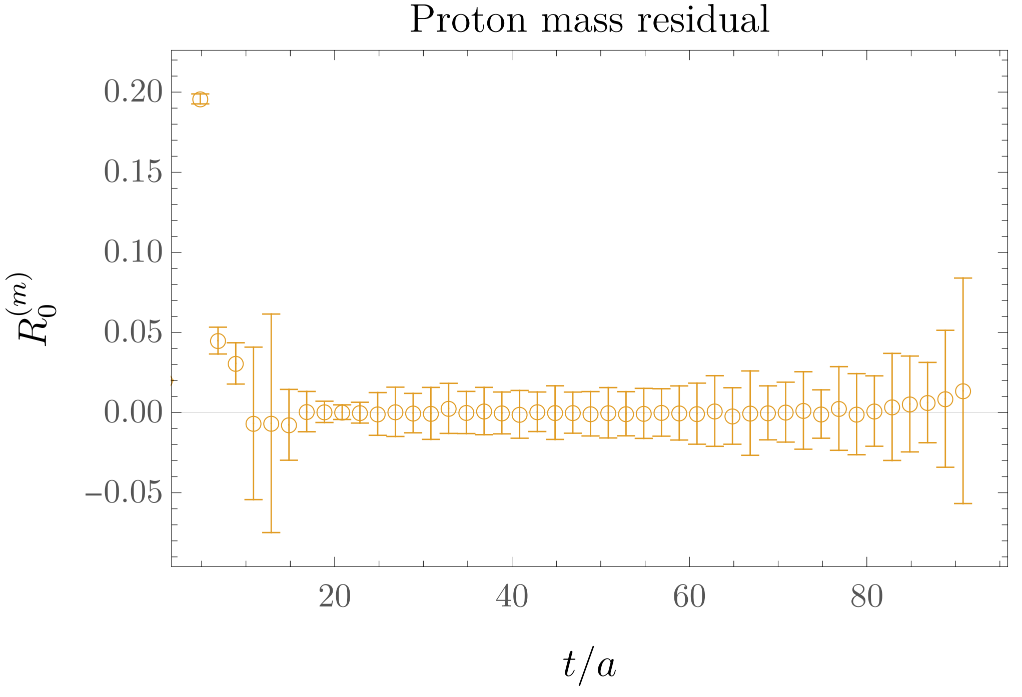
Questions

- Are there other diagnostics for saturation of variational bounds?

- Can we quantify excited-state uncertainties better in variational methods?

- How should we present Lanczos approximation error bounds (~systematic uncertainties) that come with statistical uncertainties?

$$a^2|E - E_0^{\mathrm{Lanczos}}|^2 < 0.0004(67)$$



- Are there methods from robust statistics that can reduce uncertainties arising from spurious eigenvalue outliers?