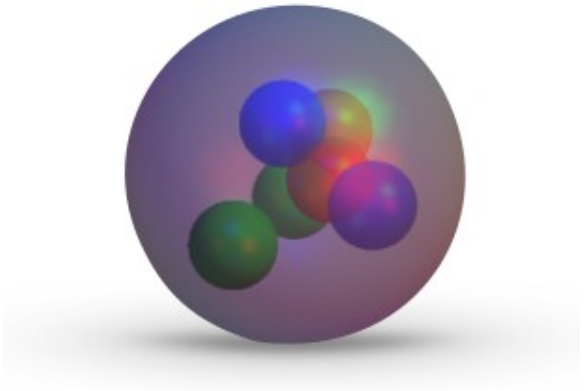
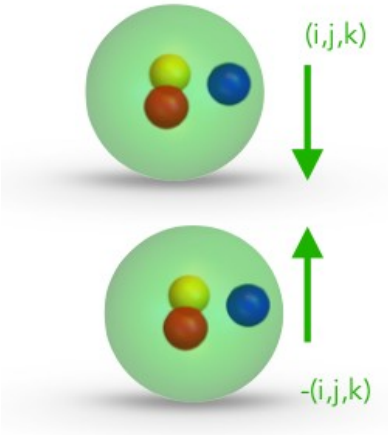
Massachusetts Institute of Technology

Systematic uncertainties in two-nucleon spectroscopy





Robert Perry for NPLQCD
Will Detmold, Zohreh Davoudi, Anthony Grebe, Dan Hackett, Marc Illa, Assumpta Parreno, Mike Wagman, Phiala Shanahan
Nov 7, Lattice 2025, Mumbai, India

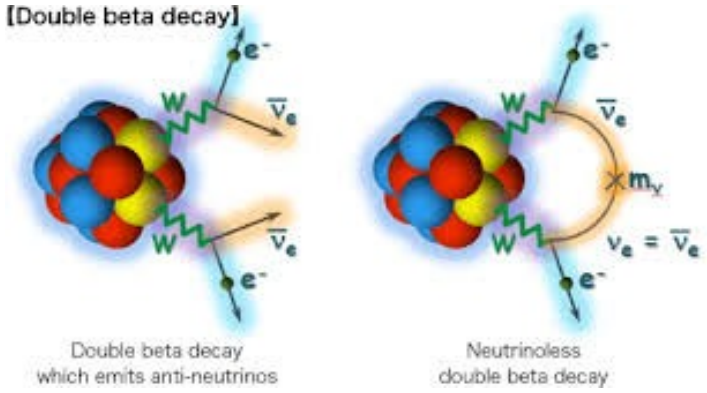
Lattice QCD and nuclear physics

Understand emergence of nuclear complexity from the quarks and gluons.

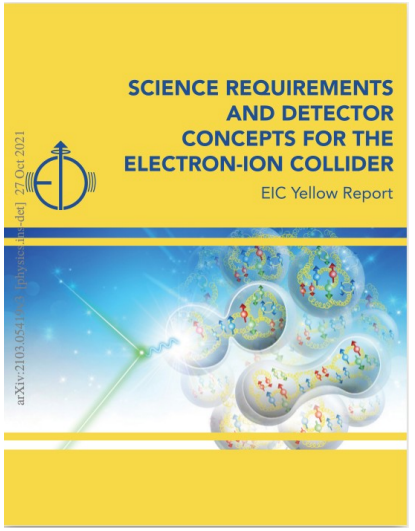
Nuclear objects often targets in BSM searches

large source of systematic uncertainty

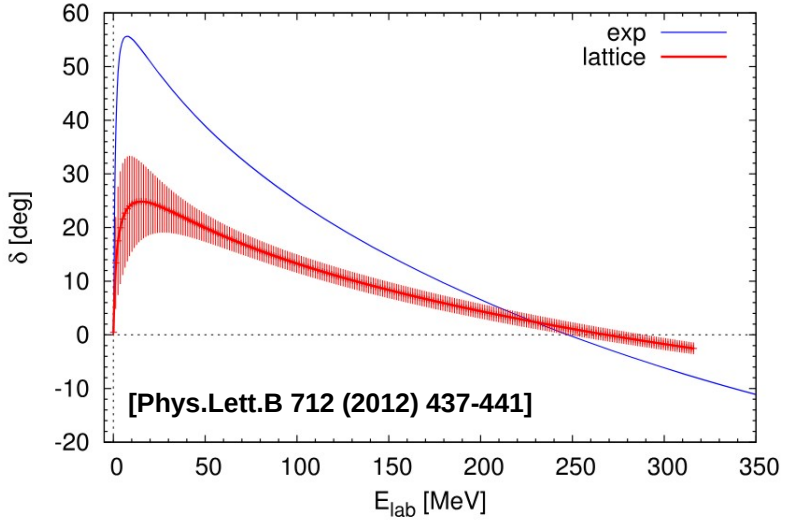
IF we can demonstrate control of systematics, LQCD can contribute!

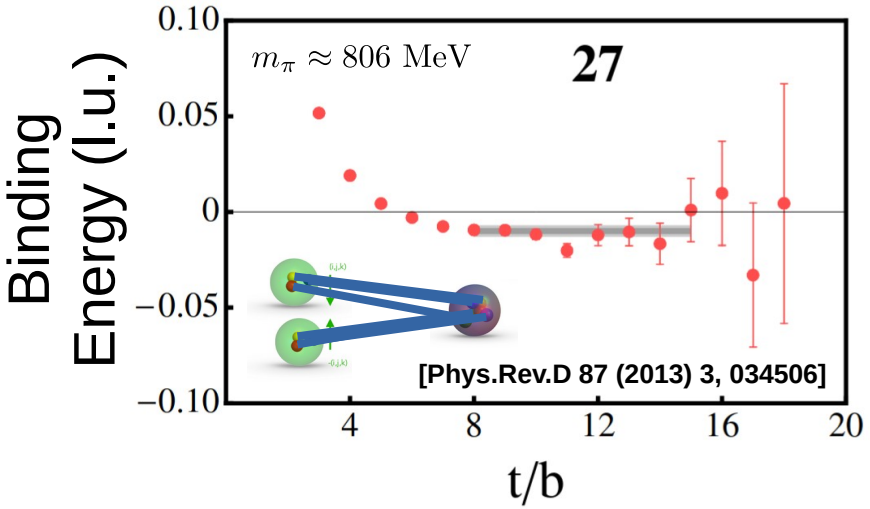


DEEP UNDERGROUND NEUTRINO EXPERIMENT



NN interactions: a one slide history





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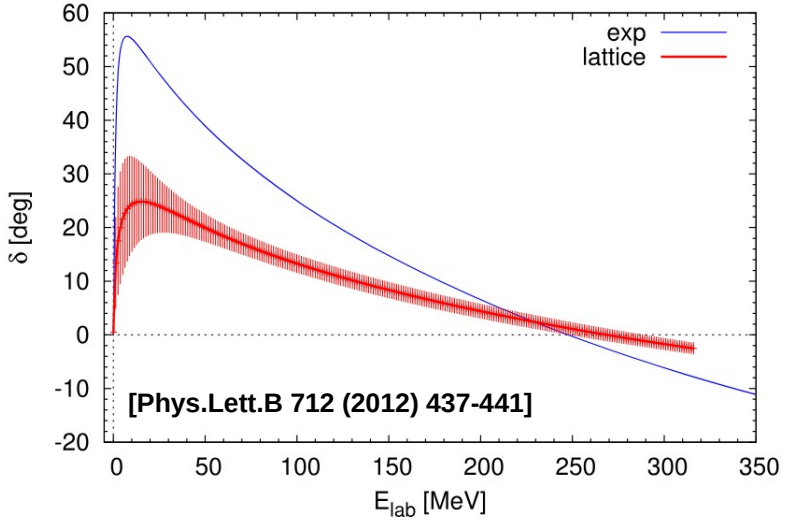
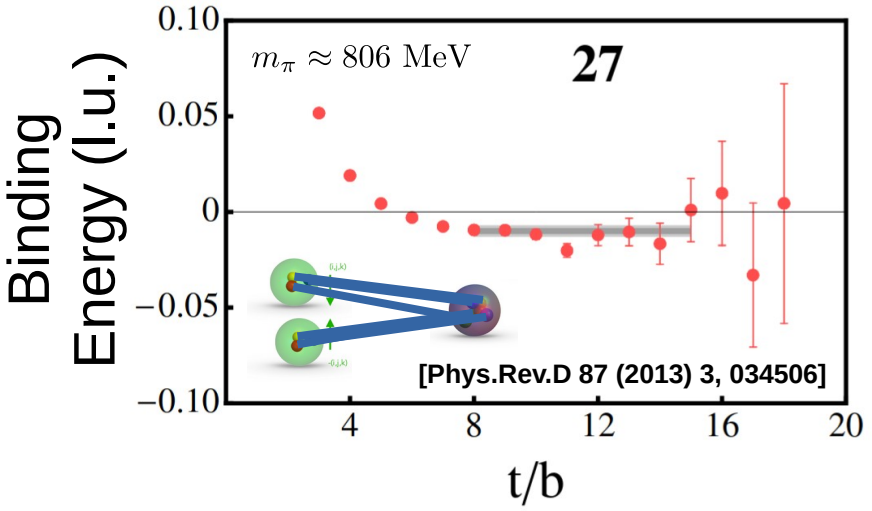
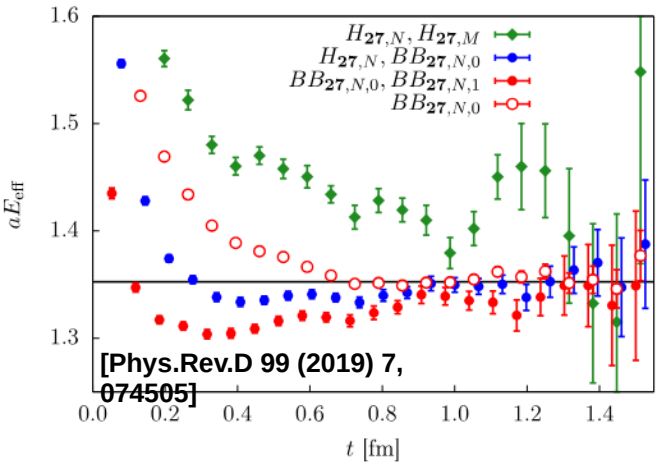
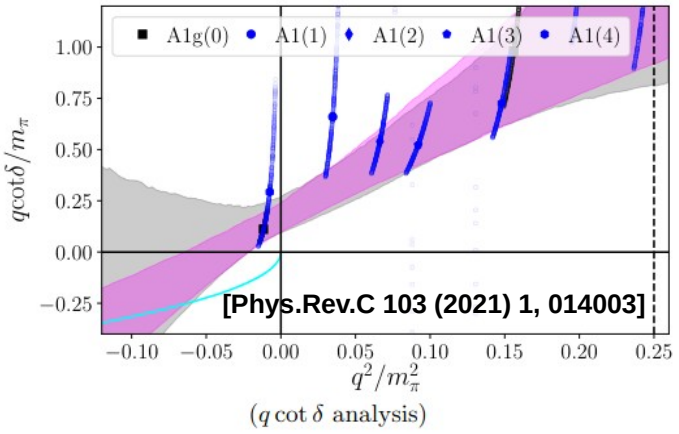
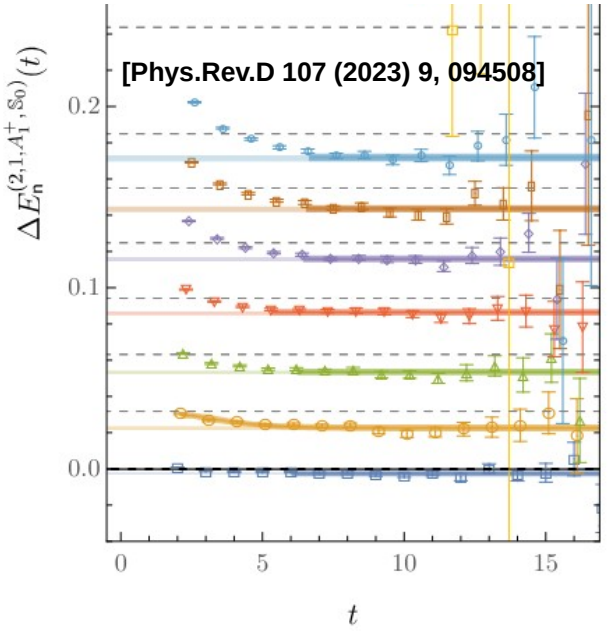


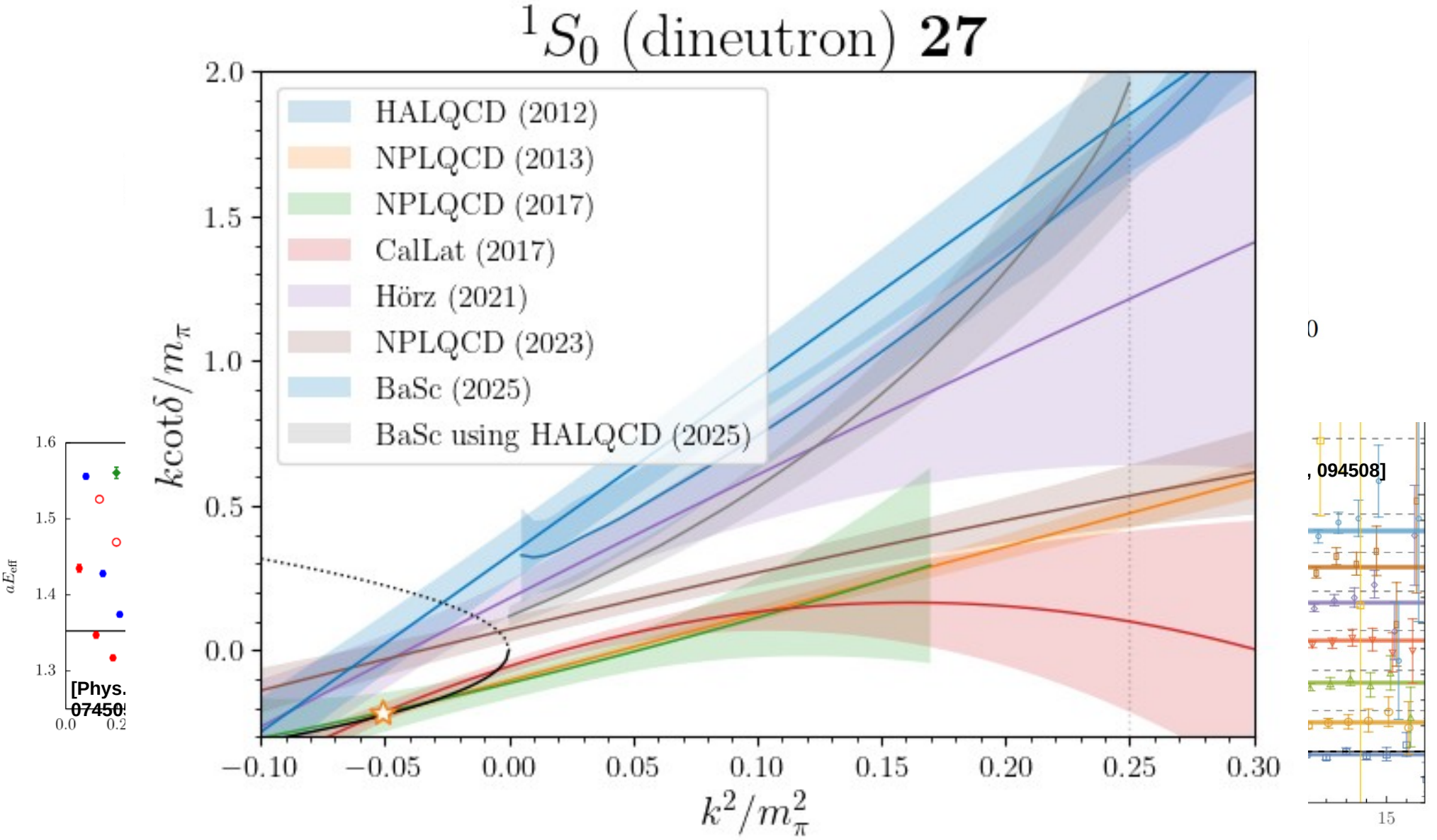






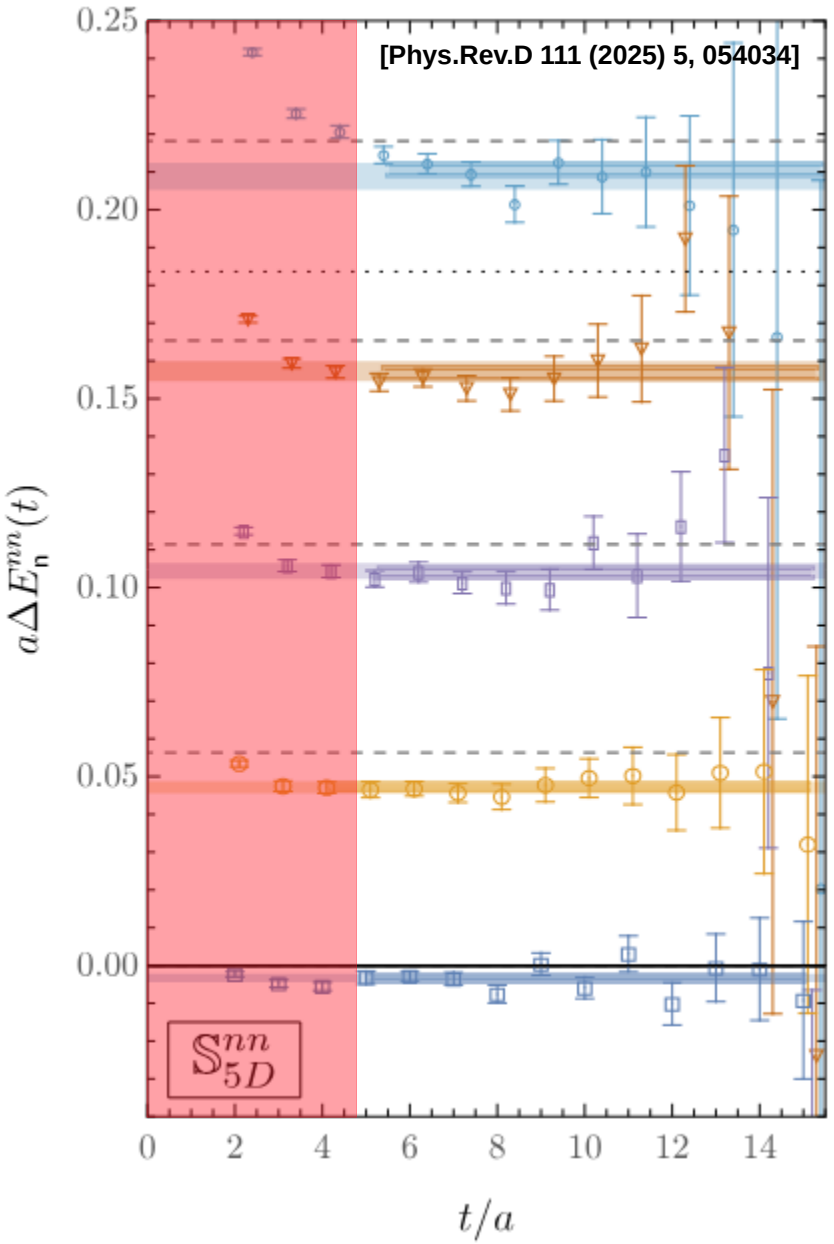


A one-slide history



Should agree: **underestimated systematic errors**

Assumption: N-state saturation



***N*-state saturation**

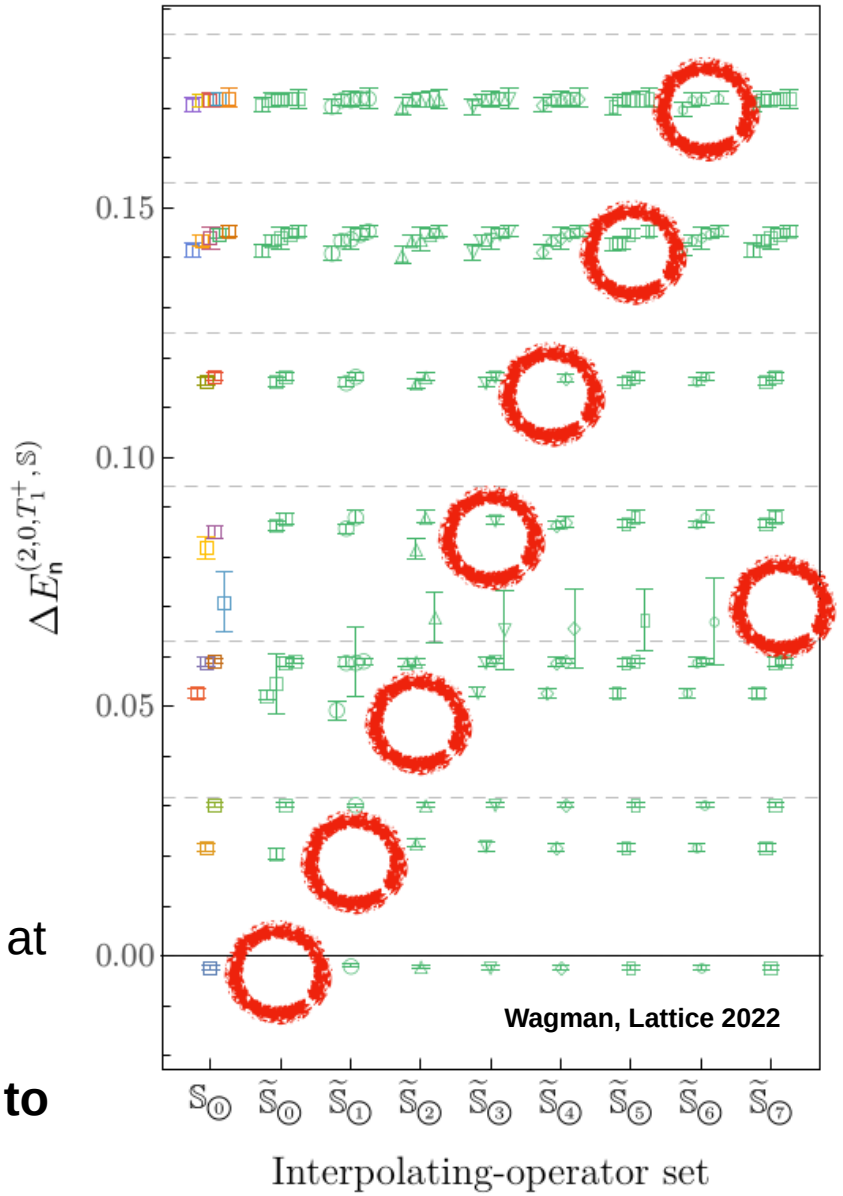
There exists a region of Euclidean time where the correlator (matrix) is accurately described by a truncated spectral decomposition containing *N* states.

Assumption: No missing states

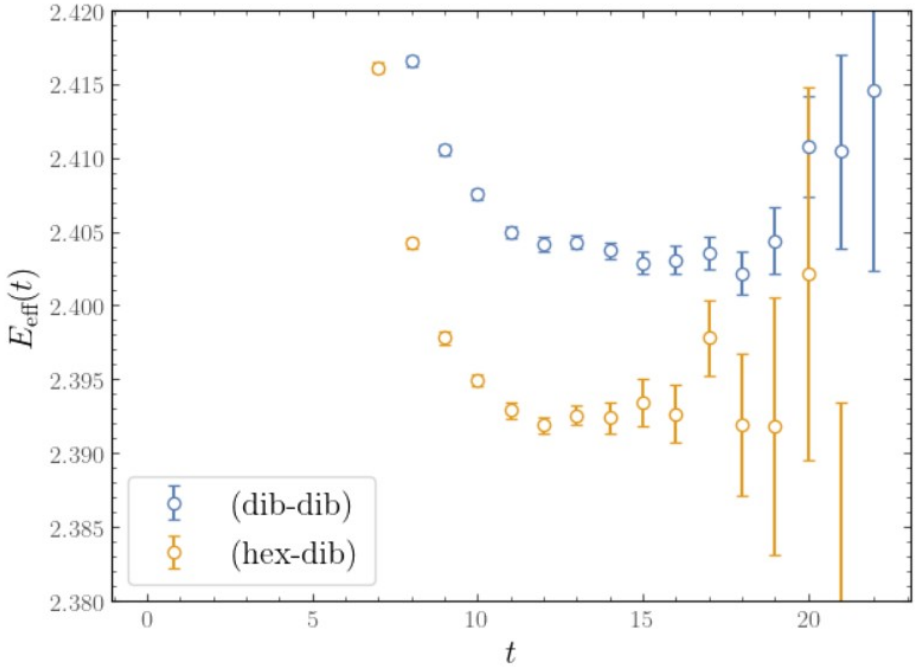
No missing states

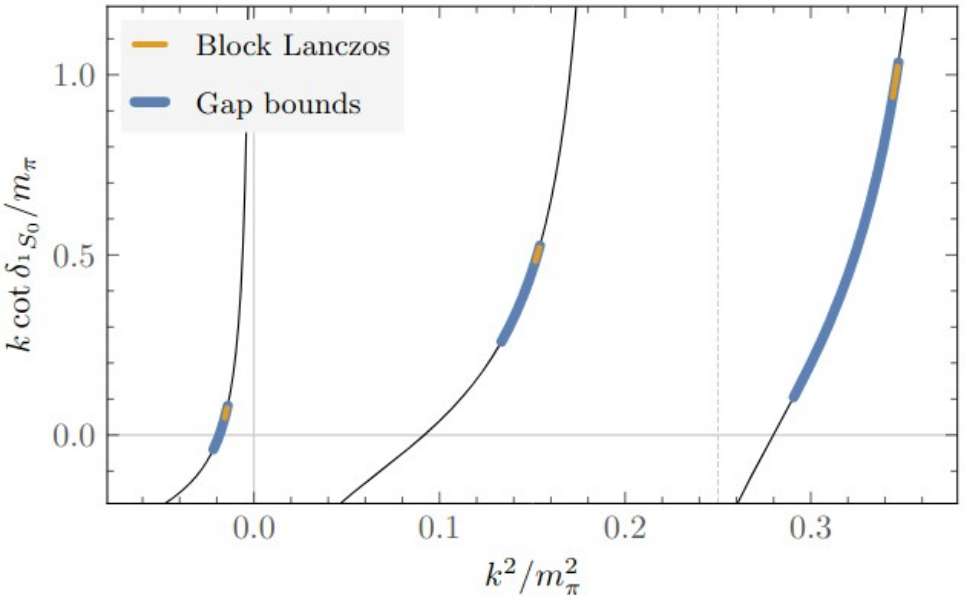
There are exactly N states with energy less than a threshold E_{gap} that make non-zero contributions to a correlator (matrix).

Can be violated: Evidence that at finite statistics, choosing “right” operator set is important; **hard to know when you’re done**



High-statistics study of two-nucleon spectroscopy



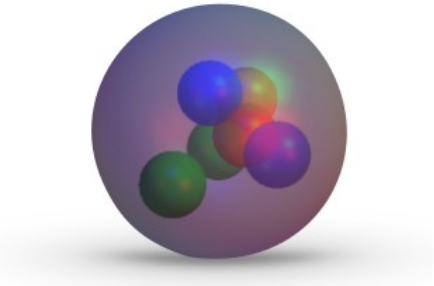


Lattice Details

$(L/a)^3 \times (T/a)$	β	am_q	a [fm]	L [fm]	T [fm]	$m_\pi L$	$m_\pi T$
$24^3 \times 48$	6.1	−0.2450	0.1453(16)	3.4	6.7	14.3	28.5

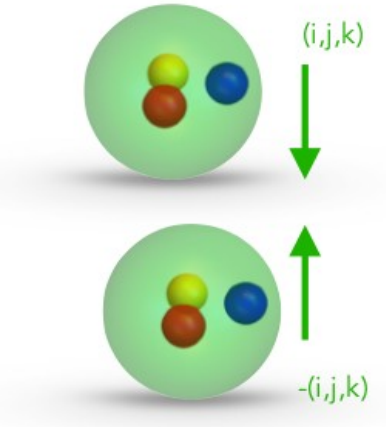
20 Million propagators

Employed **sparsened** propagators [Phys.Rev.D 104 (2021) 3, 034502]



Local hexaquark operators

Six Gaussian smeared quarks at a point

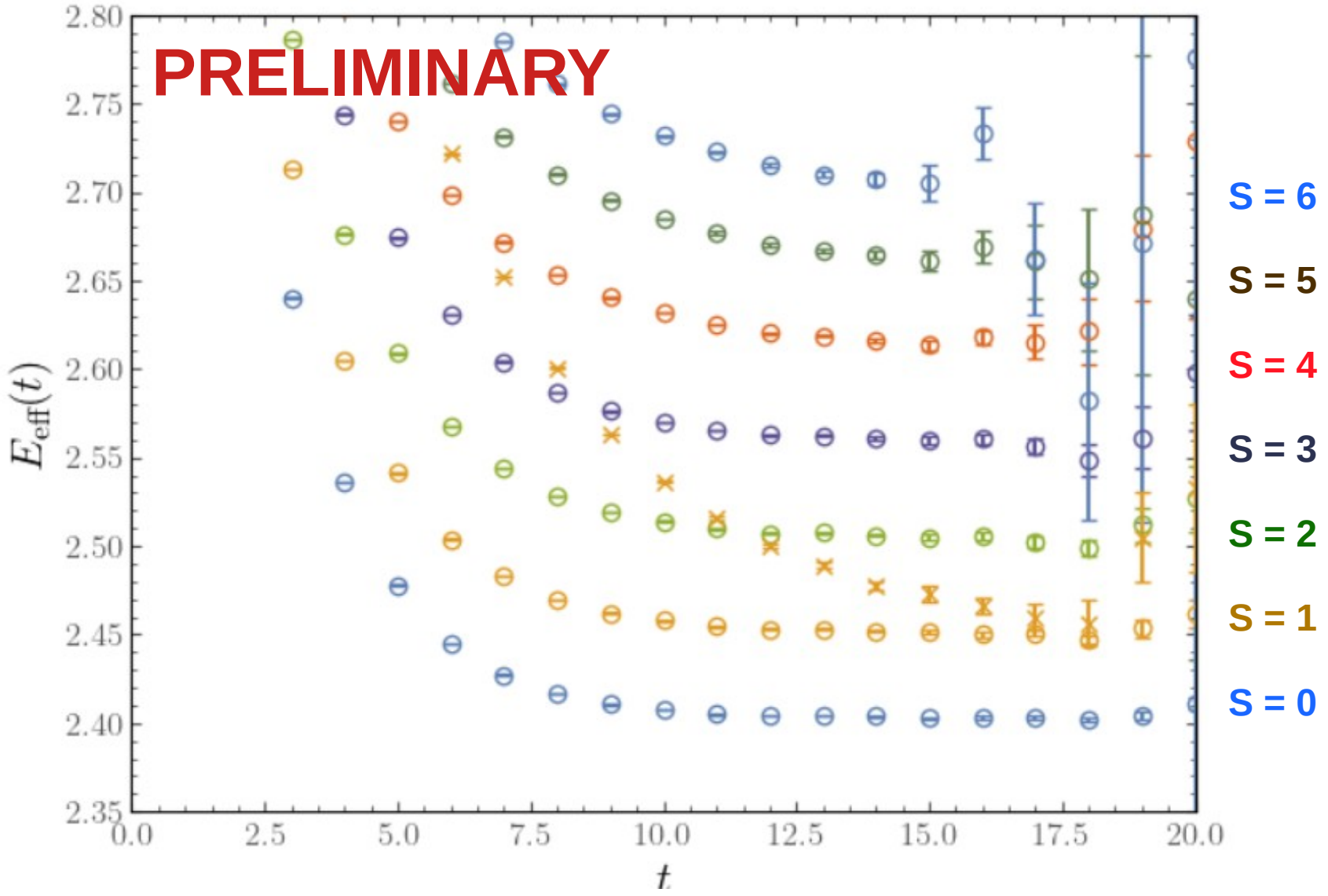


Dibaryon Operators

Two spatially-separated plane-wave baryons with relative momenta

Relative momentum: up to six units → 7 operators

Data quality: dineutron



Brute force with 20 Million propagators

Hypothesis: asymmetric correlation function contains delicate cancellation between ground- and excited states

Formally: should converge to true ground state for $t \to \infty$

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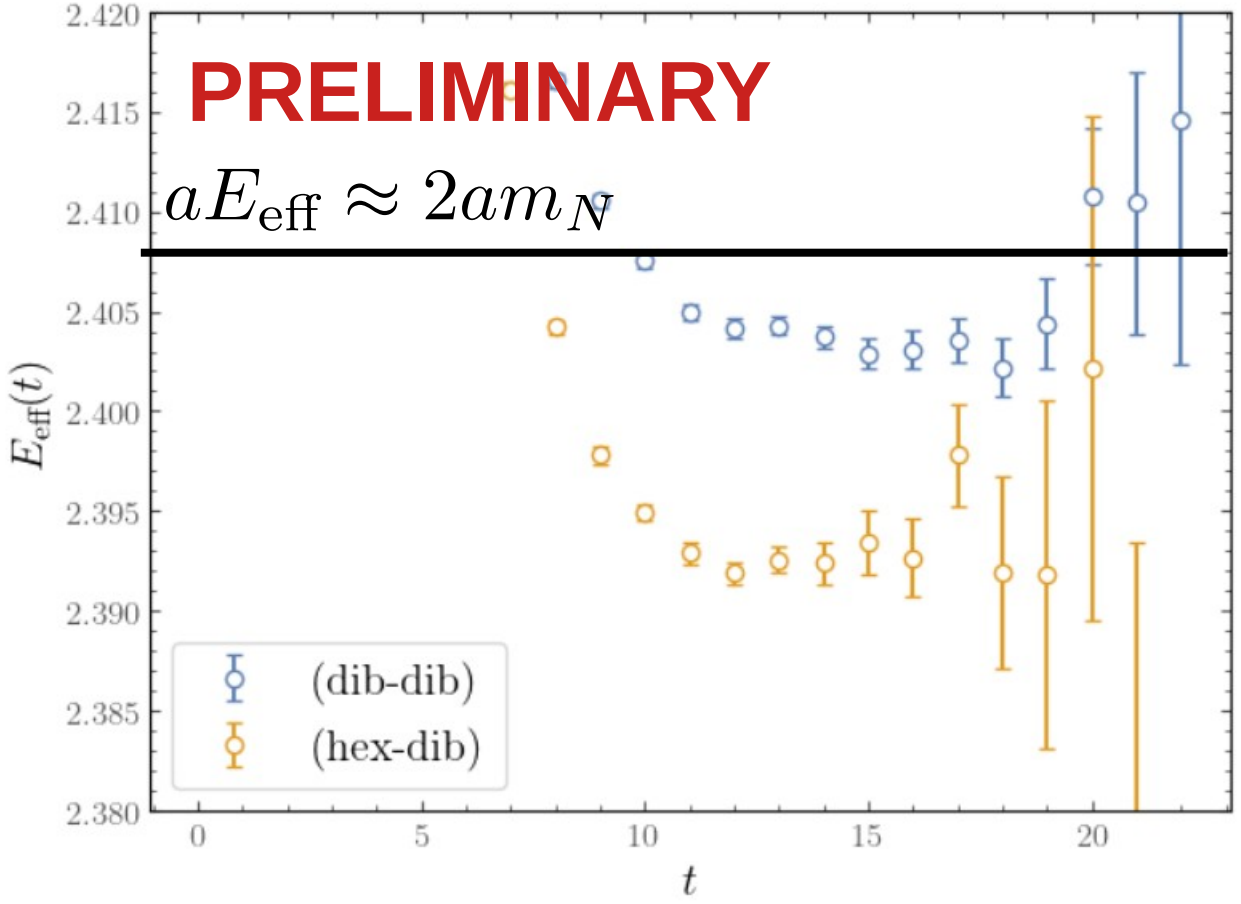

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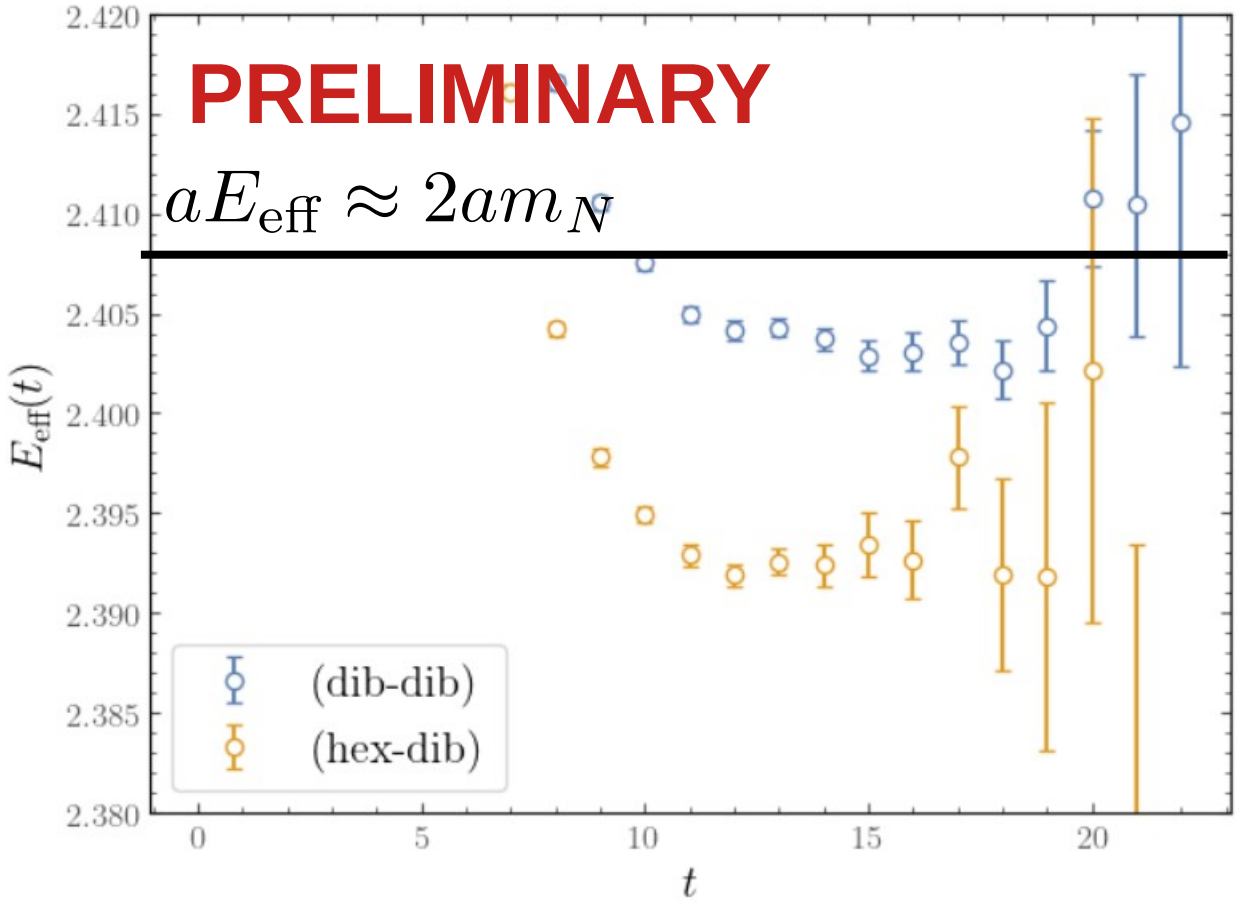

Comparable plateau quality for **symmetric** and **asymmetric** correlation functions

Lanczos method

[Phys.Rev.Lett. 134 (2025) 24, 241901]

Phys.Rev.D 112 (2025) 5, 054506

[Phys.Rev.D 112 (2025) 1, 1]

[e-Print: 2503.17357 [hep-lat]]

Discrete time-translation due to transfer matrix

$$\mathcal{O}_i(t) = T^t \mathcal{O}_i T^{-t}$$

Eigenvalues of transfer matrix can be related to energies

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

Then correlation functions are just matrix elements of powers of T:

$$C(t) = \langle 0|\phi(t)\phi^\dagger(0)|0\rangle = \langle \phi|T^t|\phi\rangle$$

Compute Hankel matrix constructed from correlation function

$$\mathbf{H}^{(p)}_{st} = \mathbf{C}(p+s+t)$$

In practice, j**ust another GEVP…**

$$\sum_t H^{(1)}_{st} v^n_t = \lambda_n \sum_t H^{(0)}_{st} v^n_t$$

Lanczos method provides two-sided bounds

[Phys.Rev.Lett. 134 (2025) 24, 241901]

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Residual bounds: eigenvalue guaranteed to exist in two-sided window

$$\lambda_k^{(m)} \pm \sqrt{B_k^{L/R(m)}}$$

where

$$B_k^{R/L(m)} = \frac{\langle y_k^{R/L(m)} | [T - T^{(m)}]^2 | y_k^{R/L(m)} \rangle}{\langle y_k^{R/L(m)} | y_k^{R/L(m)} \rangle}$$

Gap bounds: When gaps between states are (approximately) known,

$$\lambda_k^{(m)} \pm \frac{B_k^{L/R(m)}}{G_k^{(m)}}$$

Where $G_k^{(m)}$ is gap to first “missing” state.

$$\hat{G}_k^{(m)} \equiv \left| e^{-E_{\text{miss}}} - \lambda_k^{(m)} \right|$$

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Reasonable to assume at the physical point

Approximate from non-interacting levels

Calibrating gap bounds in toy model

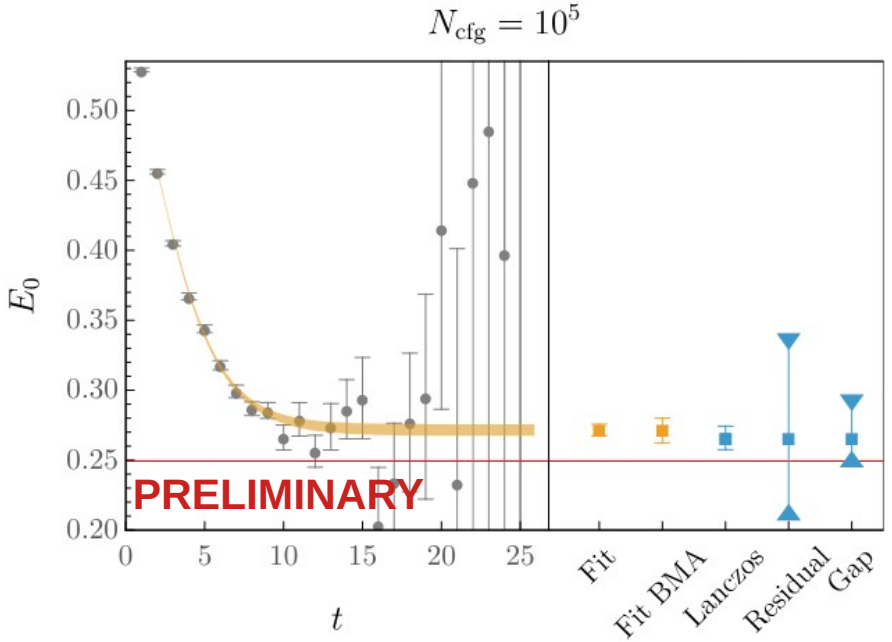
Calibrate on simple solvable model: complex harmonic oscillator (0+1d QFT)

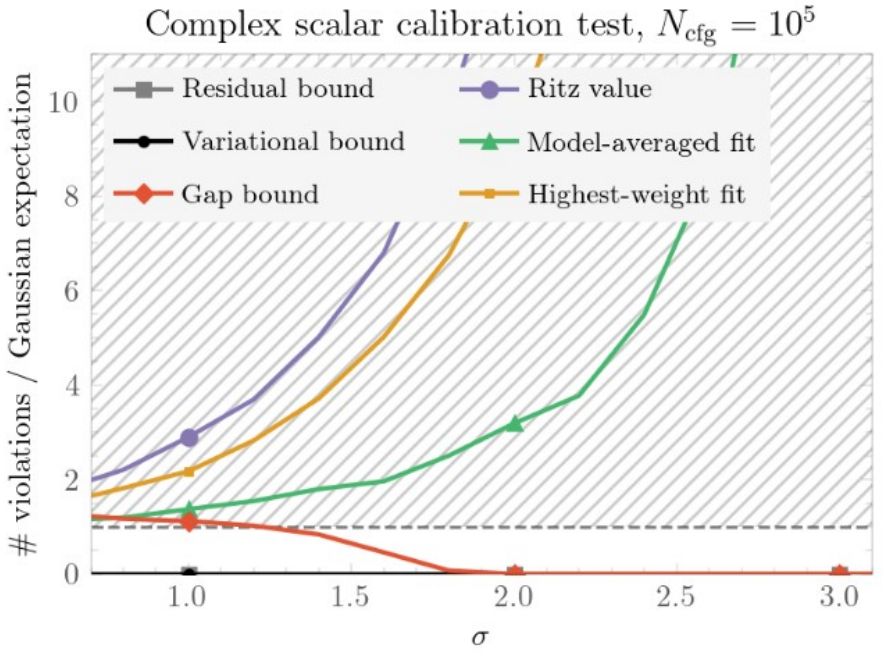
$$S = \sum_{t=0}^{L_t-1} \varphi(t)^* \left[-\varphi(t+1) + 2\varphi(t) - \varphi(t-1)\right] + M^2|\varphi(t)|^2$$

Compute two-point correlator

$$C_{\mathcal{O}}(t) = \langle \mathcal{O}_\varphi(t)\mathcal{O}_\varphi(0)^* \rangle \qquad \mathcal{O}_\varphi(t) = e^{\varphi(t)} - 1$$

Exhibits excited state contamination, exponentially bad signal-to-noise:





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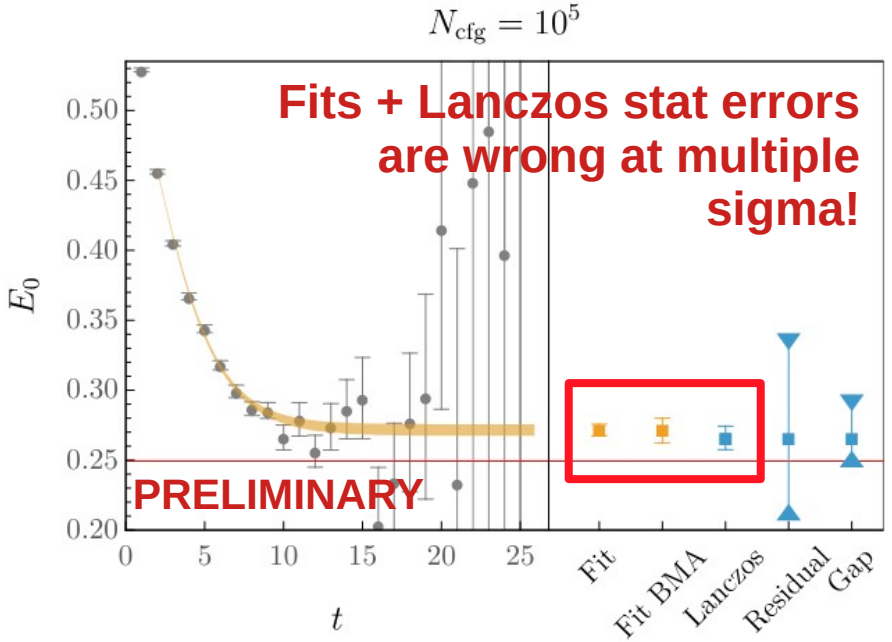

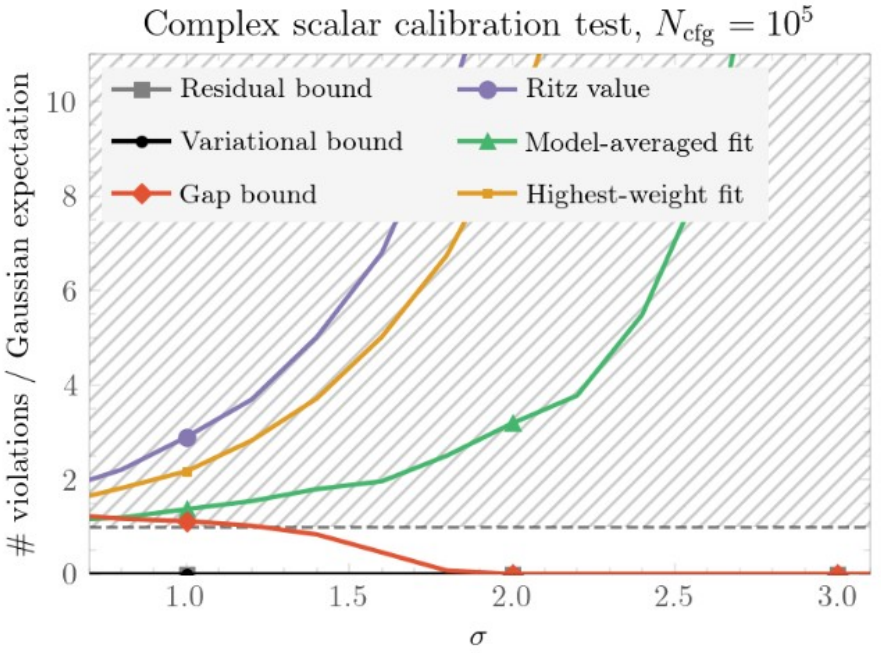

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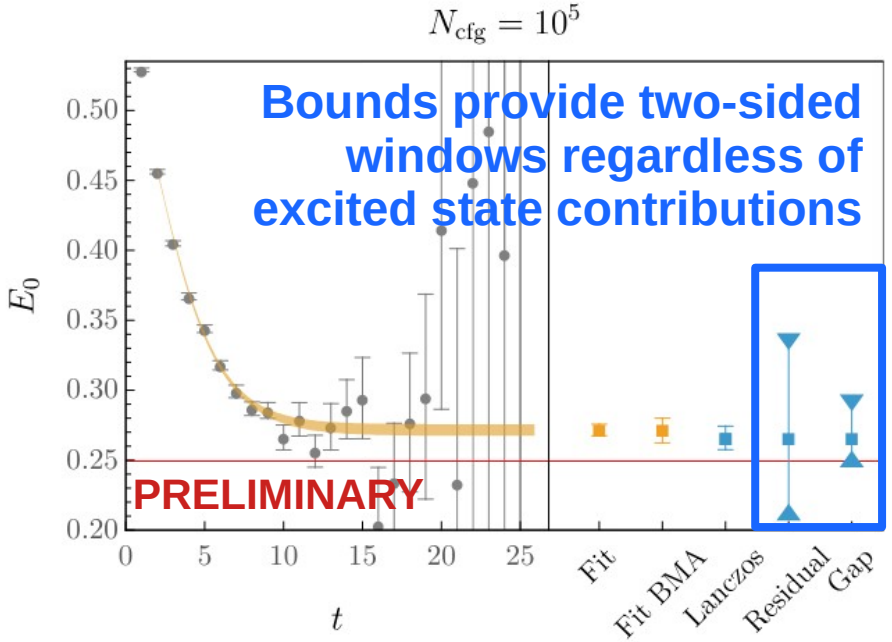
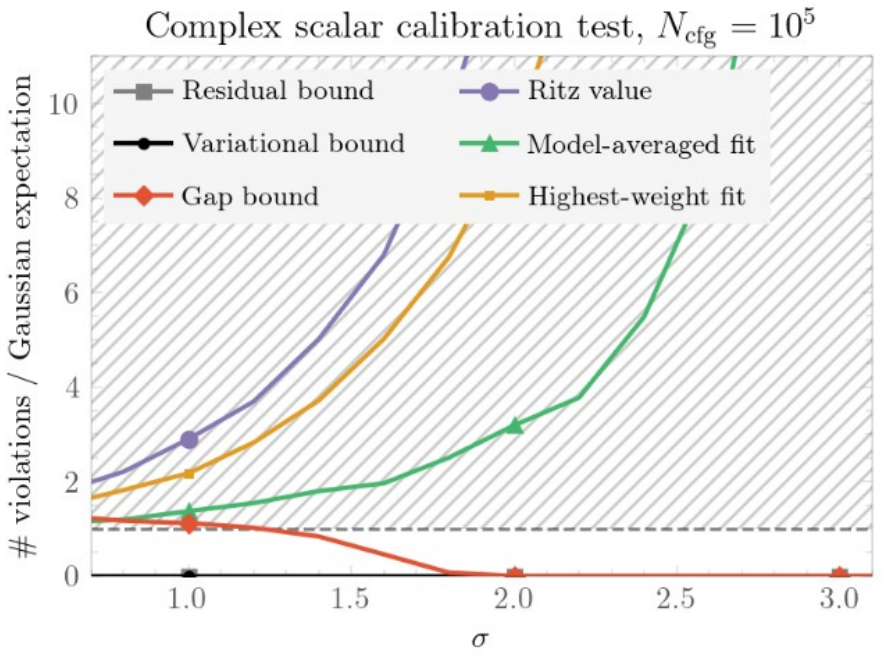
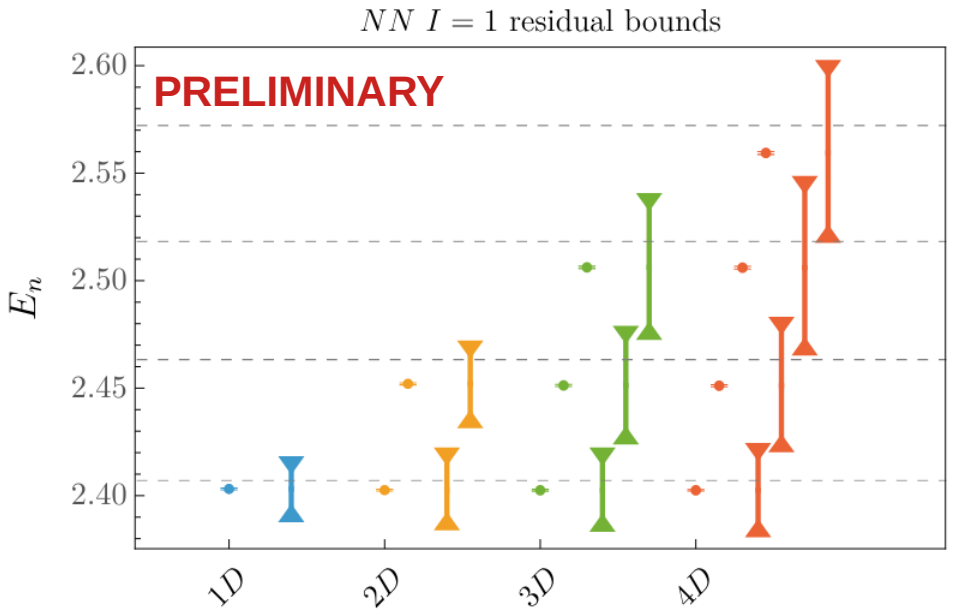
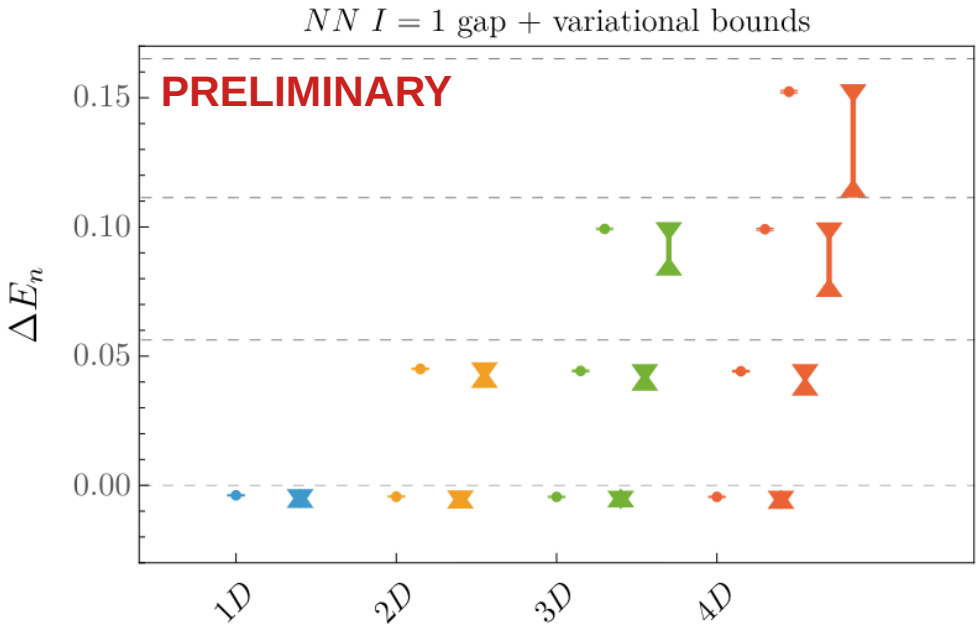




Summary of Lanczos results

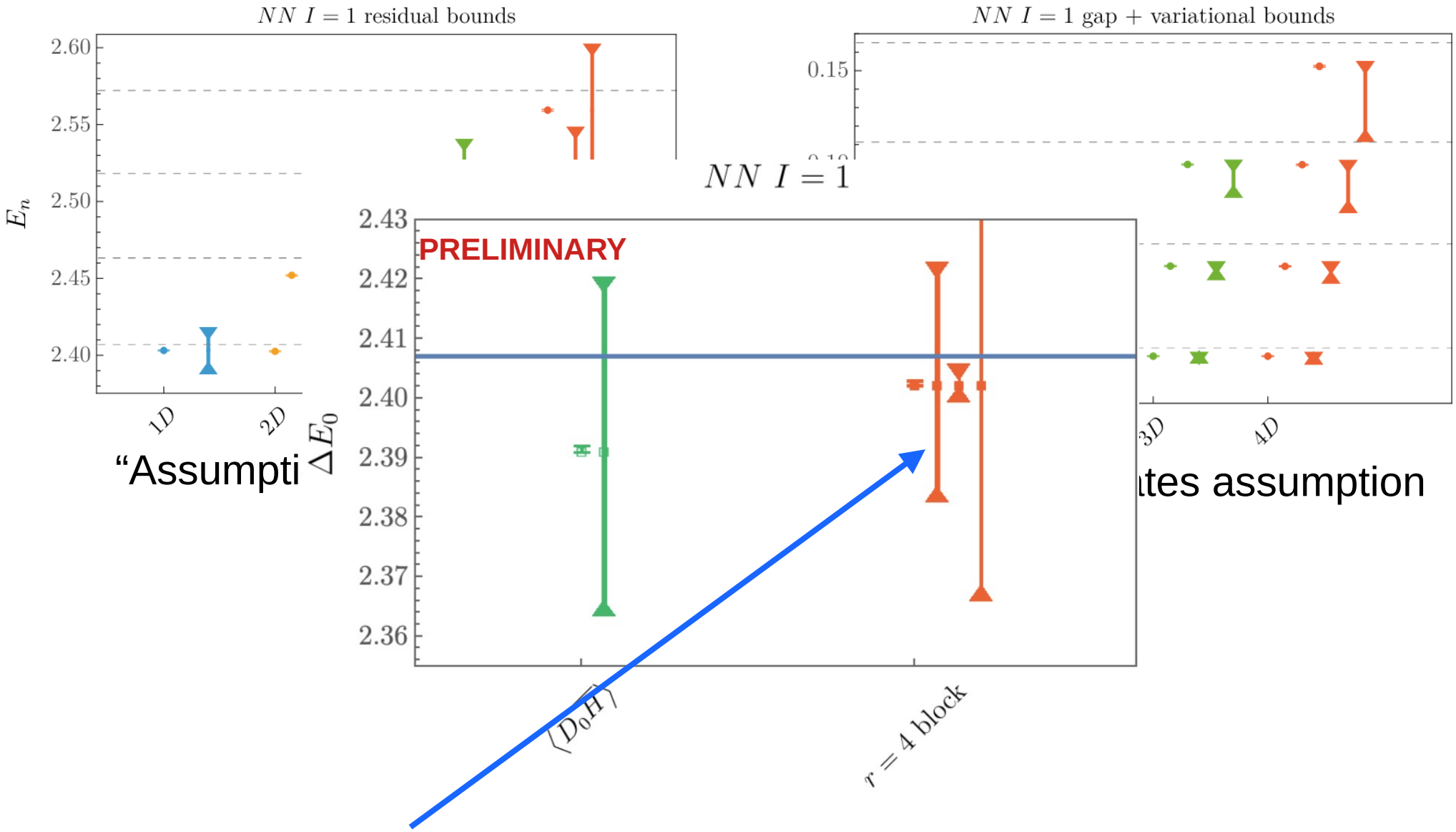


"Assumption free" spectrum



No missing states assumption (assumes no bound state)

Summary of Lanczos results



"Assumpti

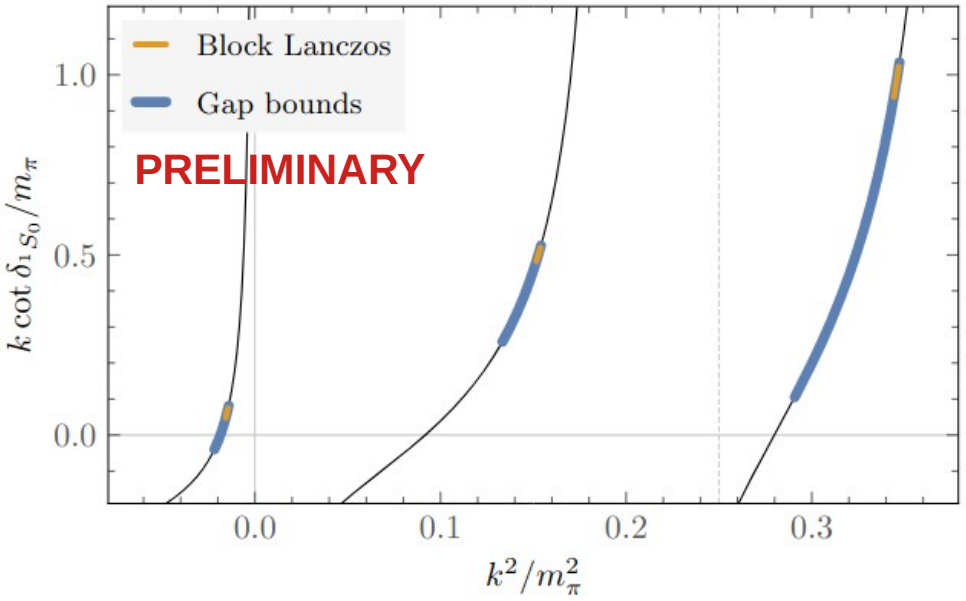
ıtes assumption

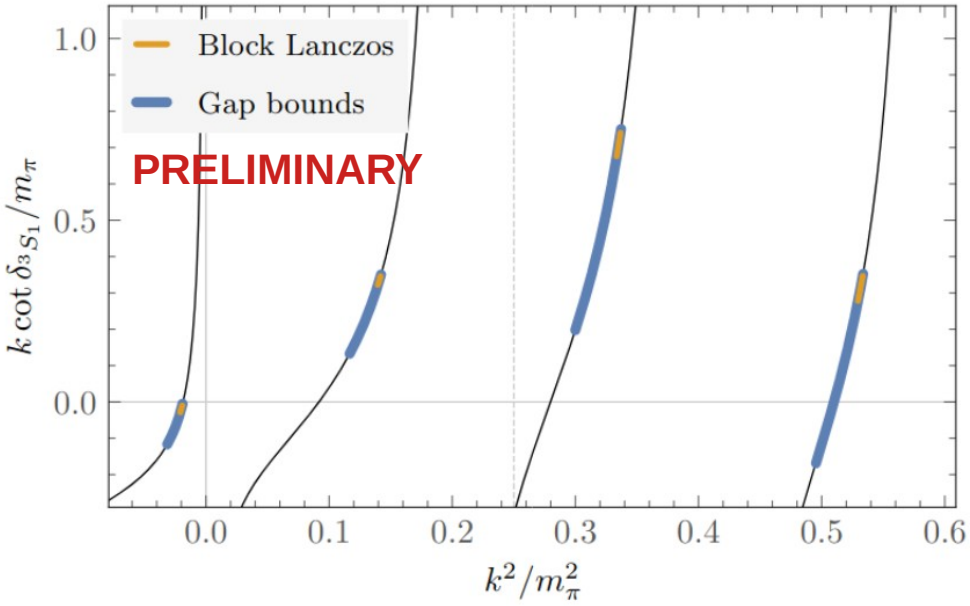
Residual bound encompasses **both** ground state scenarios...

Phase-shift determination

...But constraints on phase-shifts possible without assuming **N-state saturation**

Must assume **no missing states**





Conclusions

Muli-hadron observables have small excitation gaps & exponentially bad signal-to-noise: Challenging!

Spectroscopy is often regularized by assuming ***N*-state saturation** & **No missing states**

NPLQCD generated very high-statistics dataset at 800 MeV

“Brute force” approach does not show evidence for upwards curvature of hex-dibaryon correlator to threshold

Lanczos provides two-sided bounds on energy eigenvalues: Residual bounds require no additional assumptions, gap bounds require no missing states assumption

Multi-Hadron Spectroscopy
Backup slides

Excited state contamination

Two-point correlator in thermal field theory:

$$C_{ab}(t) = \langle \mathcal{O}_a(t) O_b^\dagger(0) \rangle = \sum_{m,n} \langle m|\mathcal{O}_a|n\rangle \langle n|\mathcal{O}_b^\dagger|m\rangle \, e^{-E_m(L_t-t)} e^{-E_n t}$$

Lattice data provides us with a **finite-precision** and **finite-length** sequence

Two expansion parameters:

$$e^{-\delta_r t} \qquad\qquad e^{-E_0 L_t}$$

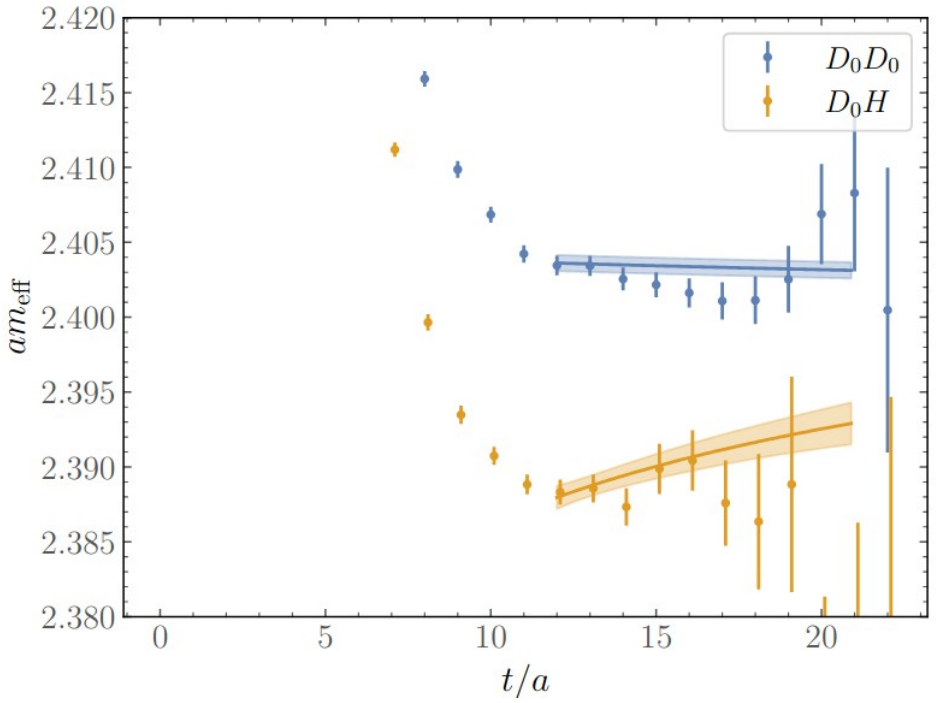
If these are small, then can truncate spectral sum

$$C_{ab}(t) = \sum_{n=0}^{N} \langle 0|\mathcal{O}_a|n\rangle \langle n|\mathcal{O}_b^\dagger|0\rangle \, e^{-E_n t} + \mathcal{O}(e^{-\delta_r t}) + \mathcal{O}(e^{-L_t E_0})$$

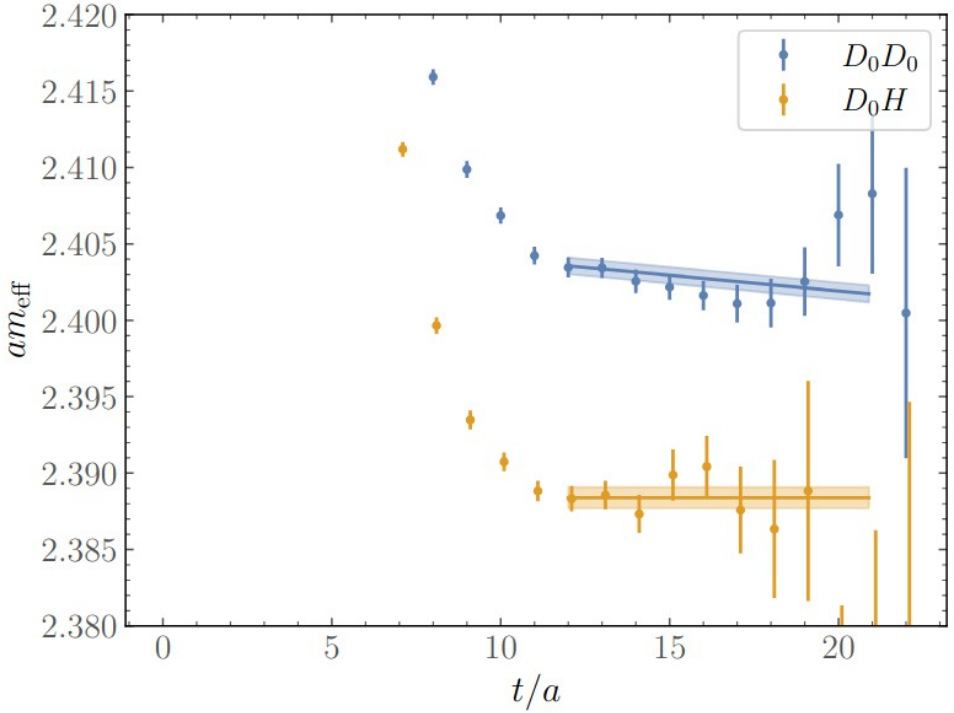
Useful to **explicitly state** assumptions underlying spectroscopy

Can hypothesis tests distinguish?

Can we distinguish these scenarios with goodness of fit? Bayes factors? Hypothesis tests?



"Scattering state solution"



"Bound state solution"

Hypothesis tests inconclusive. AIC weights exhibit slight preference for scattering state when counting constrained parameters

Lanczos and bounding methods

Residual bounds

[Phys.Rev.Lett. 134 (2025) 24, 241901, Phys.Rev.D 112 (2025) 5, 054506, Phys.Rev.D 112 (2025) 1, 1, arXiv:2503.17357]

~~N-state saturation assumption~~

~~No missing states assumption~~

“Assumption free”, but often conservative

Guarantees presence of genuine transfer-matrix eigenvalue within two-sided window

Gap bounds

[arxiv:2512.XXXX]

~~N-state saturation~~

No missing states

Calibrated(?) systematic error

No need to assume excited state contamination small