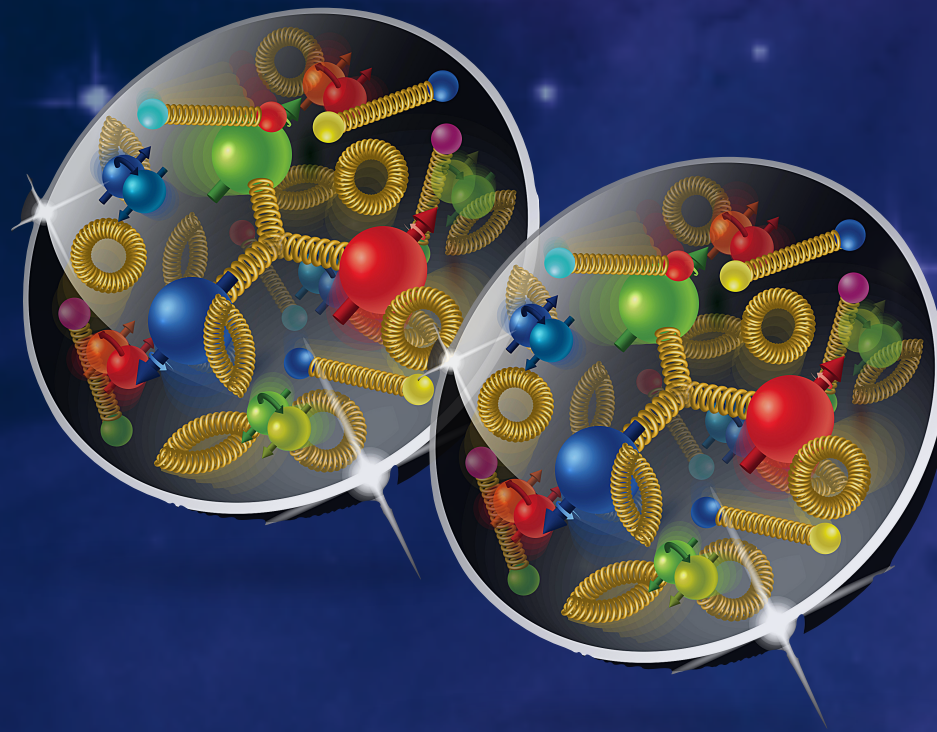


Spectral bounds and interpolating operator dependence

Will Detmold (MIT)

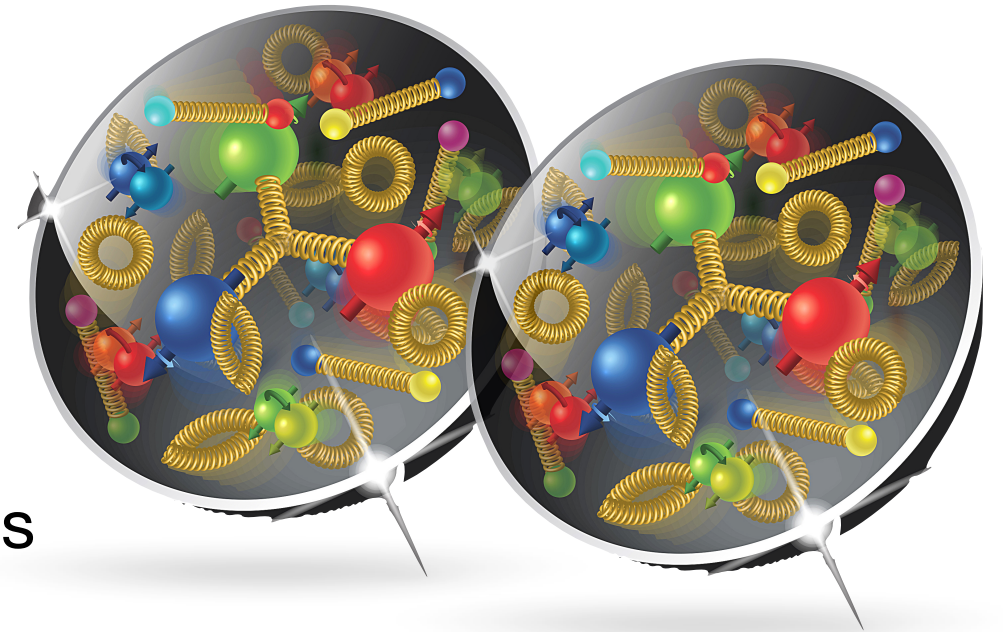


Massachusetts
Institute of
Technology

Lattice QCD for baryon interactions

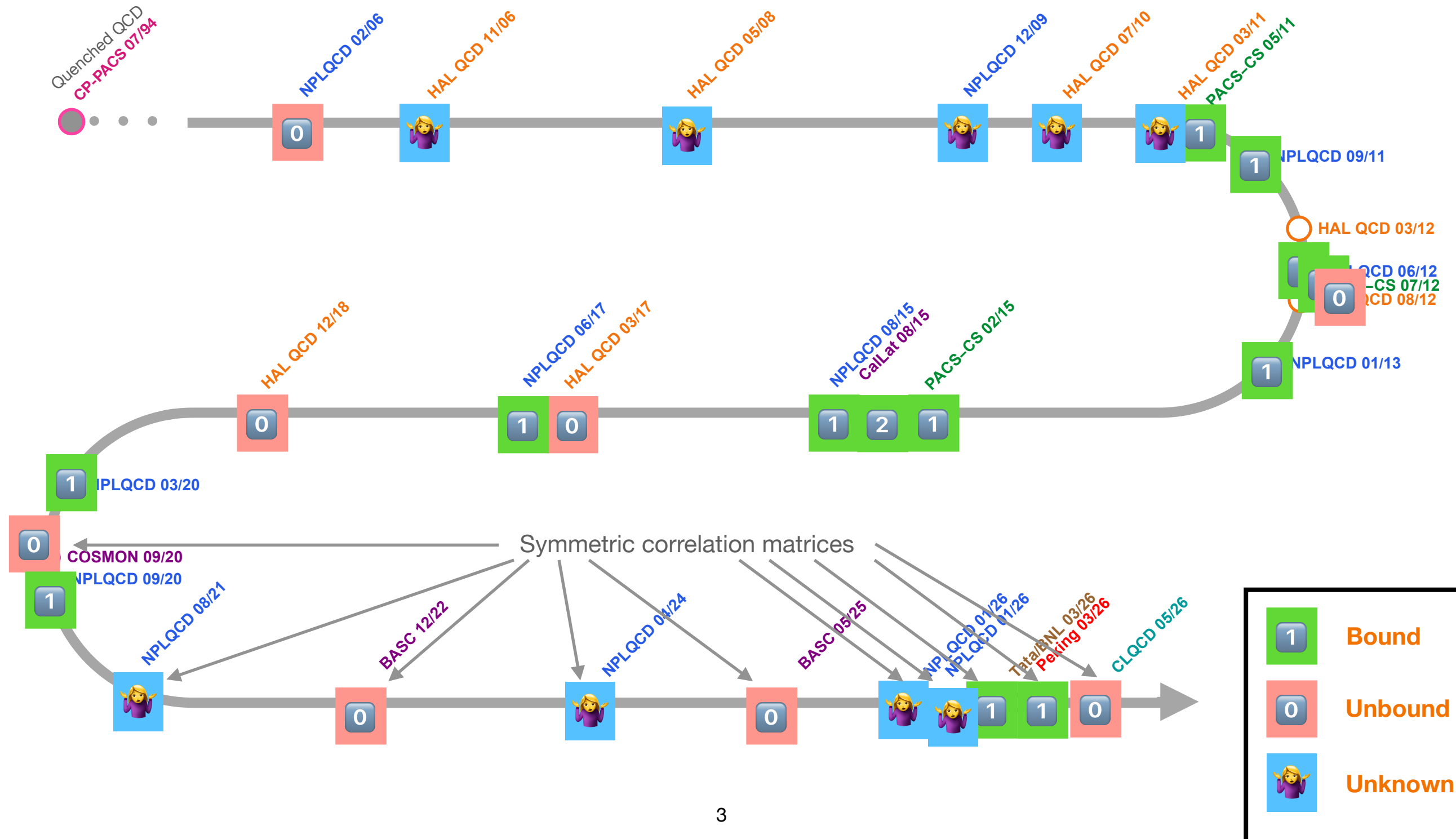
The nuclear frontier

- Baryon interactions are key to many physical processes and the origin of nuclei
- Many unanswered questions in nuclear physics
 - Hyperon-nucleon interactions important in neutron star interiors but hard to probe experimentally
 - Nuclear interactions with (B)SM currents needed for DUNE, $0\nu\beta\beta$ searches, dark matter searches, ...
- Natural to try to determine from the underlying Standard Model
 - ➔ Accessing NN scattering from first principles LQCD is a key goal
 - A **benchmark** for LQCD
 - A finely-tuned **challenge**



The “NN controversy” after 20 years

Is there a bound state at heavy quark masses?



High statistics calculations

2601.22272/3 - NPLQCD

- Very high statistics calculation on one ensemble at coarser lattice spacing

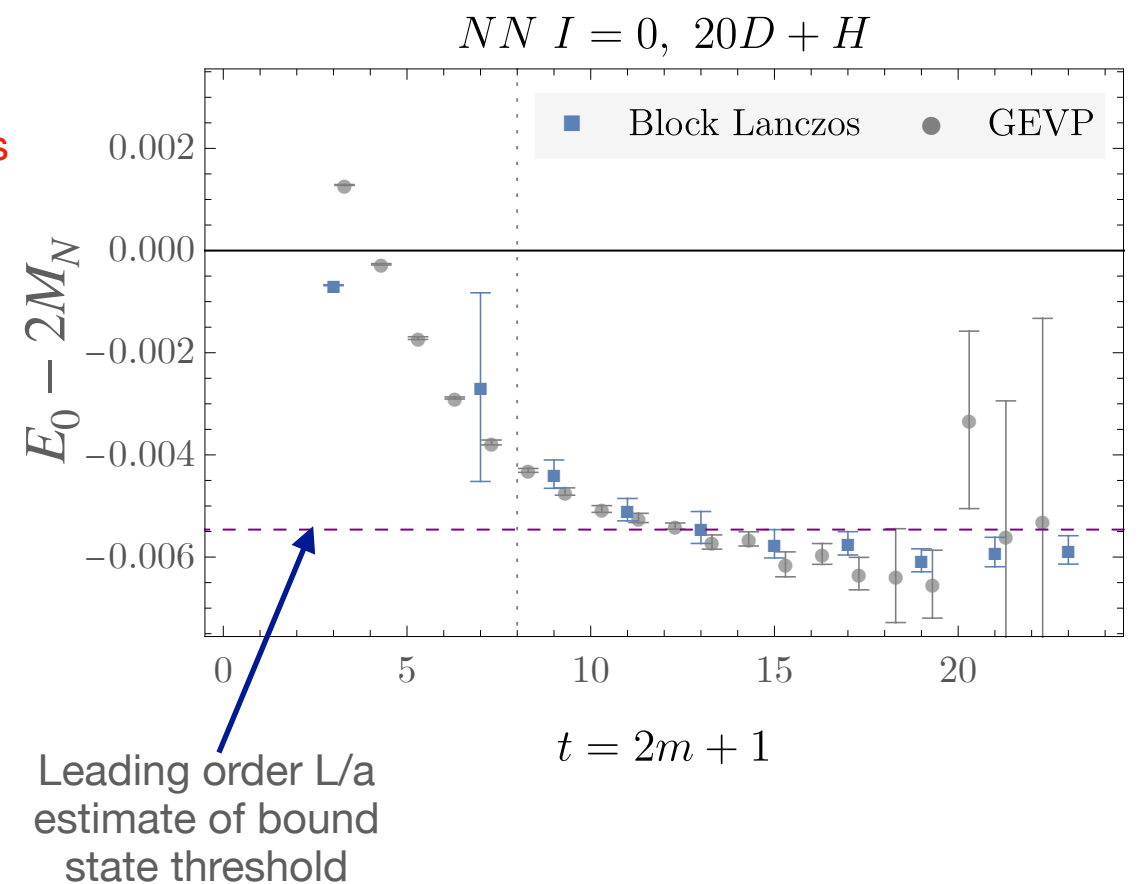
Paper	Method	N_{cfg}	$N_{\text{prop}}/N_{\text{cfg}}$	Measurements
NPLQCD2013	Asymmetric	3800	72	273600
		3000	48	144000
		1,900	54	102600
NPLQCD2017	Asymmetric	3822	96	366912
		3,050	72	219600
		1,905	54	102870
NPLQCD2023	Variational	727	512	372000
NPLQCD2025	Variational	469	216	101304
NPLQCD (in prep)	Variational	16000	1296	20736000

50x stats

- Symmetric correlator matrix from large set of operators in rest frame
- Both bound and unbound consistent with data
- Scattering lengths are unnatural

$$|a_{1S_0}|, |a_{3S_1}| \geq 10m_\pi^{-1}$$

so NN systems are fine tuned at heavy masses



High statistics calculations

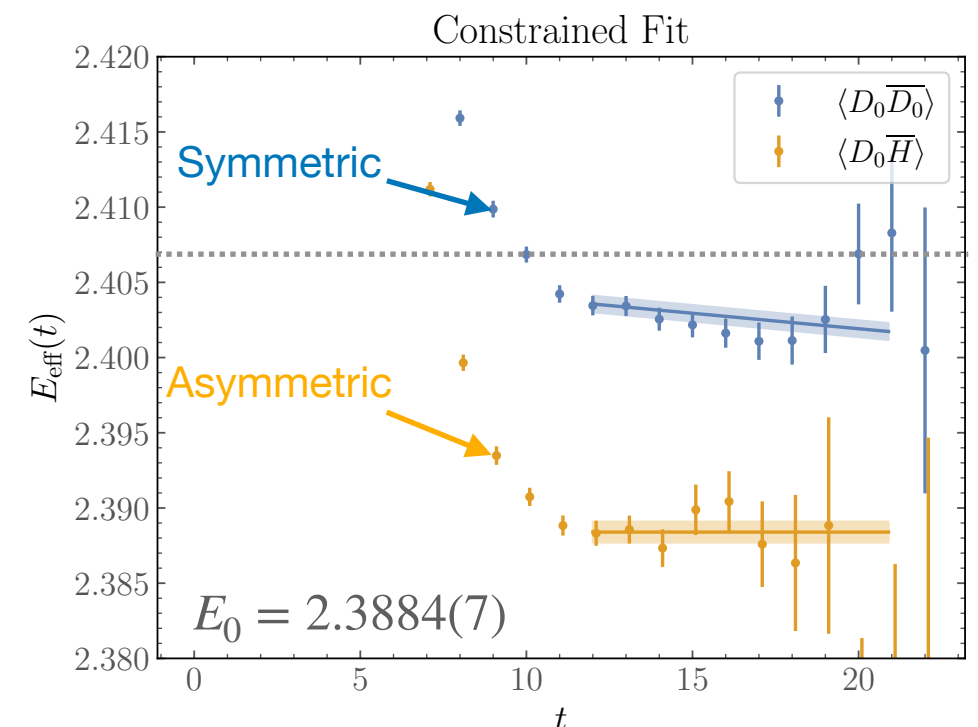
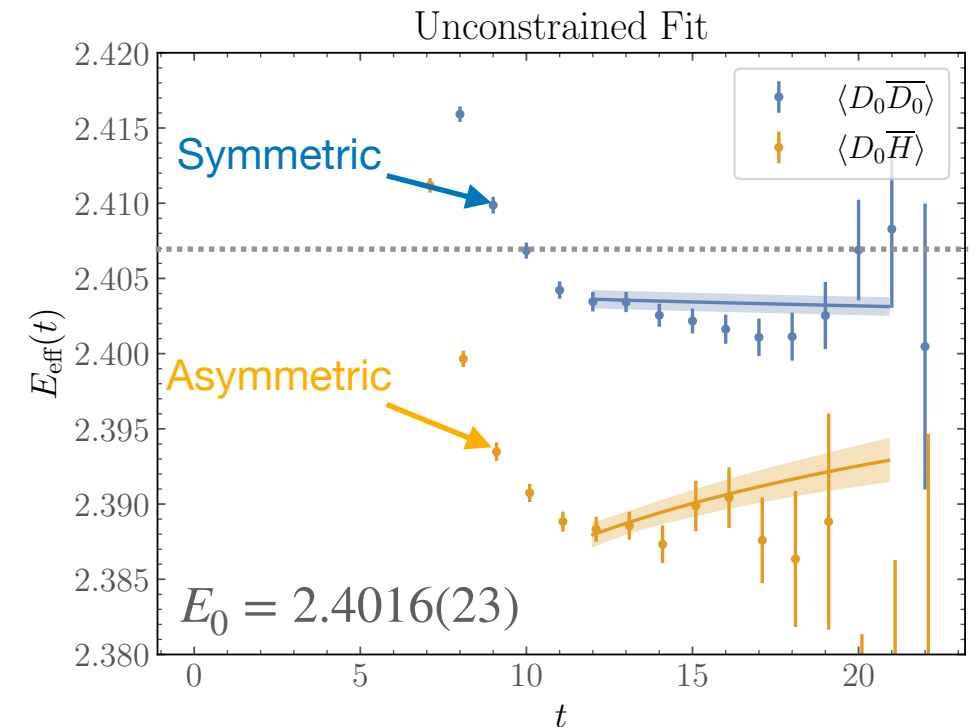
Symmetric vs asymmetric

- Asymmetric correlators can in principle couple to a ground state missed by diagonal correlators
 - Requires particular arrangement of small overlaps (ε model)
- Coupled fits to diagonal and off-diagonal hexaquark/dibaryon ops

1. Unconstrained fit

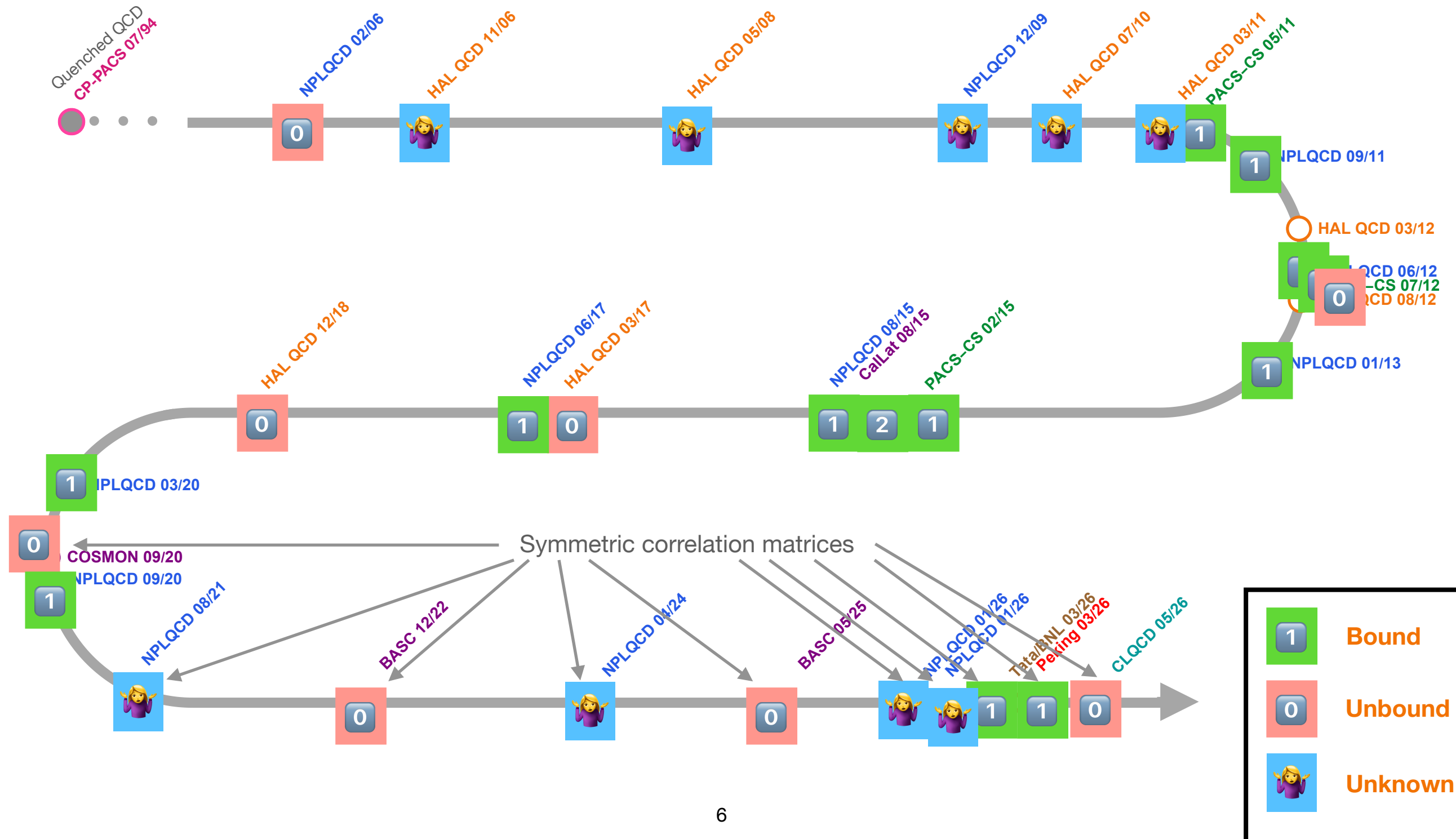
2. Constrained fit with ε overlap

- Statistically indistinguishable quality of fit and AIC
- Bayesian and frequentist hypothesis test do not reliably prefer either model
- Data alone do not answer bound vs unbound



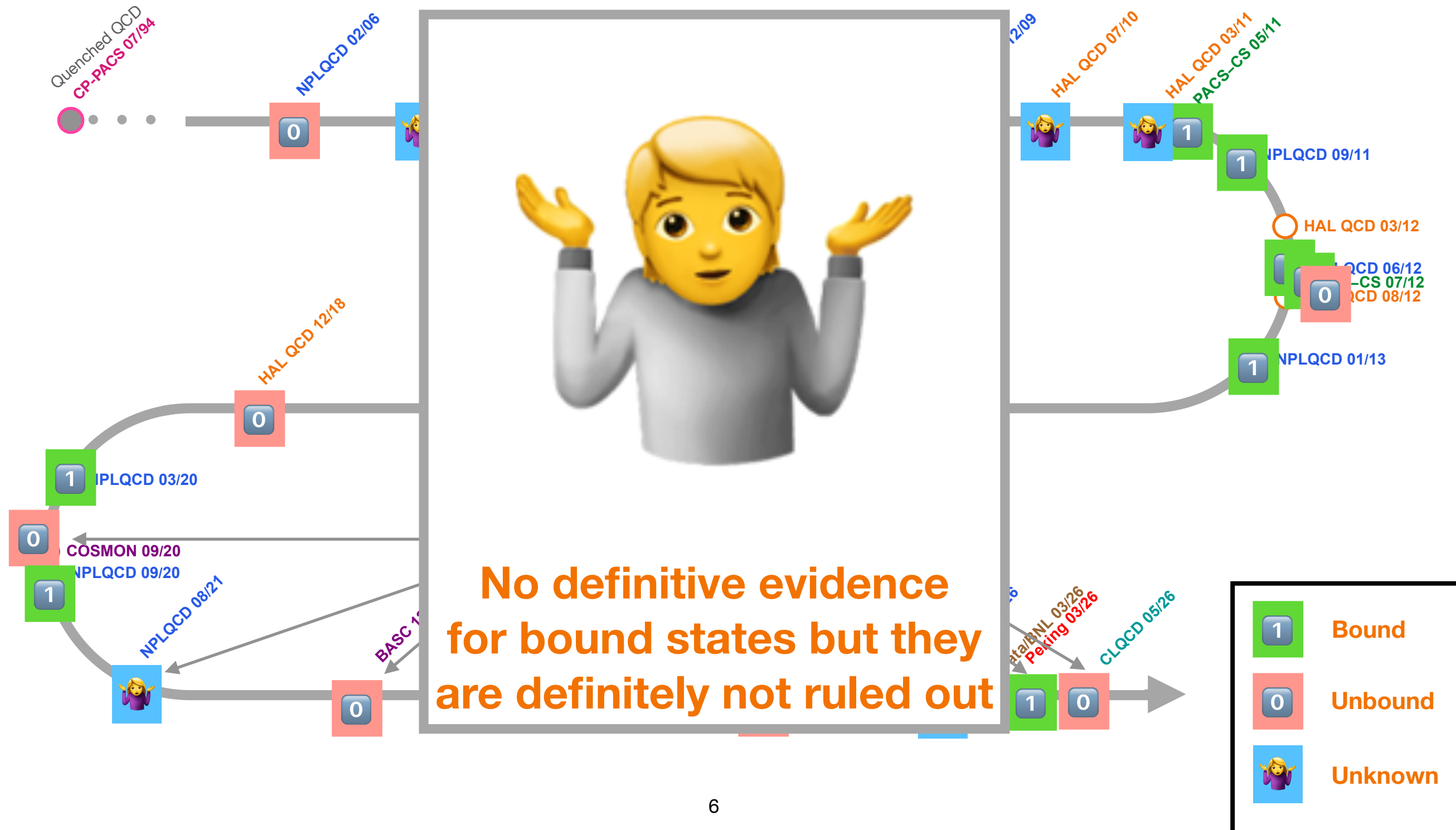
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Is there a bound state at heavy quark masses?



The “NN controversy” after 20 years

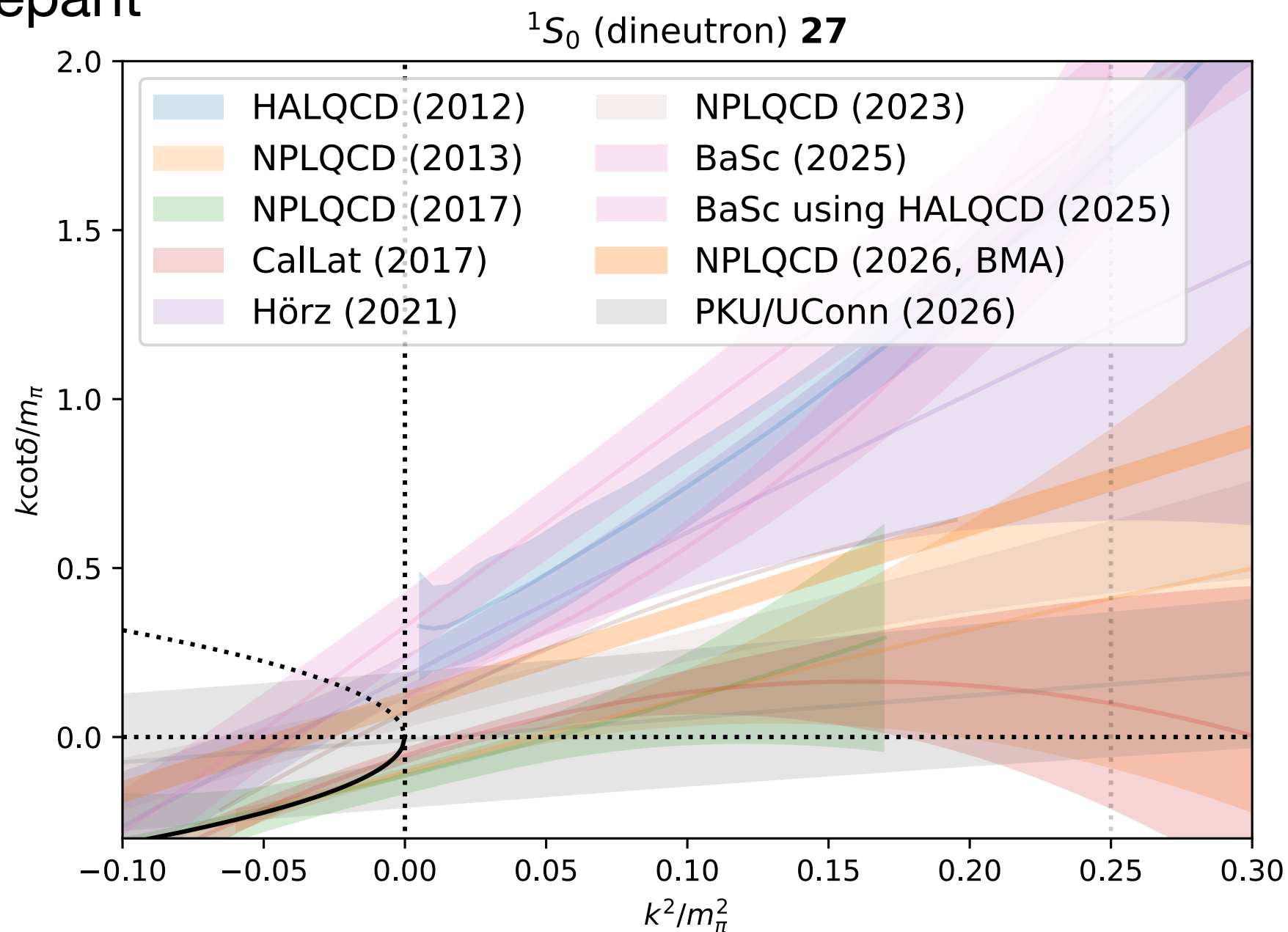
Is there a bound state at heavy quark masses?



The “NN controversy”

Phase shifts

- The problem does not end there: phase shifts are rather discrepant



How did we get here?

Challenging calculations even at the exascale

- Computationally challenging systems to study [$\mathcal{O}(10V)$ harder than proton]
- Statistically challenging systems to study [Exponentially harder than proton]
- Systematically challenging systems to study
 - Excited-state contamination in spectrum [Existentially! worse than proton]
 - Small volumes make t -channel cut relevant as quark masses approach physical mass
 - Discretisation, isospin-breaking, QED effects likely also important
- And really it is the interplay between all of the above

QCD from lattice QCD

Limits and extrapolations

- Numerical LQCD calculations are necessarily performed at finite UV and IR cutoffs
- Continuum limit arises as fixed point of RG flow and perturbative QCD determines the asymptotic scaling towards the fixed point
- For QCD, confinement and χ SB guarantee the infinite volume limit exists and χ PT controls the scaling towards this limit in many cases
- Under mild assumptions, LQCD data at a set of lattice spacings and volumes allows for extrapolation to the infinite volume, continuum limit
 - Corrections are suppressed by small parameters $a\Lambda_{\text{QCD}}$, $e^{-m_\pi L}$, ...
 - Systematically improvable 😊



QCD from lattice QCD

Limits and extrapolations

- Hilbert space of LQCD is infinite dimensional: extraction of physics from correlation functions also requires extrapolation
- Simple two-point function

$$C(t) = \langle \Omega | \chi(t) \chi^\dagger(0) | \Omega \rangle = \sum_{\mathcal{N}} Z_{\mathcal{N}} \exp(-E_{\mathcal{N}} t) = Z_0 e^{-E_0 t} \left(1 + \sum_{\mathcal{N} \neq 0} \tilde{Z}_{\mathcal{N}} e^{-\Delta E_{\mathcal{N}} t} \right)$$

which is an infinite sum over states

$$\Delta E_{\mathcal{N}} = E_{\mathcal{N}} - E_0$$

- Initially an ill-posed inverse problem as $t \in \{0, 1, \dots, N_t\}$ is discrete and finite
- However for $t \gg \Delta E_{\mathcal{N}}^{-1} \log(Z_0/Z_{\mathcal{N}}), \forall \mathcal{N}$

$$\log(C(t)/C(t+1)) \rightarrow E_0$$

QCD from lattice QCD

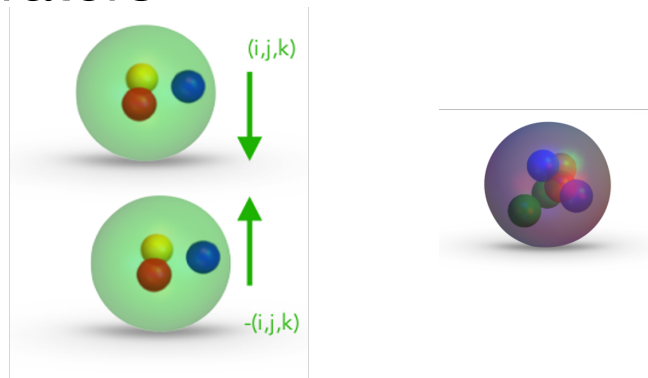
Limits and extrapolations

- Unfortunately this limit does not exist for many practical situations
 - QCD + QED; calculations near the chiral limit; two-hadron systems in the large-volume limit
 - **No small expansion parameter for extrapolation**
- Even worse, $t \gg \Delta E_{\mathcal{N}}^{-1} \log(Z_0/Z_{\mathcal{N}})$, $\forall \mathcal{N}$ depends on knowledge of $Z_{\mathcal{N}} = \langle \Omega | \chi(0) | \mathcal{N} \rangle$ for every state
 - Must **assume** this ∞ set of constraints from entirely user-chosen operators is satisfied!
 - **Is LQCD even systematically improvable?** 🤖
- Recent developments show rigorous statements about spectroscopy can be made even when $t \not\gg \Delta E_{\mathcal{N}}^{-1}$ without reference to operator-state overlaps

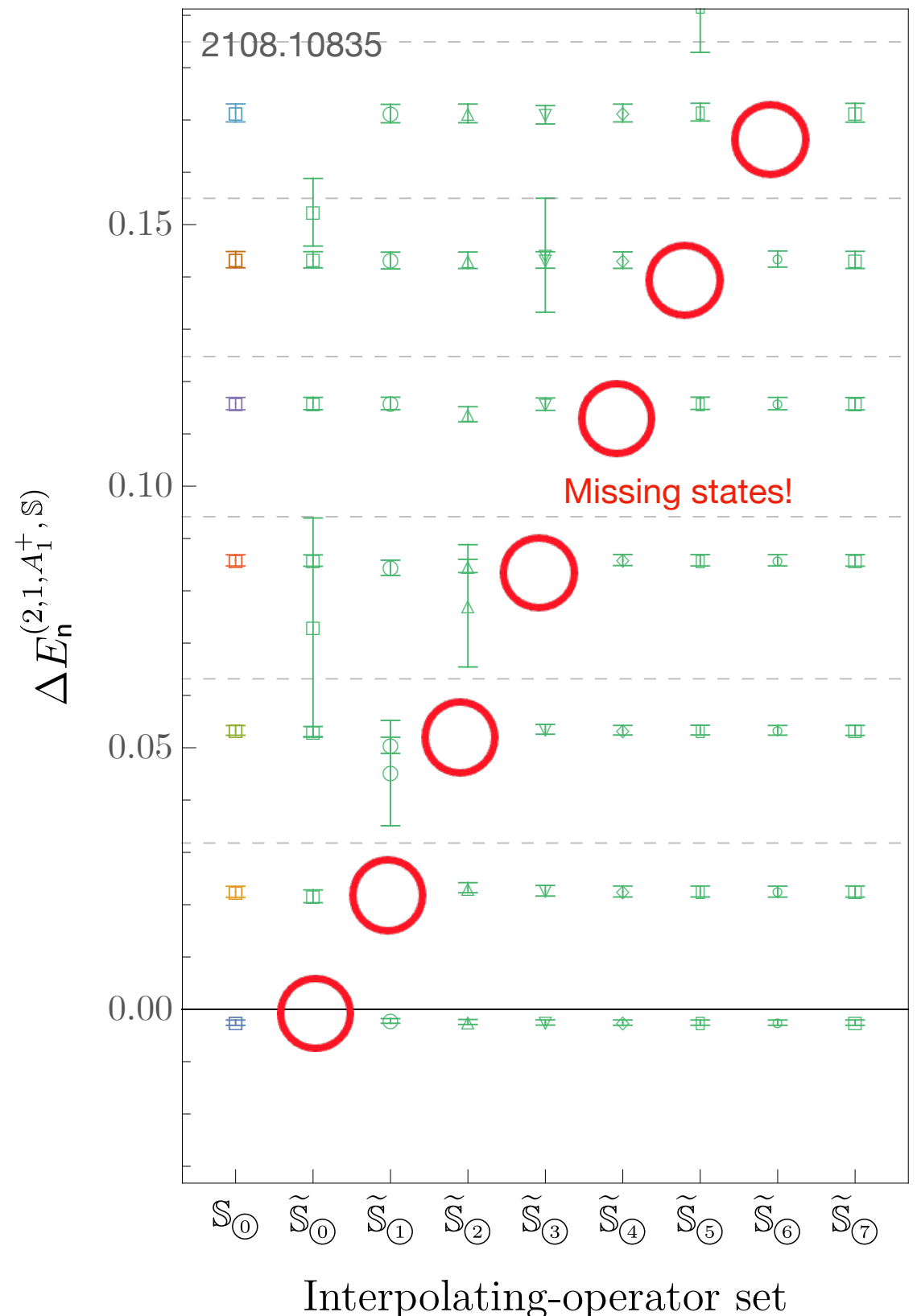
Operator dependence

nn example

- Different sets of plane-wave projected dibaryon operators and hexaquark operators



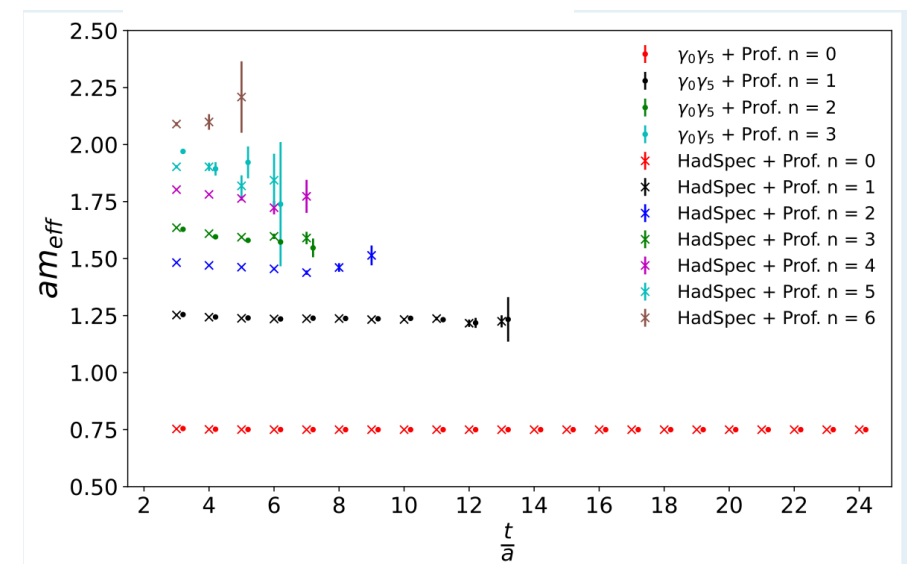
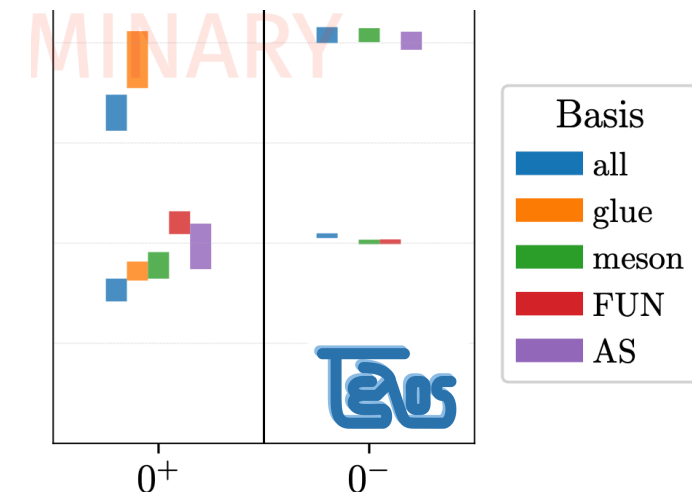
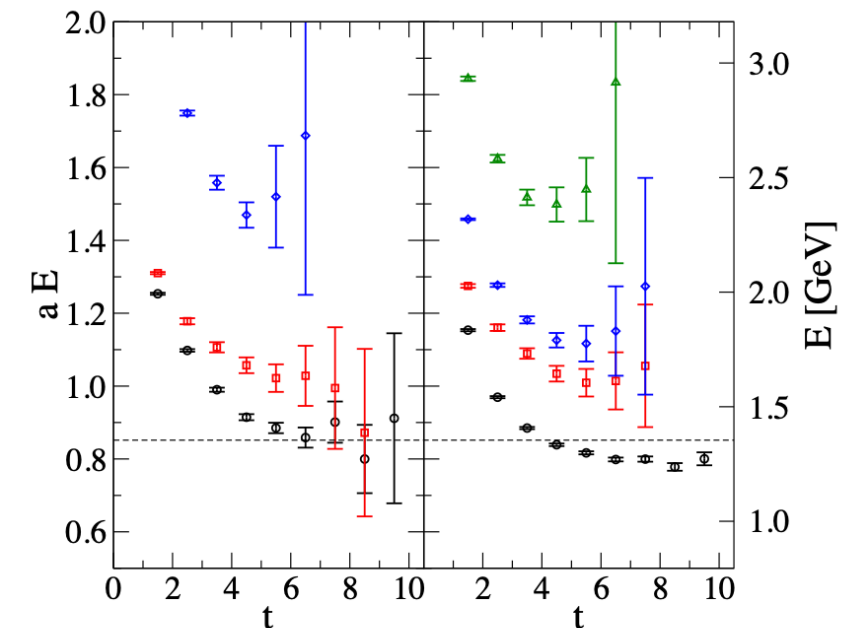
- Spectrum from GEVP of symmetric correlation matrix with very careful fitting systematics included
- At $t \rightarrow \infty$ these must agree on lowest states
- Choice of operator set **dramatically alters spectrum**
- As with asymmetric correlators, **symmetric correlators** also have **false plateaus**



Operator dependence

Many other examples

- $I=1 \pi\pi$: HadSpec 2013; $N\pi$: Lang & Verduci 2013 (1212.5055)
- 0^+ operators in $Sp(4)$ gauge theory with $N_F=2$, $N_{AS}=3$ fermions [Britto Tues 2pm]
- Charmonium and global states [Urrea-Niño Mon 2pm]
- Results only valid when interpreted as **variational upper bounds**
- A posteriori: large systematic operators we leave out. What about operators we have not put in?
- Cautionary note: choice of operators to use is obvious until it is not (QCD is devious and NN is fine-tuned)



Spectral bounds

Matrix approximation theorems [2601.22272]

- Spectroscopy $\implies$ determination the eigenvalues $\{\lambda_k\}$ of the *transfer matrix* $\hat{T}$, an ∞ -dimensional operator that generates discrete imaginary time evolution: $\hat{T} \xrightarrow{a \rightarrow 0} \exp(-a\hat{H})$
- Matrices of correlation functions probe finite-dimensional projections $\hat{T}^{(m)}$ of $\hat{T}$
 - Classic linear algebra problem: given spectrum $\{\lambda_k^{(m)}\}$ of $\hat{T}^{(m)}$ what is $\{\lambda_k\}$?
 - **Residual bounds** (Wagman 2024, see also Weinstein criterion [1934]):
$$\min_{\lambda \in \{\lambda_n\}} \left| \lambda_k^{(m)} - \lambda \right| \leq \sqrt{B_k^{(m)}} \quad \text{with } B_k^{(m)} \equiv \left| \left[\hat{T} - \hat{T}^{(m)} \right] \left| y \right\rangle \right|^2 \text{ for } |y\rangle = \chi^\dagger |\Omega\rangle$$
 - **Gap bounds:** *Davis-Kahan* [1970] and recent developments by *Haas-Nakatsukasa* [2025]
$$\min_{\lambda \in \{\lambda_n\}} \left| \lambda_k^{(m)} - \lambda \right| \leq \frac{B_k^{(m)}}{G_k^{(m)}} \left[1 + O(B) \right] \quad \text{with } \hat{G}_k^{(m)} \equiv \left| e^{-\hat{E}_{\text{miss}}} - \lambda_k^{(m)} \right|$$

where $\hat{E}_{\text{miss}}$ is the energy below which one assumes no states are missed by computed correlation functions

Spectral bounds

Eigenvalue bound windows [2601.22272]

- **Bound windows**: one or more true eigenstates of $\hat{T}$ is within the given window but say nothing about other regions
- Bound windows are computable from correlation functions and do not rely on $t \rightarrow \infty$ limit
- **Residual bounds** only rely on **Hermiticity**
- **Gap bounds** require a **no-missing-states assumption**: the set of operators used couples to all states below some energy threshold
 - Purely spectral (no constraint on sizes of overlaps)
 - Can be priored with experimental input at physical quark masses
- Bound windows provide **well-calibrated uncertainties** in solvable models
- Bound windows resolve spectral discrepancies between operator choices

Assumptions in spectroscopy

2601.22272/3

N-state saturation

There exists a region of Euclidean time in which the correlator (matrix) is accurately described by a truncated spectral decomposition with $M \geq N$ states, where N states approximate genuine energy eigenstates up to statistical noise (e.g., the N lowest-energy states).

Symmetric/asymmetric

Assumptions on Z 's & E 's

BMA fits/Lanczos are energy extractions

Known to fail!

No-missing-states

There are exactly N states with energy less than a specified threshold E_{miss} that make non-zero contributions to a correlator (matrix), neglecting thermal effects.

Symmetric

Assumptions on E 's

Two-sided gap bounds contain true eigenvalues

Often well-calibrated

Hermiticity

The correlator (matrix) is Hermitian positive definite on ensemble average.

Symmetric/asymmetric

No assumptions on Z 's & E 's

Two-sided residual bounds contain true eigenvalues

Often very conservative

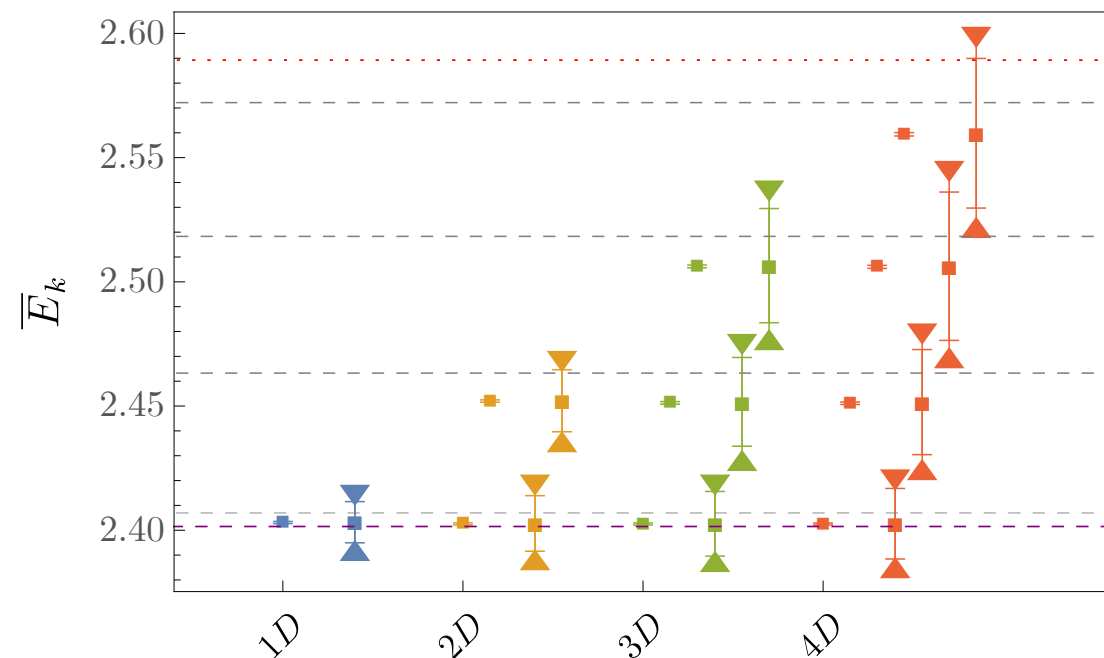
Symmetric correlators: variational upper bounds on energies

Spectral bounds

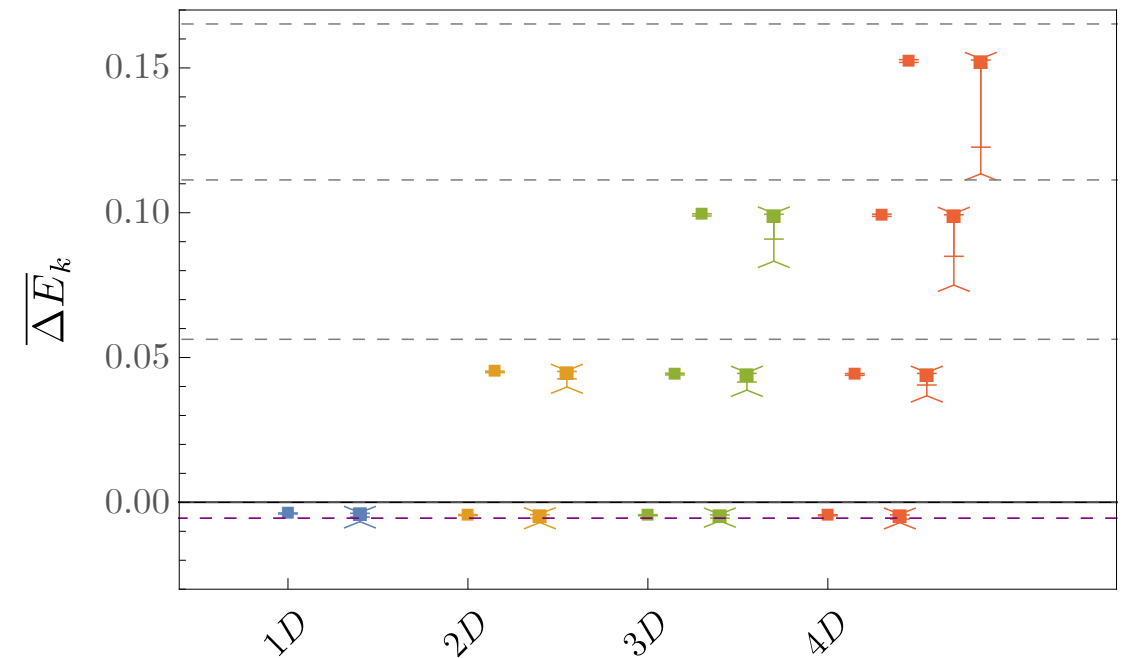
In practice [2601.22272]

- Bound windows are practical in LQCD calculations

NN $I = 1$ residual bounds

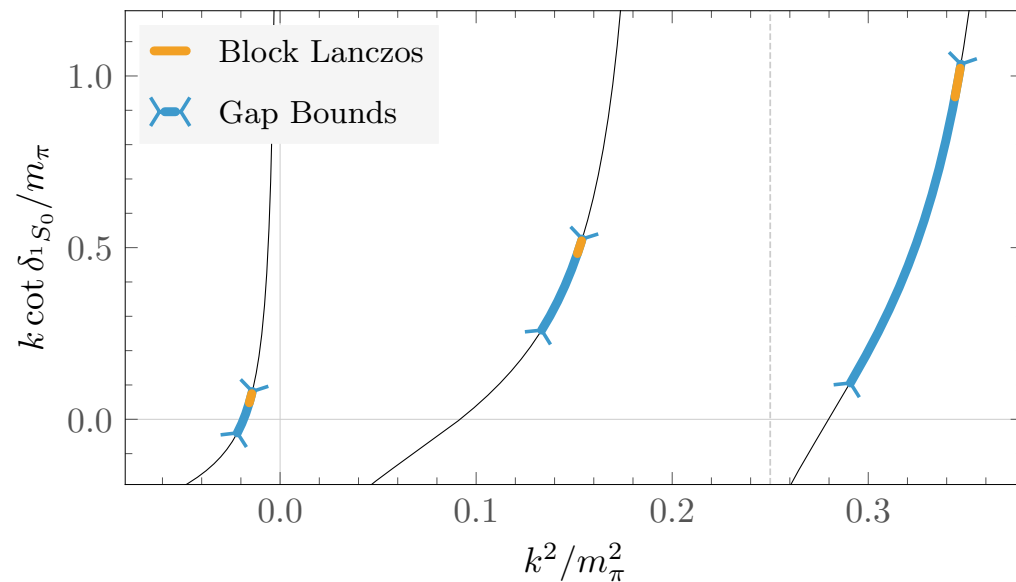


NN $I = 1$ gap + variational bounds

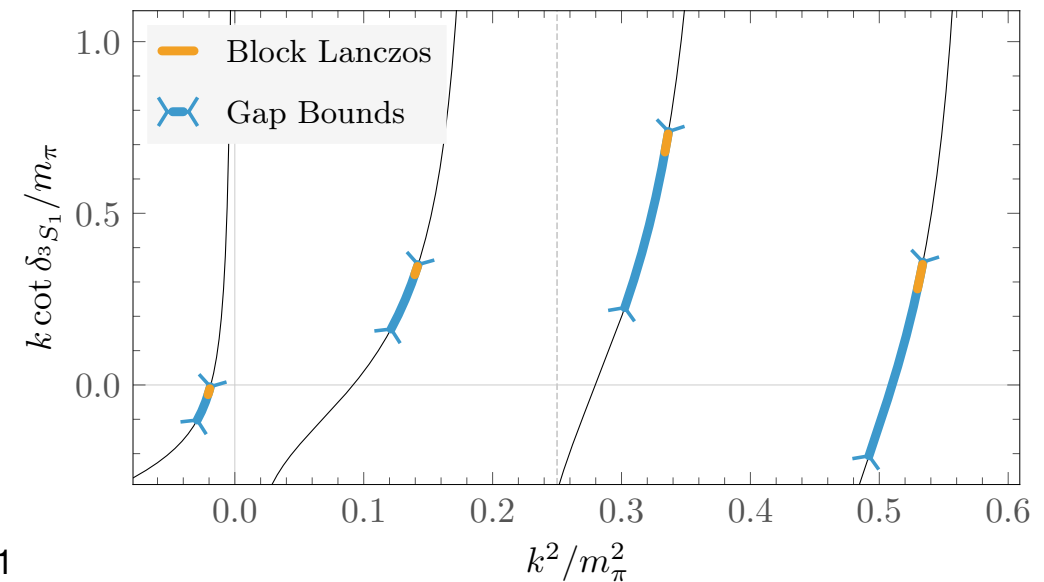


- NN scattering phase shifts from gap bounds

NN $I = 1$



NN $I = 0$

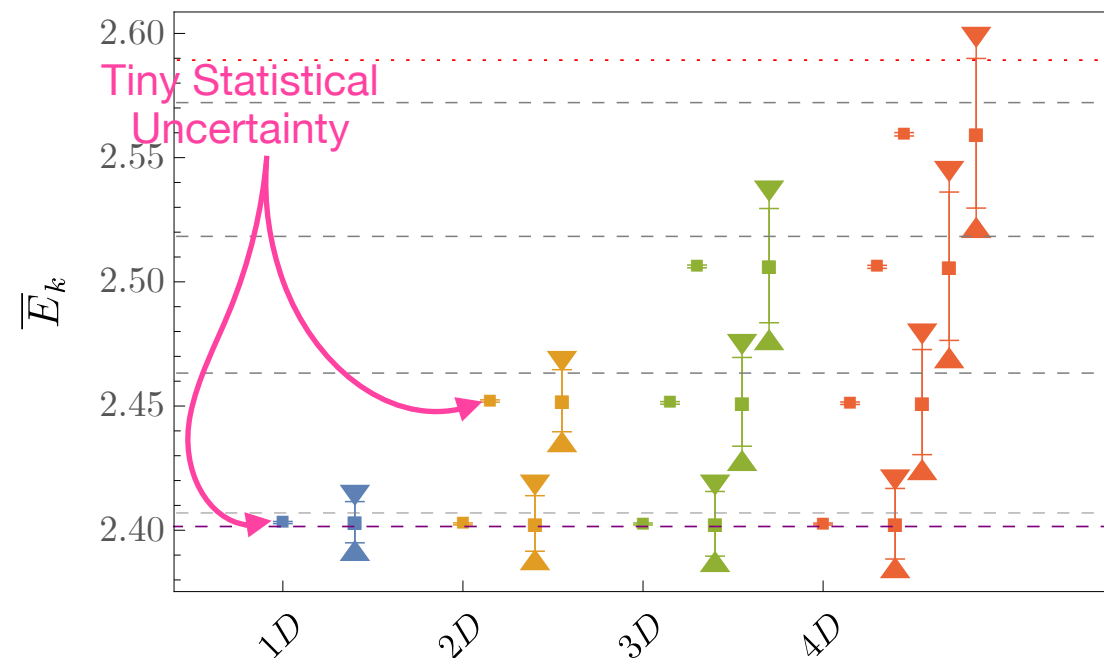


Spectral bounds

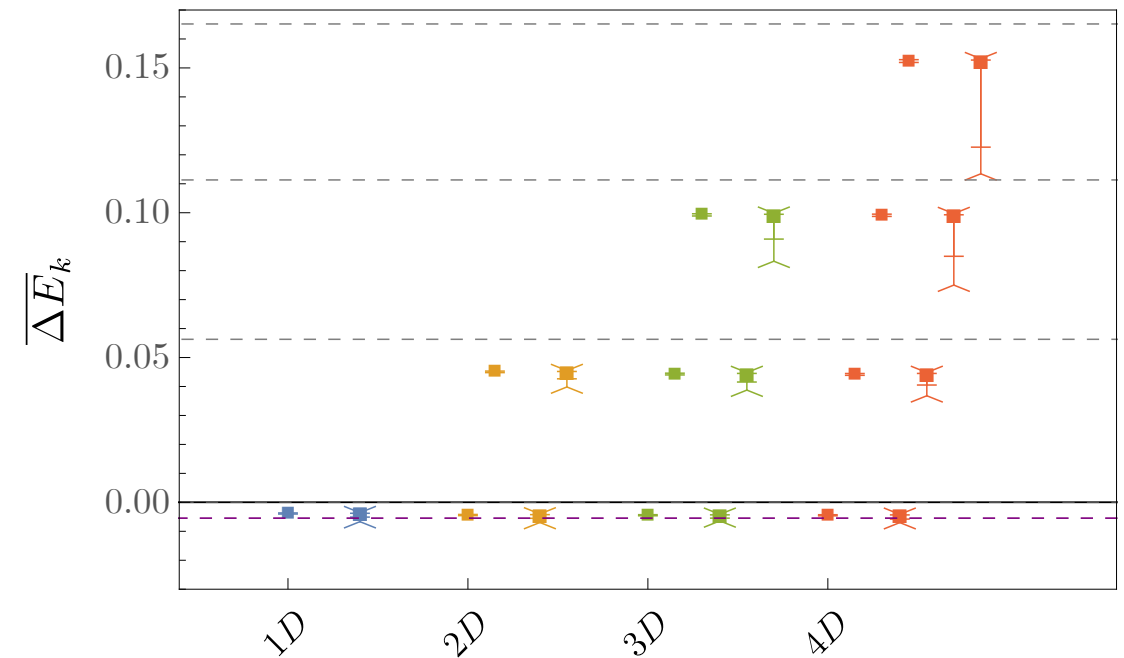
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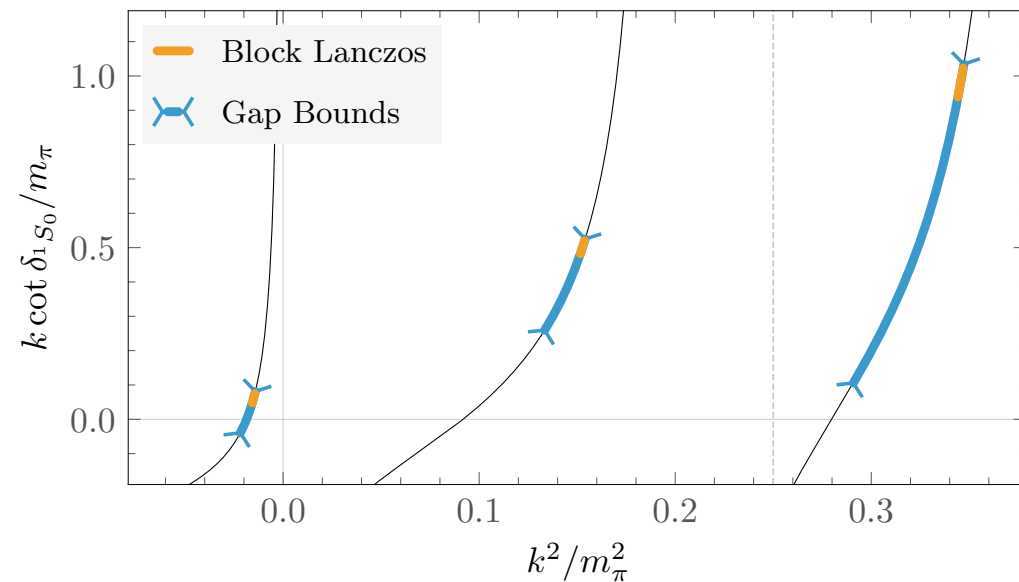


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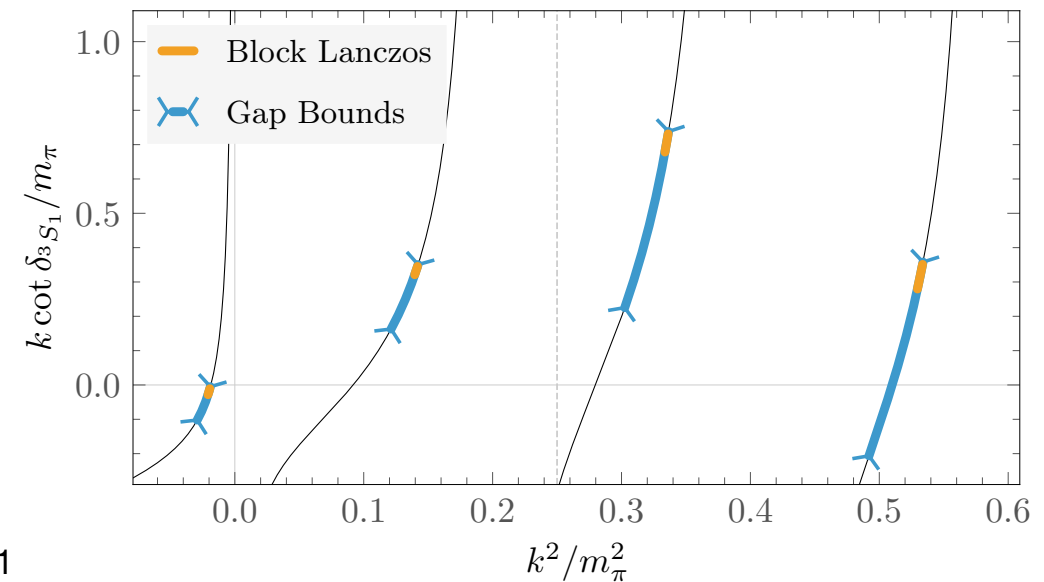


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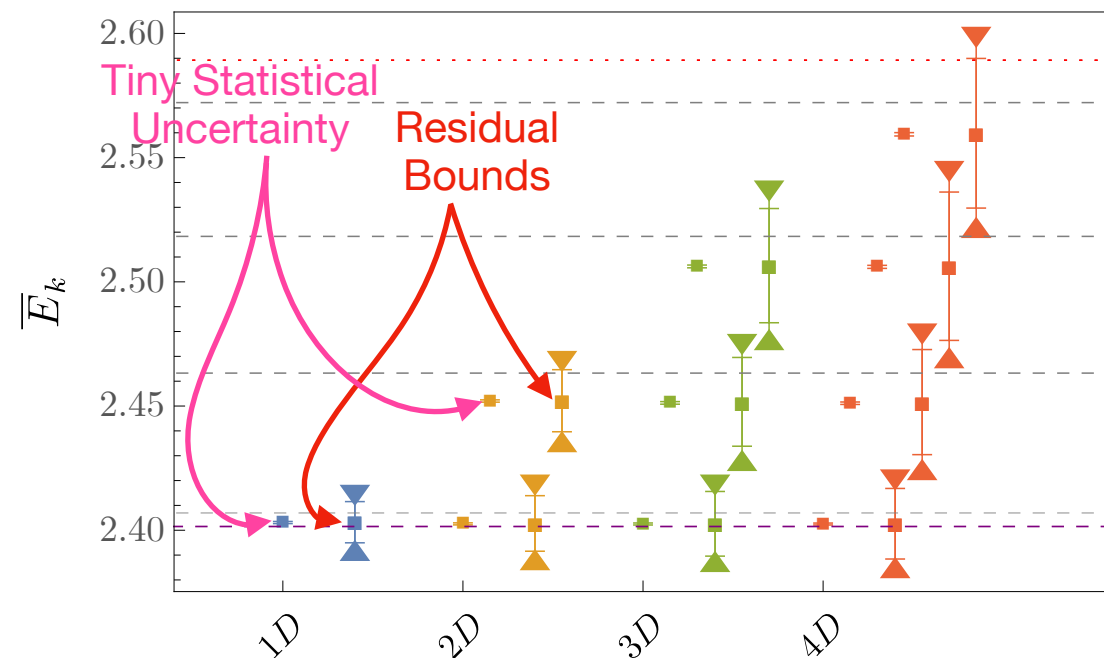


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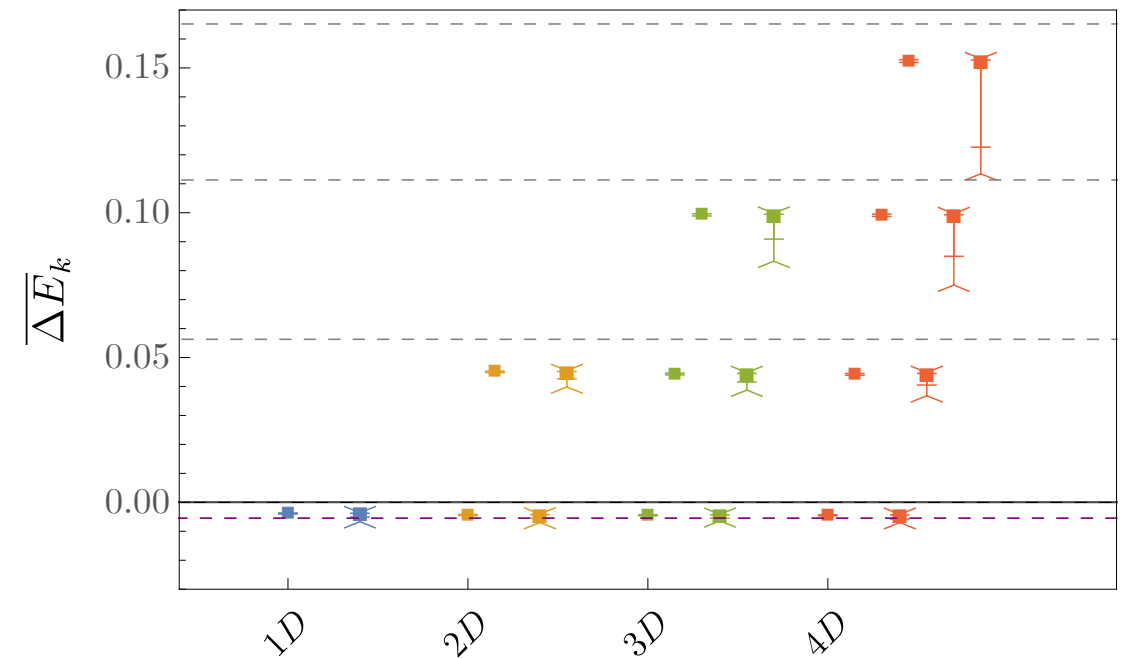
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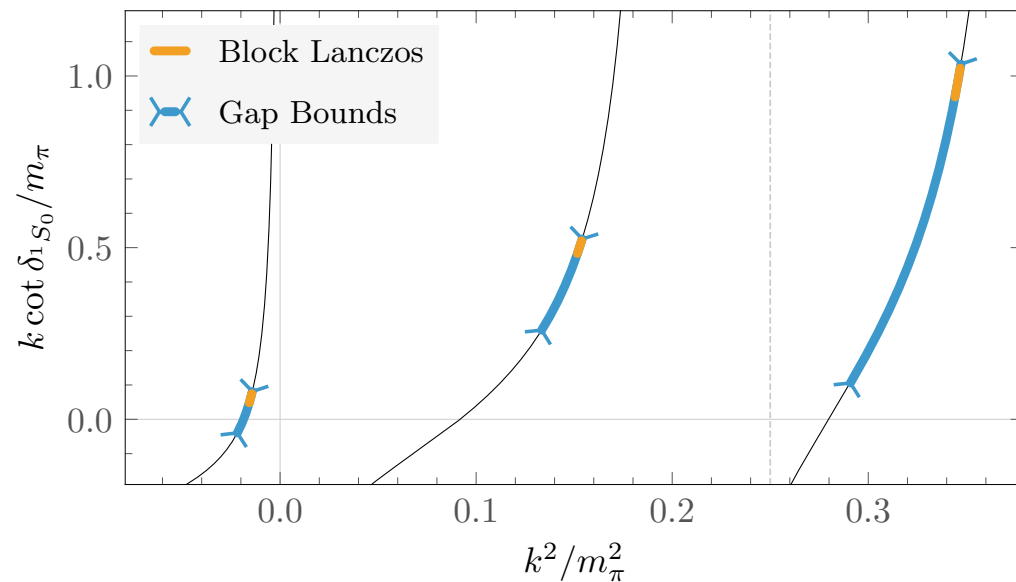


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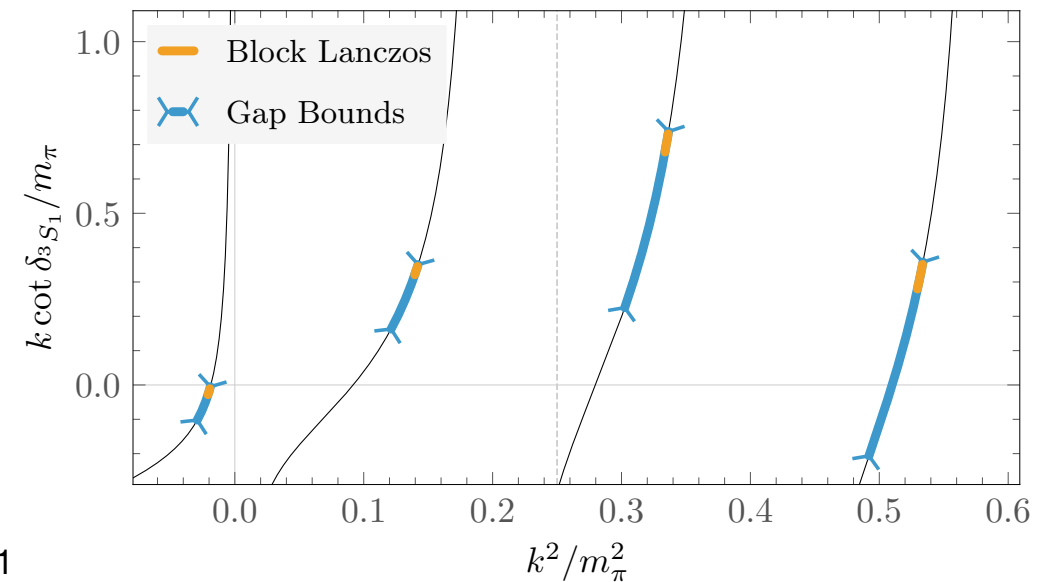


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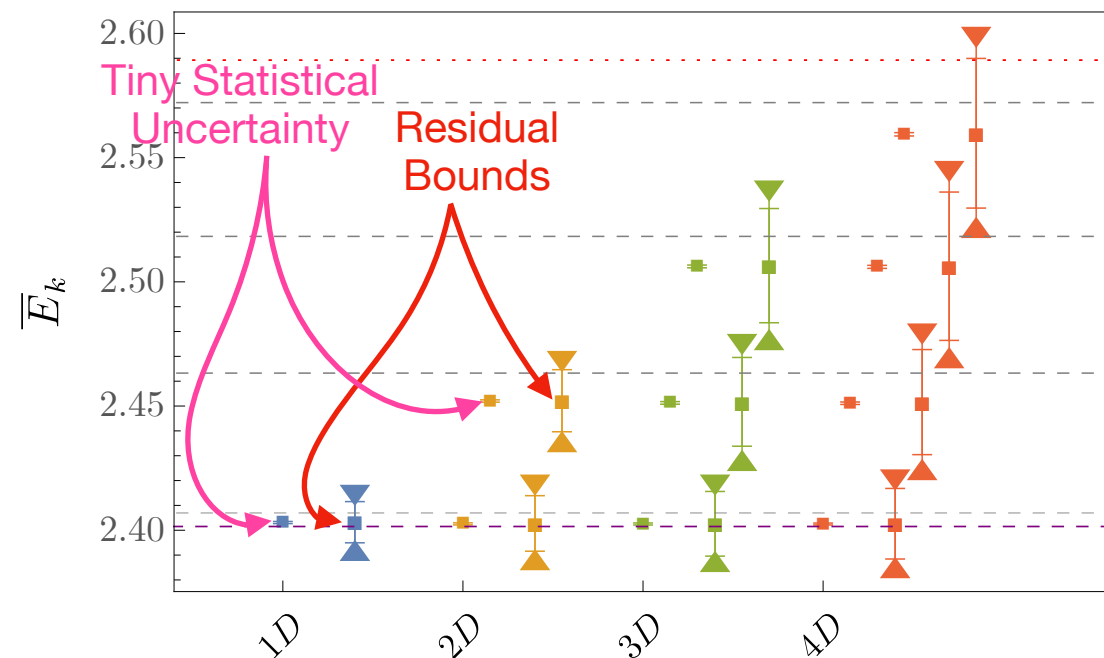


Spectral bounds

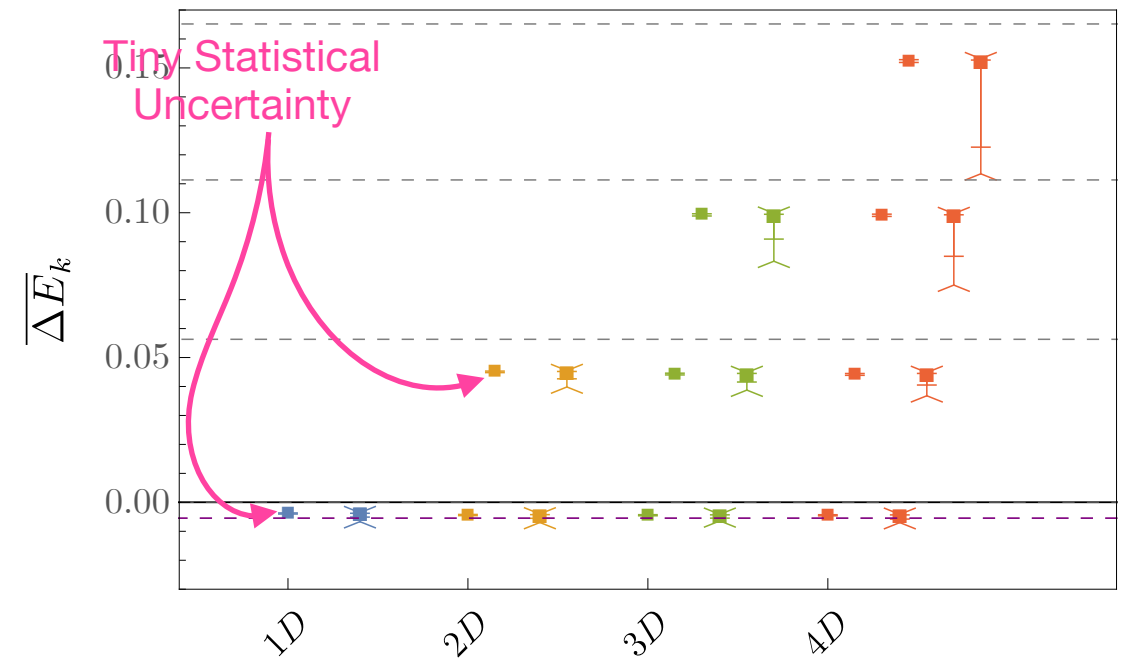
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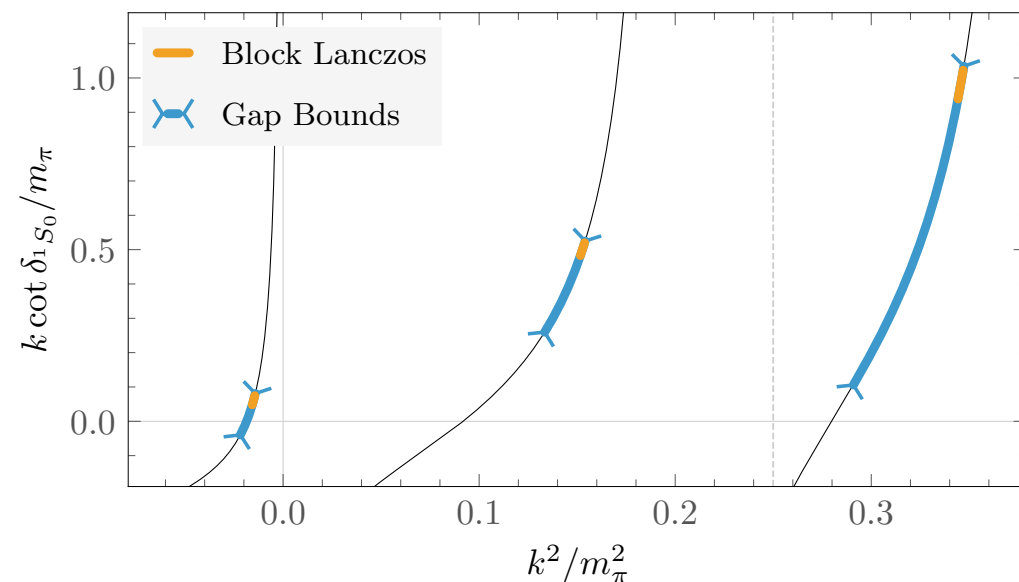


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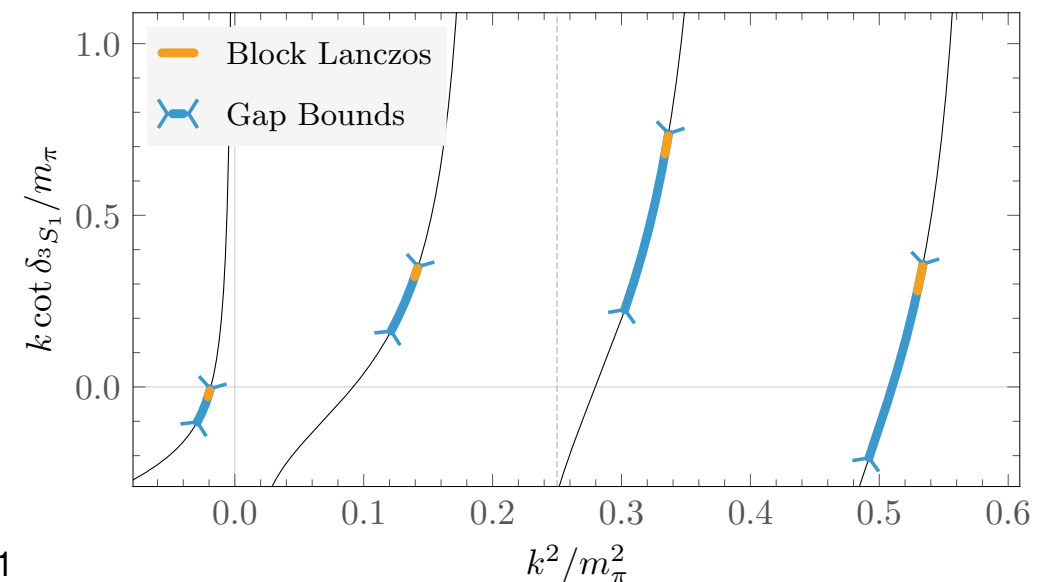


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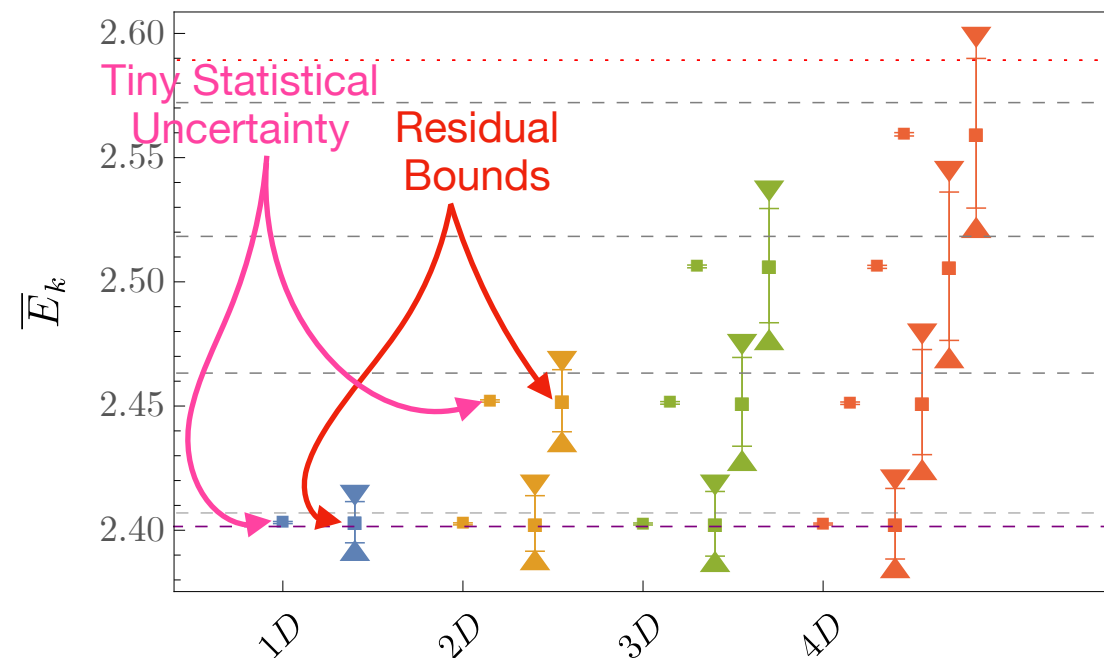


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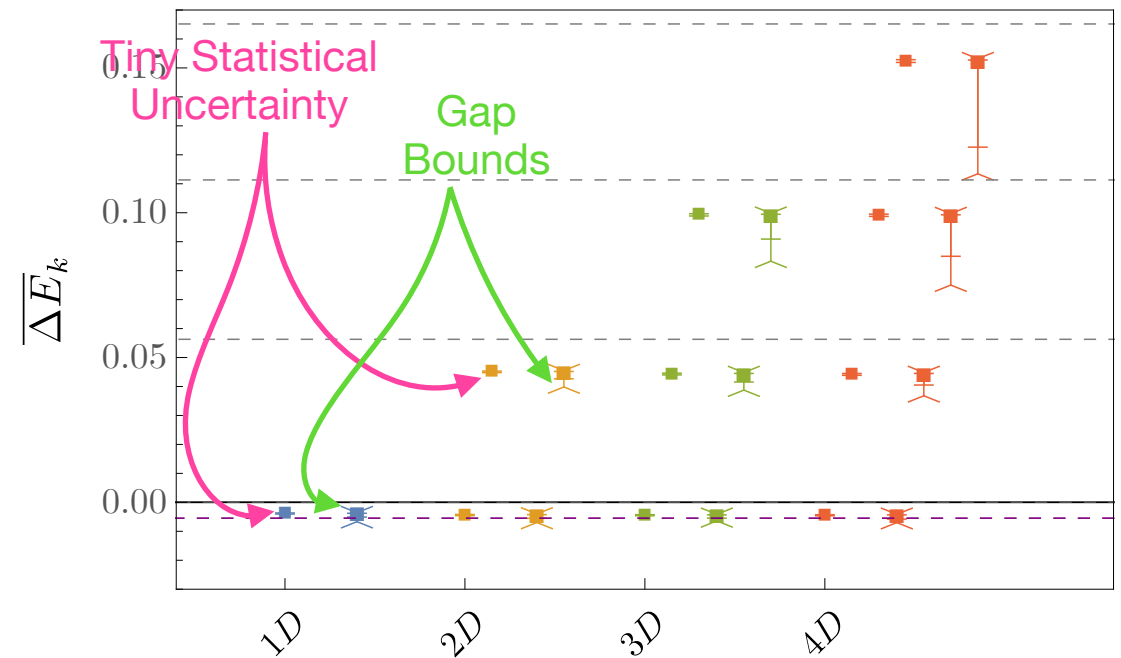
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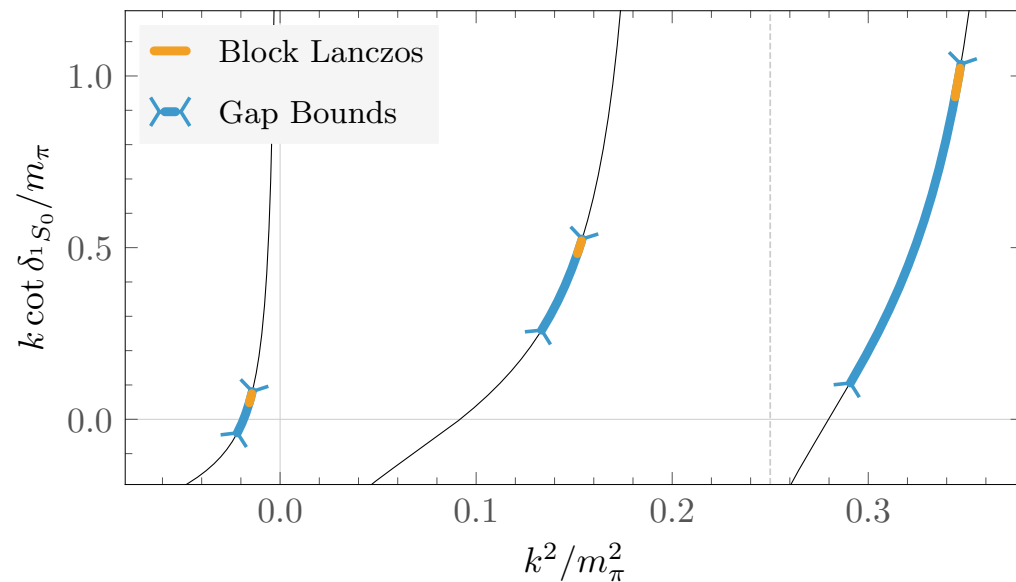


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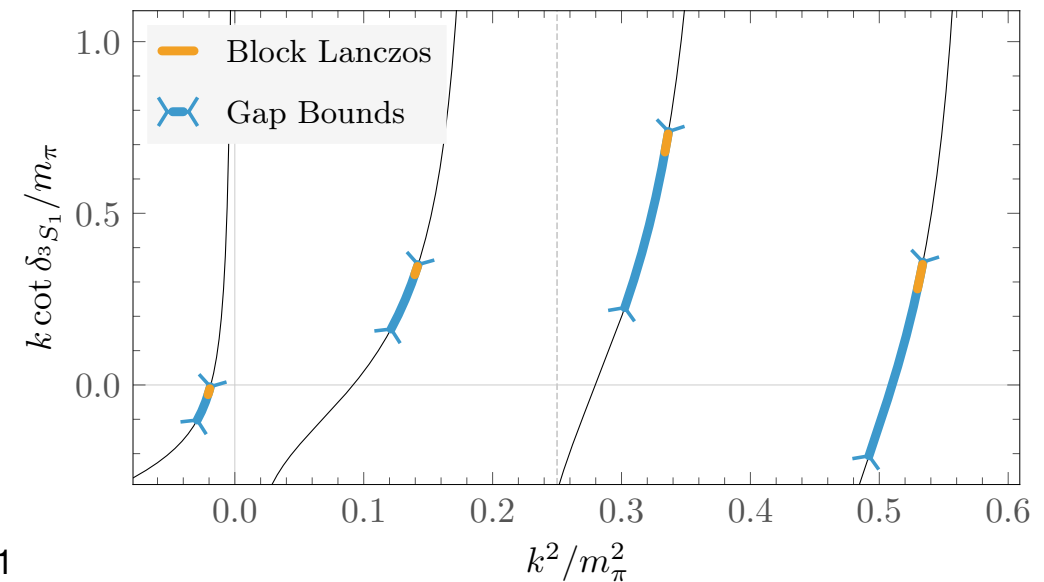


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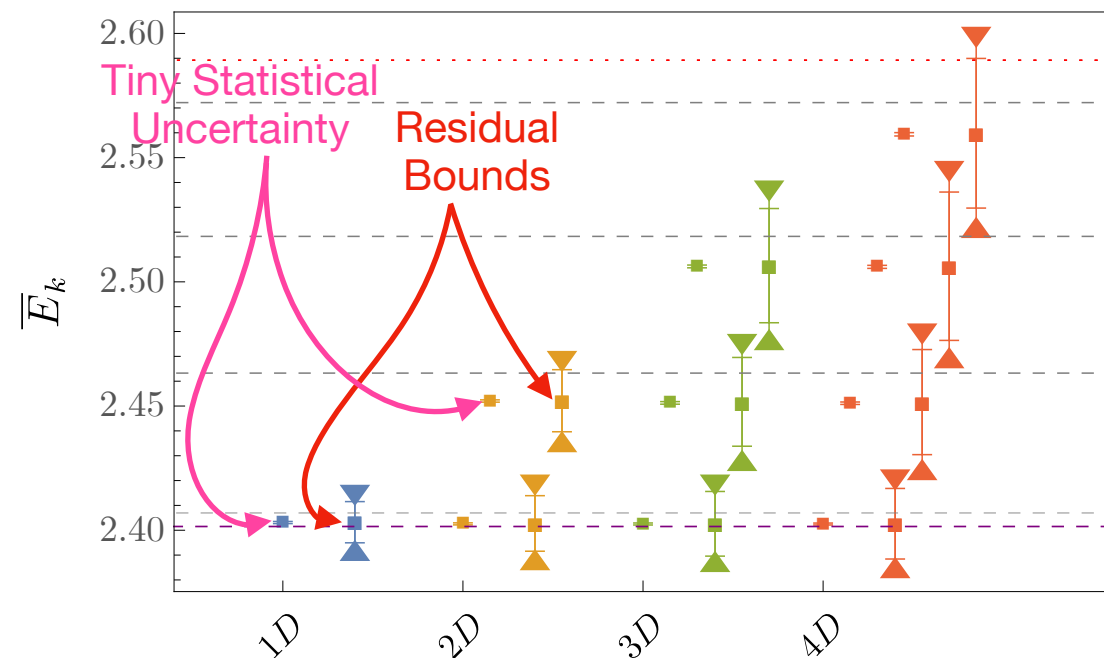


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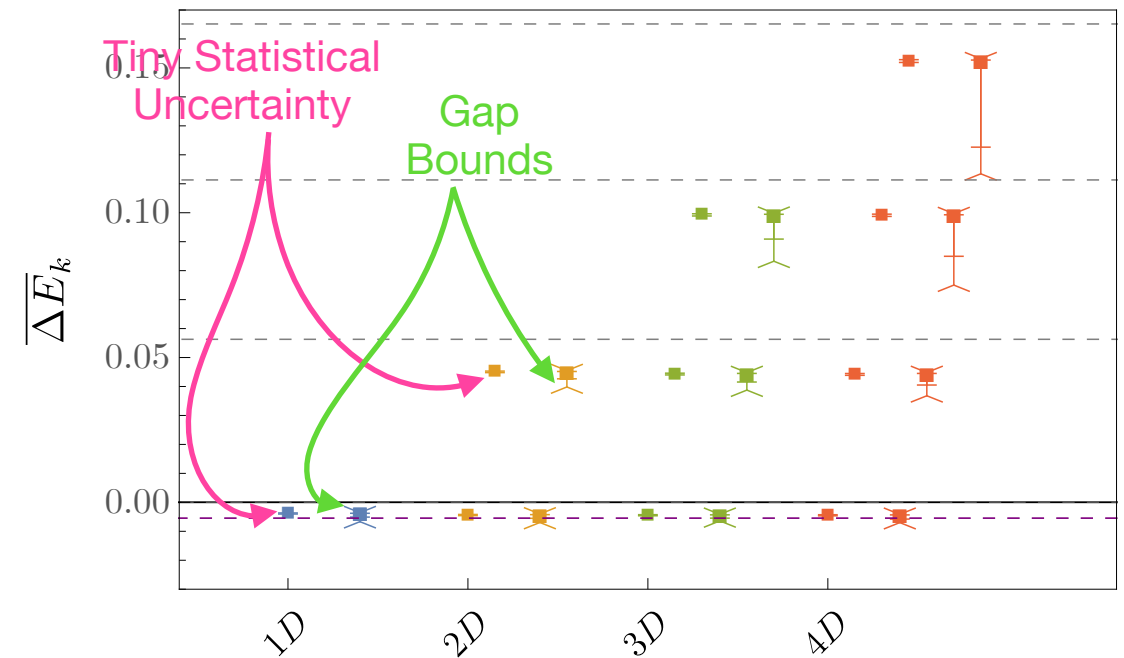
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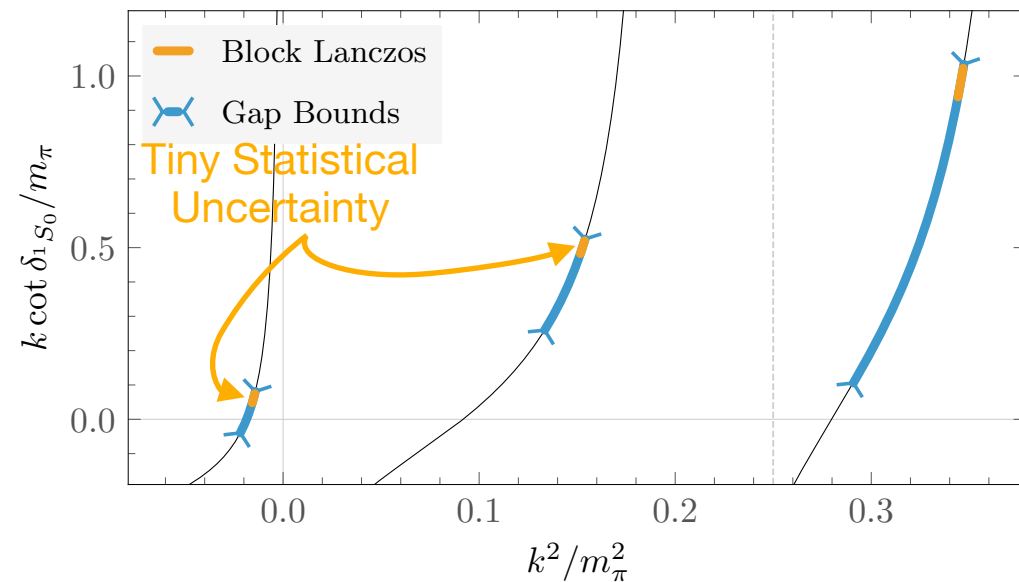


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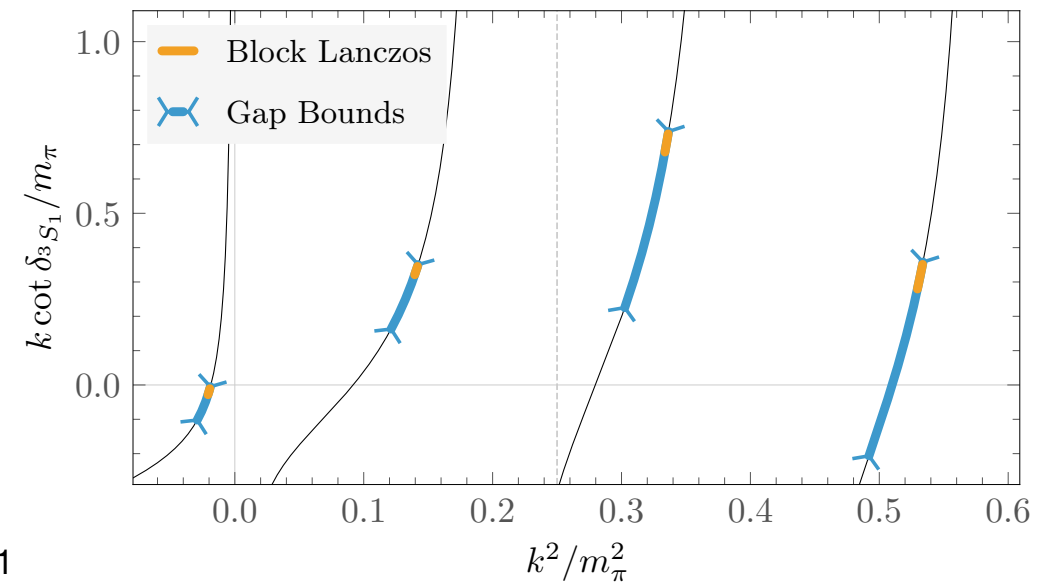


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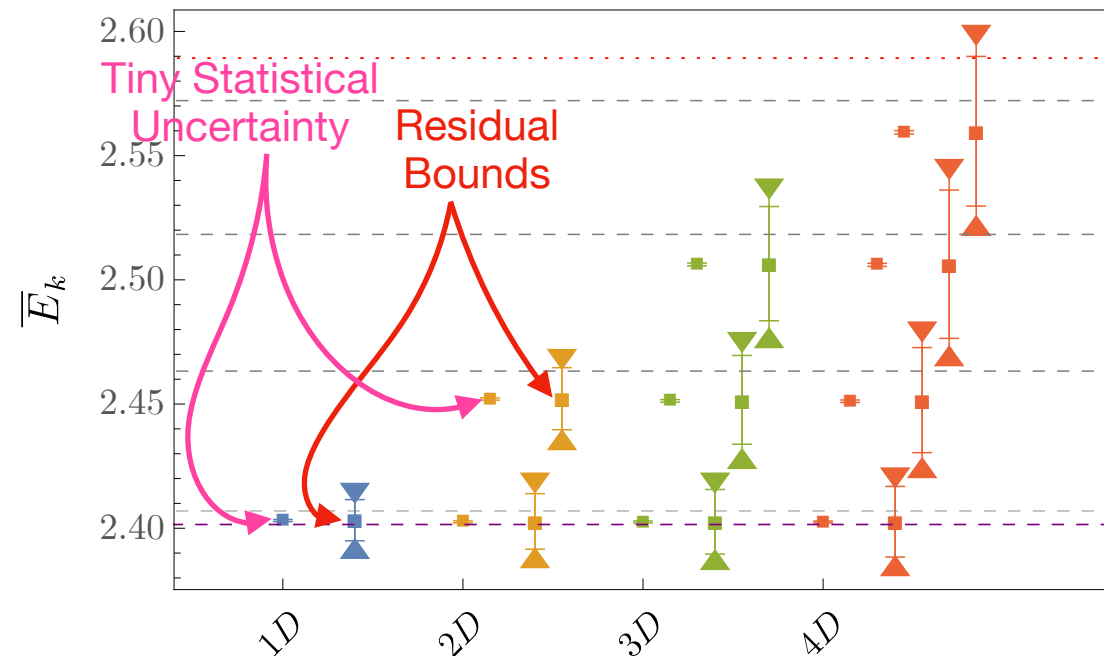


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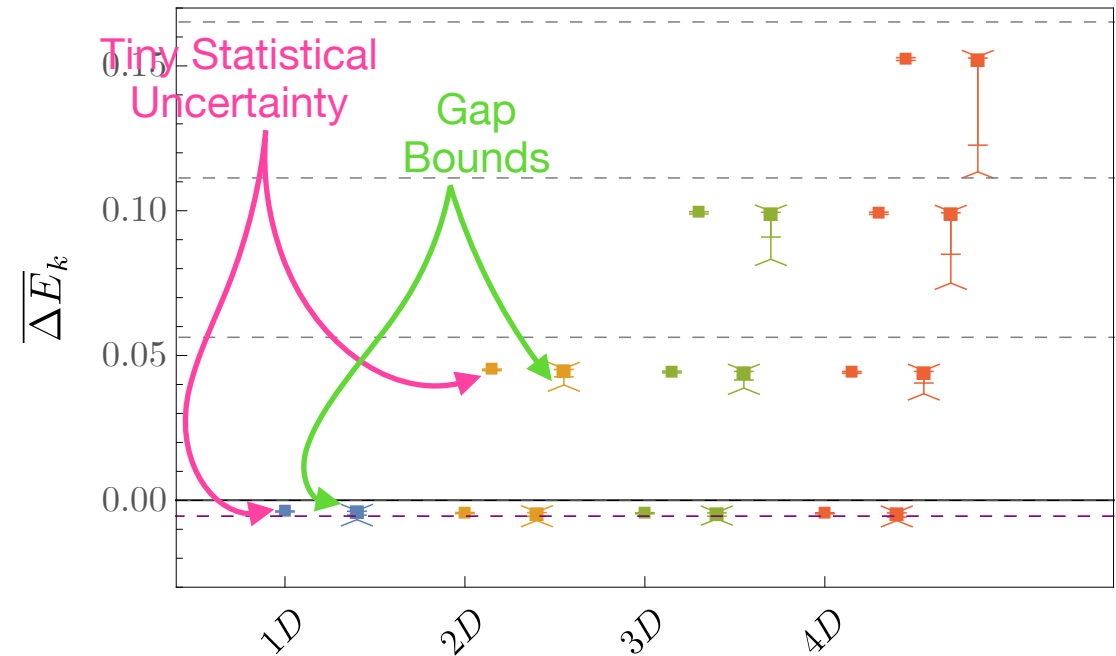
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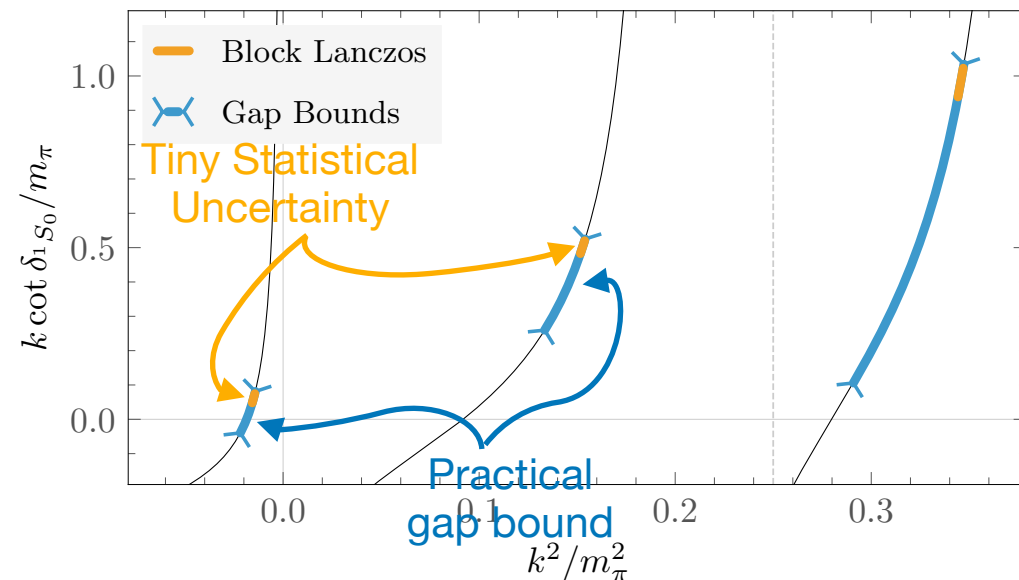


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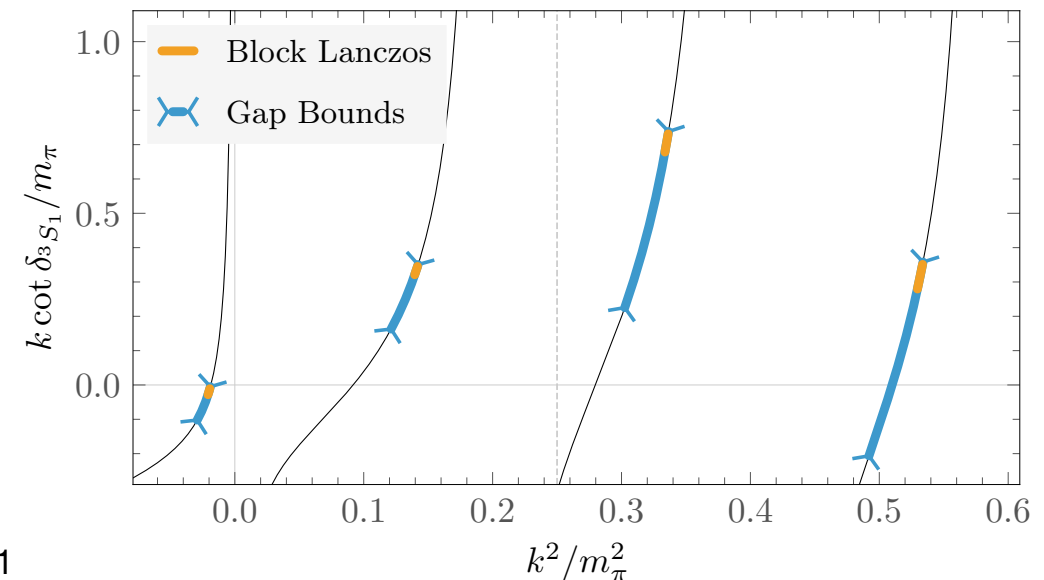


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NN $I = 1$



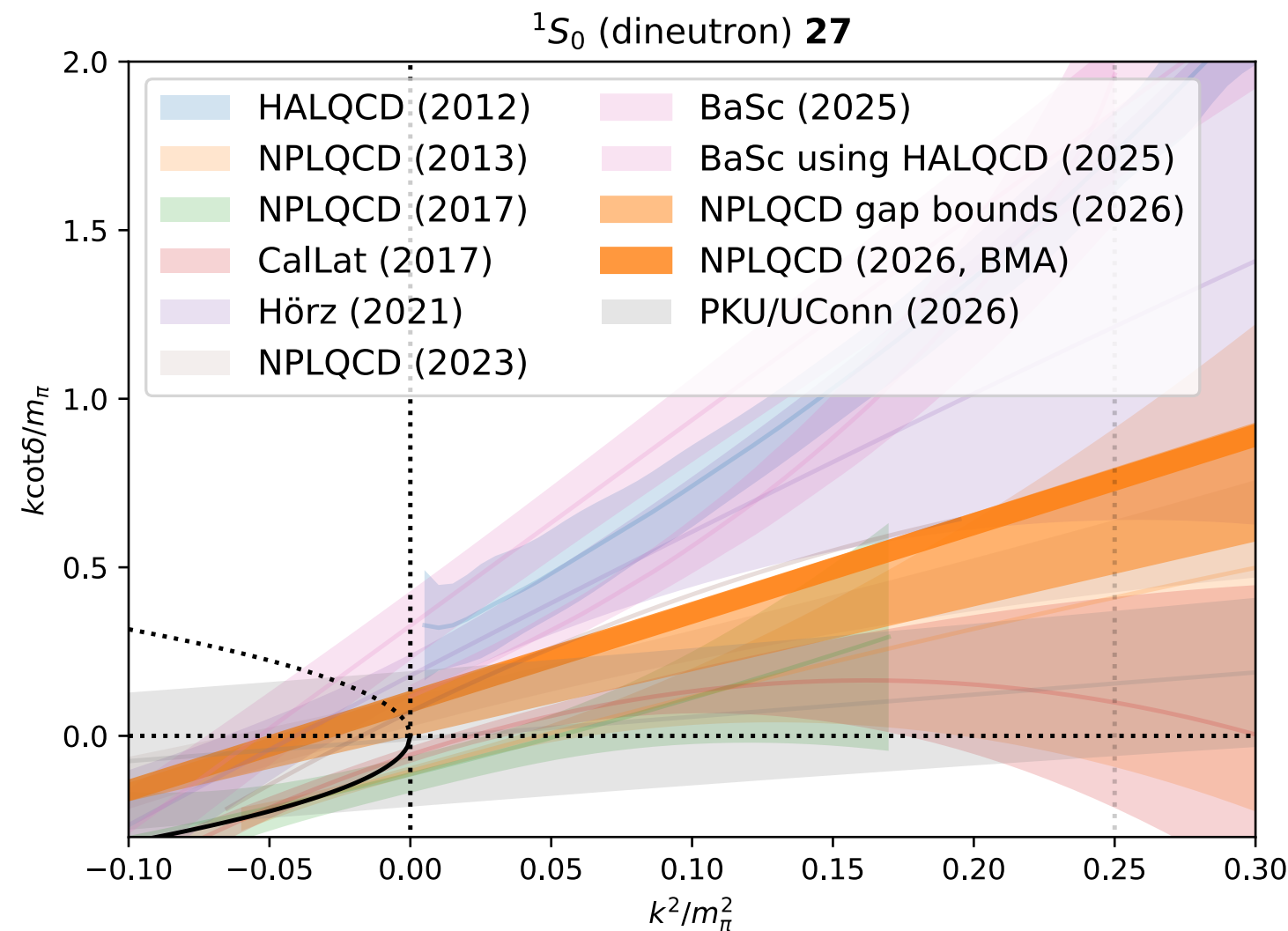
NN $I = 0$



Gap bound phase shift

Practical!

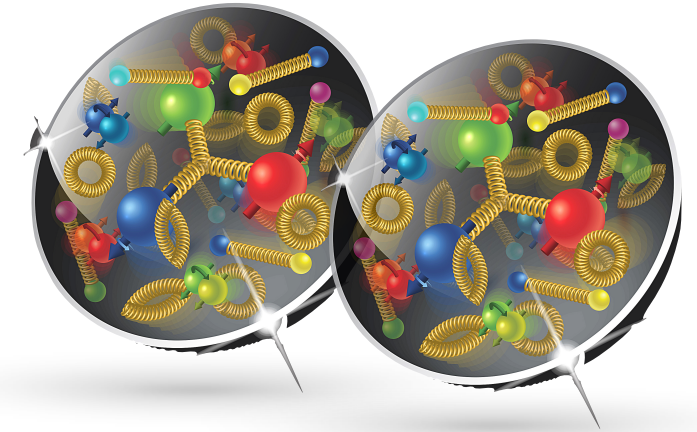
- Gap bound phase shift is constraining for high stats data



- NB: gap is priored on there NOT being a bound state in this case

What is the road forward?

Towards precision NN calculations



- NN systems in LQCD remain a confused story
 - Even after 20 years we are still not done!
- **Challenge:** Calculations with required control of statistical and systematic effects are becoming feasible
 - Without multiple volumes, lattice spacings, and more rigorous correlator analysis, confusion and discrepancies will remain
- **Opportunity:** bound windows provide new approach for operator construction
 - Can sets of operators be chosen to systematically reduce spectral bound windows?
 - Are there entirely new analysis techniques based on these tools?

Thanks!

Many thanks to NPLQCD collaboration colleagues and DOE and NSF funding agencies

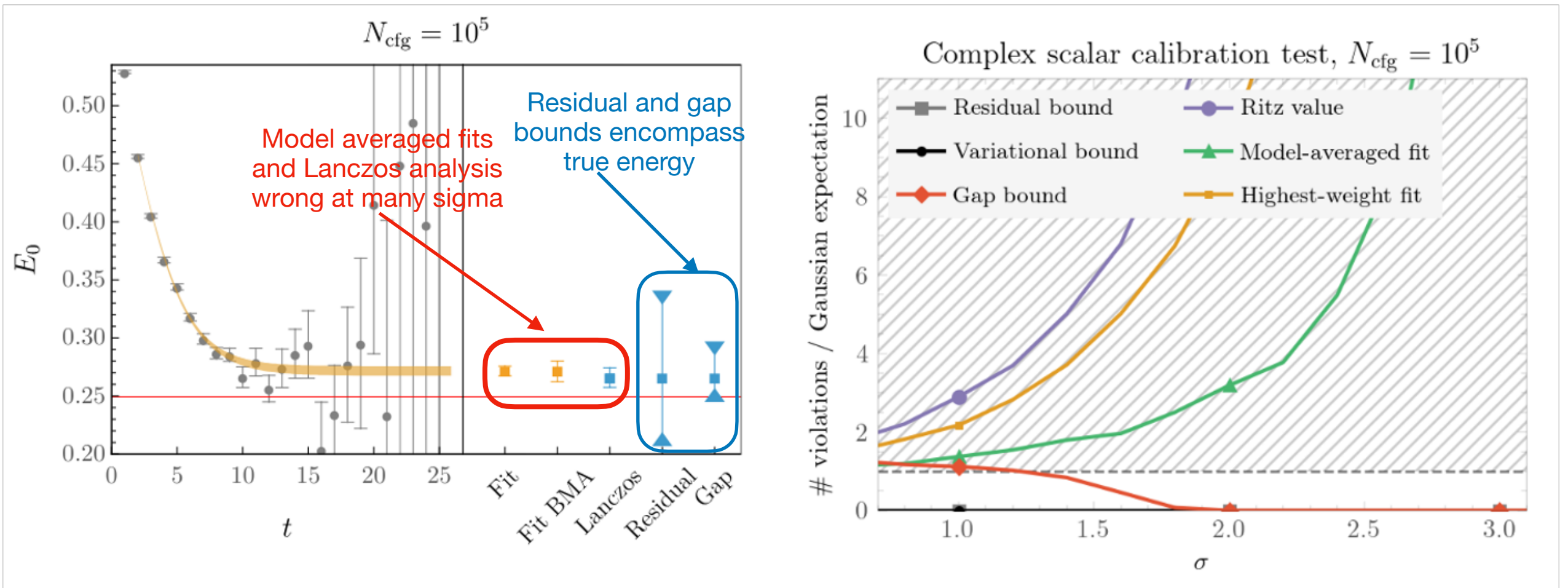
Calibrating bounds

Harmonic oscillator

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

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

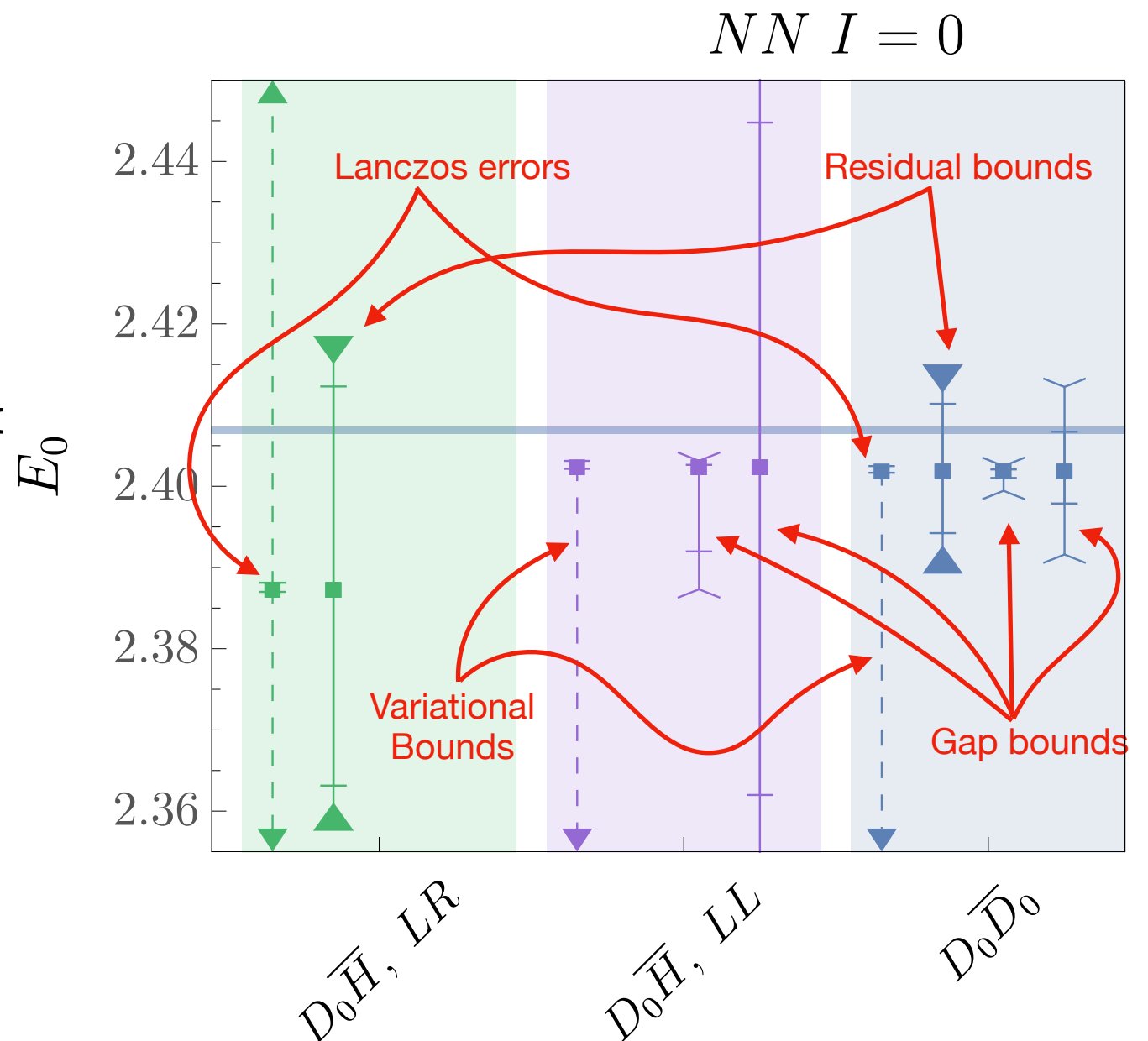
- Compute two-point correlator: $C(t) = \langle \mathcal{O}(t) \mathcal{O}^\dagger(0) \rangle$ with $\mathcal{O}(t) = e^{\varphi(t)} - 1$
- Exhibits excited state contamination, exponentially bad signal-to-noise:



Symmetric vs asymmetric correlators

Statistical errors vs spectral bounds

- Asymmetric ($D_o\bar{H}$) and symmetric ($D_0\bar{D}_0$) correlators
- Extracted energies are very very statistically discrepant
- Residual bounds on both types of correlators are consistent with $D_o\bar{H}$ and $D_0\bar{D}_0$ Lanczos errors
- Variational bounds and gap bounds require symmetric correlators
- Gap bounds are consistent with $D_o\bar{H}$ energy unless gap assumption explicitly precludes it
- Variational bounds can NEVER rule out lower energy



Variational method

Rigorous upper bounds

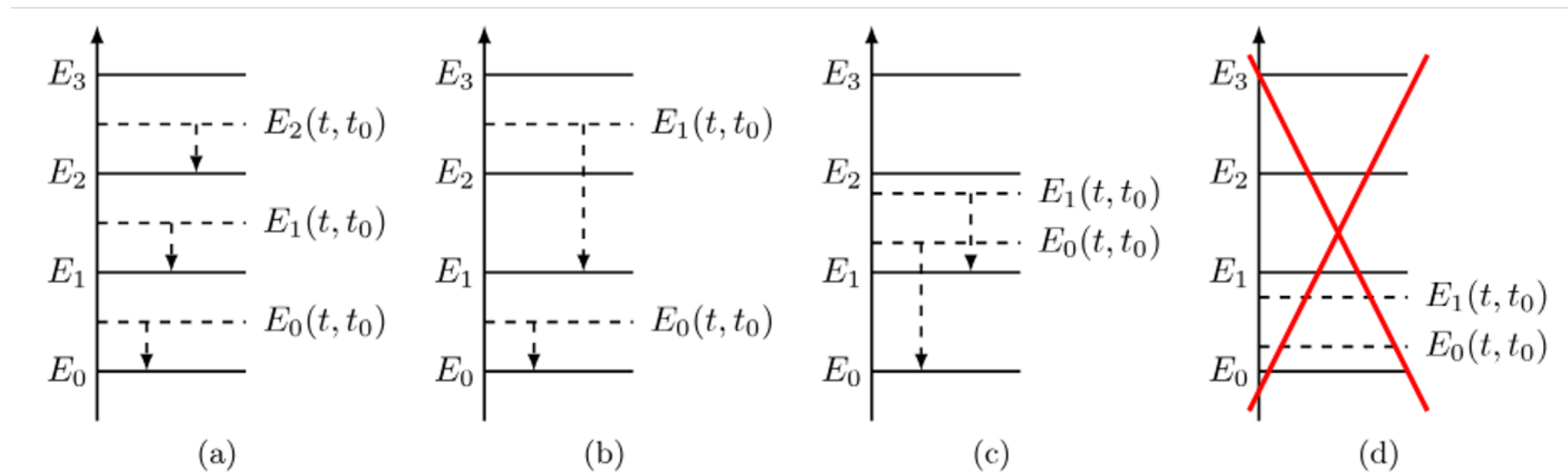
- The Rayleigh-Ritz variational method (for any $|\Psi\rangle$)

$$E_0 \leq \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

or for transfer matrix

$$E_0 \leq -\ln \frac{\langle \Psi | \hat{T} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = -\ln \frac{C(t+1)}{C(t)}$$

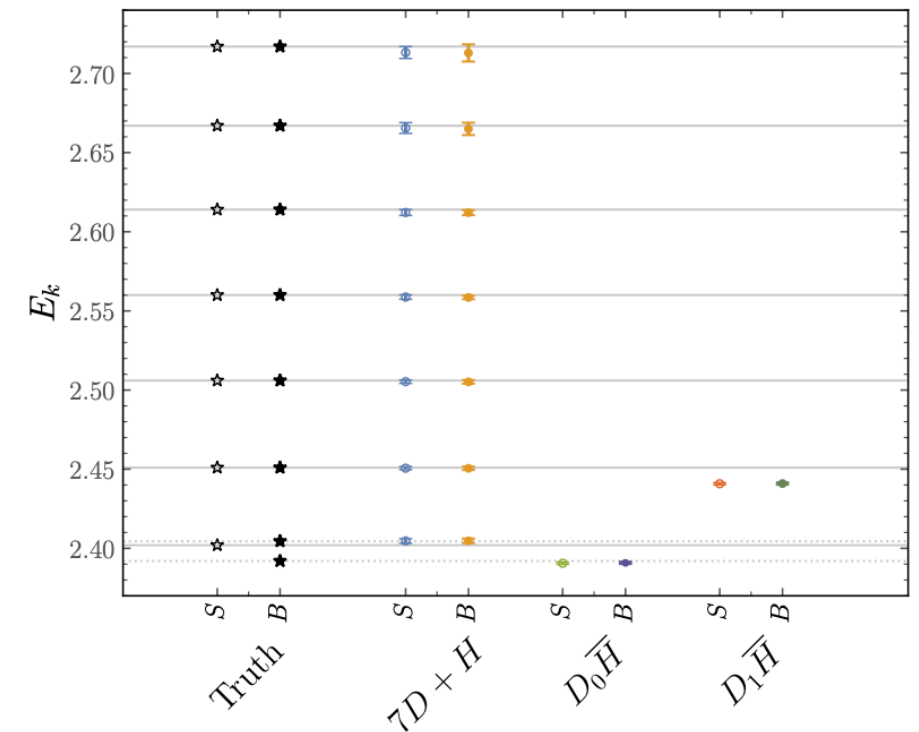
- For a correlator matrix: Cauchy Interlacing Theorem guarantees estimated (finite matrix) and true eigenvalues interleave



Failure modes of spectroscopy

Closely spaced levels

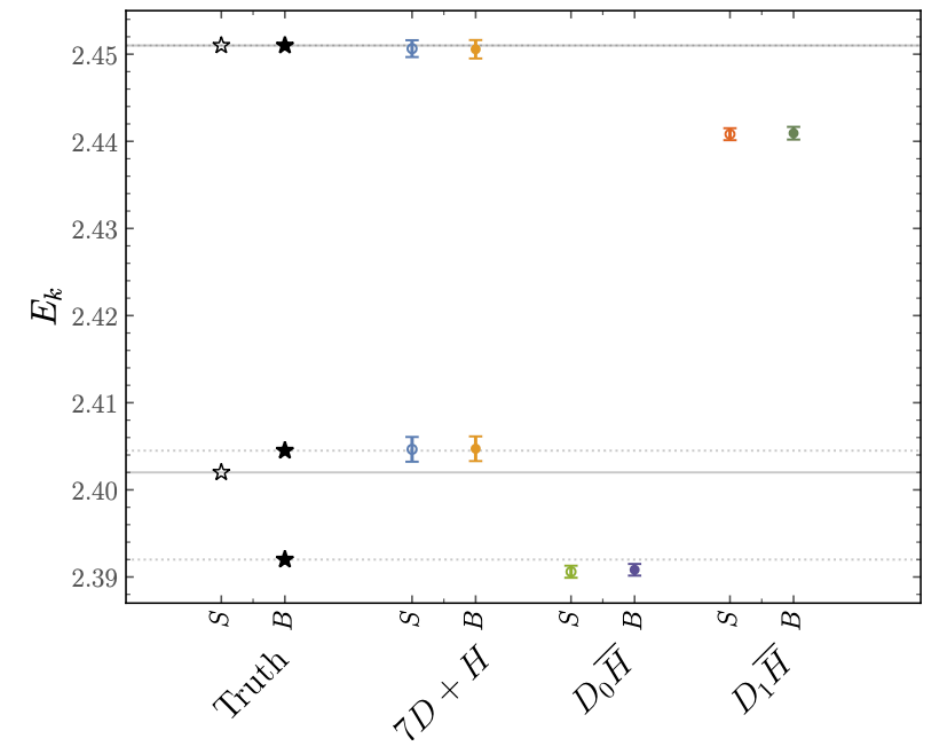
- Based on spectrum extracted in high precision calculations in 2601.022272
- Fake data based on this “truth”
 - Either single lowest state
 - Split state into 2 states based on asymmetric result (roughly divide overlaps)
- Analyse either 8x8 matrix correlator using Lanczos or analyst asymmetric hexaquark—dibaryon correlator
- Answer wrong in all cases and biased by analysis approach
- Erroneous conclusions avoided with spectral bound approaches



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- Based on spectrum extracted in high precision calculations in 2601.022272
- Fake data based on this “truth”
 - Either single lowest state
 - Split state into 2 states based on asymmetric result (roughly divide overlaps)
- Analyse either 8x8 matrix correlator using Lanczos or analyst asymmetric hexaquark—dibaryon correlator
- Answer wrong in all cases and biased by analysis approach
- Erroneous conclusions avoided with spectral bound approaches

