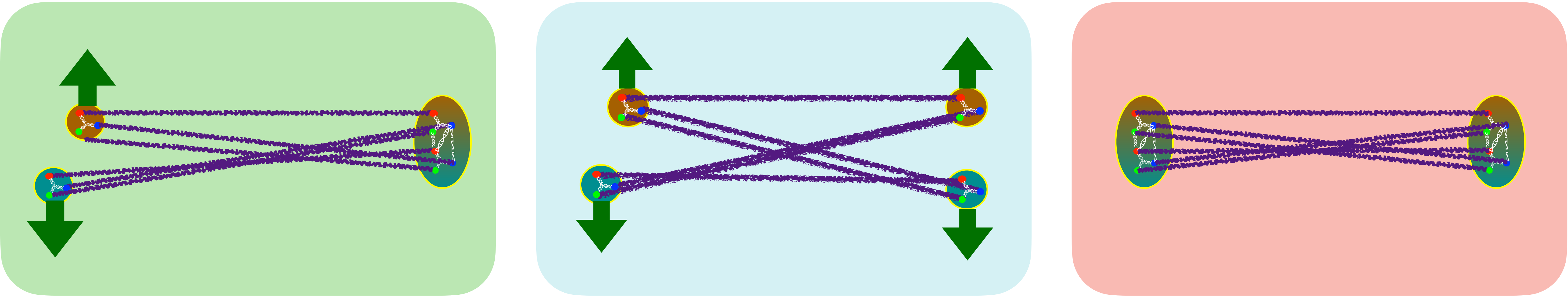
Two-baryon variational spectroscopy

Michael Wagman



with Saman Amarasinghe, Riyadh Baghdadi, Zohreh Davoudi, Will Detmold, Marc Illa, Assumpta Parreño, Andrew Pochinsky, and Phiala Shanahan

arXiv:2108.10835 and ongoing work

Lattice 2022

Bonn

August 11, 2022

Lattice QCD and nuclei

LQCD calculations of nuclear matrix elements can constrain EFTs and nuclear models relevant for precise predictions of

— electroweak reaction rates,

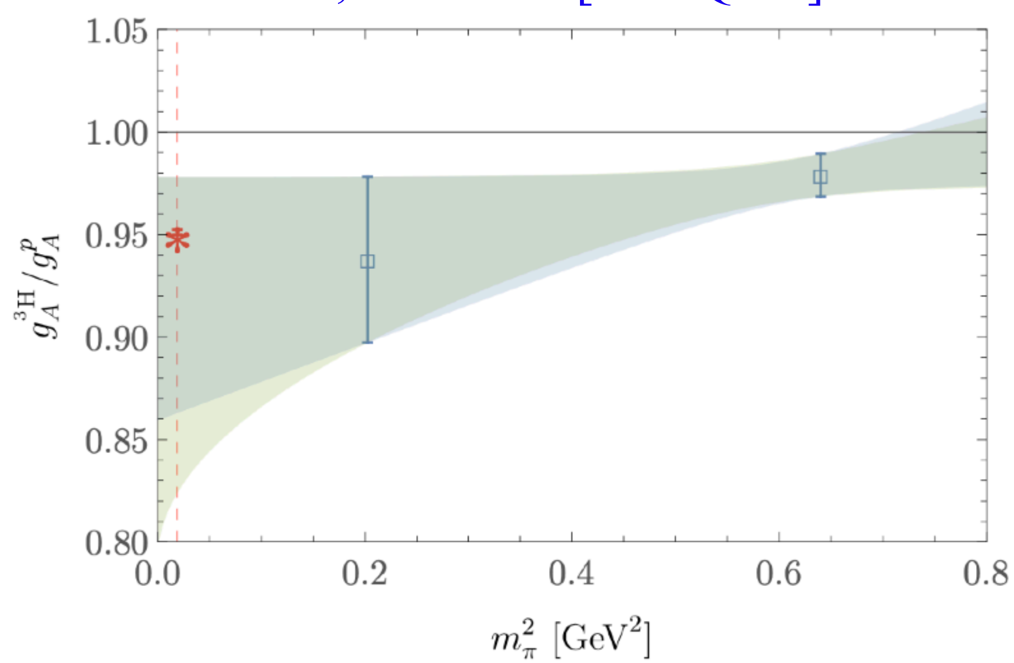
— double-beta decay,

— dark matter direct detection,

— neutrino-nucleus scattering

…

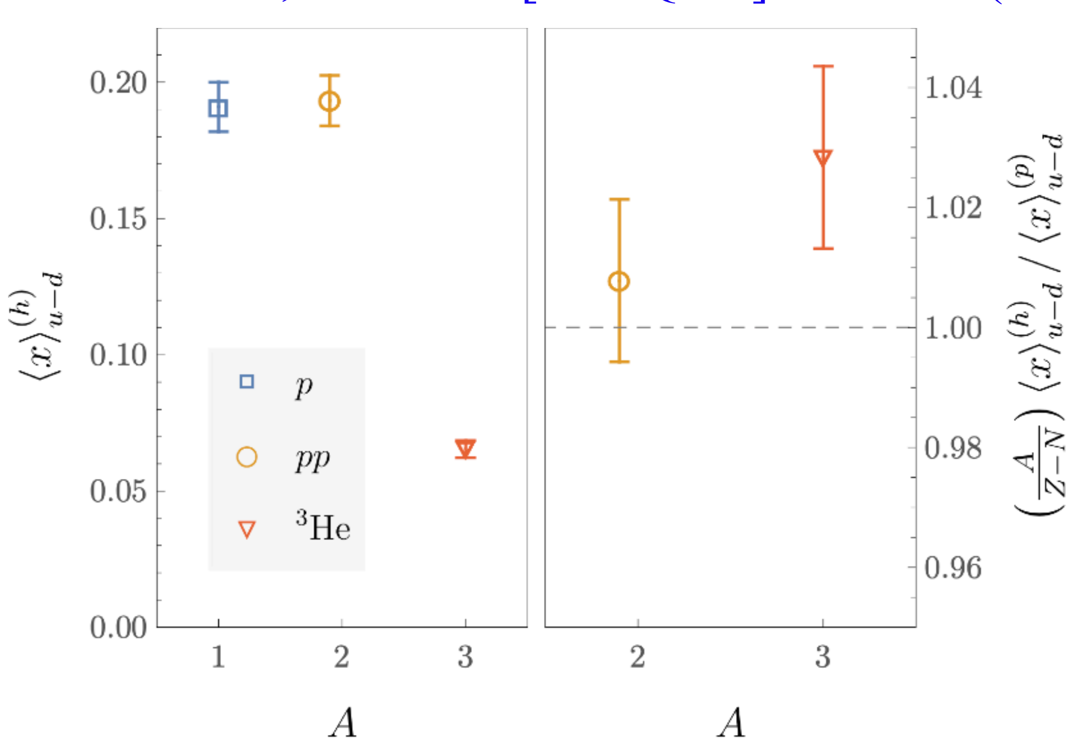
Parreño, MW et al [NPLQCD] PRD 103 (2021)



Exploratory LQCD calculations of nuclear matrix elements including axial charge and isovector quark momentum fraction of ^{3}He performed at unphysical quark masses

Although exploratory, LQCD results consistent with experimental results where available

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



Systematic uncertainties

Several systematic uncertainties remain to be quantified in detail

- 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

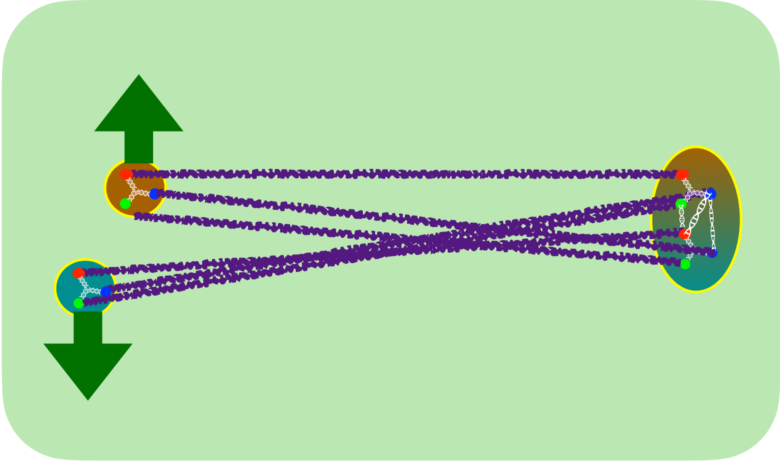
$$Z_0 e^{-E_0 t}\left(1 + \frac{Z_1}{Z_0} e^{-\delta t} + \ldots\right) \qquad \delta \equiv E_1 - E_0 \sim \frac{4\pi^2}{ML^2}$$

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)

Early studies took advantage of efficient algorithms for computing asymmetric correlation functions with local sources, results consistent with ground-state dominance

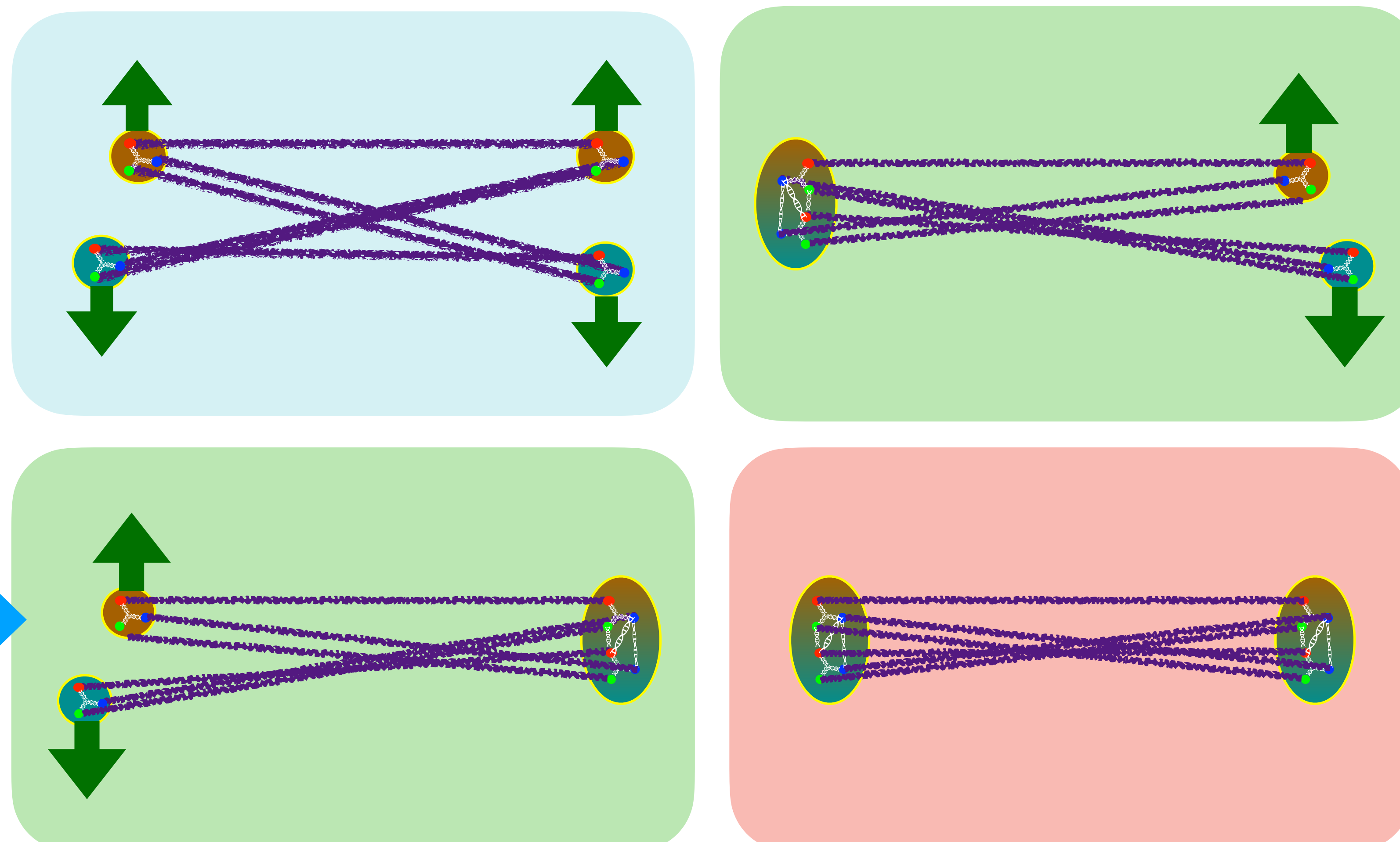
Detmold and Orginos, PRD 87 (2013)



Variational methods

Symmetric correlation-function matrices can be diagonalized to provide positive-definite correlation functions that give variational upper bounds on energies

LQCD nuclear matrix element calculations so far



First results from symmetric correlation-function matrices involving plane-wave dibaryon operators (upper-left) enabled by stochastic LapH method are in tension with previous calculations using asymmetric correlation functions

Francis et al, PRD 99 (2019)   Hörz et al, PRC 103 (2021)   Green et al, PRL 127 (2021)

Sparse all-to-all propagators

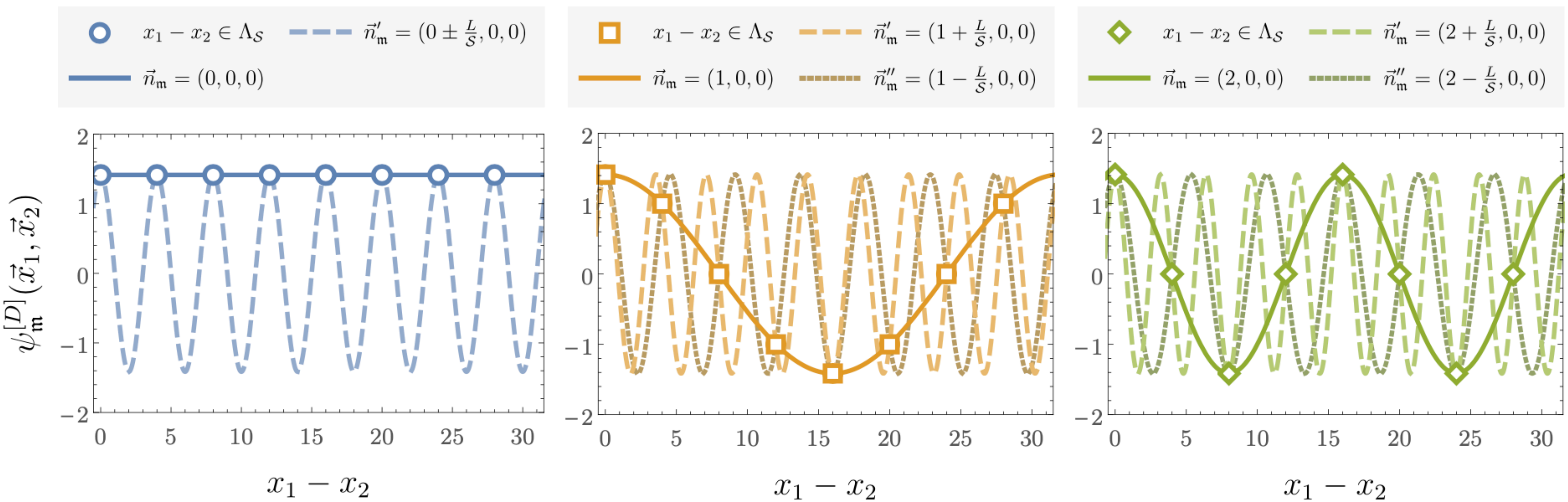
Computing (smeared) point-to-all propagators on a sparse grid of lattice sites provides explicit all-to-all quark propagators on the sparse grid

Detmold, MW et al, PRD 104 (2021)　　Li et al, PRD 103 (2021)

Allows correlation functions to be constructed for local and non-local operators

e.g. plane-wave product: $$\sum_{\vec{x}_1,\vec{x}_2\in\text{sparse grid}} e^{i\vec{k}\cdot(\vec{x}_1-\vec{x}_2)}p(\vec{x}_1,t)n(\vec{x}_2,t)$$

Leads to incomplete Fourier projection and mixing with higher modes, but degree of sparsening can be chosen so that these give negligible excited-state contamination



Interpolating operators

Known from $\pi\pi$ scattering studies near the ρ resonance that not including either local or non-local operators can lead to distortions of energy spectrum including “missing energy levels”

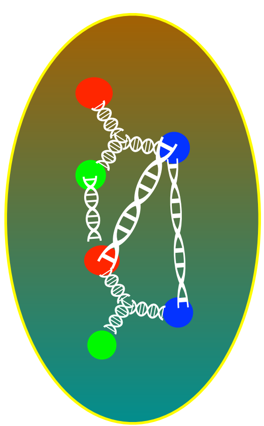
$$\overline{q}(x)\Gamma q(x) \quad \pi(\vec{p}_1)\pi(\vec{p}_2)$$

Dudek et al, PRD 87 (2013)

Wilson et al, PRD 92 (2015)

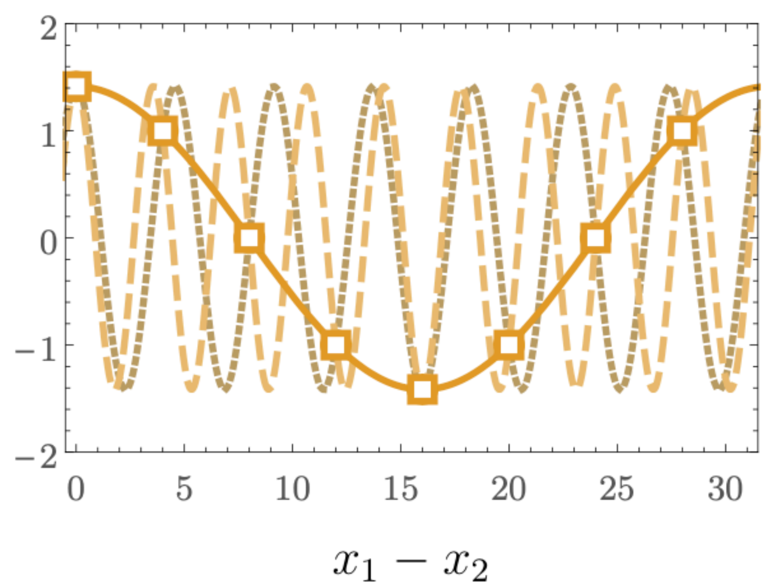
Two-nucleon systems are complicated, wide range of operators used to search for deeply bound / unbound / loosely bound states

Hexaquark:



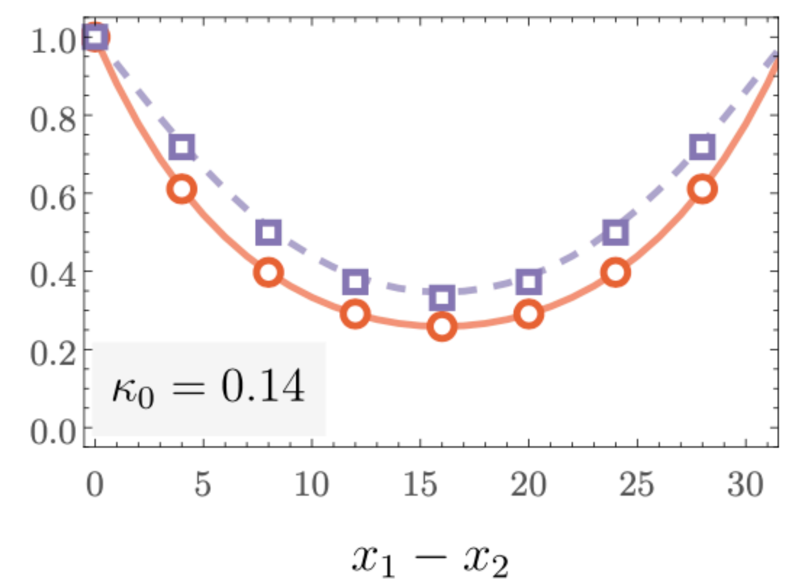
Six Gaussian smeared quarks

Dibaryon:



Two plane-wave baryons with relative momenta

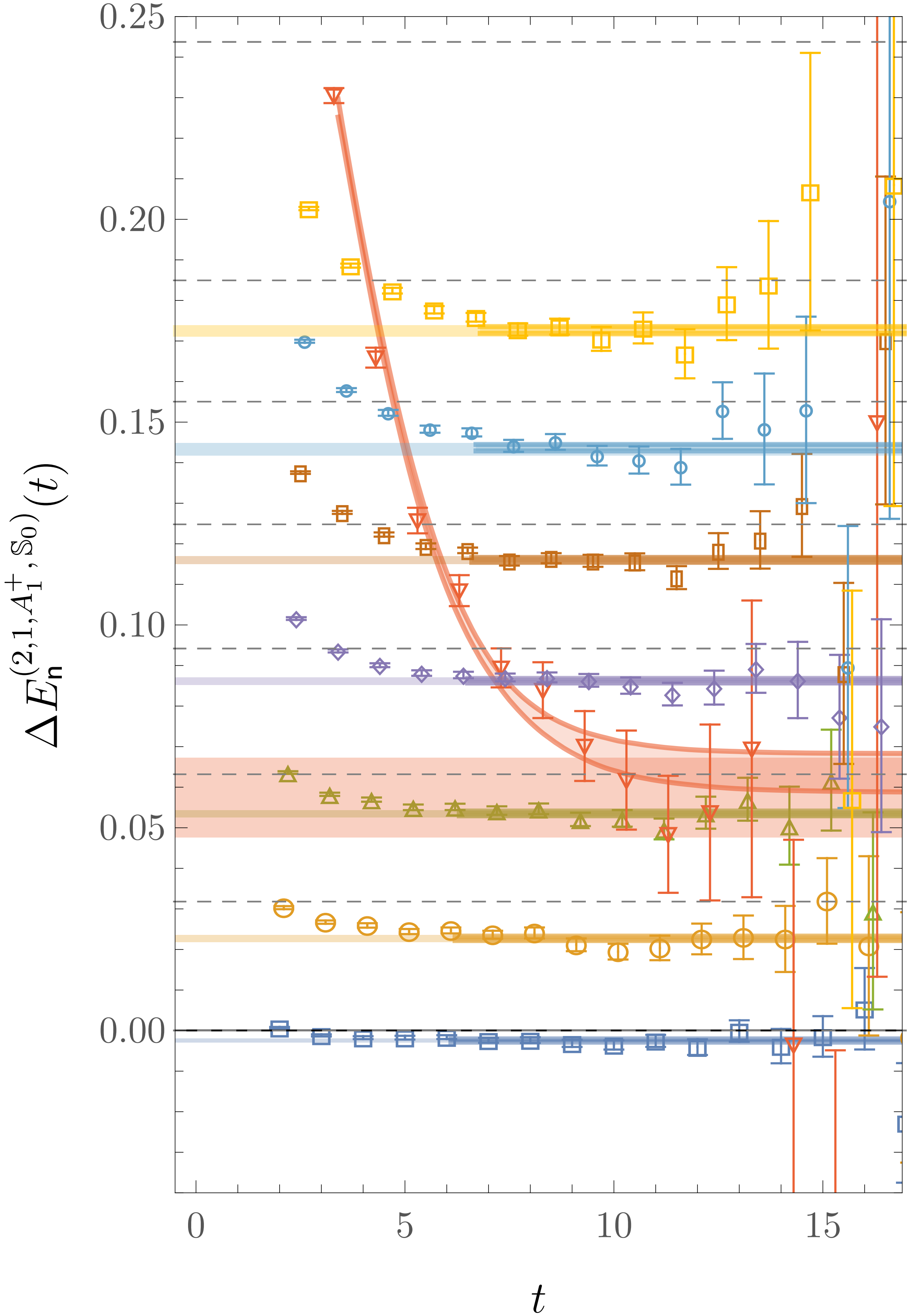
Quasi-local:



Two exponentially localized baryons

Operators constructed from products of baryon-blocks to enable efficient contractions

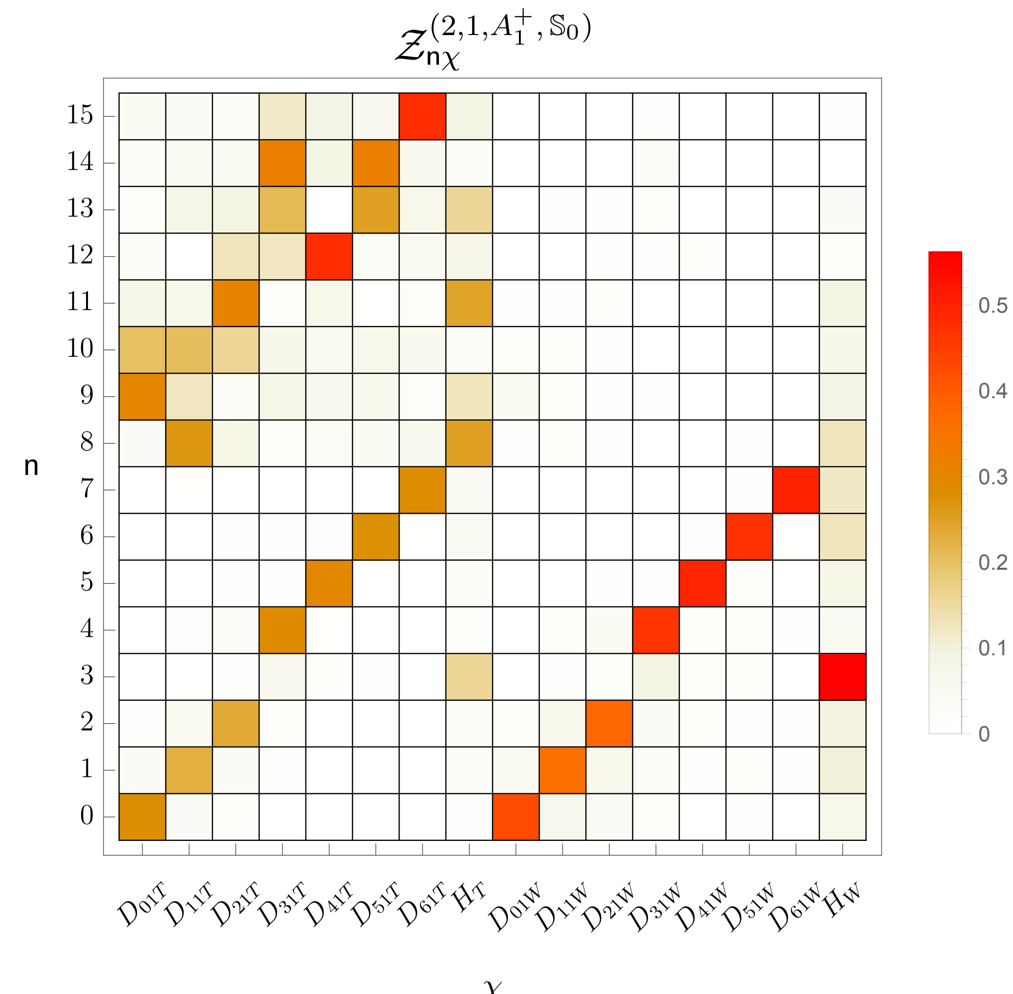
Two neutrons in a box



Variational analysis only possible for subsets of operators at current statistics, e.g. all dibaryons + hexaquark

- Consistent results obtained by replacing zero-momentum dibaryon operator with quasi-local operators

Low-energy states have majority overlap with 1 operator structure



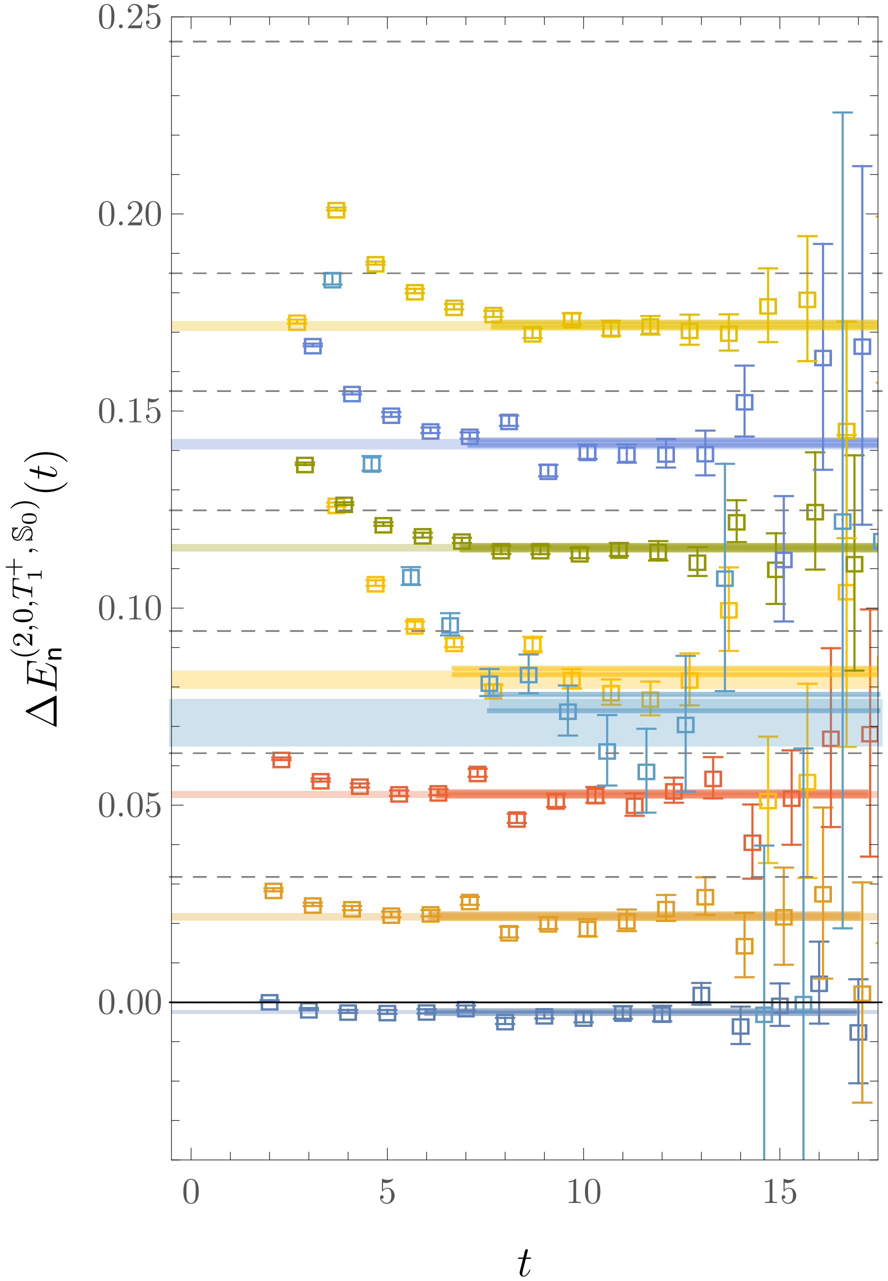
Amarasinghe, MW et al [NPLQCD], arXiv:2108.10835

The deuteron channel

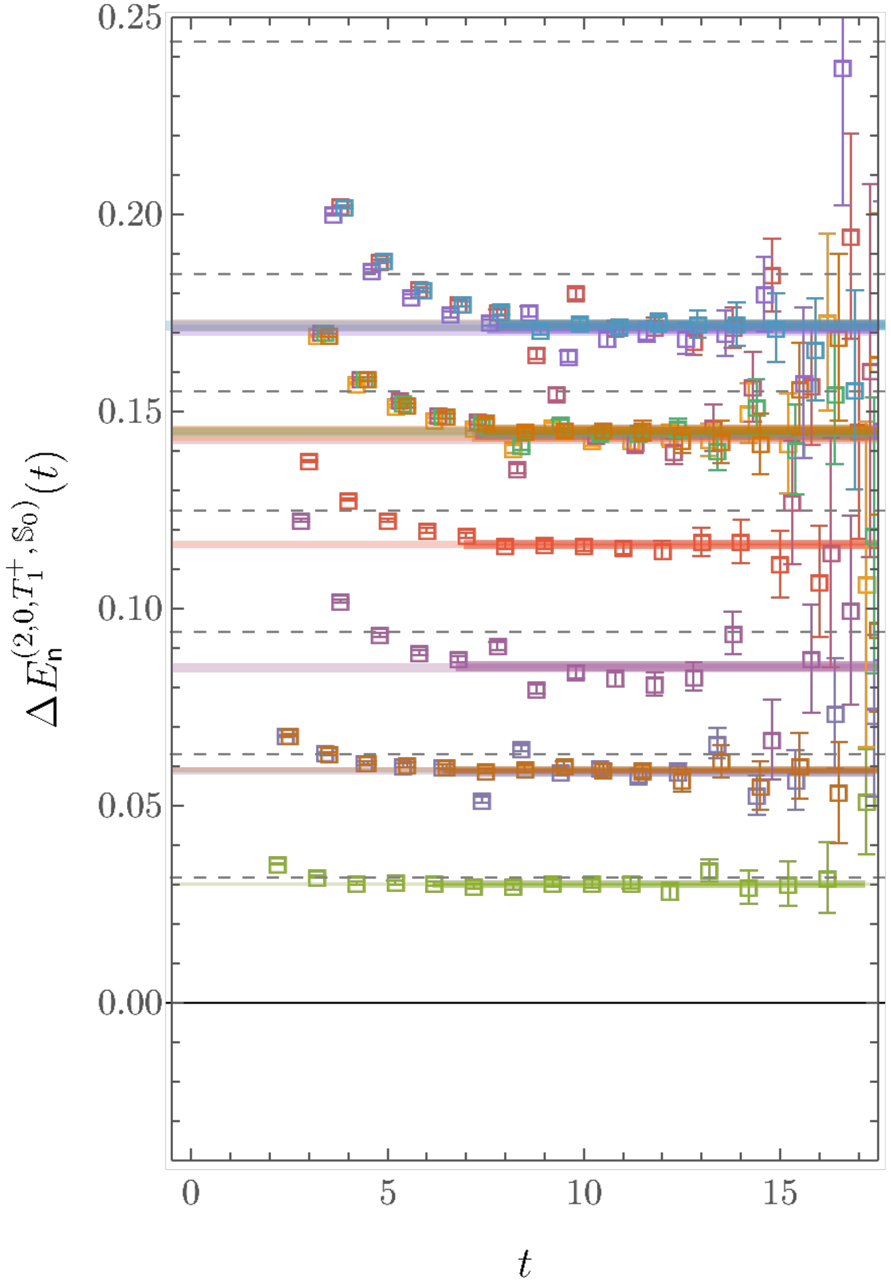
Spin-orbit coupling complicates the deuteron channel

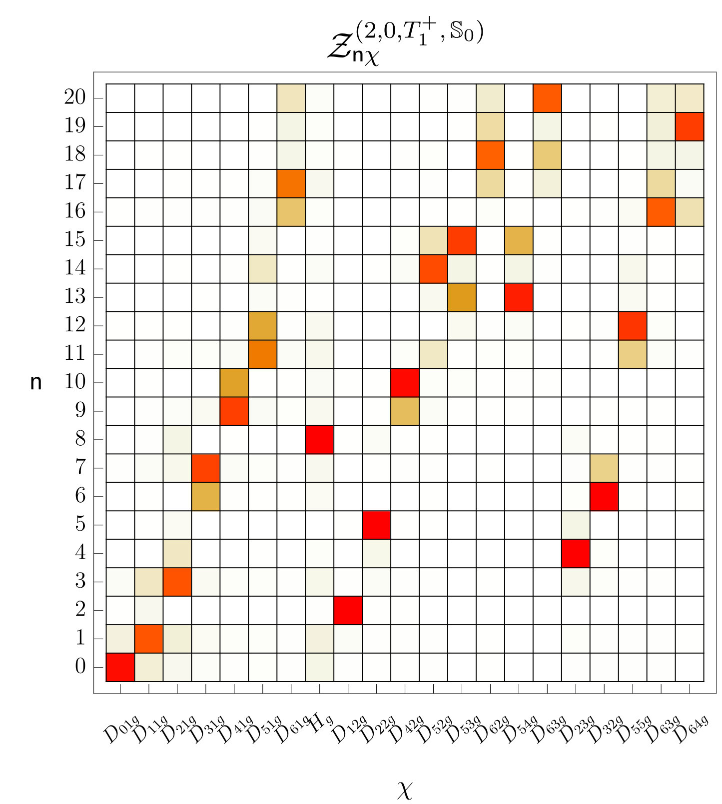
Finite-volume analogs of *S*-wave and *D*-wave operators included to provide a complete set of dibaryon operators with relative momentum $< 8(2\pi/L)$

Dominantly *S*-wave



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

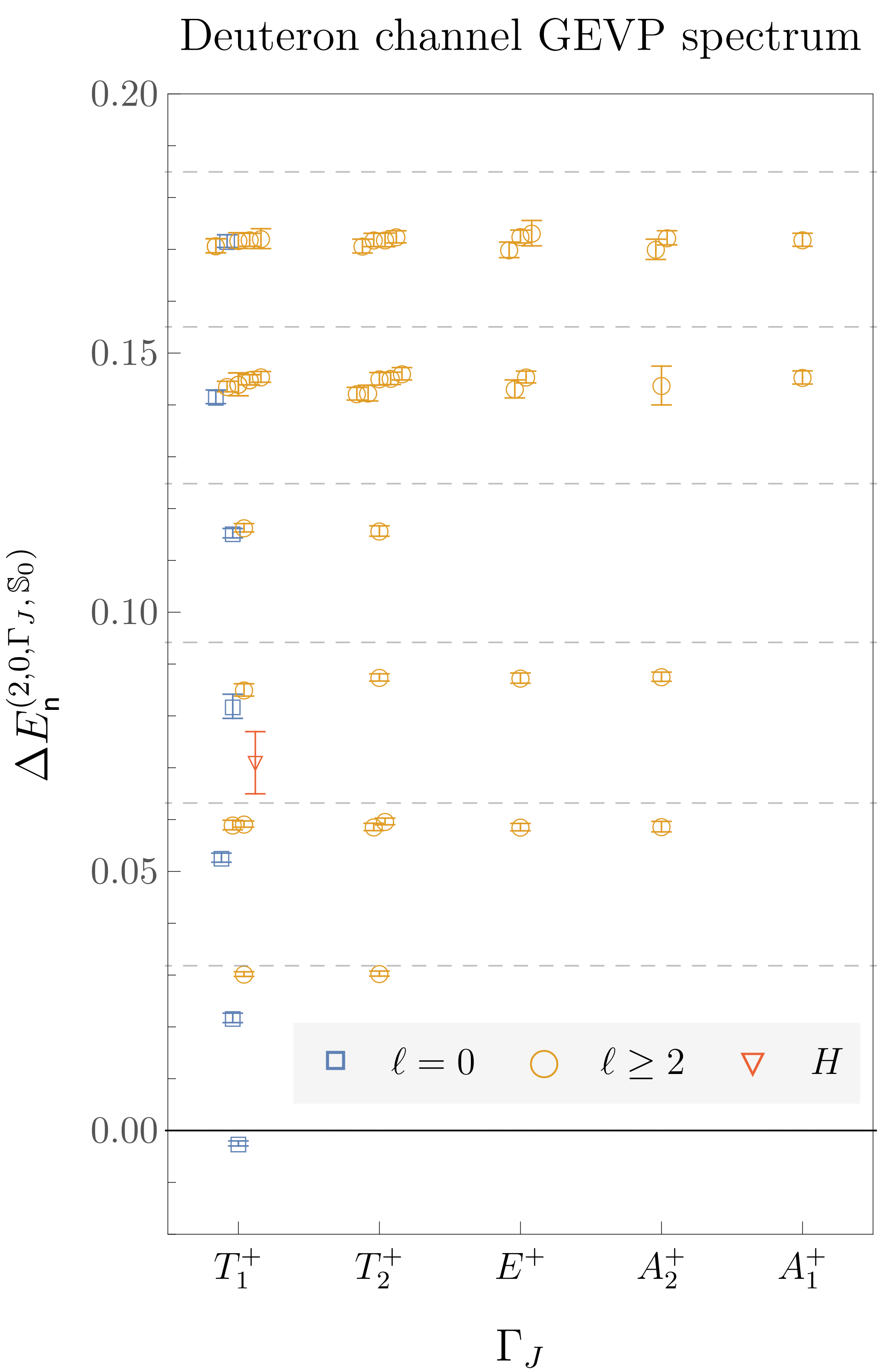




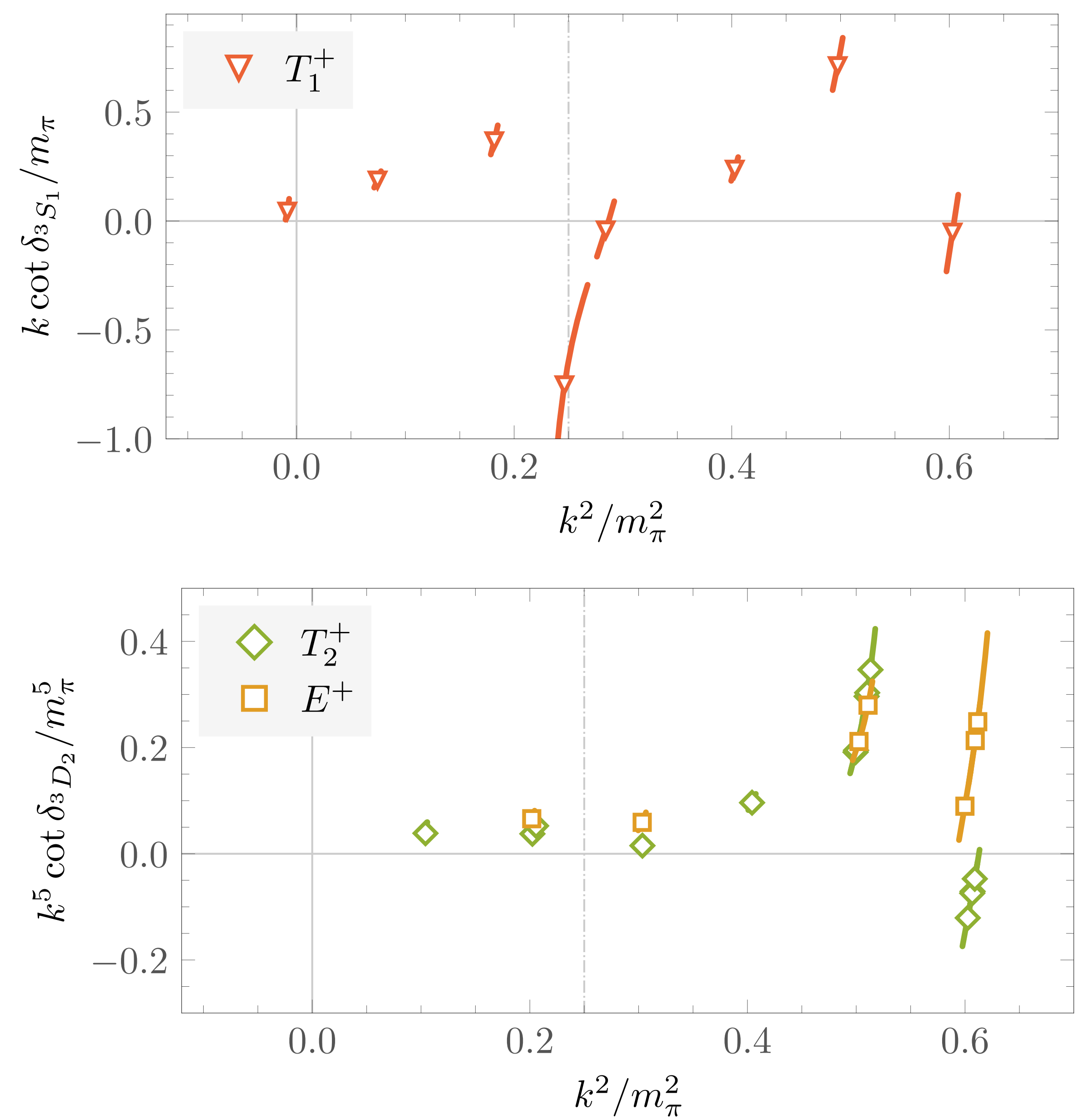
Low-energy states again have majority overlap with 1 operator structure

NN phase shifts

Generalizations of Lüscher's quantization condition map
NN finite-volume energy spectrum to phase shifts

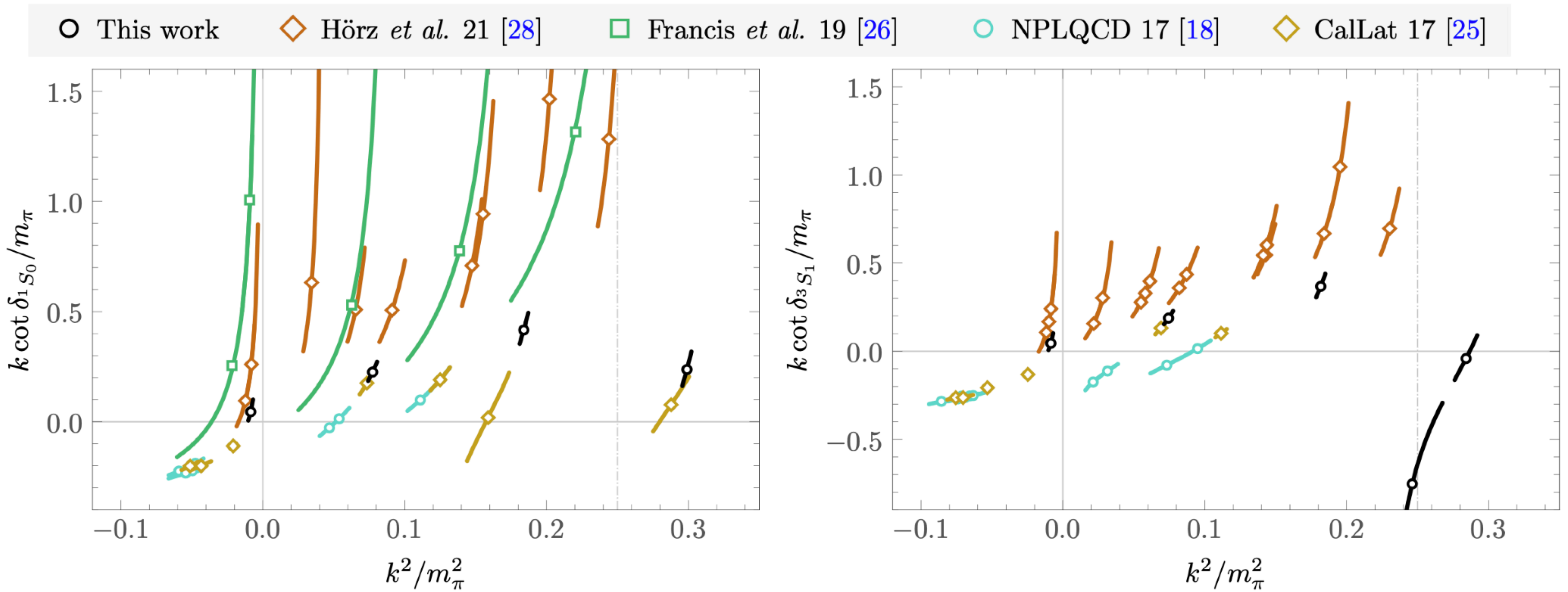


Luu and Savage, PRD 83 (2011)   Briceño, Davoudi, Luu, PRD 88 (2013)



* partial-wave mixing neglected for now

NN phase shift comparison

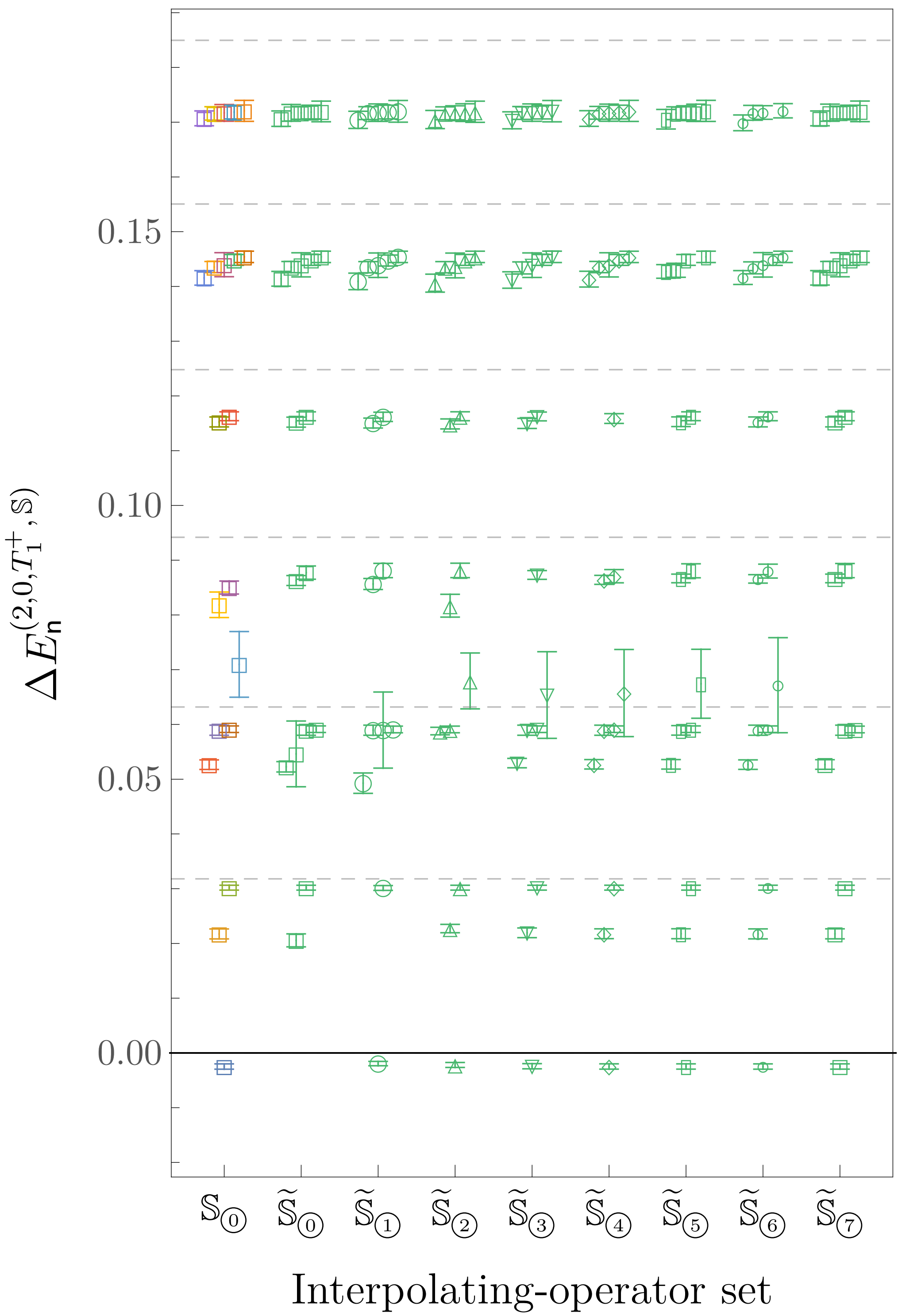


Results for two-nucleon systems with unphysically large quark masses show:

- Consistency among studies with similar interpolating operators
- Discrepancies between asymmetric correlation functions (local hexaquark source, plane-wave dibaryon sink) vs recent variational studies

Interpolating operator dependence

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



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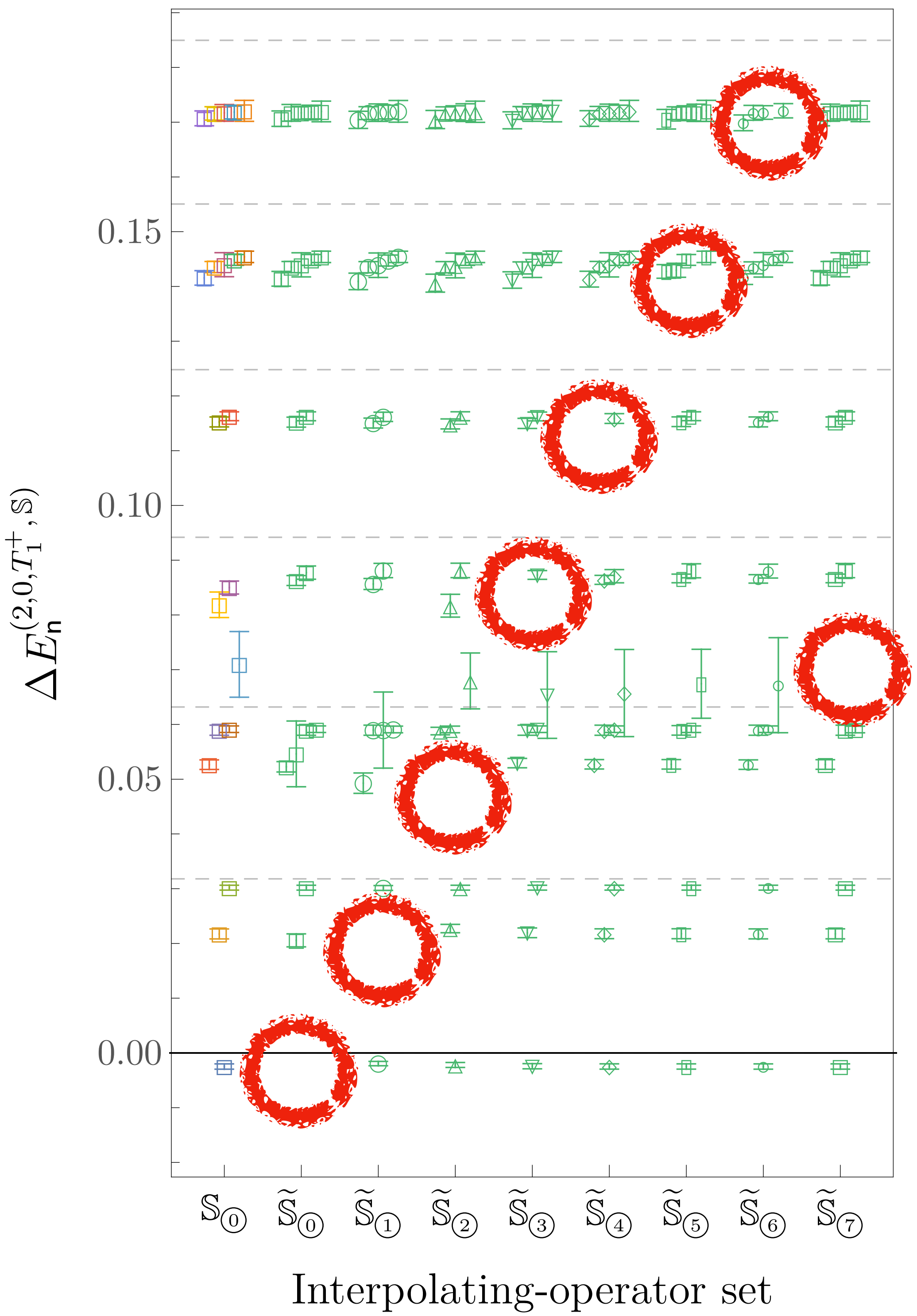
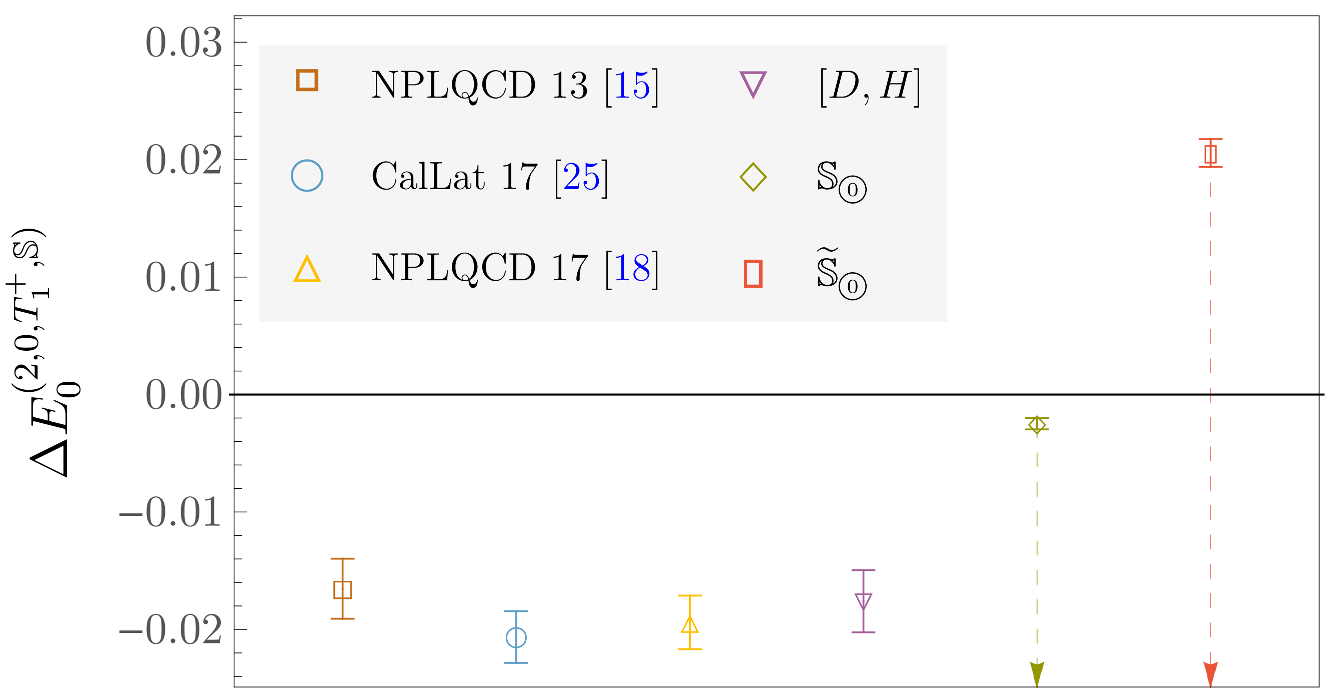


✔ **Variational upper bounds** obtained using different interpolating operator sets are consistent



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

Take-home message

If $t \lesssim 1/(E_1 - E_0)$

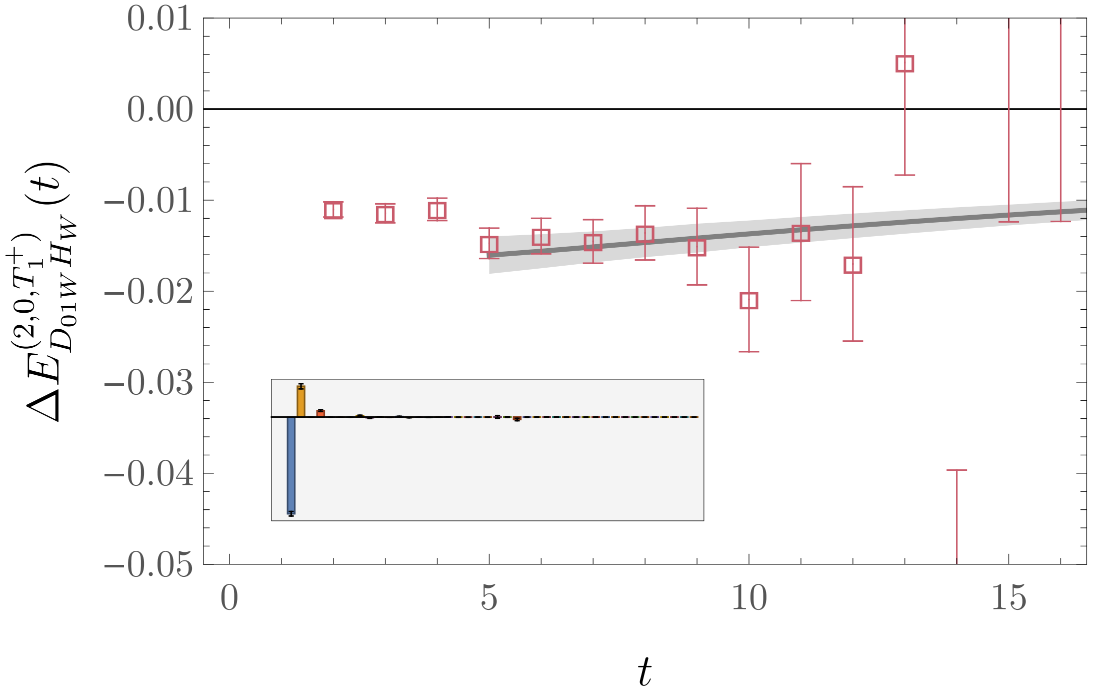
- LQCD can provide rigorous upper bounds on energies using variational methods

- Reliable energy estimates require operators with negligible overlaps to excited states below $1/t$

…but it’s hard to know if this has been accomplished

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 to -0.0025(5) for much larger

$$t \gtrsim 1/(E_1 - E_0) \approx 41$$

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 $\epsilon \ll e^{t(E_1-E_0)}$

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

Off-diagonal correlator conversely has perfect ground-state overlap

Missing bound-state operators?

Local 6-quark operators might be expected to significantly overlap with bound states

- Hilbert space is big — start with a corner we can hope to explore completely

$$H \sim T_{abcdef}(q_a^T C\Gamma_1 F_1 q_b)(q_c^T C\Gamma_1 F_2 q_d)(q_e^T C\Gamma_1 F_3 q_f)$$

A large number of color *x* spin *x* flavor tensors ($5 \times 32 \times 9 = 1440$) can be used to build hexaquark operators

e.g. 5 color tensors correspond to the 5 ways to build a singlet from 3 diquarks

$$\mathbf{1} \subset \overline{\mathbf{3}} \otimes \overline{\mathbf{3}} \otimes \overline{\mathbf{3}},$$
$$\mathbf{1} \subset \mathbf{6} \otimes \mathbf{6} \otimes \mathbf{6},$$
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Rao and Shrock, Phys. Lett. B 116 (1982)

Buchoff and MW, PRD 93 (2016)

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Quark antisymmetry greatly reduces the number of independent operators to 16 (in both isospin channels)

1	$H_{AAA,\gamma_5 P_+,\gamma_4,1,SAA}$	2	$H_{AAA,\gamma_5 P_-,\gamma_4,1,SAA}$
3	$H_{SAA,\gamma_5 P_+,\gamma_5 P_+,\gamma_5 P_+,SAA}$	4	$H_{SAA,\gamma_5 P_+,\gamma_5 P_-,\gamma_5 P_+,SAA}$
5	$H_{SAA,\gamma_5 P_+,\gamma_5 P_-,\gamma_5 P_-,SAA}$	6	$H_{SAA,\gamma_5 P_+,1,1,SAA}$
7	$H_{SAA,\gamma_5 P_+,\gamma_4,\gamma_4,SSS^{(1)}}$	8	$H_{SAA,\gamma_5 P_+,\gamma_4,\gamma_4,SSS^{(2)}}$
9	$H_{SAA,\gamma_5 P_-,\gamma_5 P_+,\gamma_5 P_+,SAA}$	10	$H_{SAA,\gamma_5 P_-,\gamma_5 P_-,\gamma_5 P_+,SAA}$
11	$H_{SAA,\gamma_5 P_-,\gamma_5 P_-,\gamma_5 P_-,SAA}$	12	$H_{SAA,\gamma_5 P_-,1,1,SAA}$
13	$H_{SAA,\gamma_5 P_-,\gamma_4,\gamma_4,SSS^{(1)}}$	14	$H_{SAA,\gamma_5 P_-,\gamma_4,\gamma_4,SSS^{(2)}}$
15	$H_{SSS,\gamma_5 P_+,\gamma_5 P_-,\gamma_5 P_+,SSS^{(1)}}$	16	$H_{SSS,\gamma_5 P_+,\gamma_5 P_-,\gamma_5 P_-,SSS^{(1)}}$

Rao and Shrock, Phys. Lett. B 116 (1982)

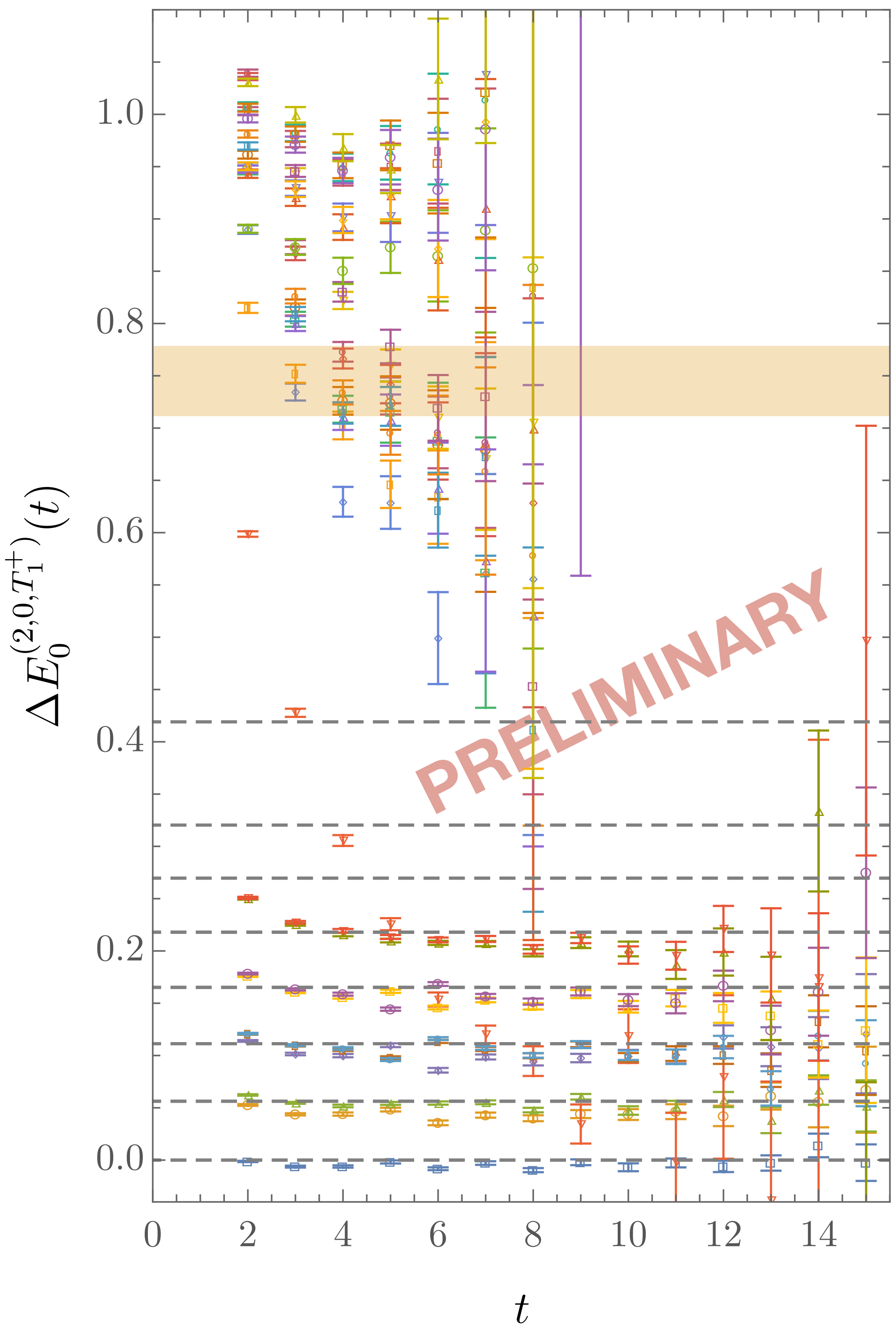
Buchoff and MW, PRD 93 (2016)

One operator (#3) is a product of color-singlet baryons, all others involve “hidden color” states not describable by color-singlet products

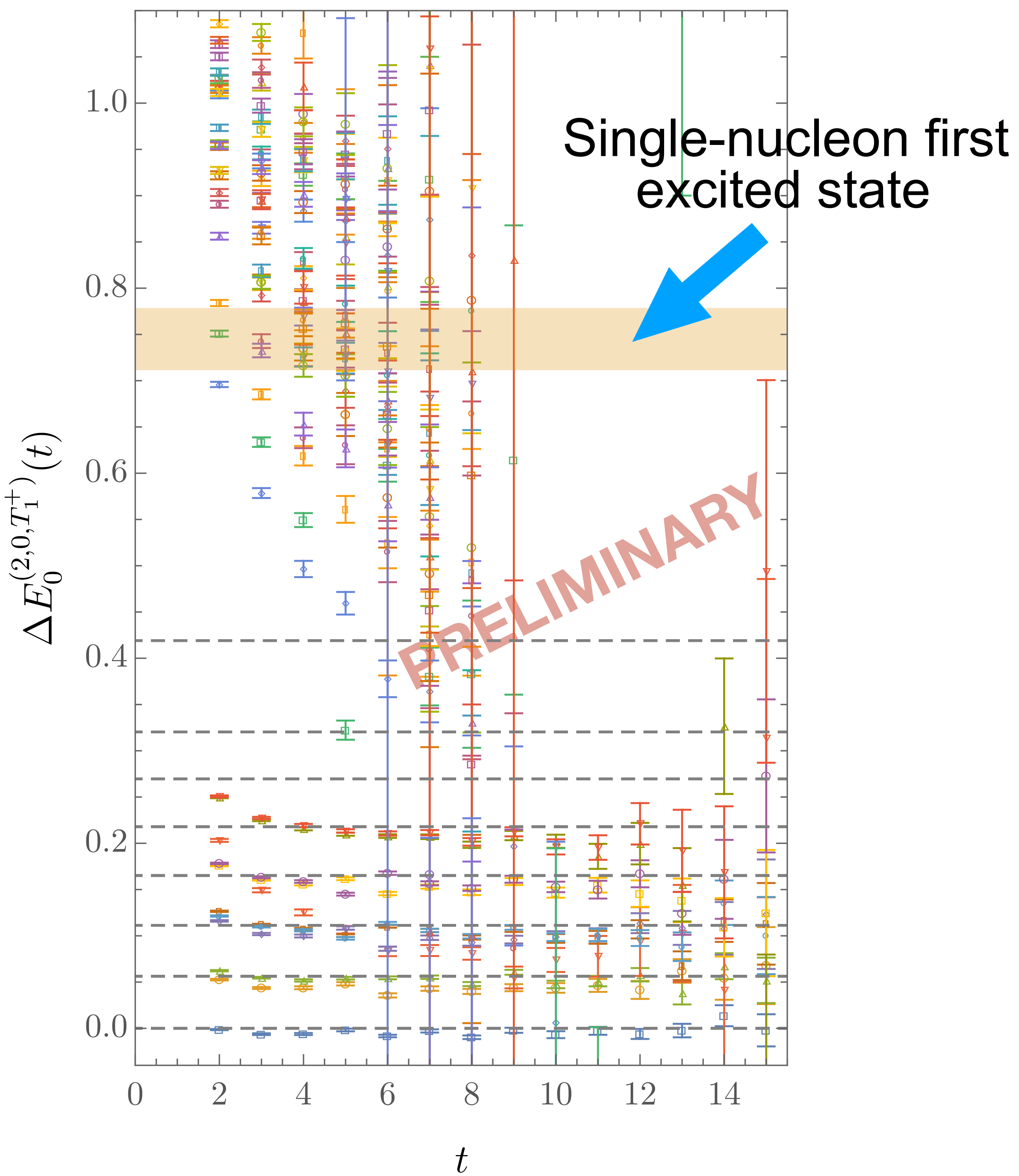
Harvey, Nucl. Phys. A 352 (1981)

Hidden-color deuteron states

Dibaryons + color-singlet-product hexaquark

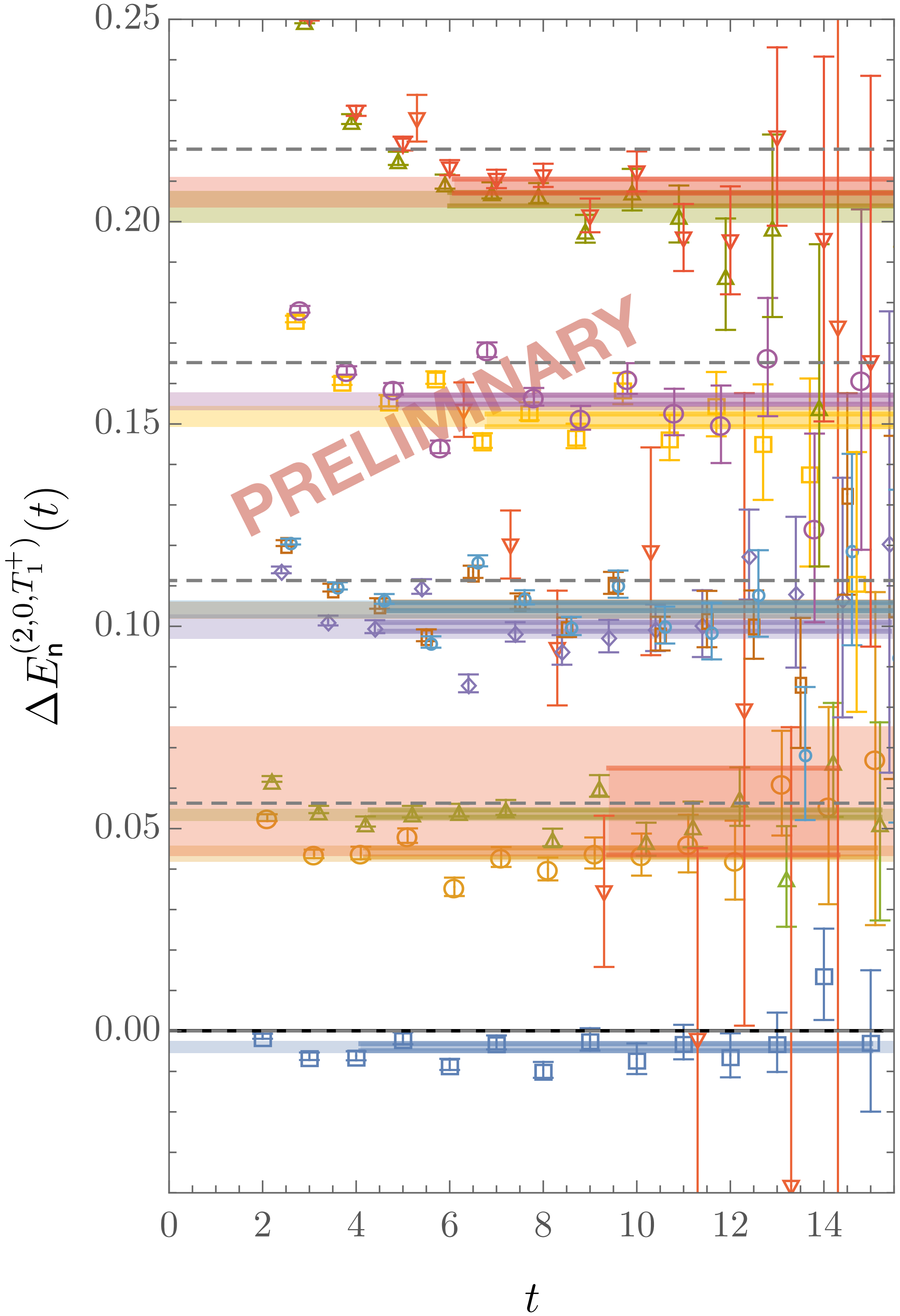


Dibaryons + complete basis of hexaquarks



Hexaquarks and the deuteron

Dibaryons + color-singlet-product hexaquark



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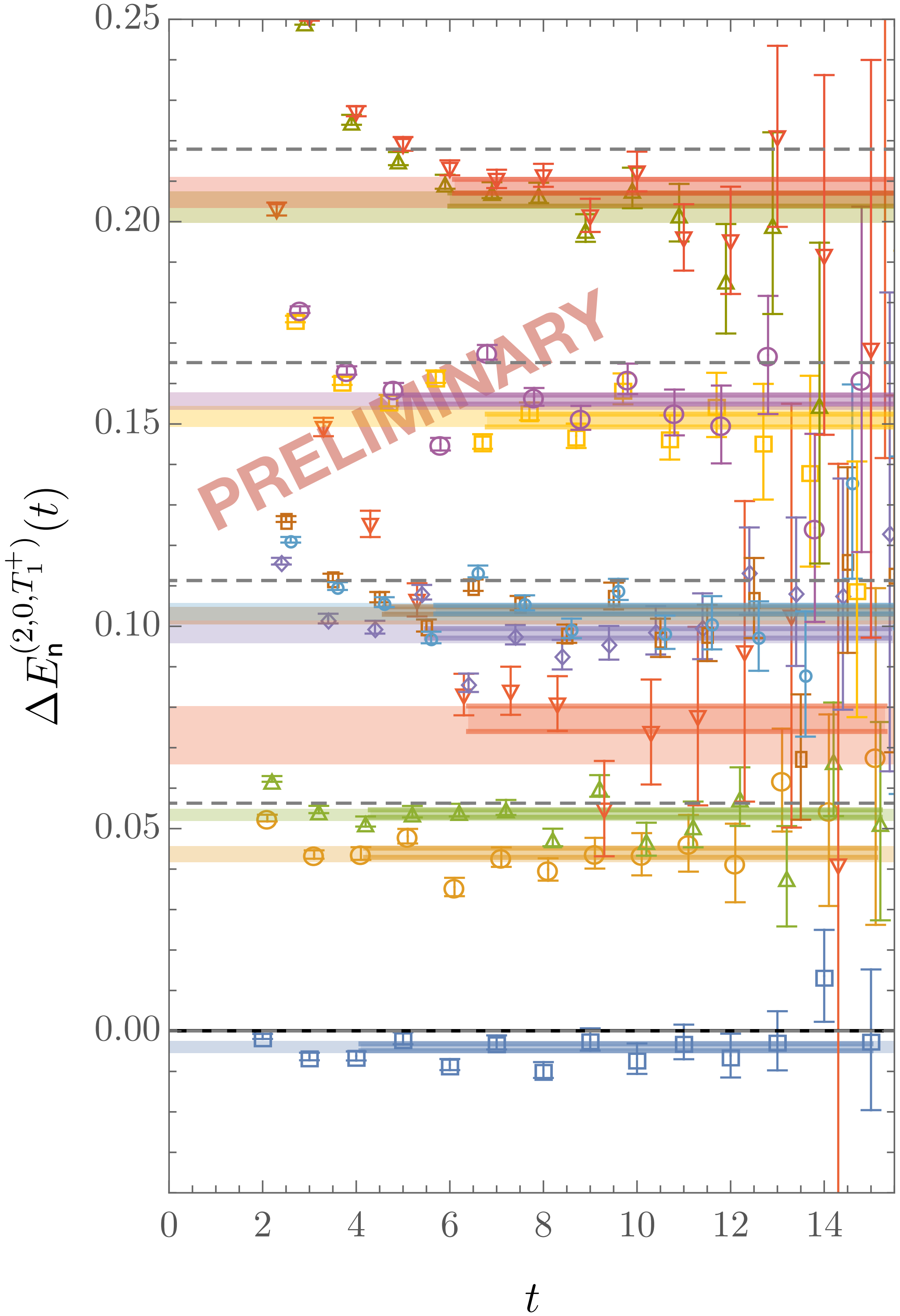
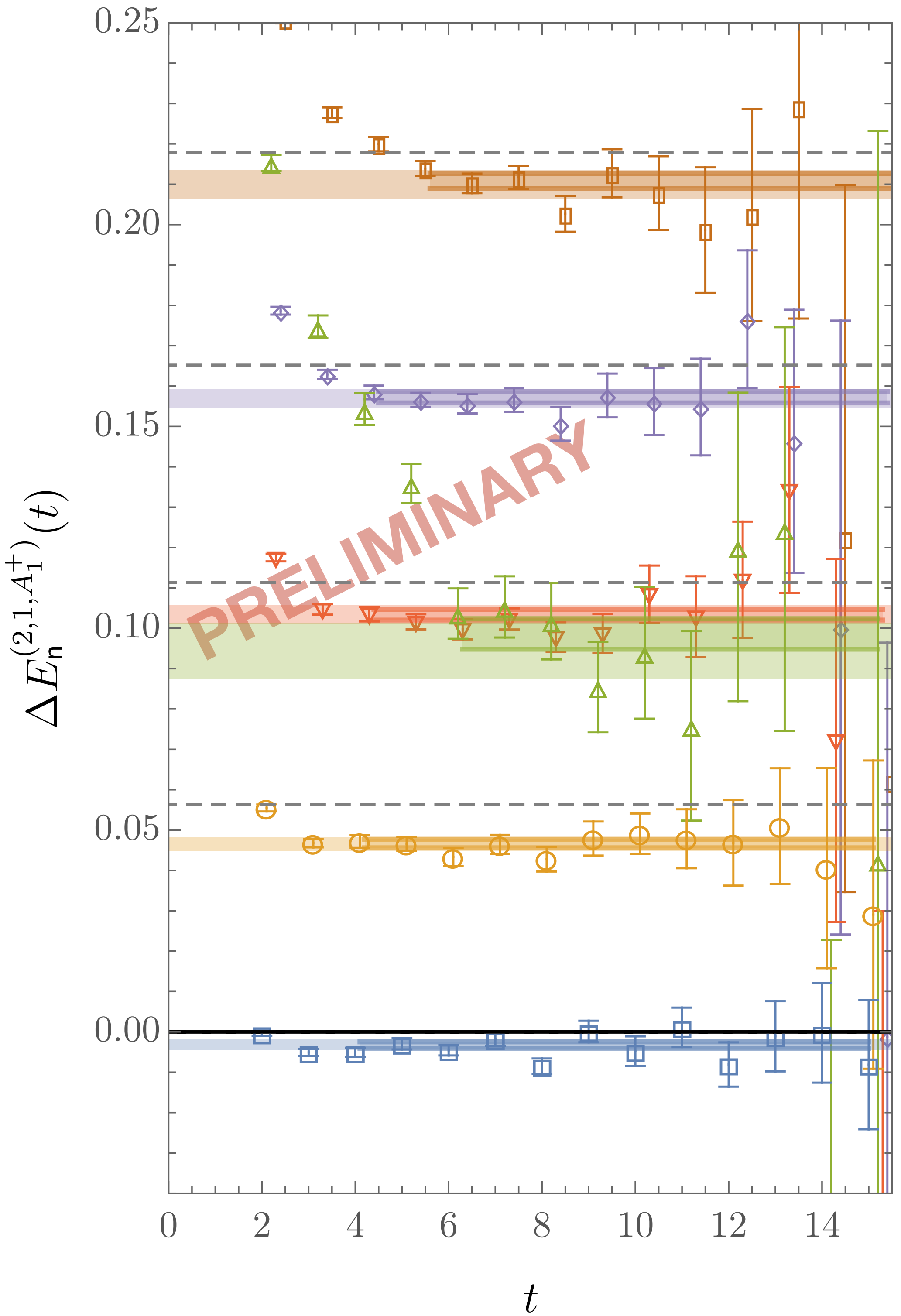
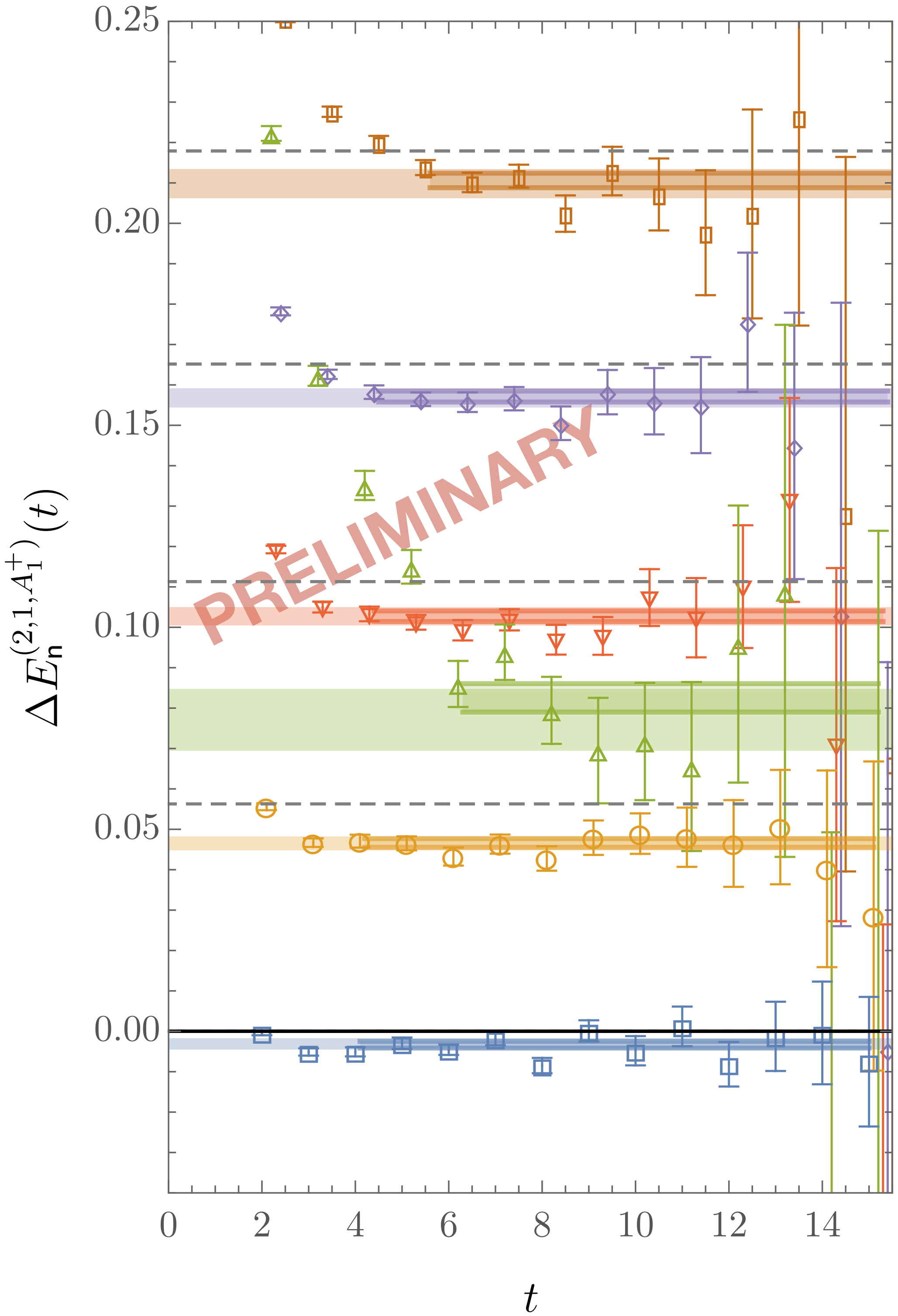


Hexaquarks and the dineutron

Dibaryons + color-singlet-product hexaquark

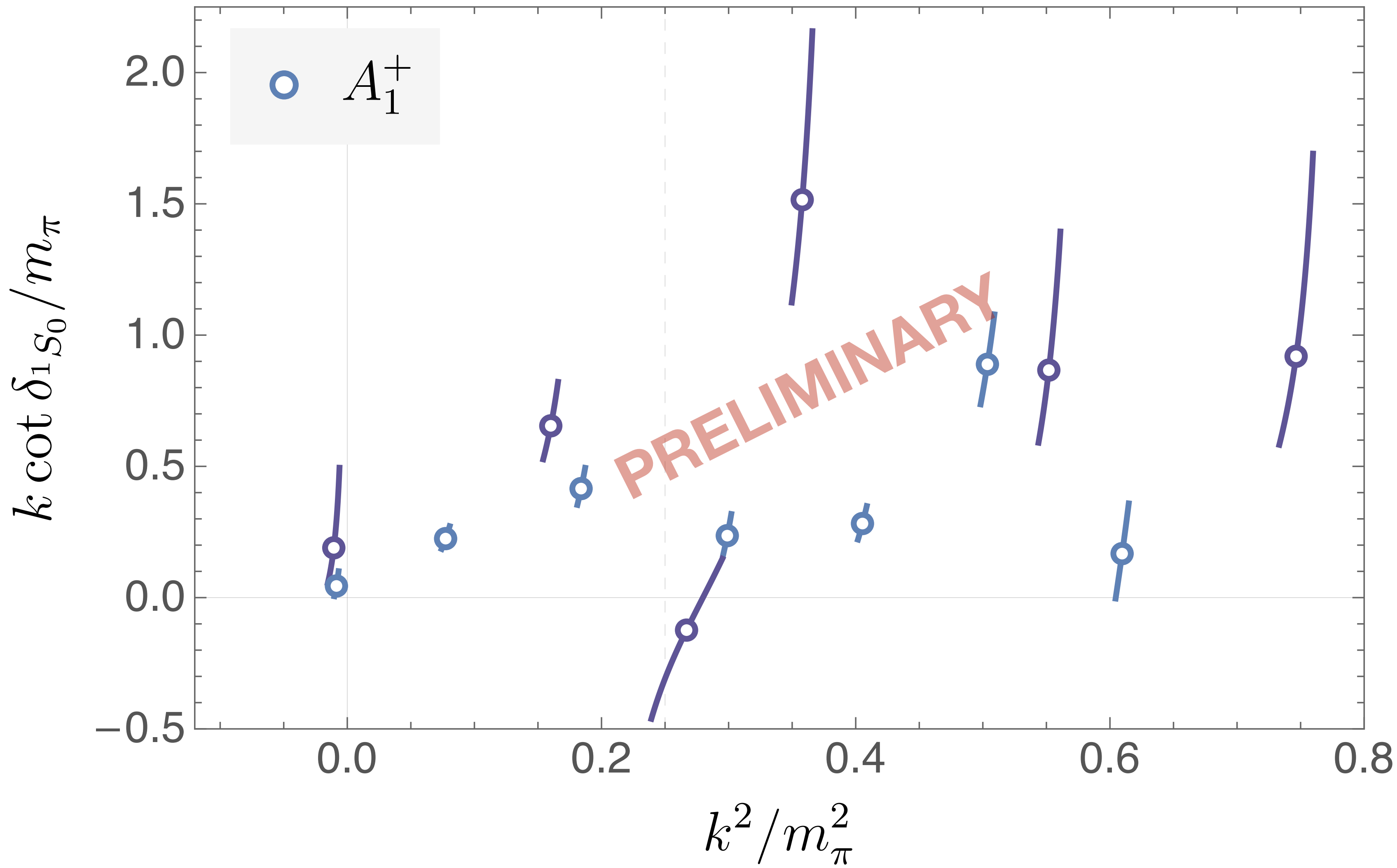


Dibaryons + complete basis of hexaquarks



Phase-shift results

Phase-shift results for $L = 32a \approx 4.6\ \mathrm{fm}$ and $L = 24a \approx 3.5\ \mathrm{fm}$ consistent, do not provide evidence for dineutron or deuteron bound states for $m_\pi \sim 800\ \mathrm{MeV}$



Suggestive of *NN* resonance near $k^2/m_\pi^2 \sim 0.3$ at this quark mass. Further analysis needed to test this and determine resonance parameters if so

Conclusions

- Variational studies have revealed significant interpolating-operator dependence in LQCD calculations of *NN* energy spectrum with unphysical quark masses
- Variational bounds don't provide conclusive evidence for (or against) bound states — including complete basis of **local** 6 quark operators, two volumes…
- Analogous studies of hyperon-nucleon and hyperon-hyperon scattering underway, stay tuned for H-dibaryon results