WILL DETMOLD

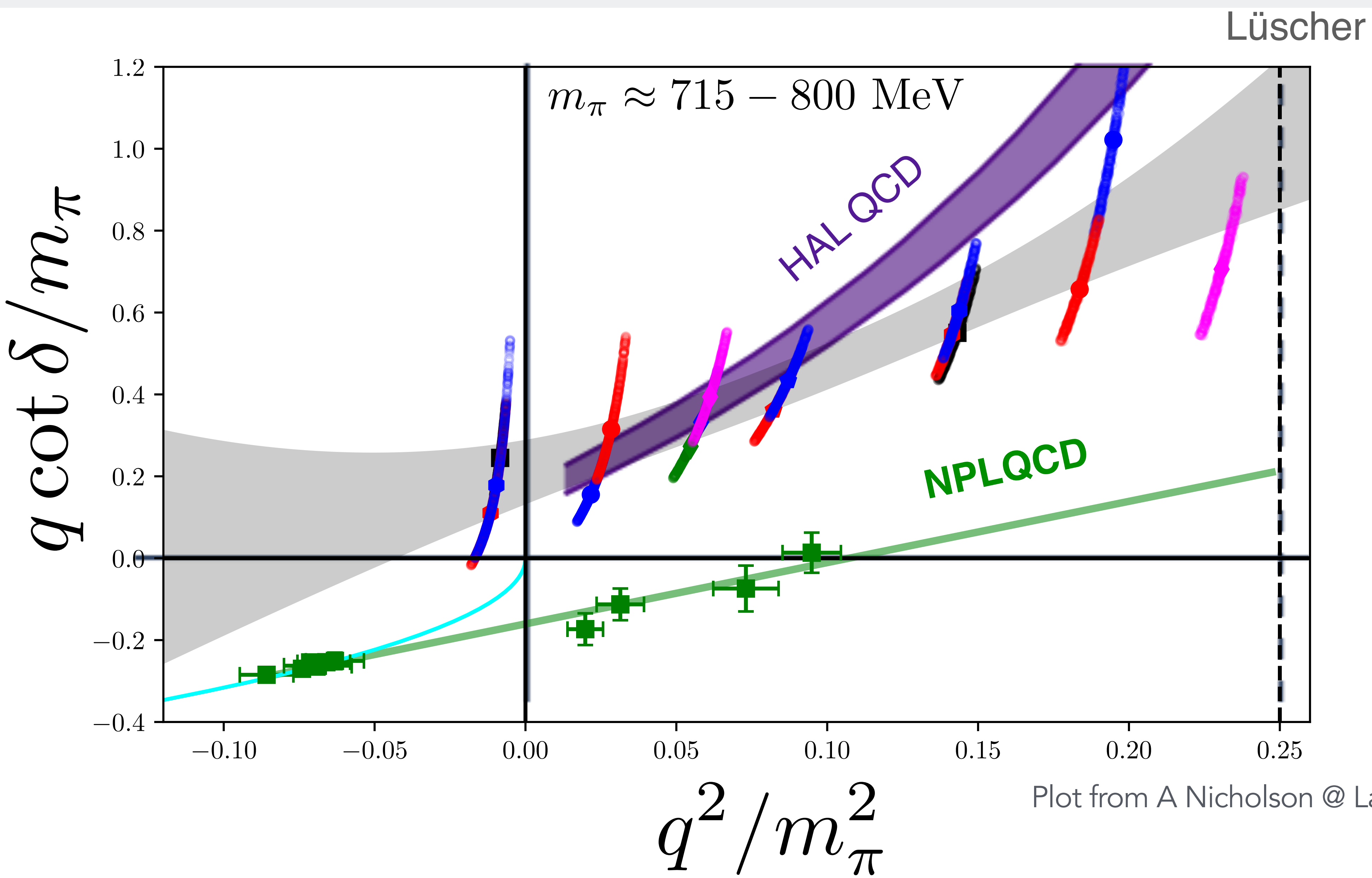
Massachusetts Institute of Technology

UNRESOLVING THE NN CONTROVERSY

Bethe Forum 2022, Bonn, Aug 18th, 2022

Resolving the NN controversy

A Nicholson, Lattice 2022: *"preponderance of evidence now shows there is no bound state at heavy pion masses"*



Plot from A Nicholson @ Lattice 2022

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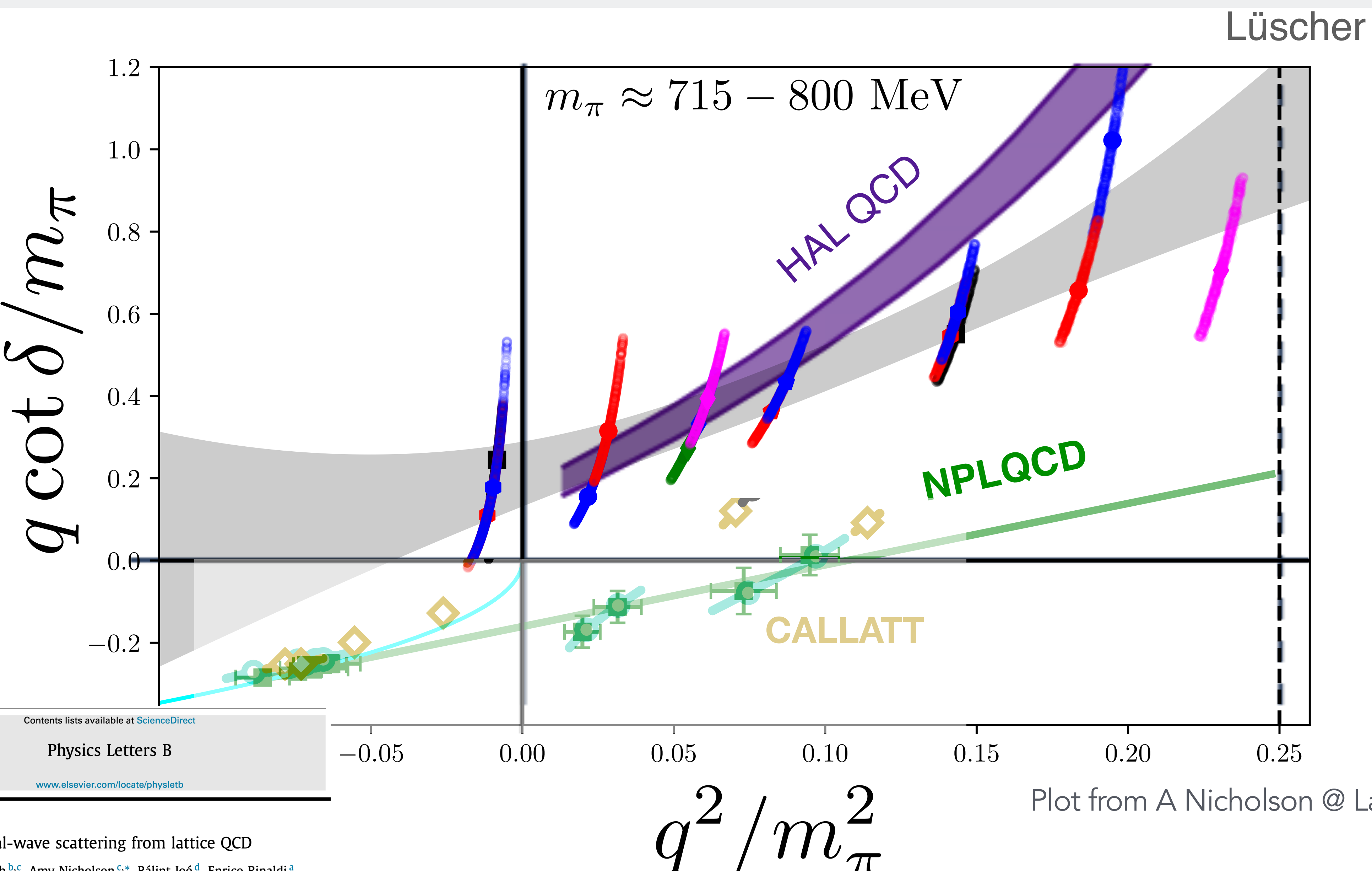

Plot from A Nicholson @ Lattice 2022

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Physics Letters B

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Two-nucleon higher partial-wave scattering from lattice QCD

Evan Berkowitz [a,*], Thorsten Kurth [b,c], Amy Nicholson [c,*], Bálint Joó [d], Enrico Rinaldi [a], Mark Strother [c], Pavlos M. Vranas [a], André Walker-Loud [b,d,e,*]

Why nuclear systems

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Lattice QCD for nuclei
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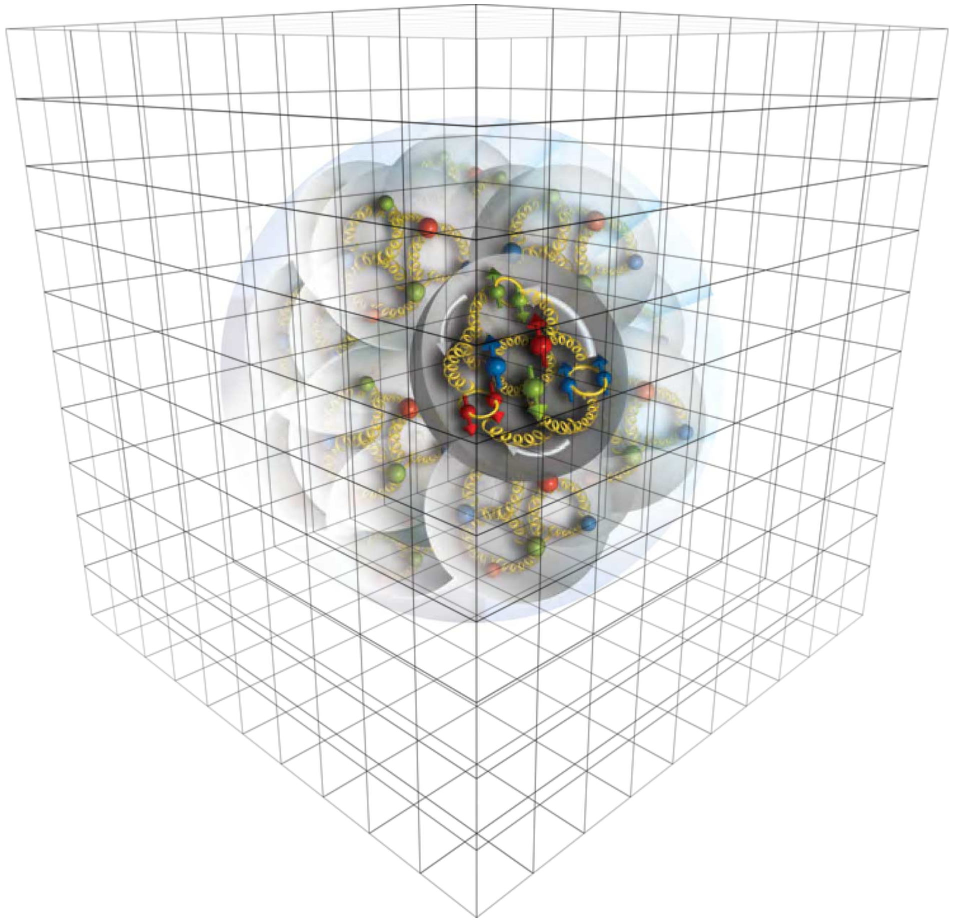
Goal: understand nuclei from first principles in the Standard Model (requires LQCD)



- Nuclei are fundamental in describing the universe around us
  - What is the structure of matter?
  - How does it depend on SM parameters
- Nuclei are important as targets for intensity frontier experiments
  - Constraining BSM physics requires nuclear inputs (some inaccessible in experiment)

Many systematics to overcome

All exisiting calculations are incomplete

Baryon-baryon (and larger A systems) are challenging

Challenges

- Reaching physical quark masses (all extrapolations are pretty coarse)
- Exponentially suppressed FV effects
- Reaching continuum limit
- Statistically noisy data (worse for baryonic systems)
- Excited state contamination

*Difficult to decouple these effects

Lattice artefacts

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Lattice artefacts are potentially important
```

- Naively lattice artefacts in NN and N correlators are correlated
  - Expect artefacts: $\Delta E = \Delta E_0(1 + (a\Lambda)\delta E_1 + \ldots)$ with $\delta E_1 \ll 1$
  - But maybe they aren't?
- Green et al.: significant lattice effects that overbind relative to continuum
  - H dibaryon, 7 ensembles with 2-3 fm volumes, 5 lattice spacings
  - Fit to ratio of variational diagonalised correlator to baryon correlator squared hence non-convex

Lattice artefacts

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Lattice artefacts are potentially important
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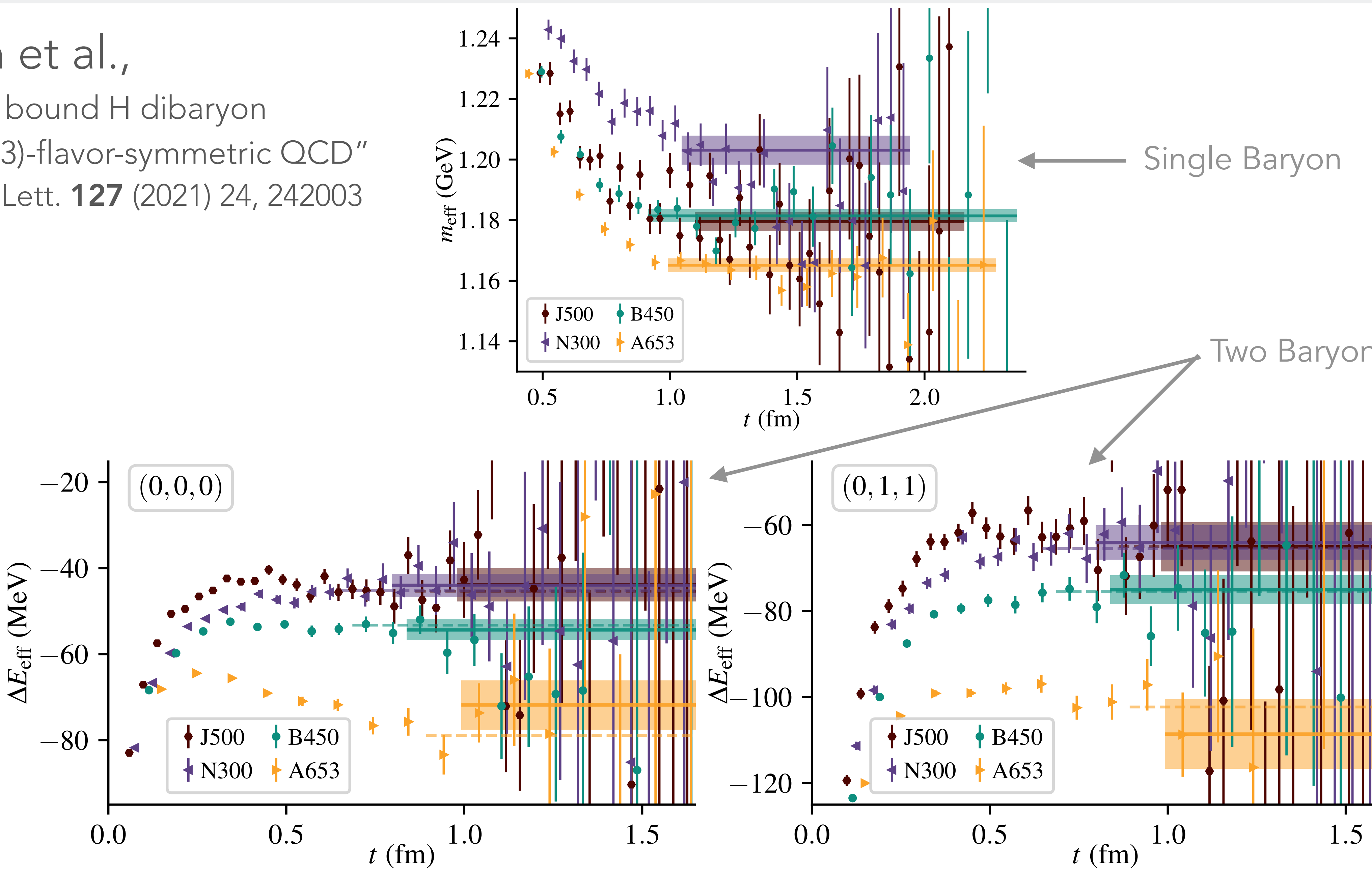
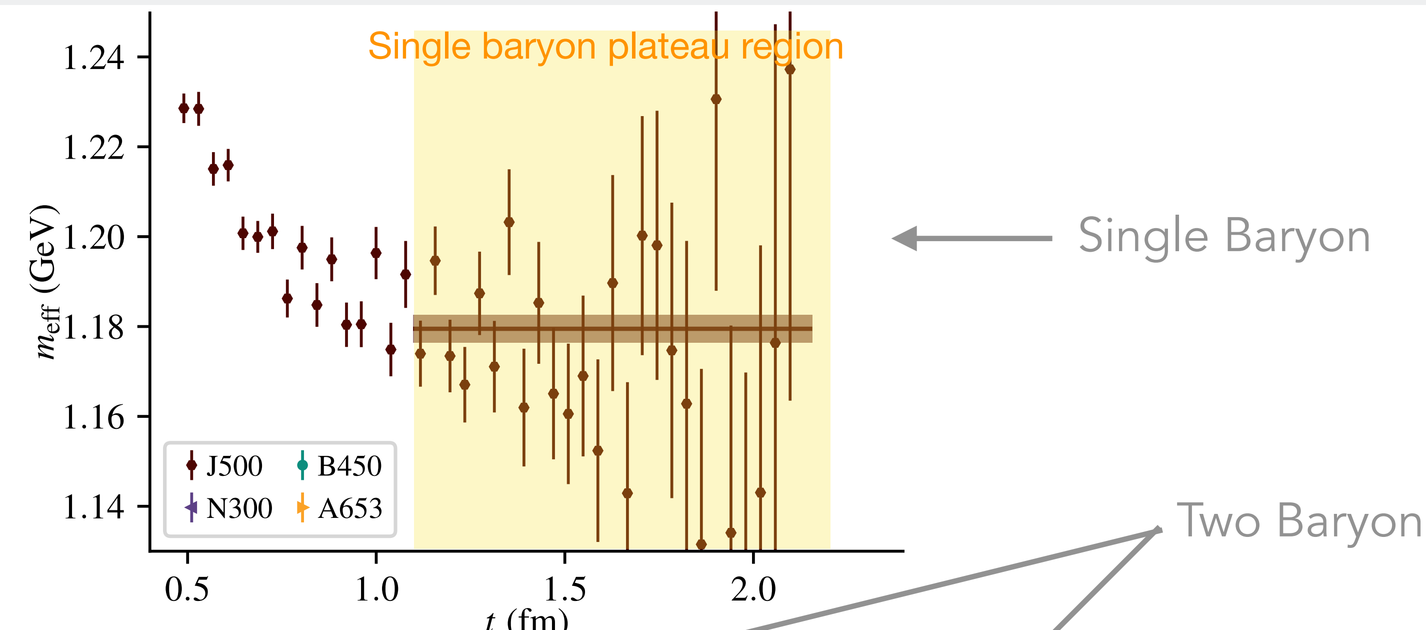
Green et al.,
"Weakly bound H dibaryon from SU(3)-flavor-symmetric QCD"
Phys.Rev.Lett. **127** (2021) 24, 242003

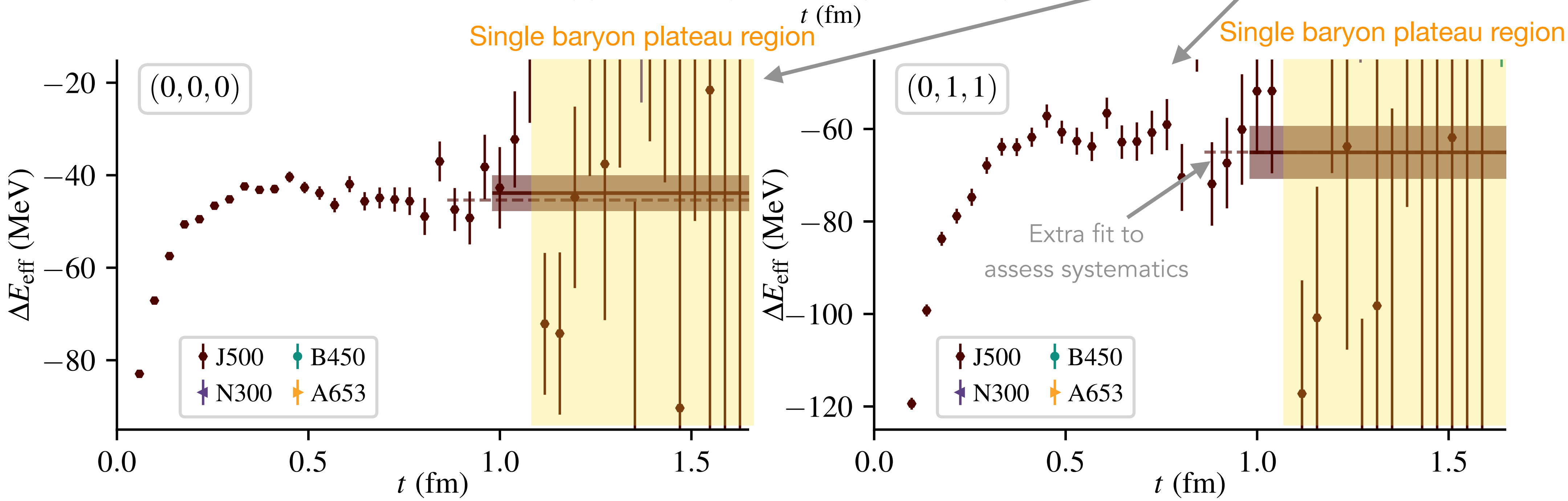


Lattice artefacts

Lattice artefacts are potentially important

J500 ensemble
(a=0.04 fm)





Lattice artefacts

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```
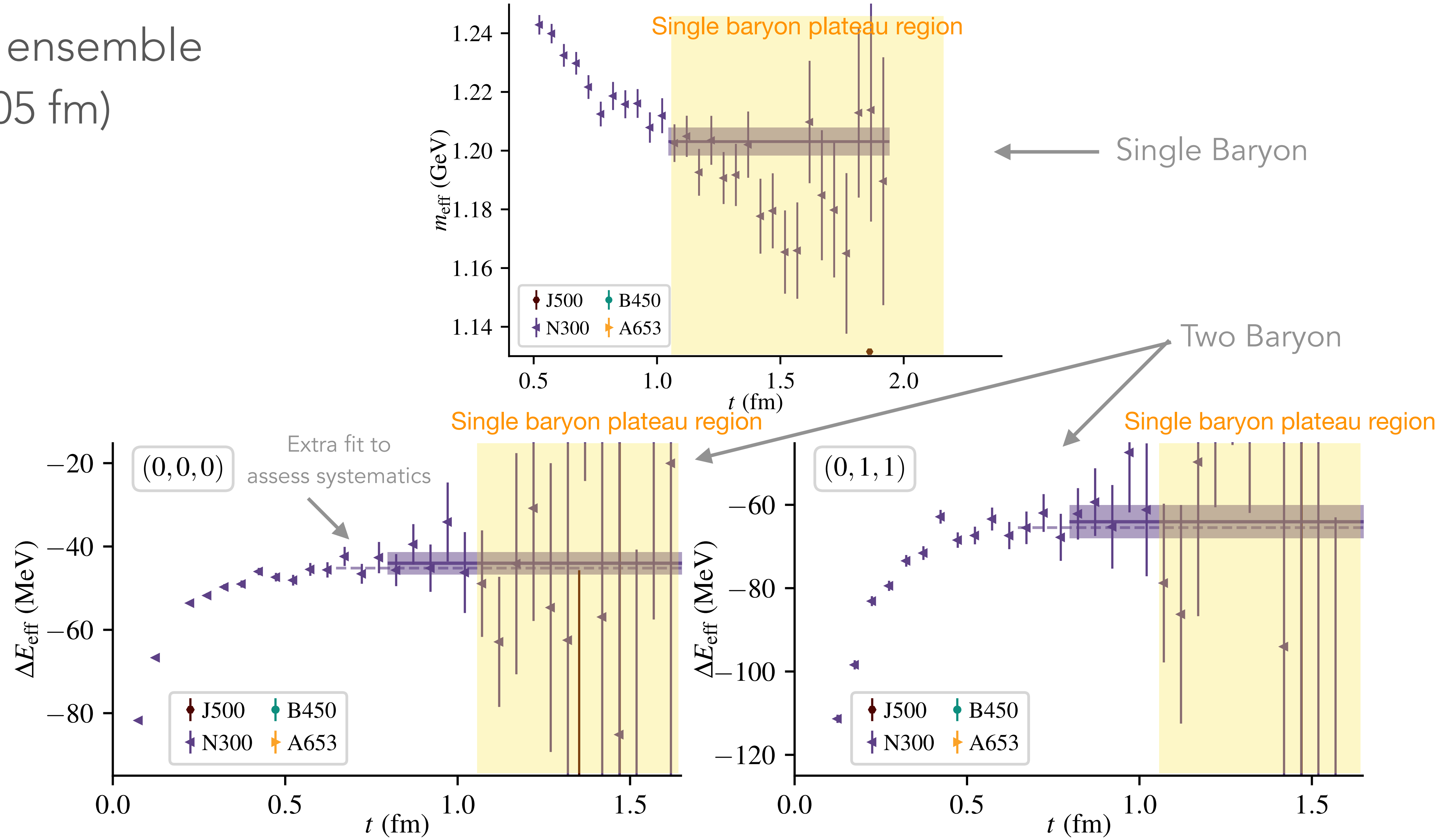

N300 ensemble
(a=0.05 fm)



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  - H dibaryon, 7 ensembles with 2-3 fm volumes, 5 lattice spacings
  - Fit to ratio of variational diagonalised correlator to baryon correlator squared hence non-convex
  - In my opinion statistical challenges cloud conclusions

Spectroscopy

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Still a challenging problem
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- Transfer matrix for given parameters has finite but very large number of discrete states in spectrum for a given set of q numbers
- Space of possible interpolating operators uncountably large but we can not use them all
- Analysis methods:
  - Variational method (GEVP)
  - Multi-state fits to Hermitian matrices of correlators
  - Multi-state fits to vector of correlators (Prony too, non-convex ☹️)
  - Ratios of correlators (non-convex ☹️, not sum of exponentials ☹️)

The variational method in LQCD

[Michael&Teasdale, NPB(1983); Lüscher&Wolff NPB(1990)]

- Derivatives of diagonalised correlators of GEVP at some ($t,t_0/t_{ref}$) are stochastic bounds on energy
  - Exact spectral bounds only in infinite statistics limit
  - Exact energies only in limit of a basis
- Sums of exponentials fitted to diagonalised GEVP correlators
  - Provide a more robust stochastic bound?
  - Fits may do strange things due to fluctuations/correlations in data
- Eventually thermal states should show up below GS

NPLQCD variational study

NPLQCD

A variational study of two-nucleon systems with lattice QCD

Saman Amarasinghe,[1] Riyadh Baghdadi,[1,2] Zohreh Davoudi,[3]
William Detmold,[4,5] Marc Illa,[6] Assumpta Parreño,[6]
Andrew V. Pochinsky,[4] Phiala E. Shanahan,[4,5] and Michael L. Wagman[7]

2108.10835v1

Largest operator set to date

- Technological improvements
  - Sparse propagators (timeslice-to-all on coarse grid)
  - `tiramisu` code generator makes contractions efficient

2108.10835v2

167→727 configs

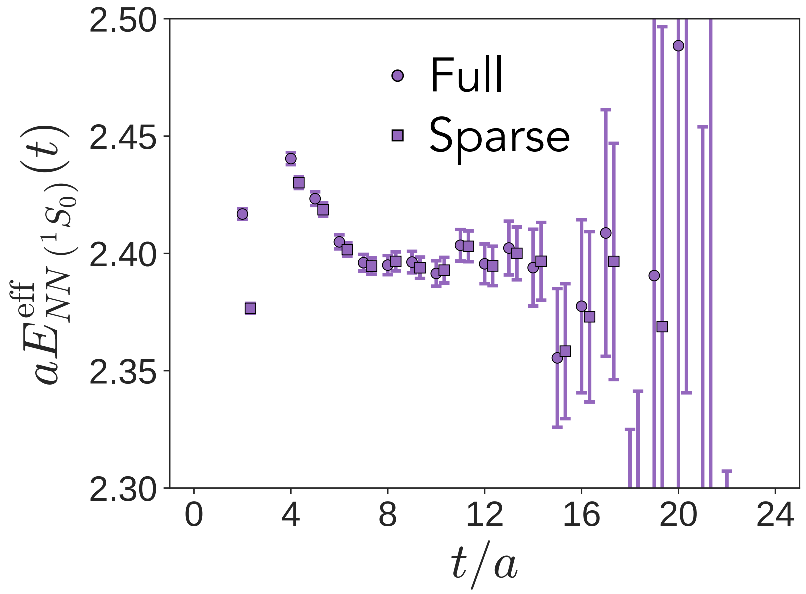
22XX.XXXX

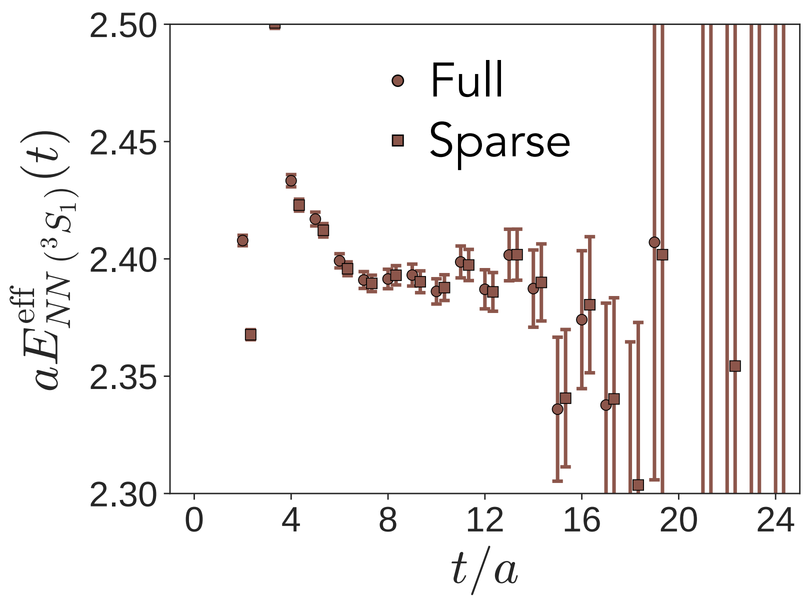
- Multi-exponential fits cf GEVP
- Additional volumes
- Enlarged operator set

Sparse propagators

[Detmold et al. Phys. Rev. D **104**, 034502 (2021)]

- Isotropic O(a) improved action: a=0.14 fm, L^3xT=32^3x48, heavy SU(3) symmetric quarks
- Sparse grid of independent sources every *S* sites in each spatial direction (2 different smearing)
- Project propagator solutions to coarse spatial grid: timeslice-to-all 8^3x48 propagator
    - Many ways to do projection (decimation, random subset choice, convolution,…)
    - No modification of eigenstates but slightly modifies couplings to excited states
- Enables O(V^4) calculations





Operator construction

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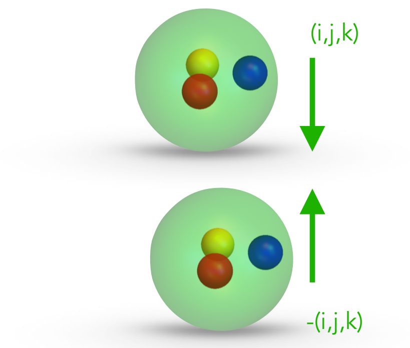
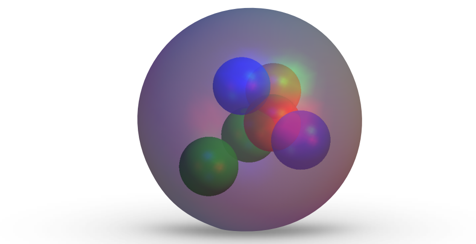
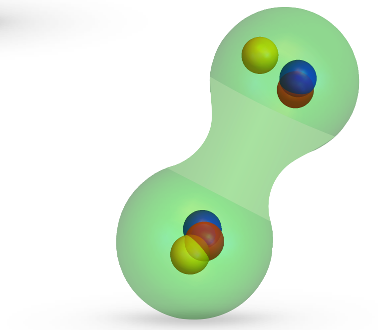
Nuclear physics is fine tuned: intuition beware!
```

Three types of operators considered

1. Dibaryons  (projected to cubic irreps)

2. Hexaquarks 

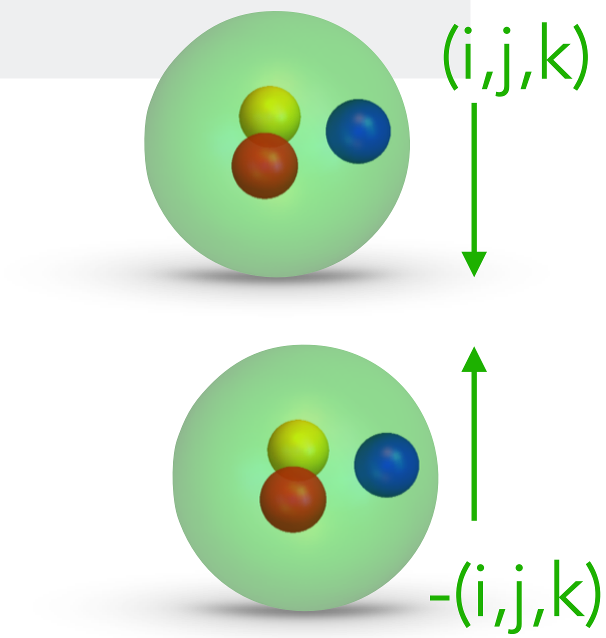
3. Quasi-local operators 

Zero total momentum, two different smearing at source and sink

Operator construction: dibaryons

```
Two momentum-projected colour-singlet baryons
```

$$D_{\rho\mathfrak{m}g}(t) = \sum_{\vec{x}_1,\vec{x}_2\in\Lambda_{\mathcal{S}}} \psi^{[D]}_{\mathfrak{m}}(\vec{x}_1,\vec{x}_2) \sum_{\sigma,\sigma'} v^{\rho}_{\sigma\sigma'} \frac{1}{\sqrt{2}} \left[p_{\sigma g}(\vec{x}_1,t)n_{\sigma' g}(\vec{x}_2,t) + (-1)^{1-\delta_{\rho 0}} n_{\sigma g}(\vec{x}_1,t)p_{\sigma' g}(\vec{x}_2,t)\right]$$



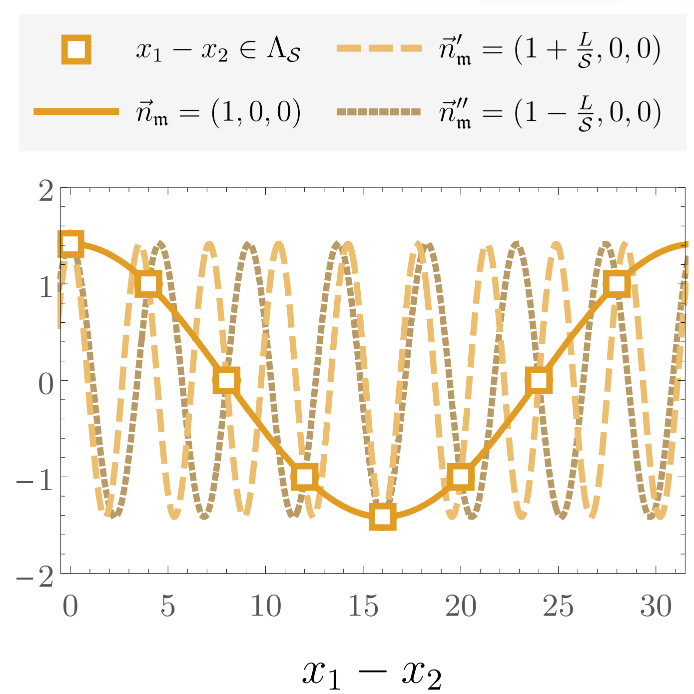
With plane-wave product wave functions

$$\psi^{[D]}_{\mathfrak{m}}(\vec{x}_1,\vec{x}_2) = e^{i\vec{k}_{\mathfrak{m}}\cdot(\vec{x}_1-\vec{x}_2)} \qquad \vec{k}_{\mathfrak{m}} = \frac{2\pi\vec{n}_{\mathfrak{m}}}{L}$$

Express nucleons in terms of quark fields

Sparse quark propagators lead to incomplete Fourier projection and mixing with higher modes

- Leading contamination from n=(8,0,0): irrelevant



Operator construction: hexaquarks

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Local product of six quarks
```
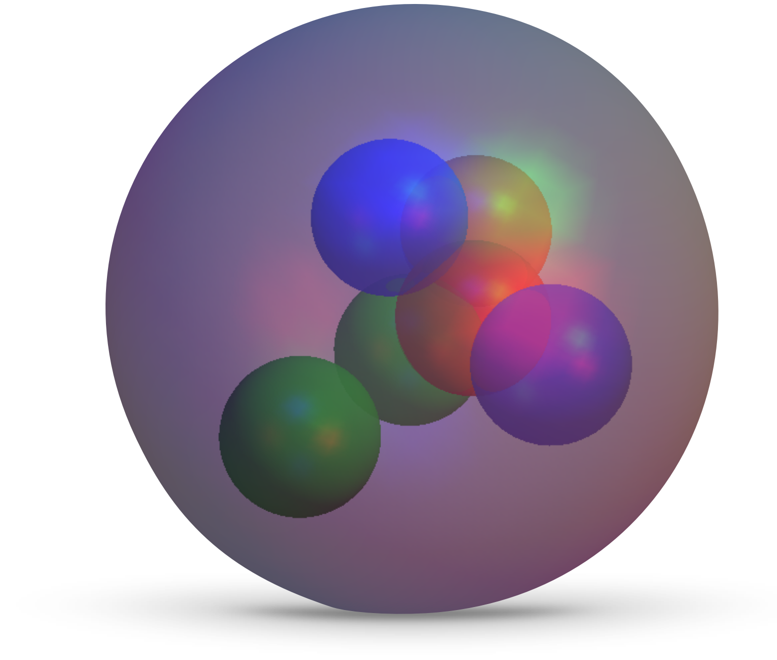

Choose product of 2 colour-singlet baryons: eg I=1, S=0 dinucleon

$$H_{0\mathfrak{c}g}(t) = \sum_{\vec{x}\in\Lambda_S} \psi_{\mathfrak{c}}^{[H]}(\vec{x}) \frac{1}{2} \left[p_{0g}(\vec{x},t) n_{1g}(\vec{x},t) - p_{1g}(\vec{x},t) n_{0g}(\vec{x},t) \right.$$
$$\left. + n_{0g}(\vec{x},t) p_{1g}(\vec{x},t) - n_{1g}(\vec{x},t) p_{0g}(\vec{x},t) \right]$$

Express nucleons in terms of quark fields:

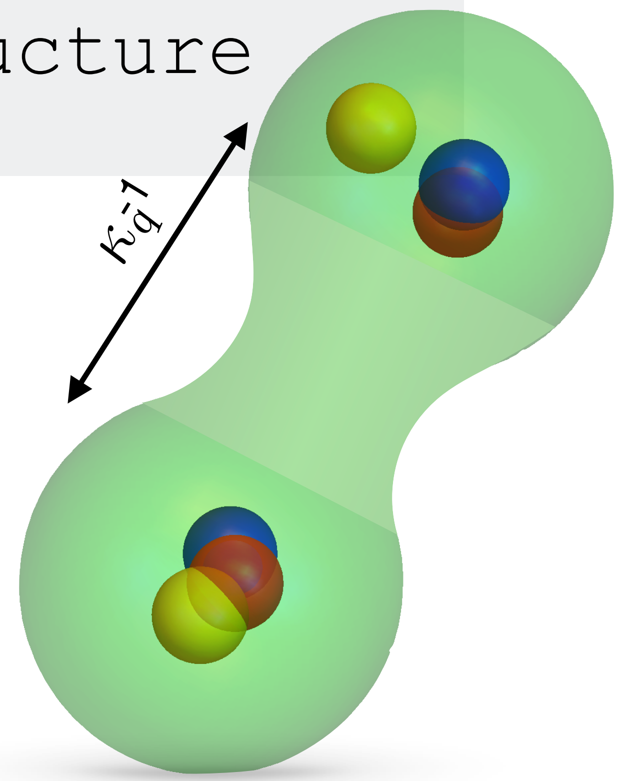


$$H_{\rho\mathfrak{c}g}(t) = \sum_{\vec{x}\in\Lambda_S} \psi_{\mathfrak{c}}^{[H]}(\vec{x}) \sum_{\alpha} w_{\alpha}^{[H]\rho} u_g^{i(\alpha)}(\vec{x},t) d_g^{j(\alpha)}(\vec{x},t) u_g^{k(\alpha)}(\vec{x},t)$$
$$\times\, d_g^{l(\alpha)}(\vec{x},t) u_g^{m(\alpha)}(\vec{x},t) d_g^{n(\alpha)}(\vec{x},t)$$

Wavefunction specified by table of weights w

Operator construction: quasi-local

NN EFT motivated deuteron-like structure



Loosely bound system: FV EFT wavefunction

$$\sum_{\vec{n}\in\mathbb{Z}_3} e^{-\kappa|\vec{x}_1-\vec{x}_2+n\vec{L}|}\left(\frac{\mathcal{A}}{|\vec{x}_1-\vec{x}_2+\vec{n}L|}+\ldots\right)$$

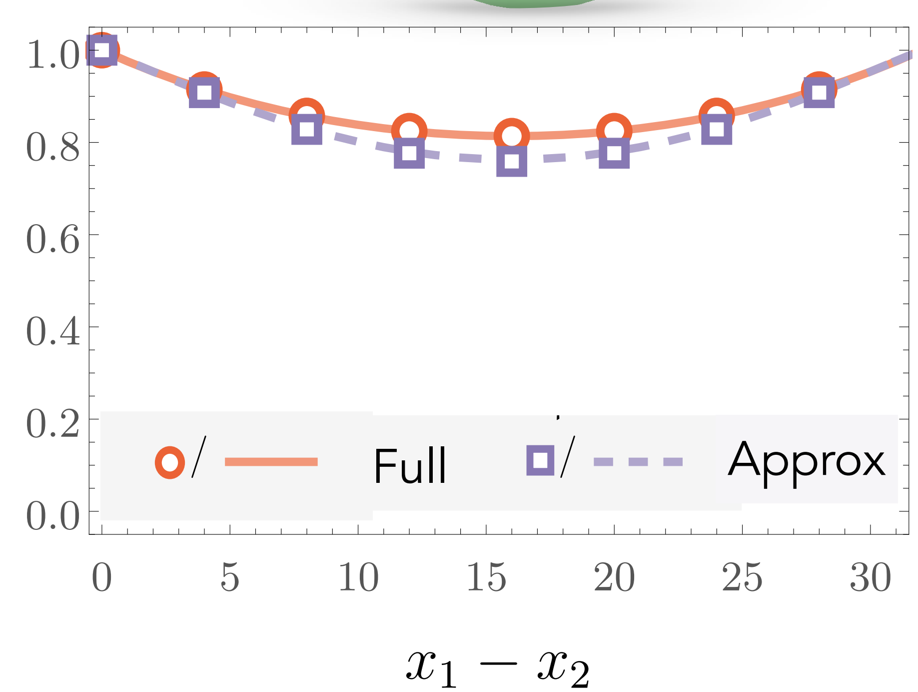
Factorisable approximation is

$$\psi_{\mathfrak{q}}^{[Q]}(\vec{x}_1,\vec{x}_2,\vec{R}) = \frac{1}{V_{\mathcal{S}}}\sum_{\tau\in\mathbb{T}_{\mathcal{S}}} e^{-\kappa_{\mathfrak{q}}|\tau(\vec{x}_1)-\vec{R}|}e^{-\kappa_{\mathfrak{q}}|\tau(\vec{x}_2)-\vec{R}|}$$

Use to build operators

$$Q_{\rho\mathfrak{q}g}(t) = \sum_{\vec{x}_1,\vec{x}_2\in\Lambda_{\mathcal{S}}} \psi_{\mathfrak{q}}^{[Q]}(\vec{x}_1,\vec{x}_2,\vec{R})\sum_{\sigma,\sigma'} v^{\rho}_{\sigma\sigma'}\frac{1}{\sqrt{2}}\left[p_{\sigma g}(\vec{x}_1,t)n_{\sigma' g}(\vec{x}_2,t) + (-1)^{1-\delta_{\rho 0}} n_{\sigma g}(\vec{x}_1,t)p_{\sigma' g}(\vec{x}_2,t)\right]$$

Use 3 different values of width κ_q



Fitting technology

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Robust fitting crucial
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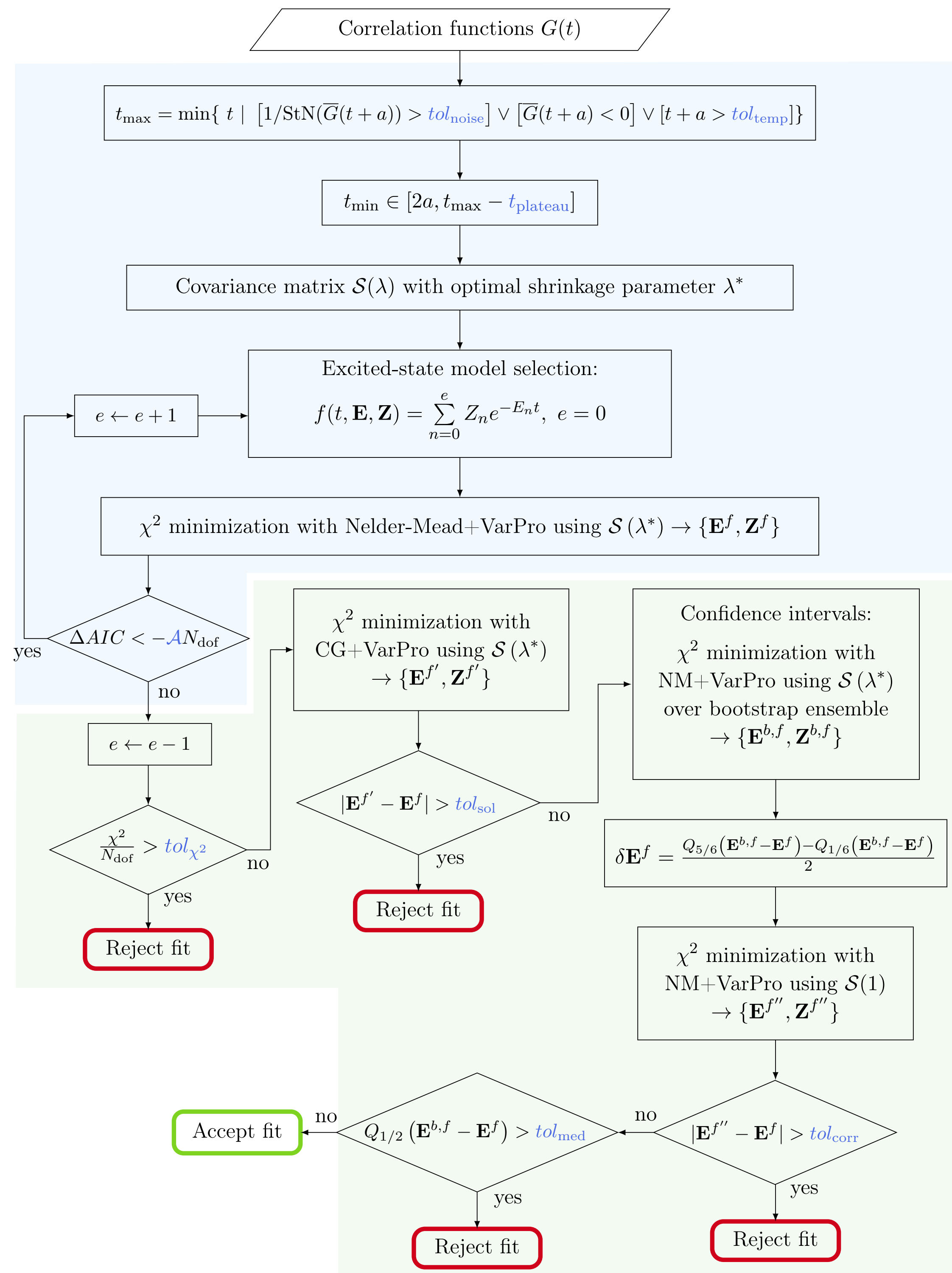
- Fits to correlators - then take correlated bootstrap differences for energy shifts
- Scan over all possible fit ranges and fit models up to 3-exp within those ranges
- Many tests of fit stability
- Final result - weighted model average

$$\overline{E}_0 = \sum^{N_{\text{success}}} w^f E_0^f, \qquad \widetilde{w}^f = \frac{p_f\left(\delta E_0^f\right)^{-2}}{\sum_{f'=1}^{N_{\text{success}}} p_{f'}\left(\delta E_0^{f'}\right)^{-2}};$$

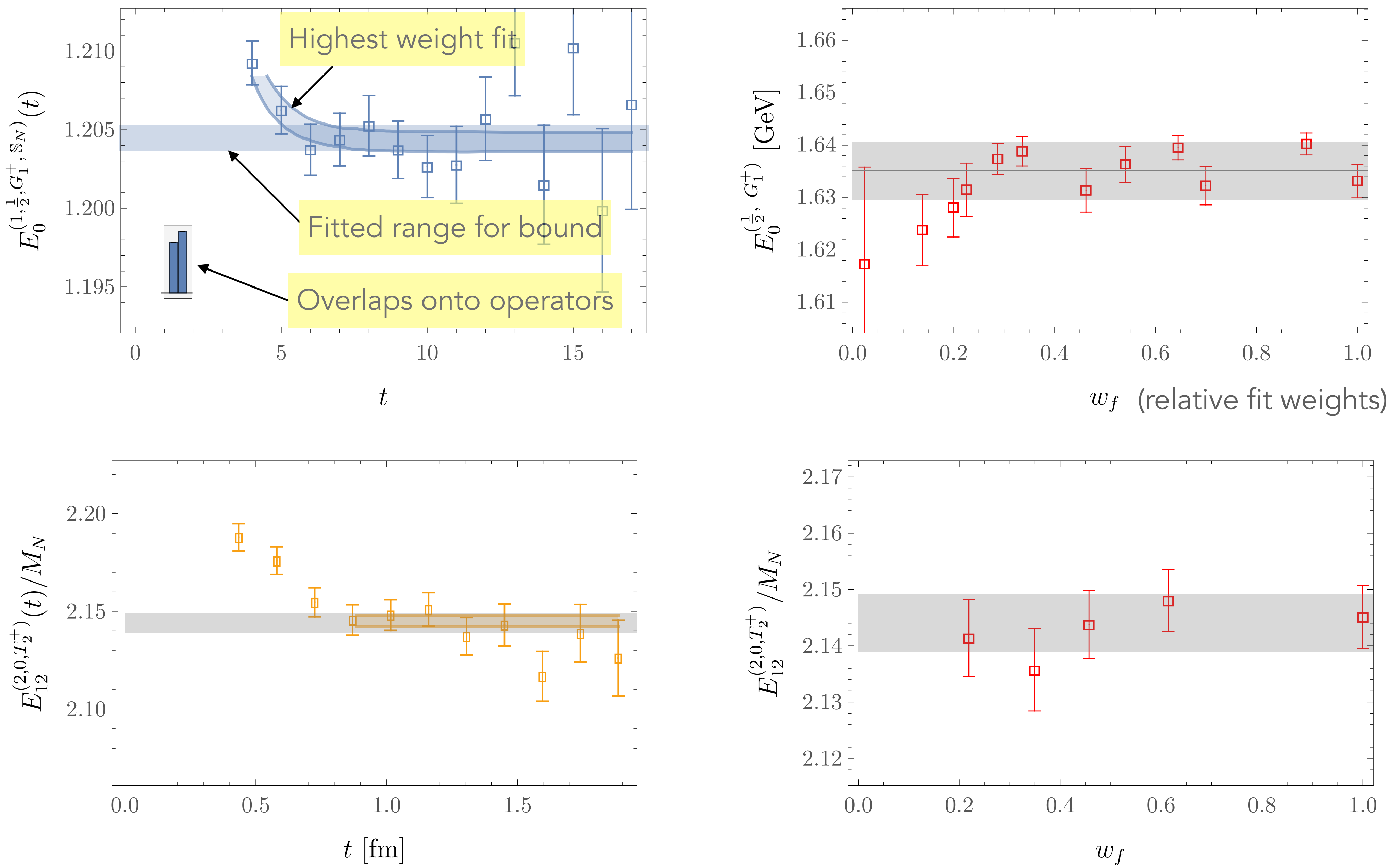
- Final uncertainties - weighted combination $\delta \overline{E}_0 = \sqrt{\delta_{\text{stat}} \overline{E}_0^2 + \delta_{\text{sys}} \overline{E}_0^2}$

$$\delta_{\text{sys}} \overline{E}_0^2 = \sum_{f=1}^{N_{\text{success}}} w^f \left(E_0^f - \overline{E}_0\right)^2, \qquad \delta_{\text{stat}} \overline{E}_0^2 = \sum_{f=1}^{N_{\text{success}}} w^f (\delta E_0^f)^2$$



Fitting methods: example

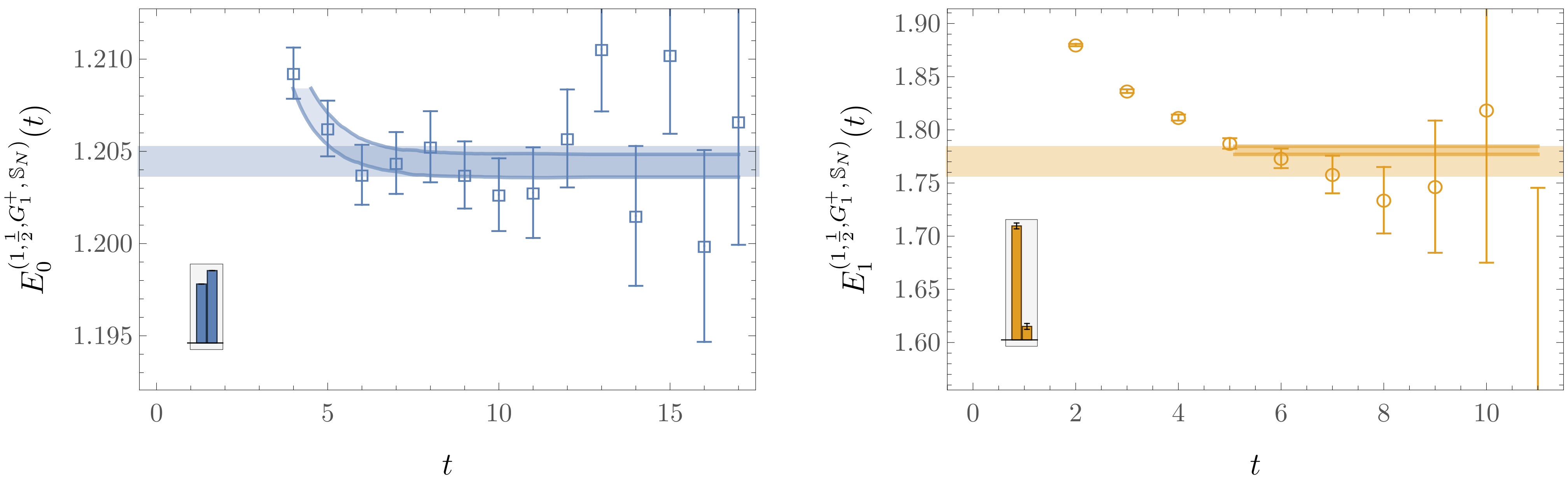
Nucleon GS and Deuteron 12th level



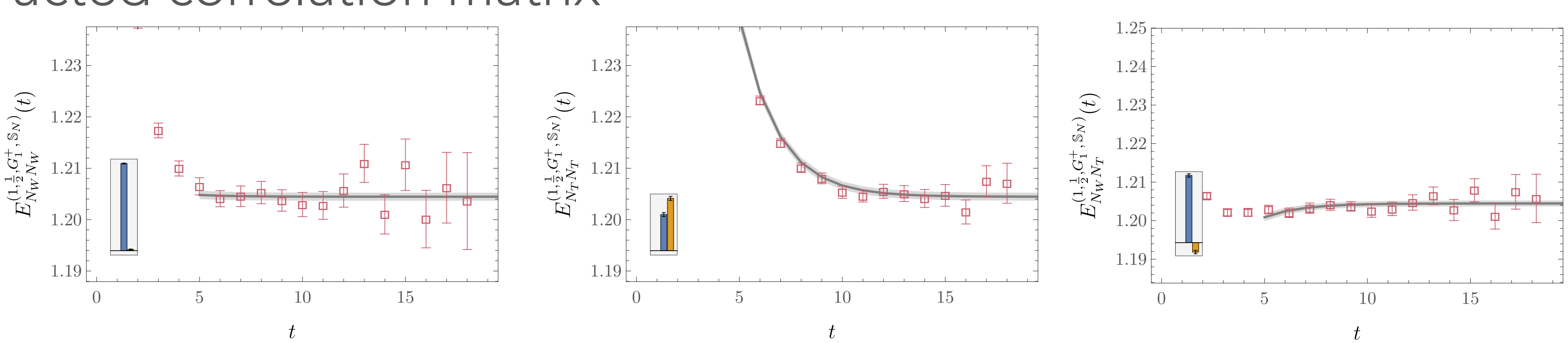
Nucleon

`2x2 correlator matrix: different smearings`

Diagonalised correlators



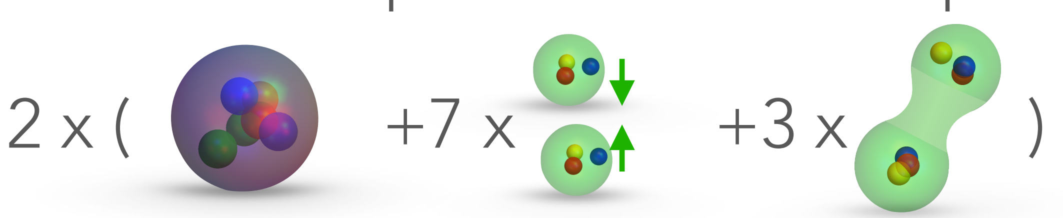
Reconstructed correlation matrix



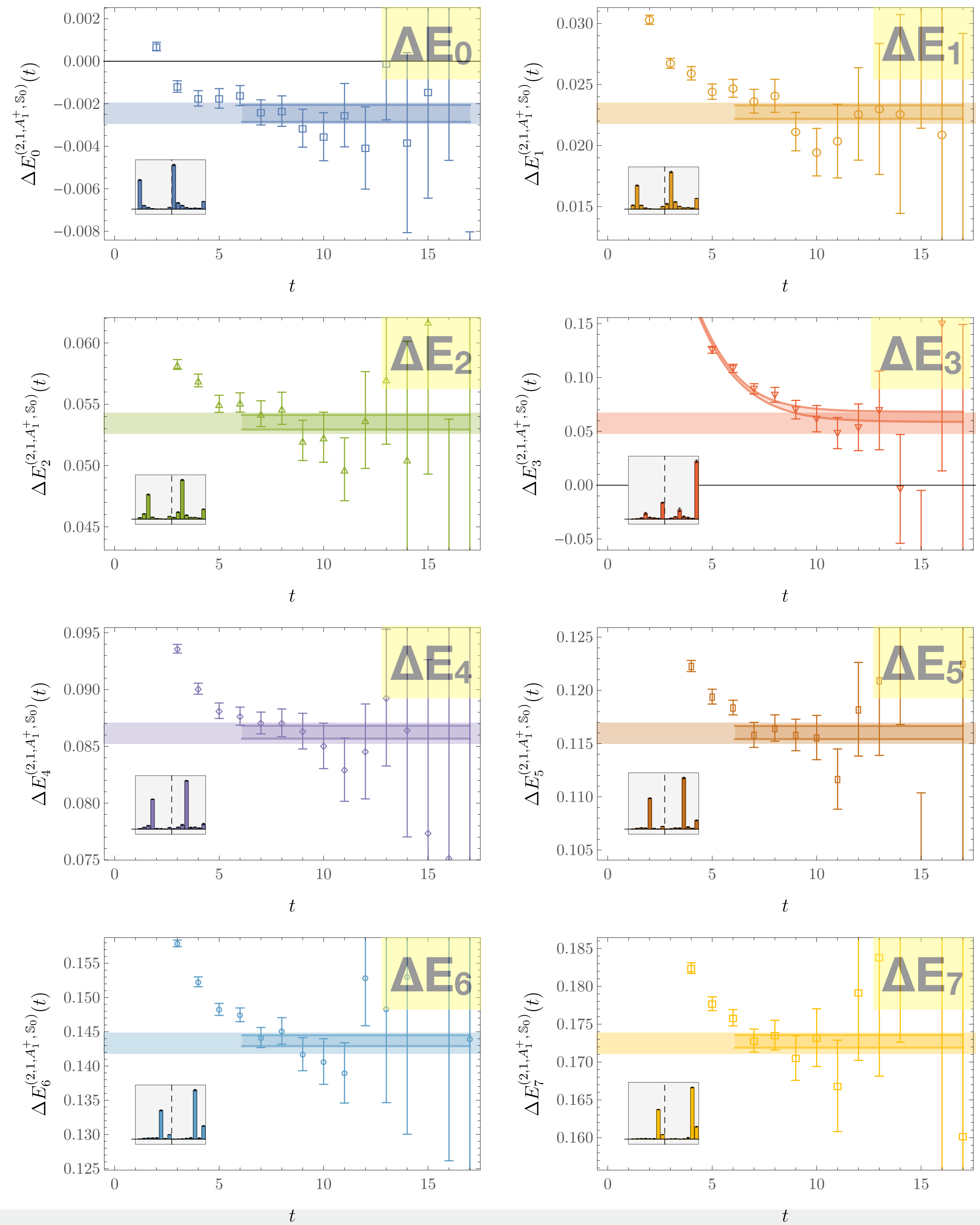
Dineutron

A1+ representation

Total of 22 operators in A1+ rep

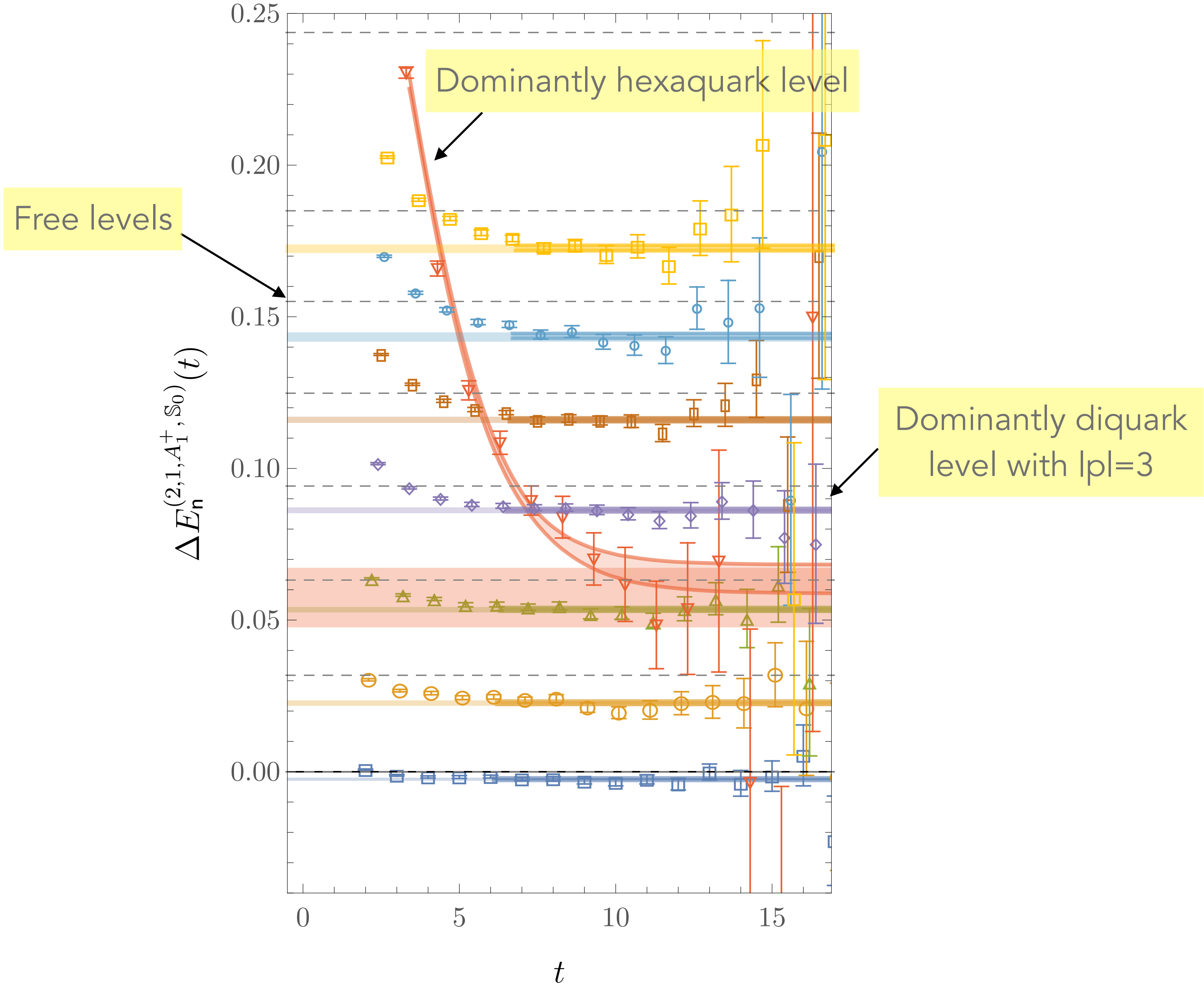


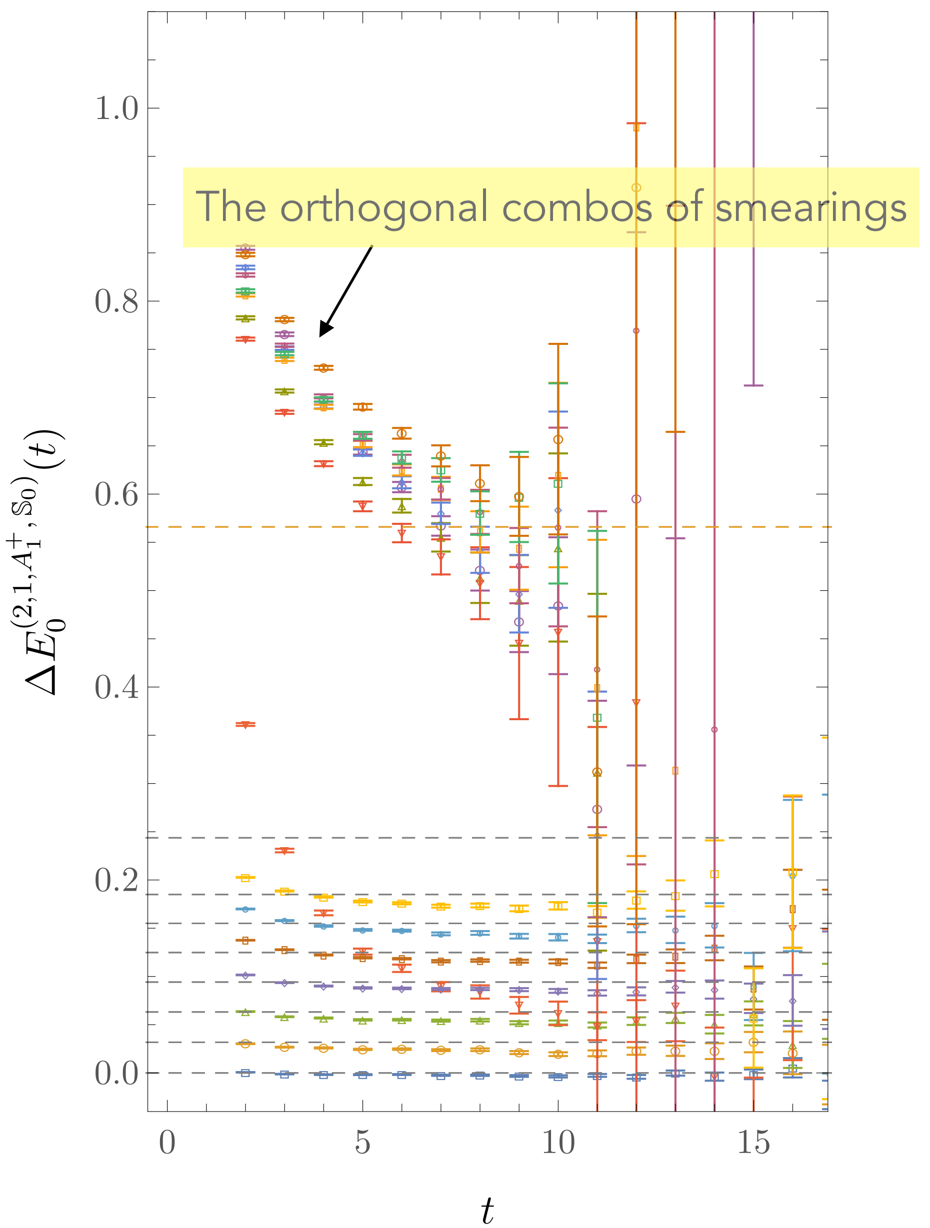
- GEVP 16-dim subset (drop quasi)
  - Lowest 8 levels shown
  - Dominant overlap onto the two smearings of each operator
  - Ground state just below threshold: ΔE~-4 MeV cf ~-20 MeV from off-diagonal corrs.



Dineutron

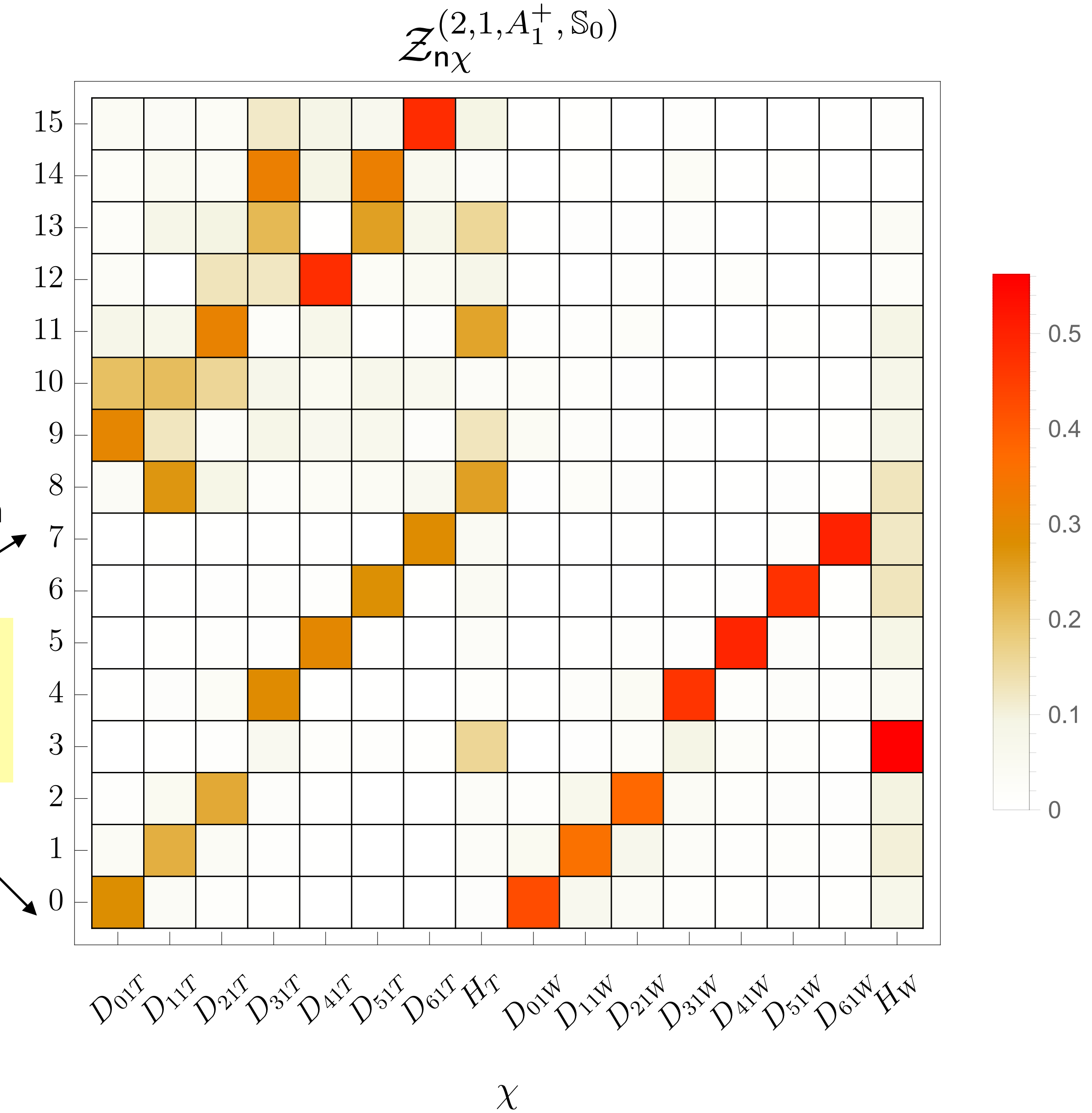
Summary of GEVP levels





Dineutron

Summary of GEVP eigenvectors



Low levels have strong overlap onto only one operator type

Dineutron

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Low-lying GEVP spectra in different irreps
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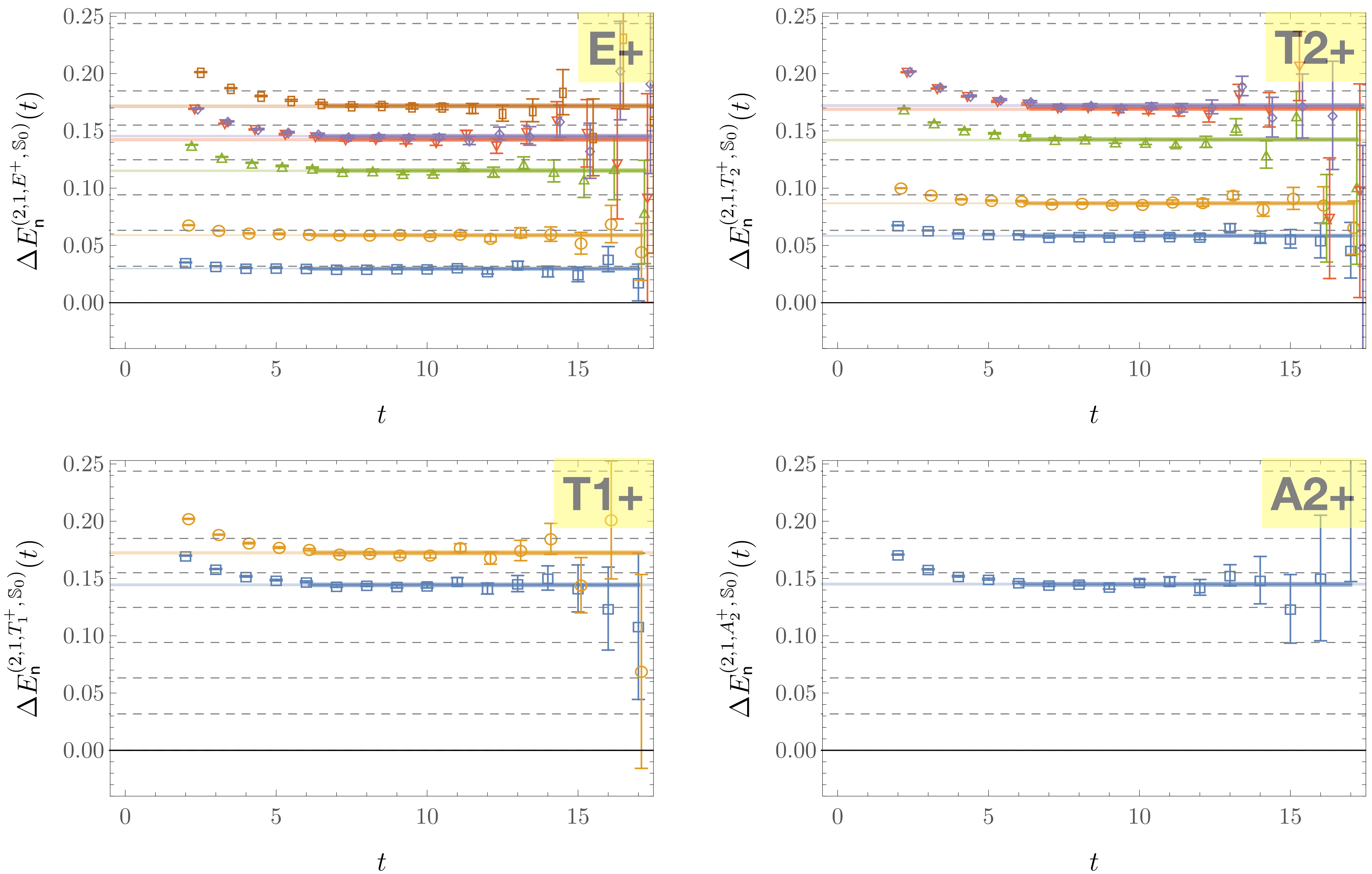
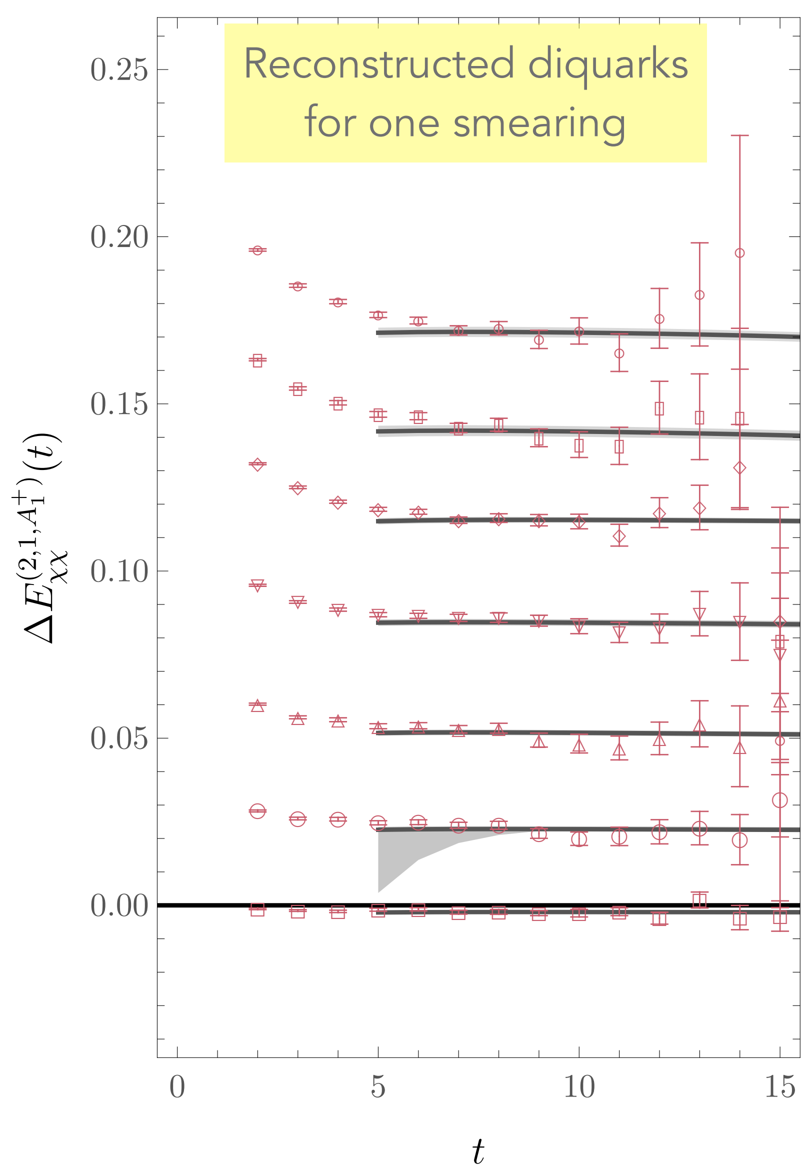


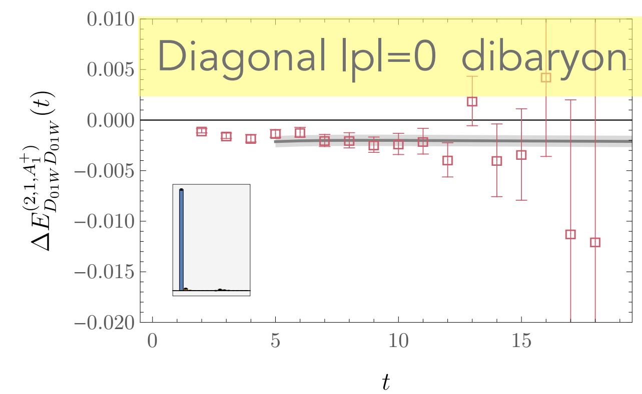
Dineutron

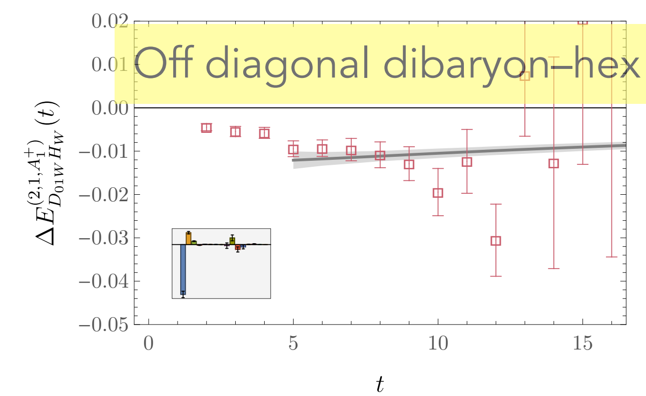
Reconstructed results describe corr. matrix

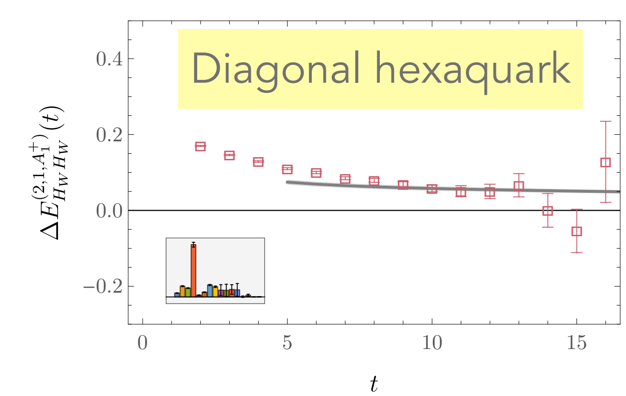
Energies and GEVP evecs allow reconstruction of correlators

- Generally good description of diagonal
- Reproductions of dibaryon-hexaquark far from perfect









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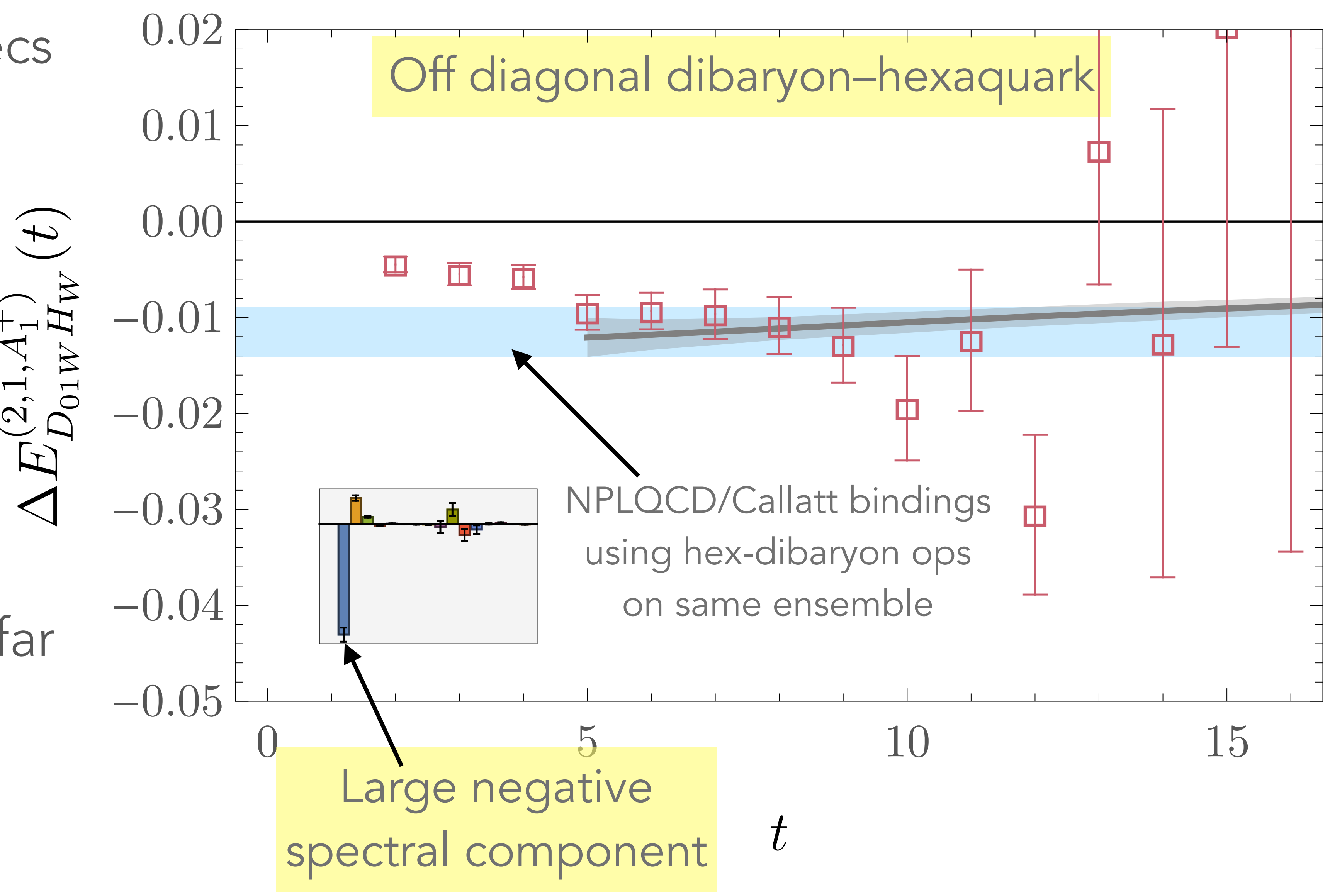


Dineutron

Operator set variation

Lowest bound stable for sets containing p=0 dibaryon OR quasi-local operator

$\mathbb{S}_{⓪}^{(2,1,A_1^+)}$ = 2 x (+7 x [|p|=0,…,6])

$\mathbb{S}_{①}^{(2,1,A_1^+)}$ = 2 x (1 x [|p|=0])

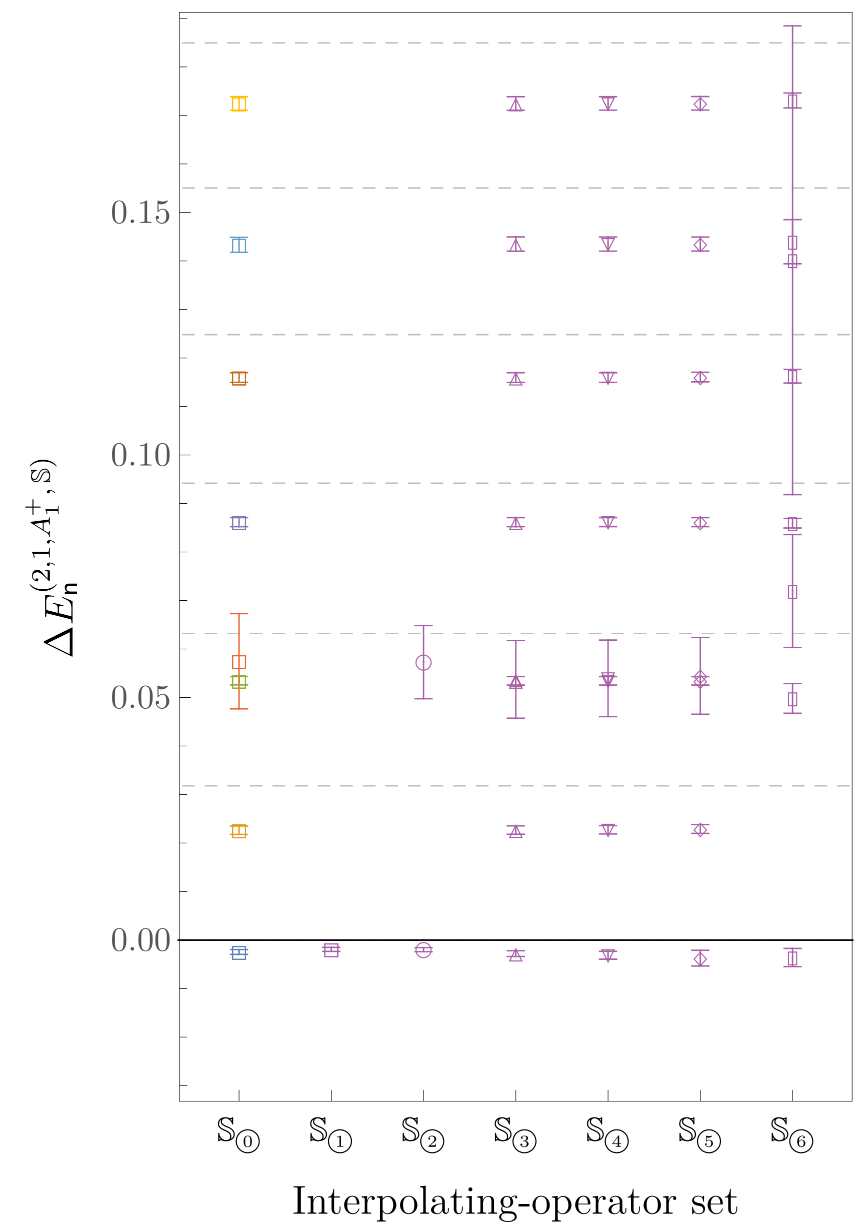
$\mathbb{S}_{②}^{(2,1,A_1^+)}$ = 2 x (+1 x [|p|=0])

$\mathbb{S}_{③}^{(2,1,A_1^+)}$ = 2 x (+6 x [|p|=1,…,6] +1 x [κ=1])

$\mathbb{S}_{④}^{(2,1,A_1^+)}$ = 2 x (+6 x [|p|=1,…,6] +1 x [κ=2])

$\mathbb{S}_{⑤}^{(2,1,A_1^+)}$ = 2 x (+6 x [|p|=1,…,6] +1 x [κ=3]

$\mathbb{S}_{⑥}^{(2,1,A_1^+)}$ = 2 x (+6 x [|p|=0,2,3,4,5,6] +1 x [κ=3])



Dineutron

```
You get what you put in
```

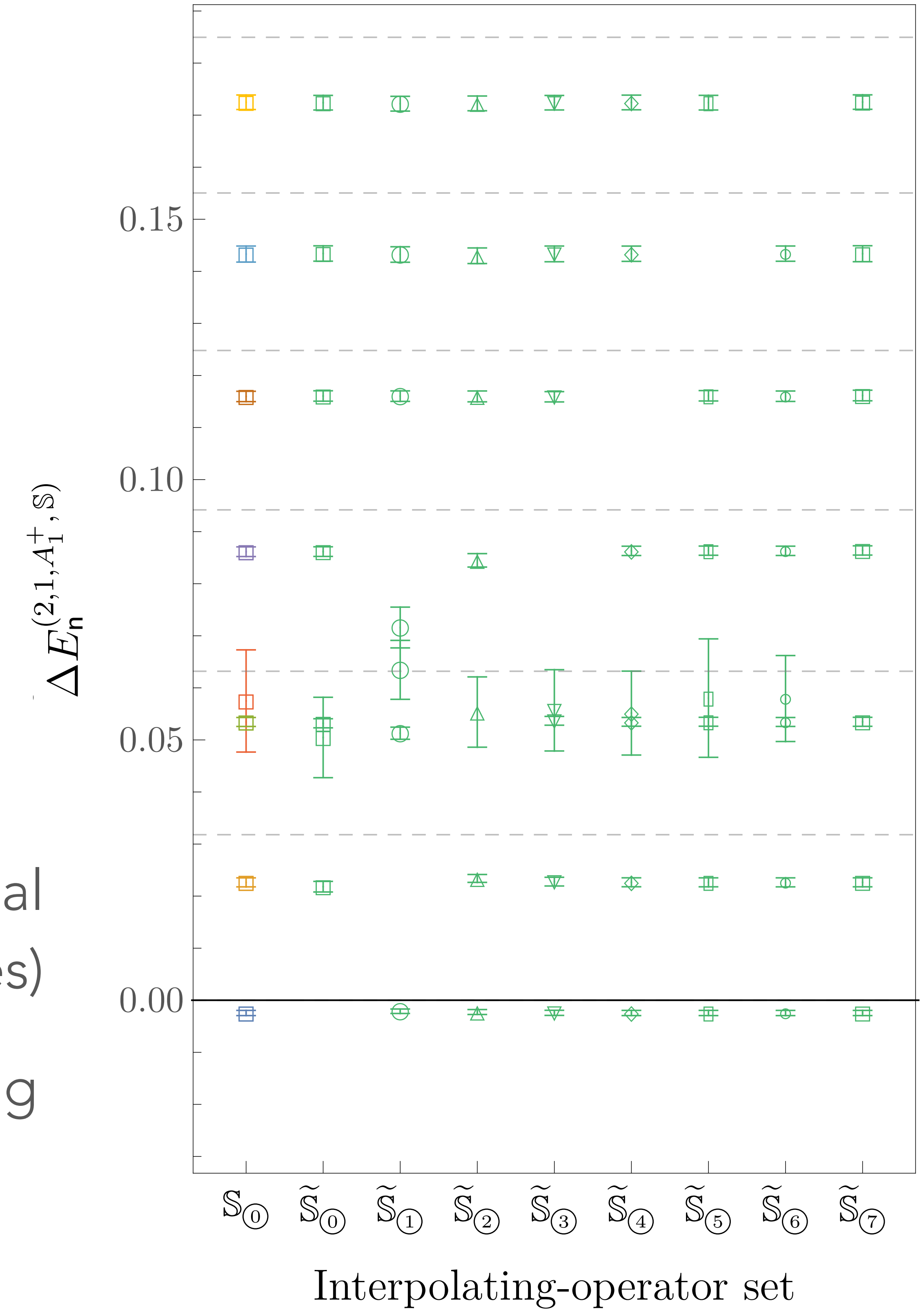
Sets without a particular dibaryon or hexaquark operator

$\mathbb{S}_{\textcircled{0}}^{(2,1,A_1^+)}$ = 2 x (+7 x [|p|=0,…,6])

$\widetilde{\mathbb{S}}_{\textcircled{m}}^{(2,1,A_1^+)}$ = 2 x (+6 x [|p|=0,…,~~m~~,…,6]) m∈{0,…6}

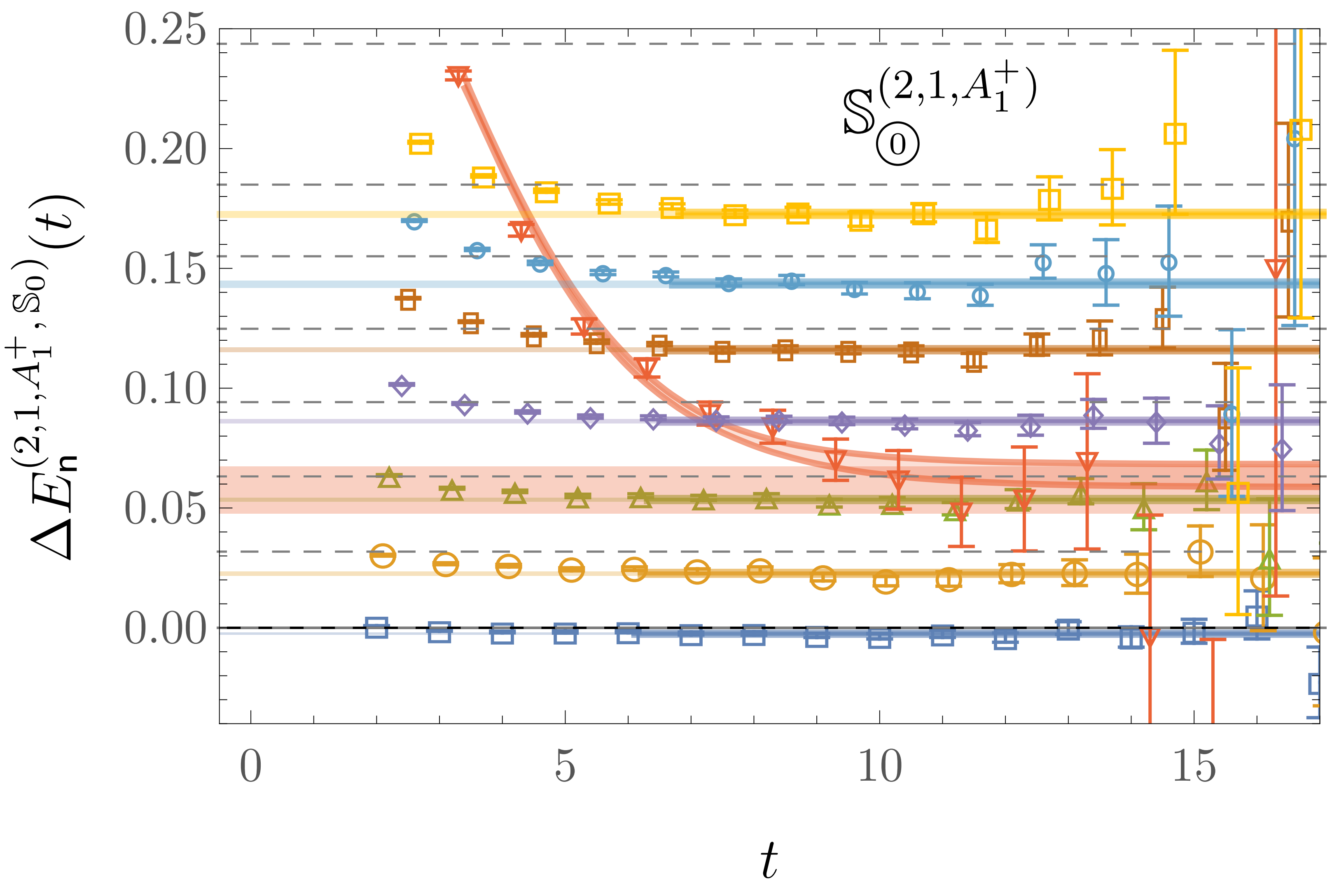
$\widetilde{\mathbb{S}}_{\textcircled{7}}^{(2,1,A_1^+)}$ = 2 x (7 x [|p|=0,…,6])

- Dibaryon operators are close to orthogonal (ie very small overlaps onto "wrong" states)
- If an operator is left out, the corresponding "right" state is not found



An extra state

"Resonant" hex-state stable vs operator set



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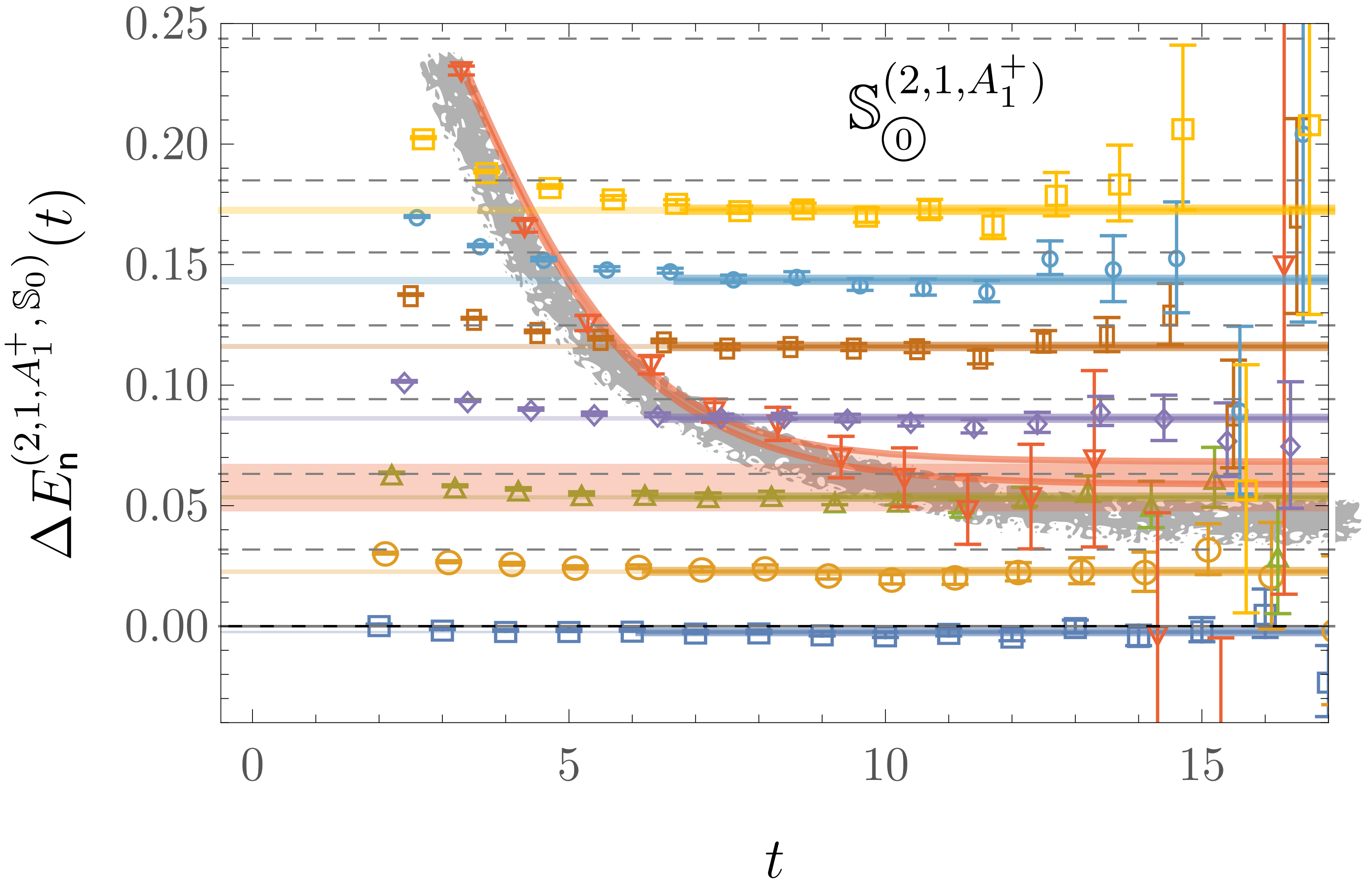

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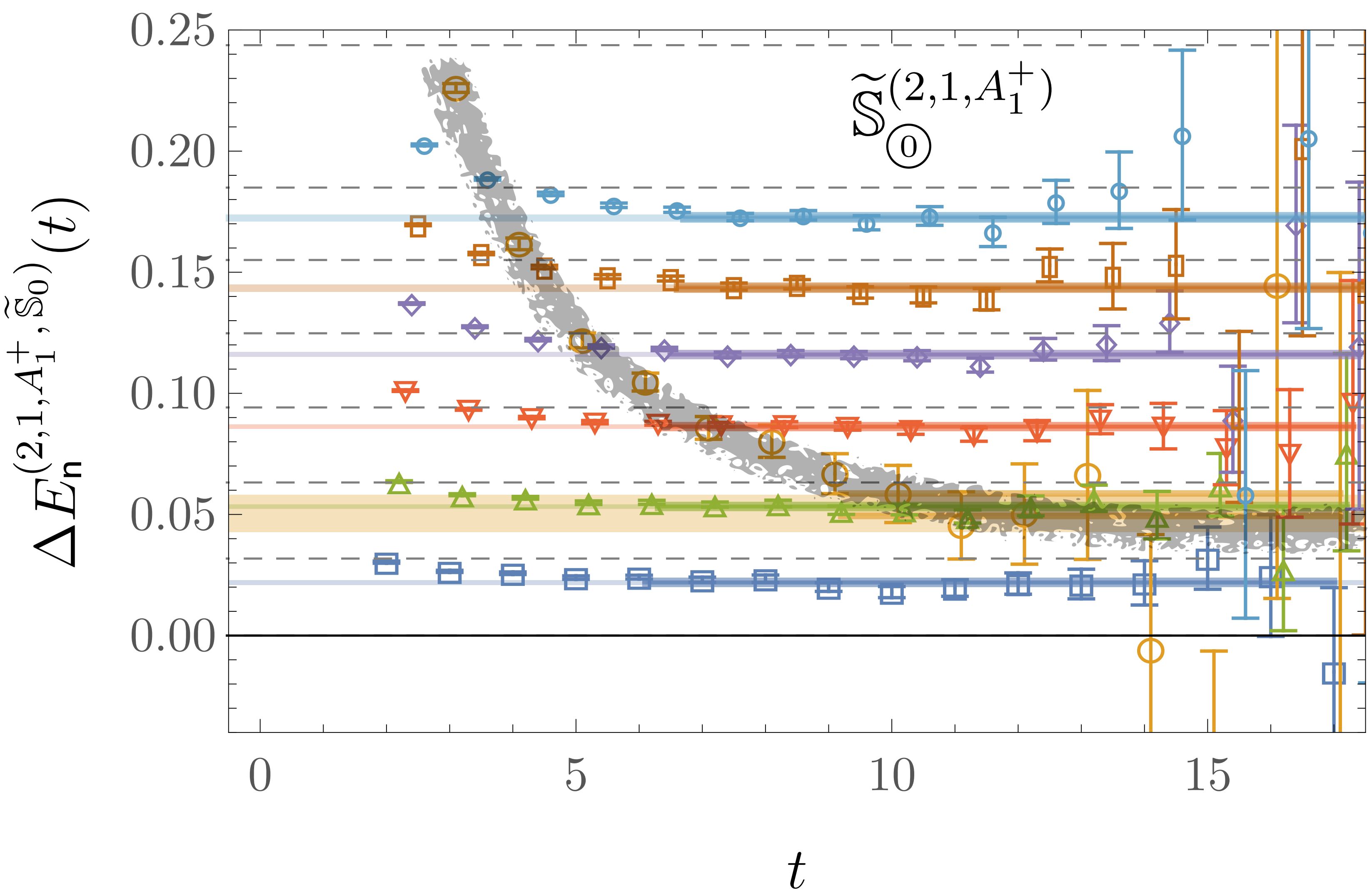

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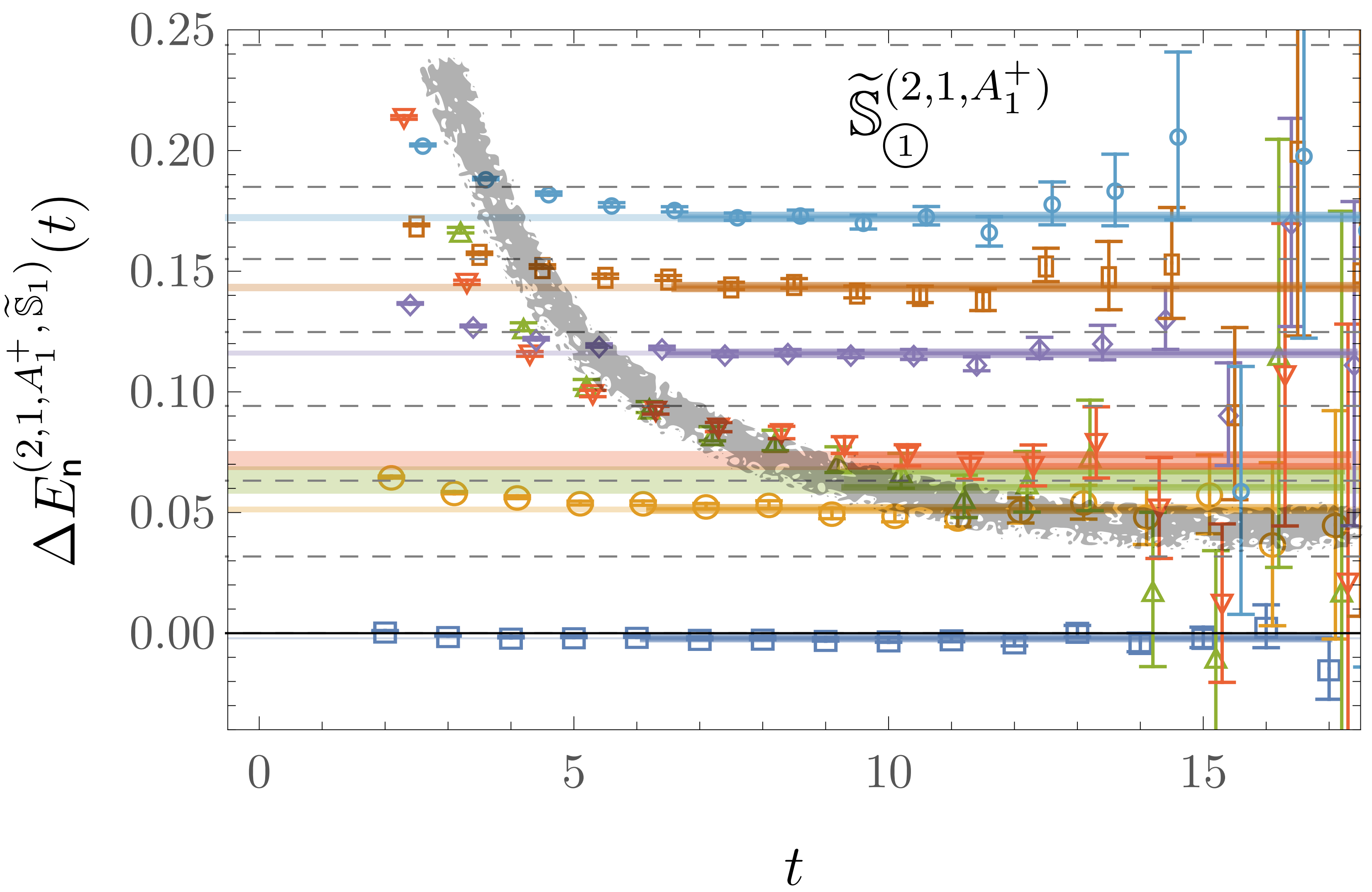

An extra state

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"Resonant" hex-state stable vs operator set
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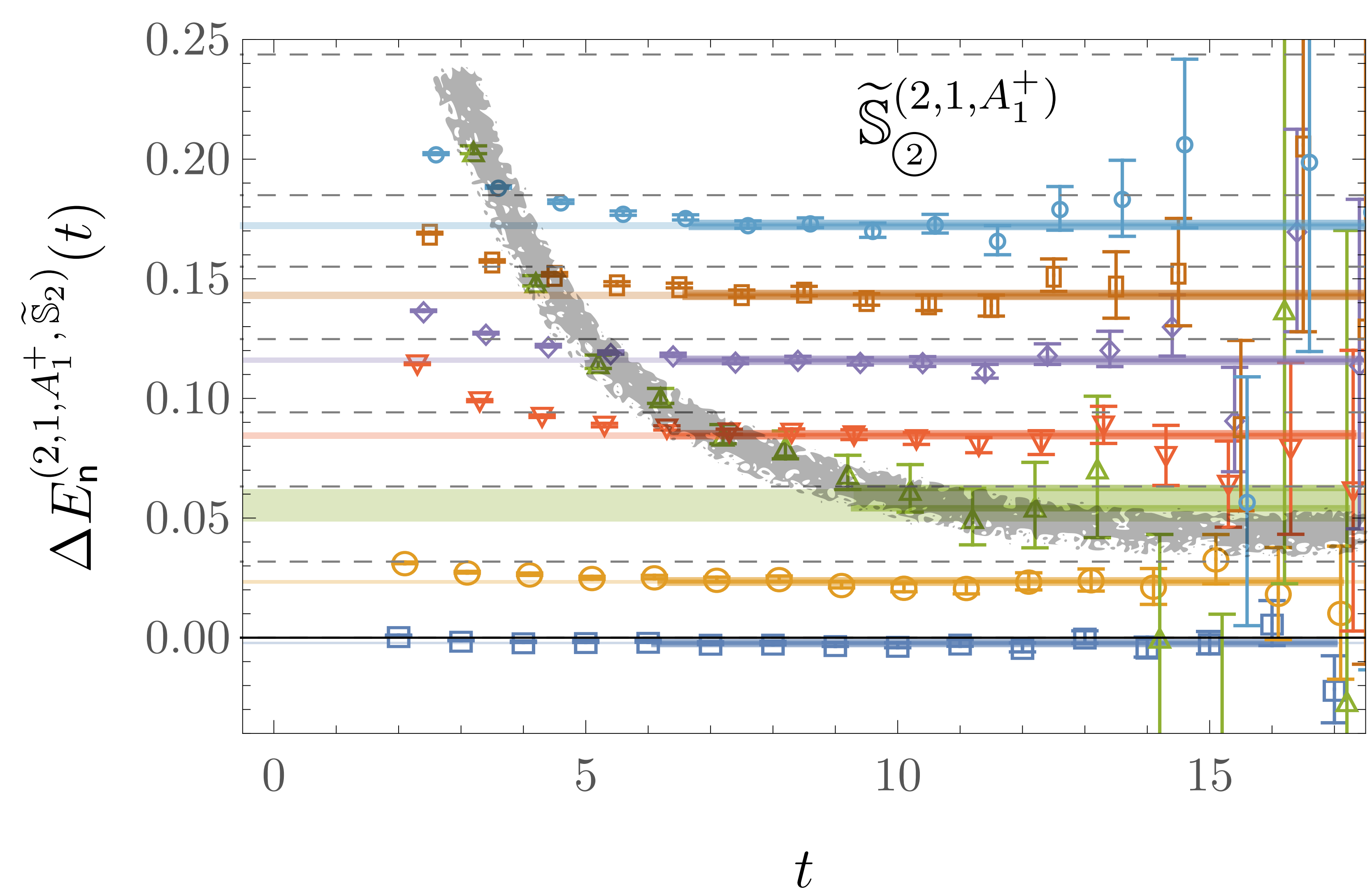

An extra state

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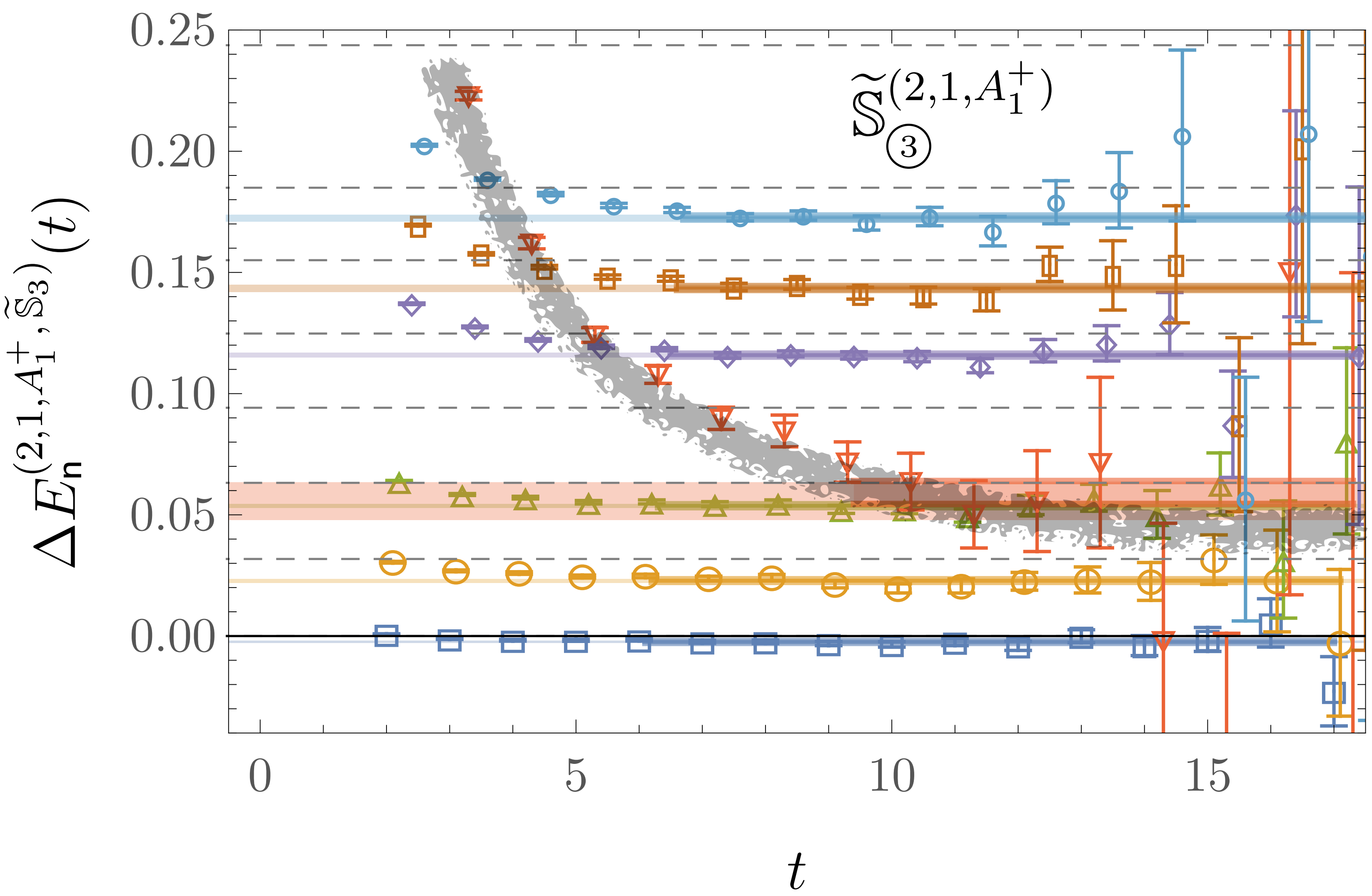
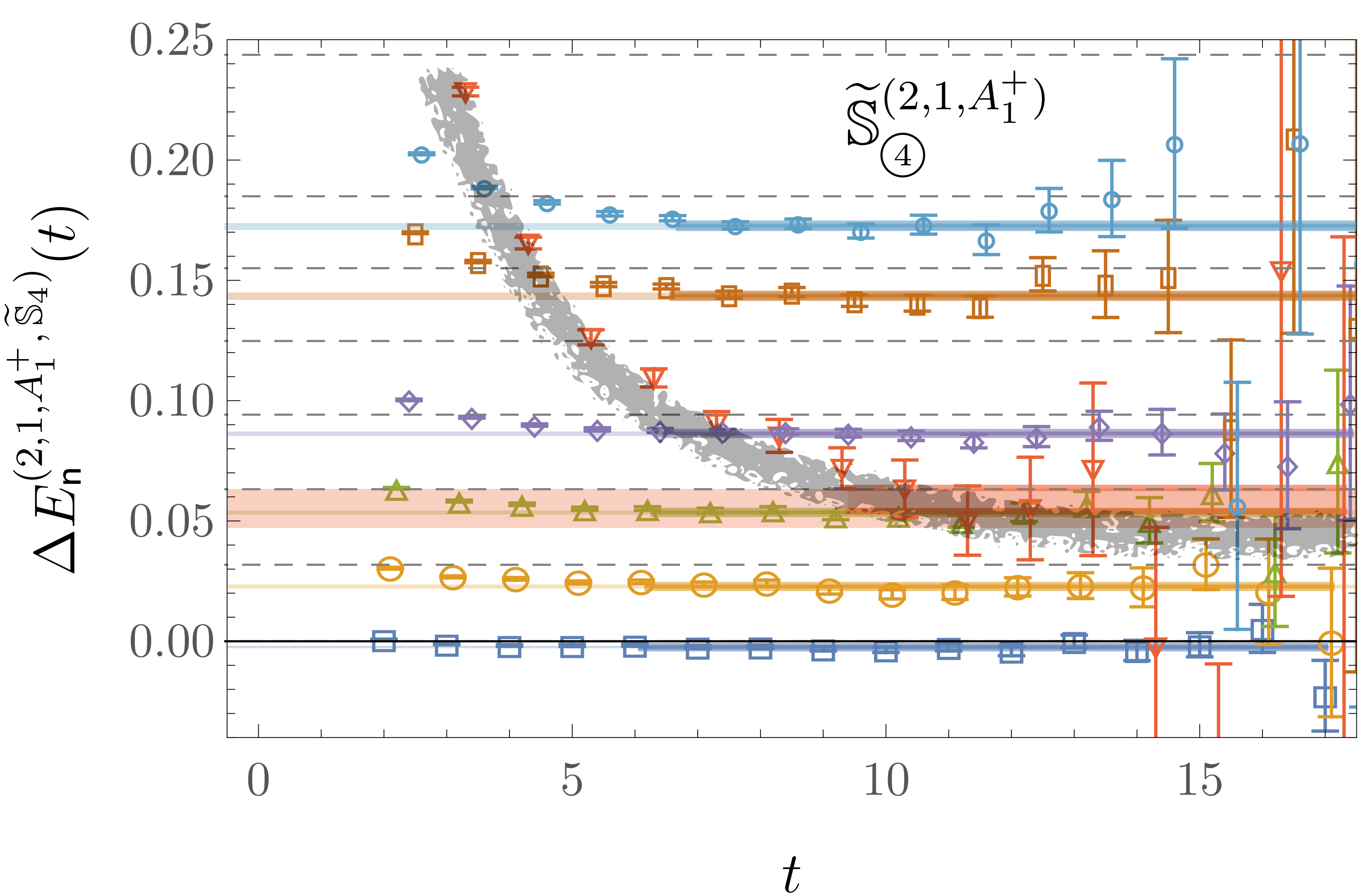


An extra state

“Resonant” hex-state stable vs operator set



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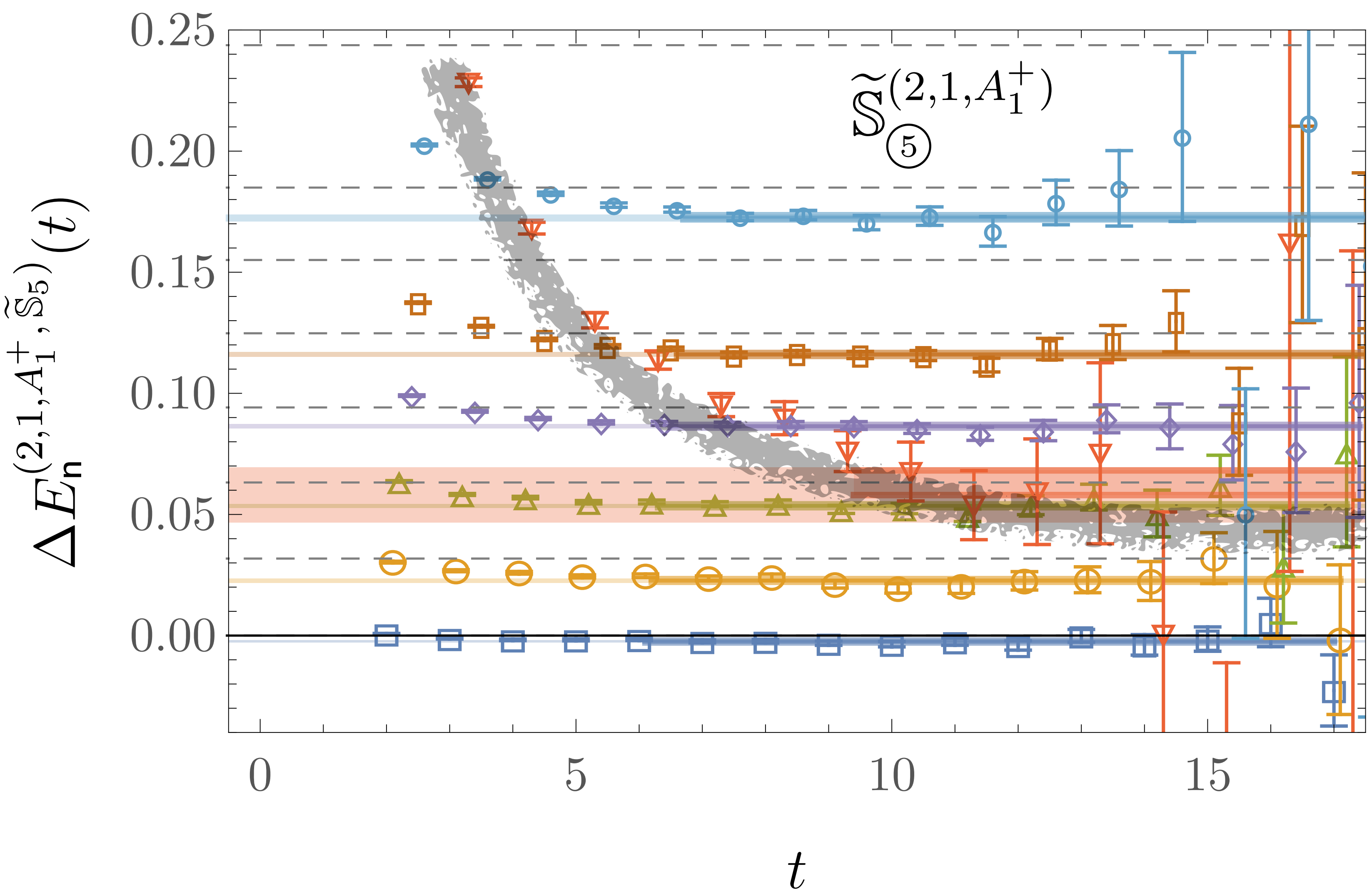
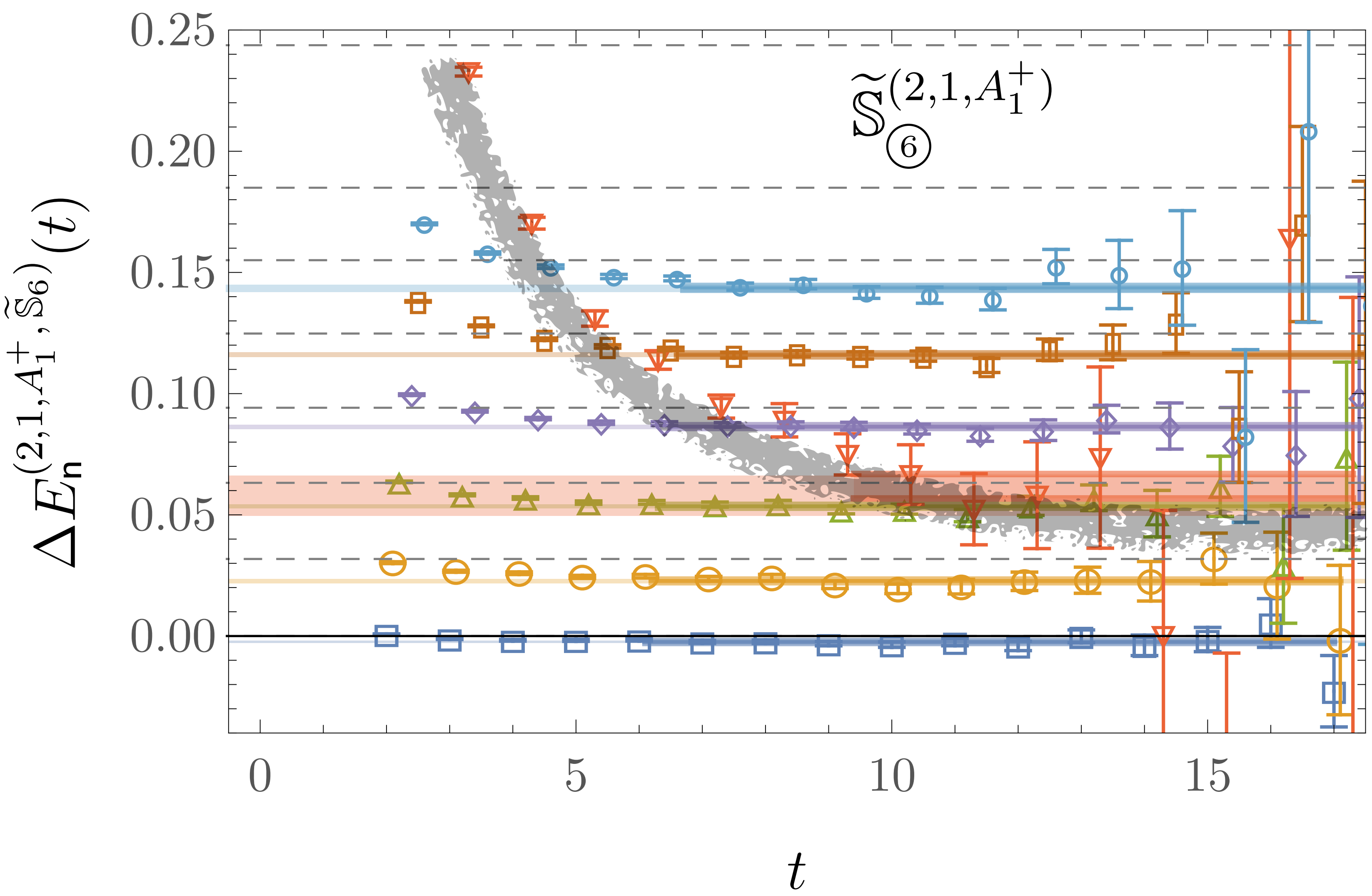


An extra state

“Resonant” hex-state stable vs operator set



An extra state

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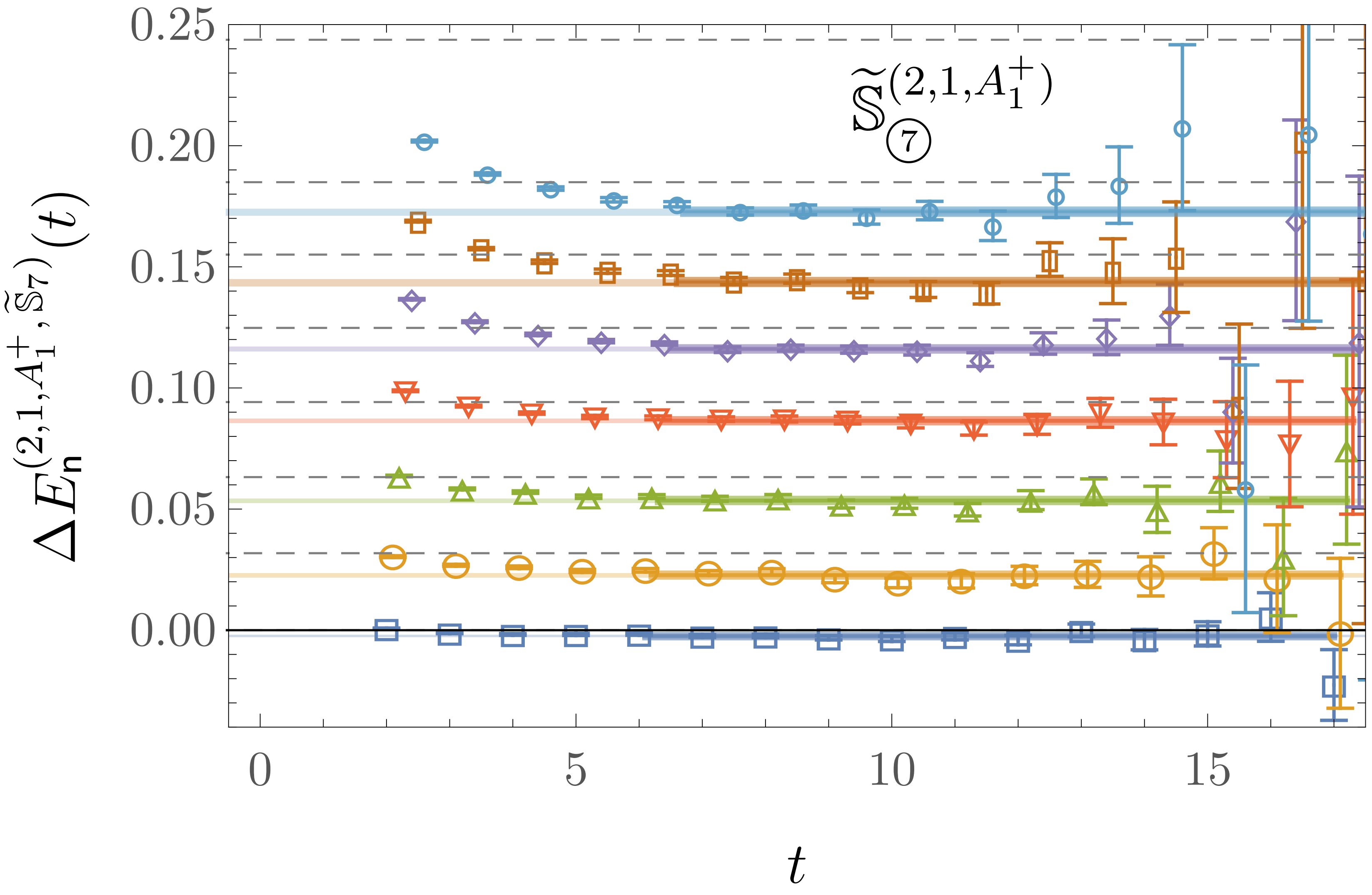
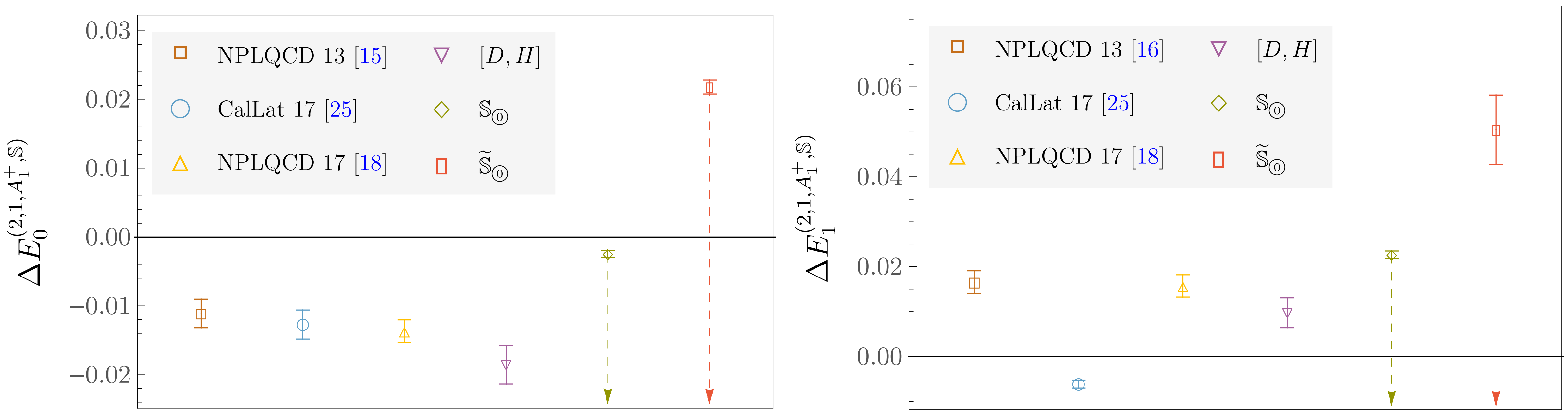
Unless remove the hexaquark operator
```



Comparisons

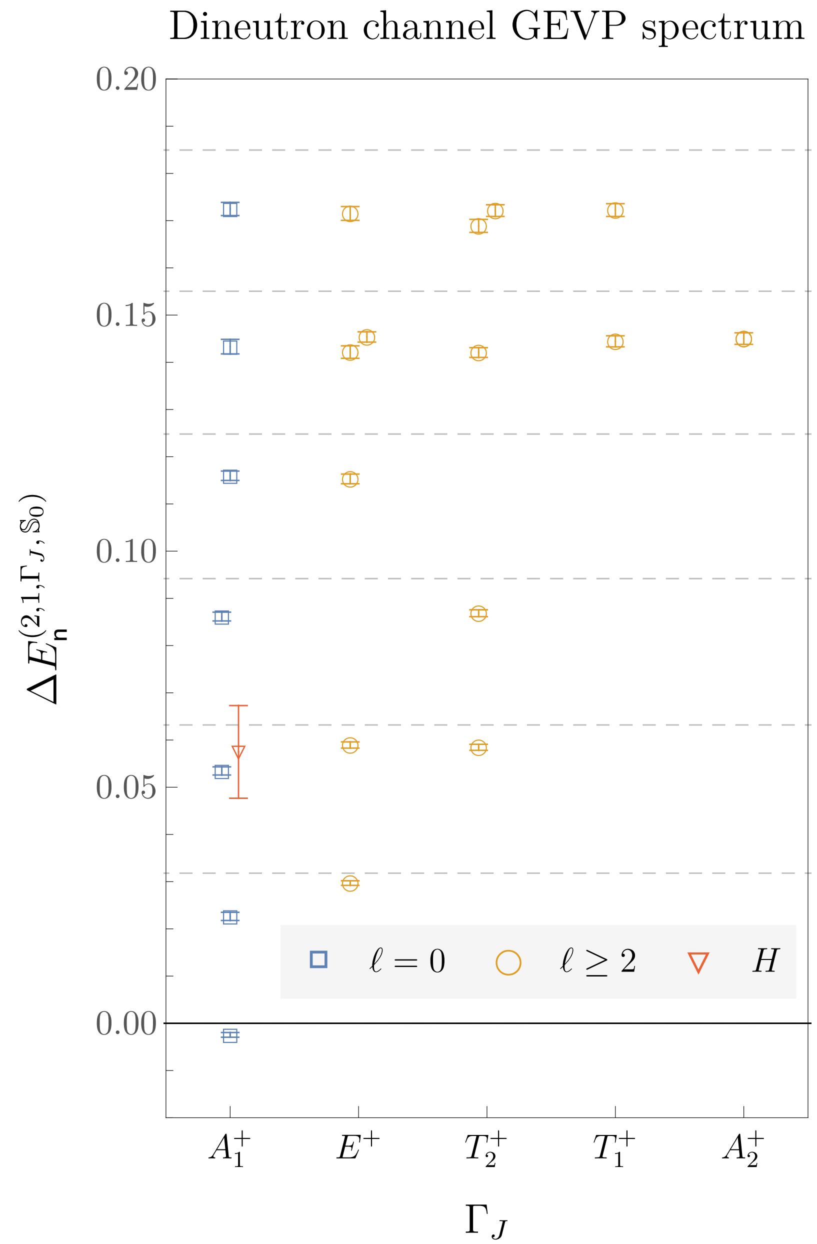
Summary of ground and first excited states

- Variational results correctly interpreted as bounds: some are better than others
- As in previous calculations, off-diagonal correlators consistent with a deeper state

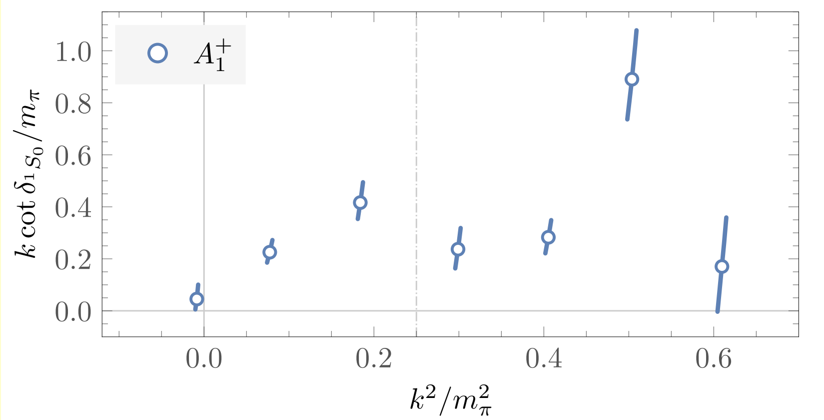


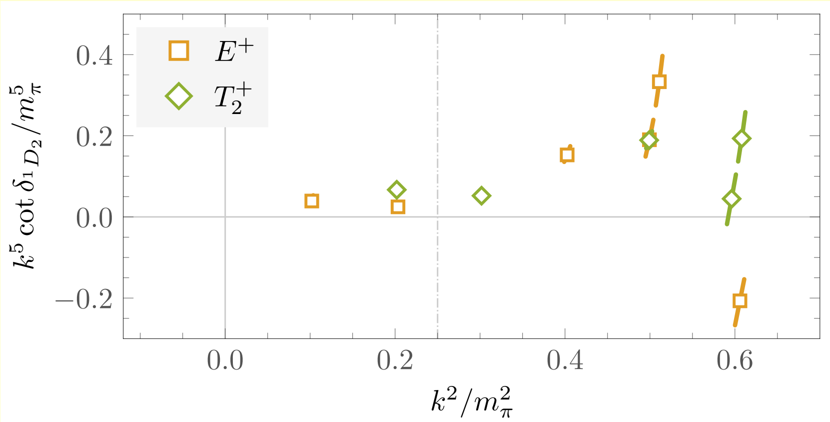
Summary

Extracted levels in all cubic irrupts



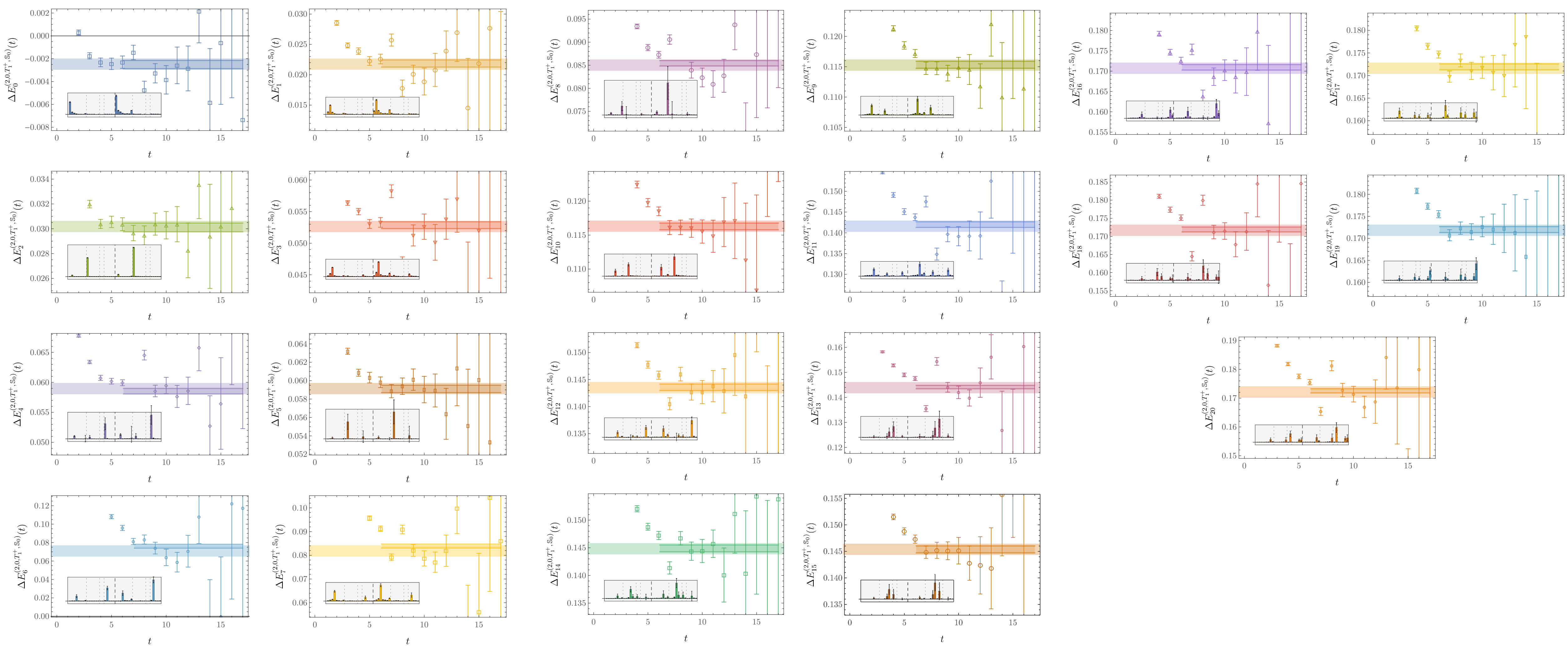
If interpret as energies rather than bounds can convert to phase shifts





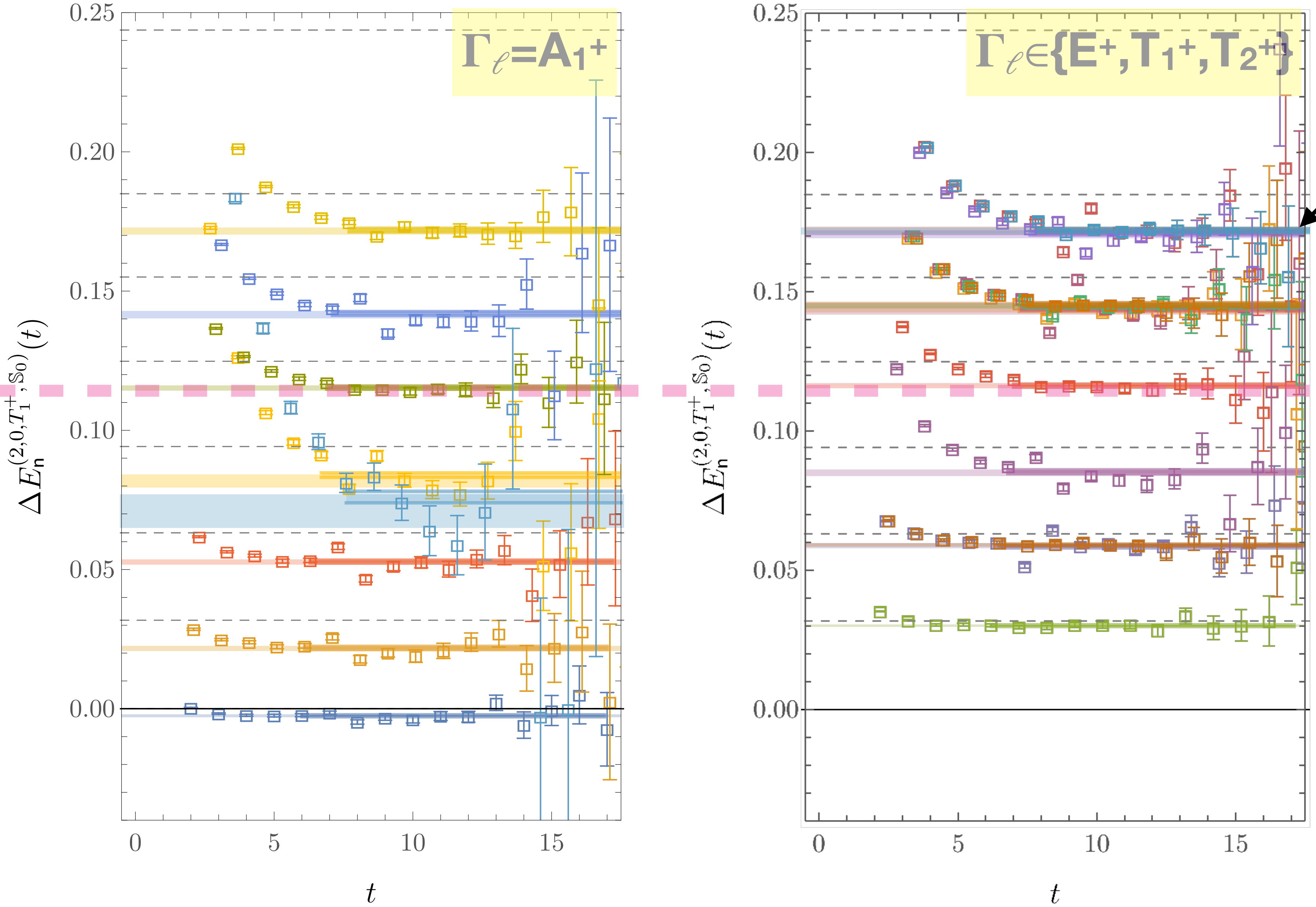
Deuteron

42 operators in largest GEVP: lots of levels!



Deuteron

Summary of GEVP Γ_J=T_1^+ levels

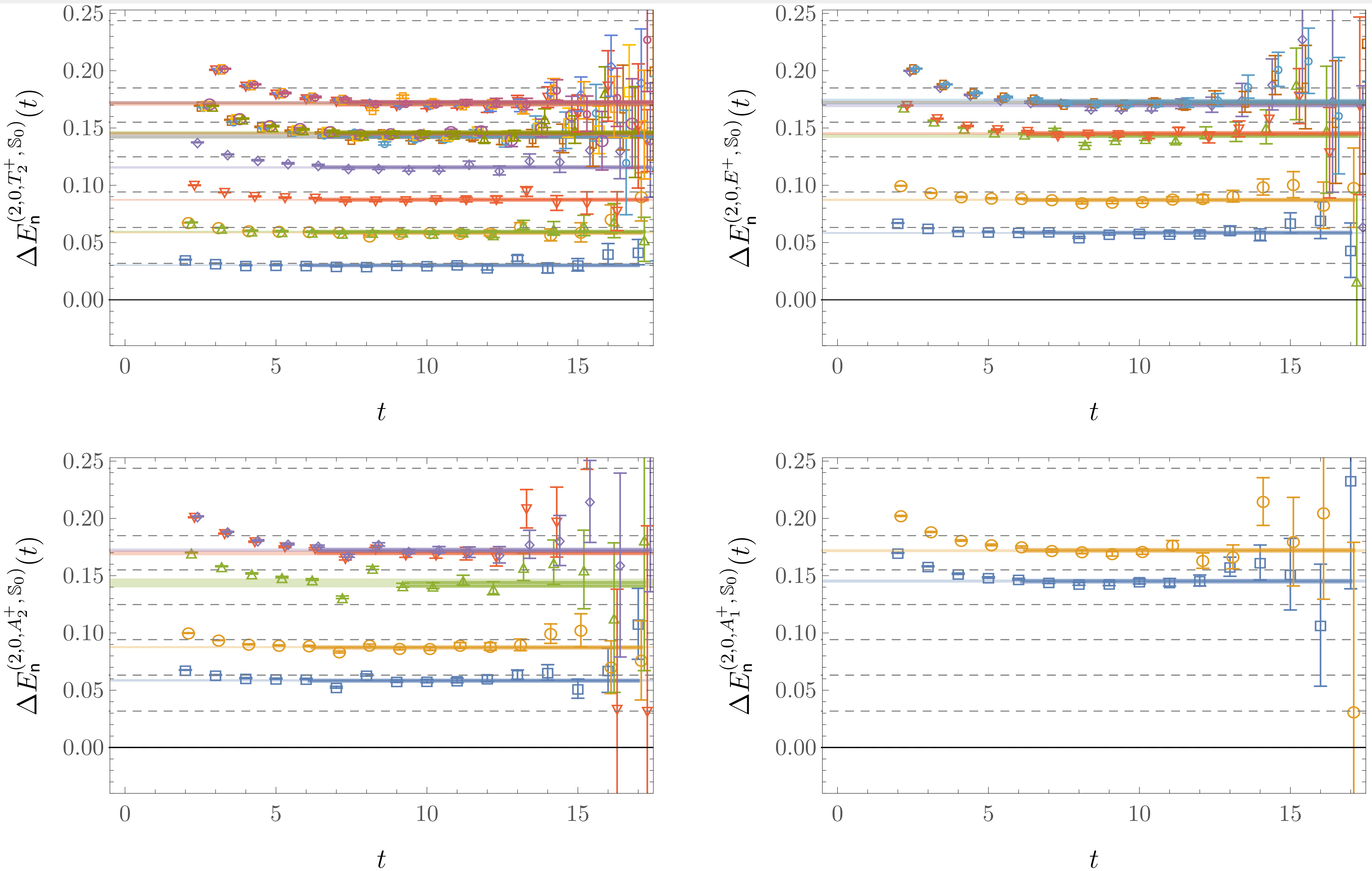


Close levels resolved between different irrepts

Multiplicities are as for free levels

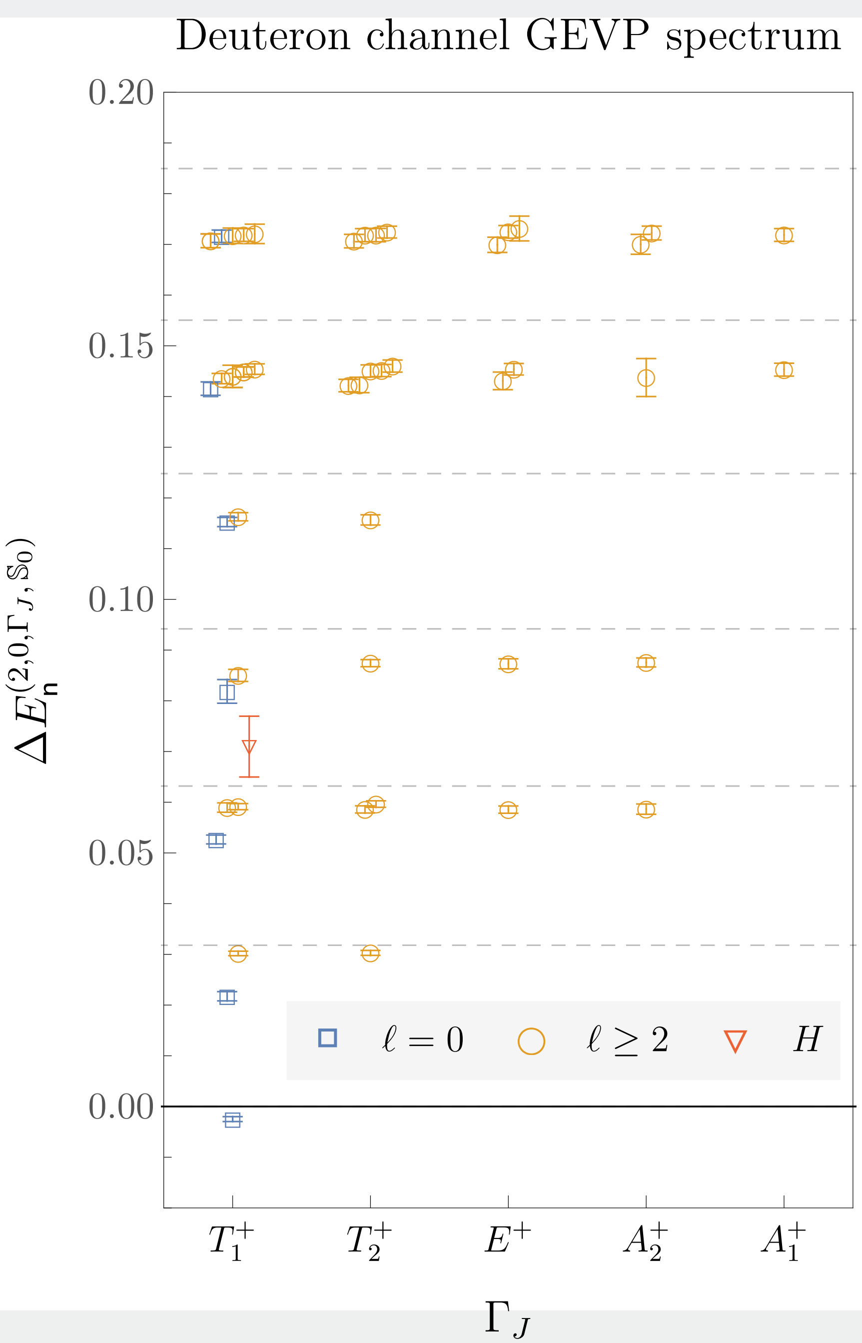
Deuteron

Other total J irreps



Deuteron

Extracted levels in various cubic irrupts



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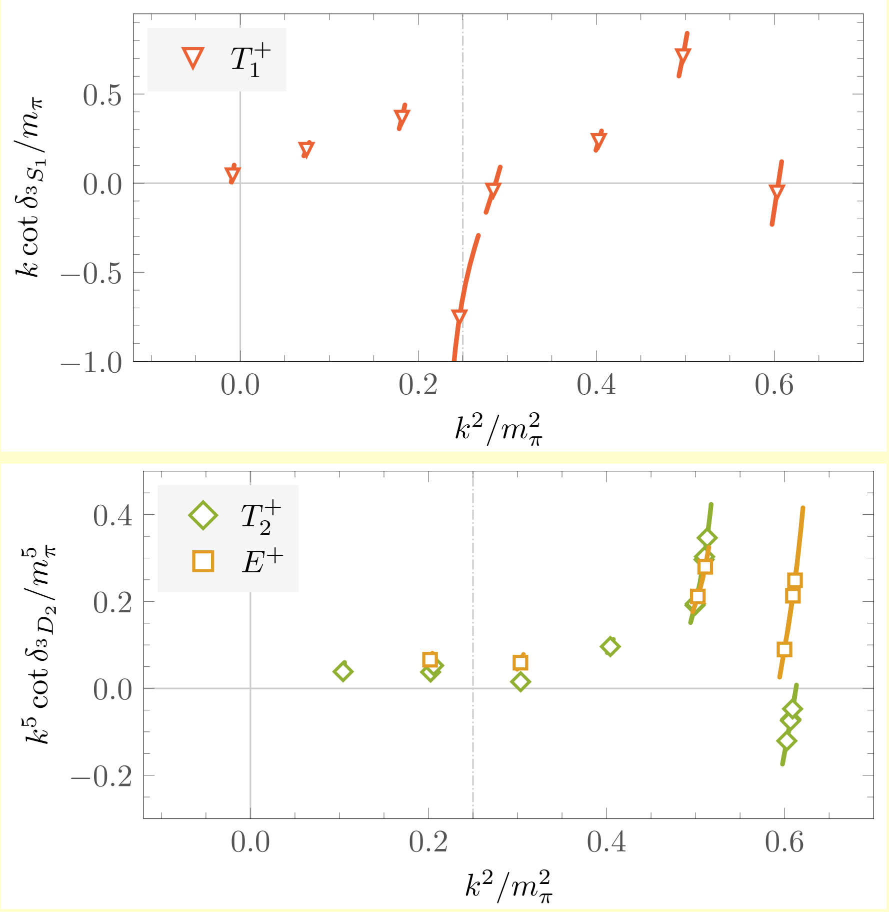
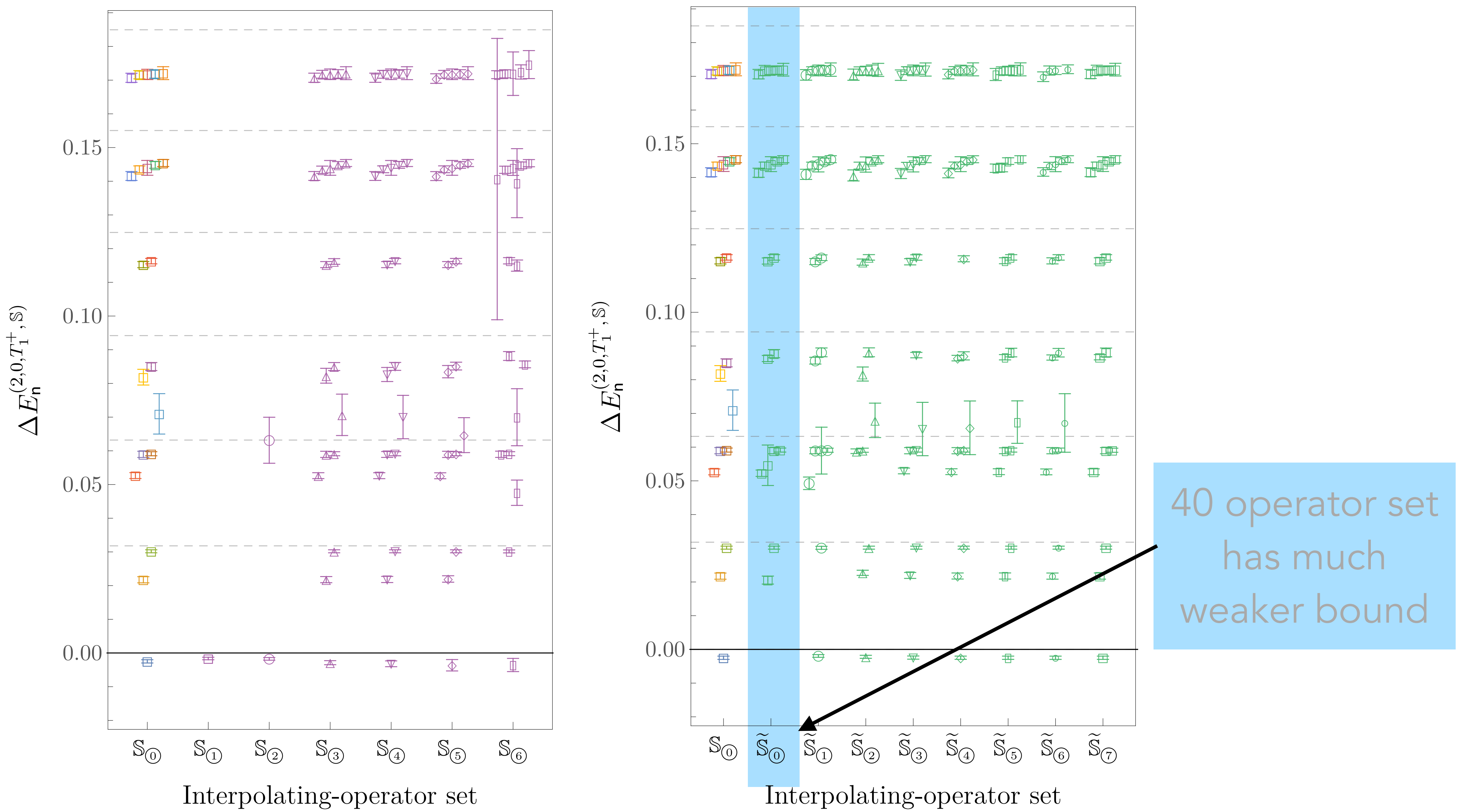


Deuteron

Similar picture on removal of operators from set



Evidence about bound states

PRO

- Off-diagonal correlators show plateau for deep states [Callatt, NPLQCD, PACS-CS]
- Same state seen in volumes that differ by a factor of 8 [NPLQCD]
  - Hard to explain by cancellations
- EFT matching show consistency between 2,3,4 body systems
- GEVP analyses do not see states unless the "right" operator is included in operator set

CON

- Variational bounds from GEVP consistent with attractive threshold state [Hörz et al, NPLQCD, Green et al.]
- Robust against some variations of operator set (but not others)
- GEVP reconstruction can approximately describe off-diagonal correlators
- HALQCD potentials also do not see bound states

A simple model

```
Can off diagonal correlators find lower state?
```

- 2x2 matrix of correlators with 3 states with energies: $E_0 < E_1 < E_2$

$$C_{ij}(t) = \vec{Z}_i^\dagger D(t) \vec{Z}_j \qquad D(t) = \mathrm{diag}(e^{-E_0(t-t0)}, e^{-E_1(t-t0)}, e^{-E_2(t-t0)})$$

- Z factors given by:

$$\vec{Z}_1 = (\epsilon, \sqrt{1-\epsilon^2}, 0)$$
$$\vec{Z}_2 = (\epsilon, 0, \sqrt{1-\epsilon^2})$$

- Diagonalisation in variational method will give GEVP eigenvalues

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

- Off diagonal correlator

$$C_{12}(t) = \epsilon^2 \exp(-E_0(t-t_0))$$

An ever so not quite as simple model

```
Zero overlaps unlikely [Nicholson, Lattice 2022]
```

- 2x2 matrix of correlators with 3 states with energies: $E_0 < E_1 < E_2$

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- Z factors given by:

$$\vec{Z}_1 = (\epsilon, \sqrt{1-\epsilon^2}, \epsilon')$$
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- Diagonalisation in variational method will give GEVP eigenvalues

$$\lambda_0(t) = \exp(-E_1(t-t_0)) + \mathcal{O}(\epsilon^2, \epsilon'^2)$$
$$\lambda_1(t) = \exp(-E_2(t-t_0)) + \mathcal{O}(\epsilon^2, \epsilon'^2)$$

- Off diagonal correlator

$$C_{12}(t) = \epsilon'[\exp(-E_1(t-t_0)) + \exp(-E_2(t-t_0))] + \epsilon^2 \exp(-E_0(t-t_0)) + \mathcal{O}(\epsilon^2\epsilon')$$

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- Off diagonal correlator

Dominated by g.s. if $\epsilon' \ll \epsilon^2$

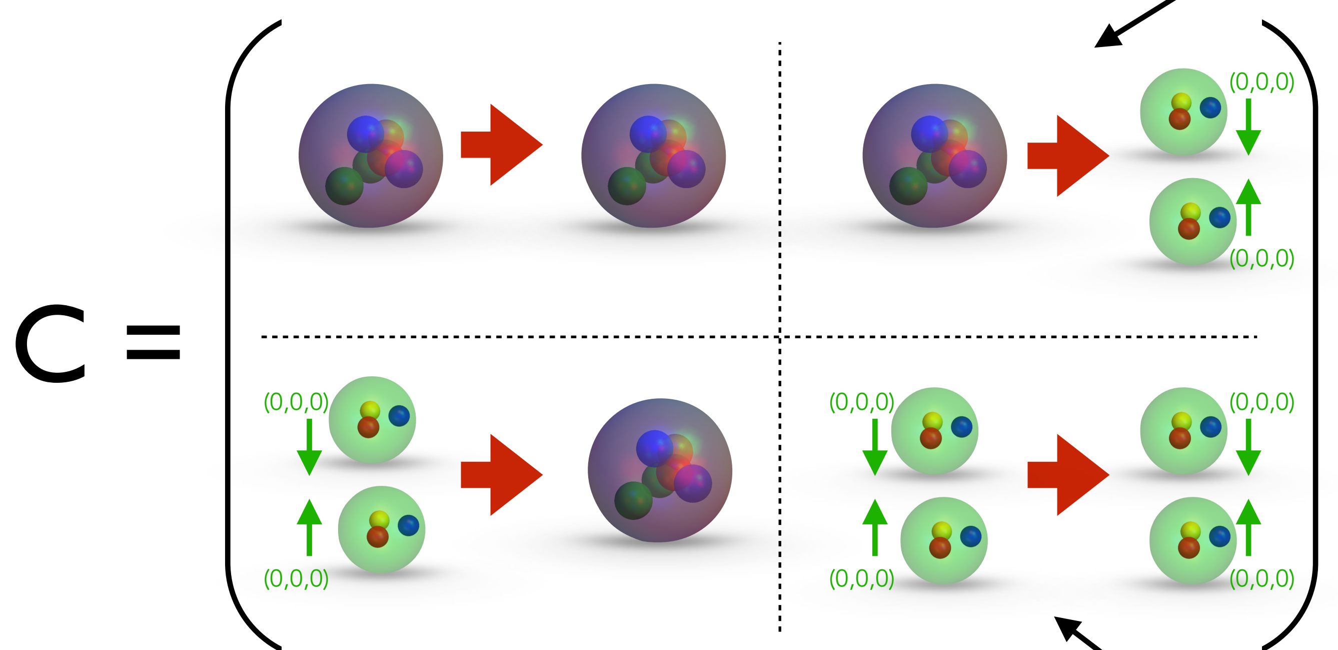
$$C_{12}(t) = \epsilon'[\exp(-E_1(t-t_0)) + \exp(-E_2(t-t_0))] + \epsilon^2 \exp(-E_0(t-t_0)) + \mathcal{O}(\epsilon^2\epsilon')$$

Model vs data

```
Exponential fits consistent with bound state
```

- Consider sub matrix of full deuteron matrix

"Sees" deep state

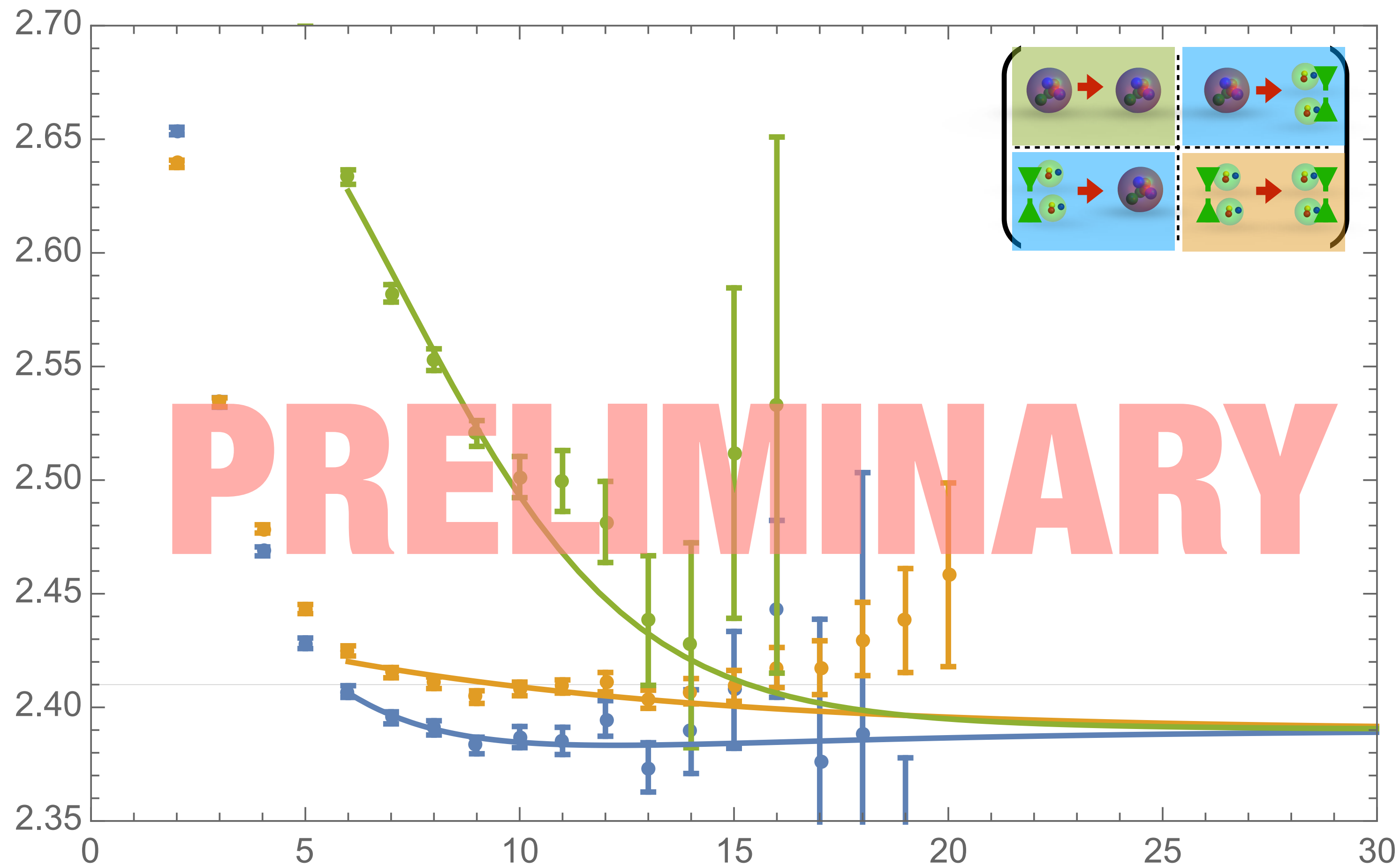


Dominates variational bound

Model vs data

Exponential fits consistent with bound state

- With larger data set, multi-exponential matrix fits work with ΔE~-20 MeV



Interpretation

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What does this all mean?
```

Conclusions are mixed

- Bounds depend on the operators used in variational set
  - Results interpreted as bounds are perfectly consistent
    - Expanding the set of operators provides more stringent bound BUT large set ≠ good set
  - Results interpreted as determination of energies have operator dependence at 20+ sigma (stats + fitting systematics)
    - A posteriori: large systematic should be assigned from operator dependence based on operators we leave out
    - What about operators we have not put in?

Interpretation

```
Two conclusions that cannot be reached currently
```

- There are bound states in the dineutron and deuteron channels
  - So far, only non-convex correlators "see" deep states
  - Multi-exponential fits to corr. matrix consistent with a bound or unbound state
  - Need a high statistics convex correlator at late times to be definitive
- There are NOT bound states in the dineutron and deuteron channels
  - This conclusion would require a basis of operators: unreachable
  - Many examples of states being missed without the "right" operators

More work is needed

```
Uncontroversial conclusion I hope
```

Adding more hexaquark operators

```
Currently working on smaller volume
```

For local hexaquark operators, a basis can be written down

- Systematically explore a tiny (but very unphysical) corner of Hilbert space!
- Hexaquark built from three diquarks [Rao and Shrock, Phys. Lett. B 116 (1982), Buchoff & Wagman PRD 93 (2016)]

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

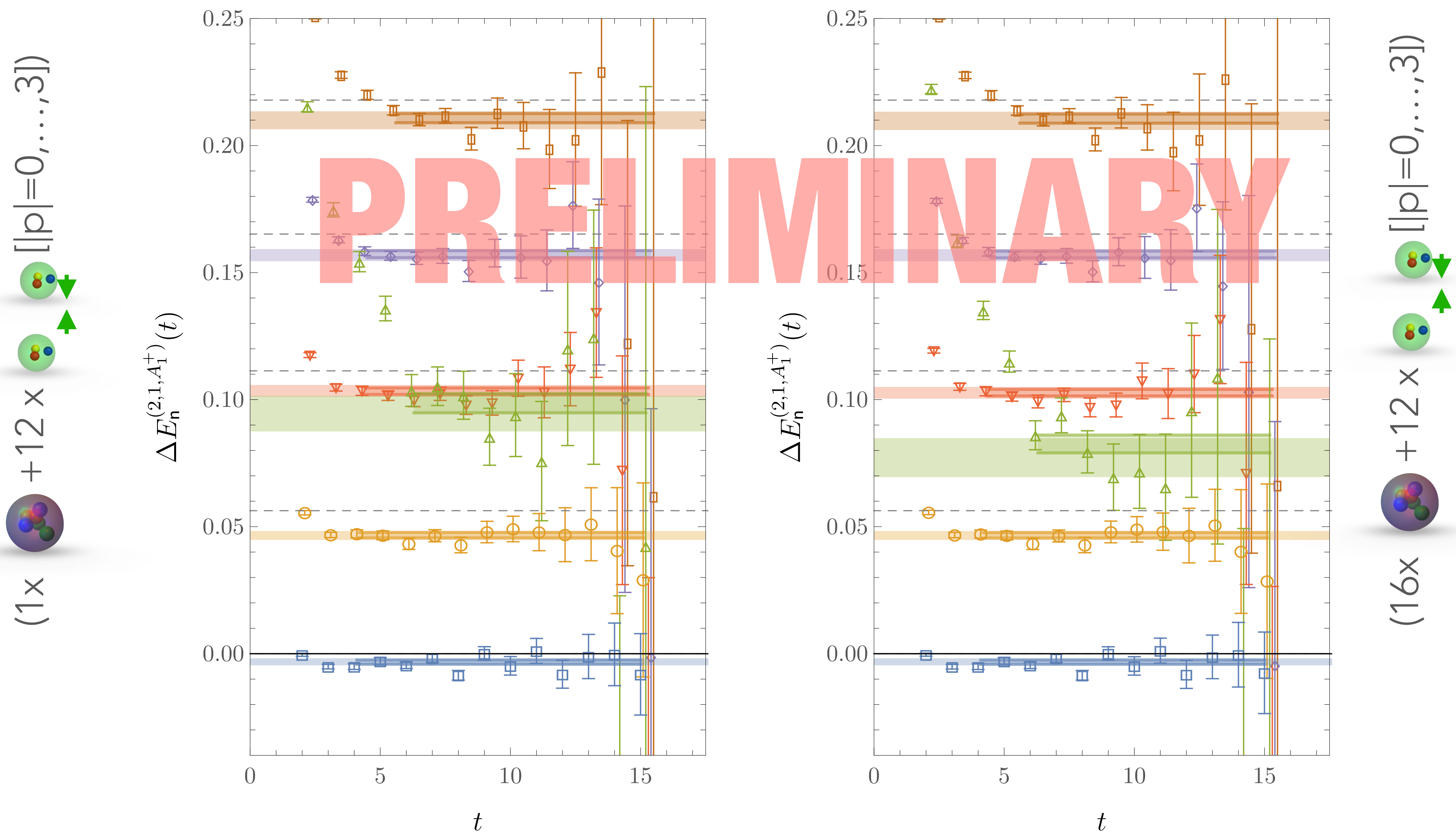
Colour x spin x flavour space =1440 possibilities

- Antisymmetry and Fierz identities reduces to 16 independent operators
- One hexaquark is baryon x baryon, others are not (hidden colour) and are much more expensive

Adding more hexaquark operators

Currently working on smaller volume

Dineutron channel (L=3.4 fm): only the extra state cares!



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