Variational study of NN systems and the H-dibaryon

Mike Wagman, FNAL ~~Phiala Shanahan, MIT~~

Saman Amarasinghe
Riyadh Baghdadi
Zohreh Davoudi
Will Detmold
Marc Illa
William Jay
Assumpta Parreño
Robert Perry
Andrew Pochinsky
Michael Wagman

NPLQCD

Image Credit: 2018 EIC User's Group Meeting

Massachusetts Institute of Technology

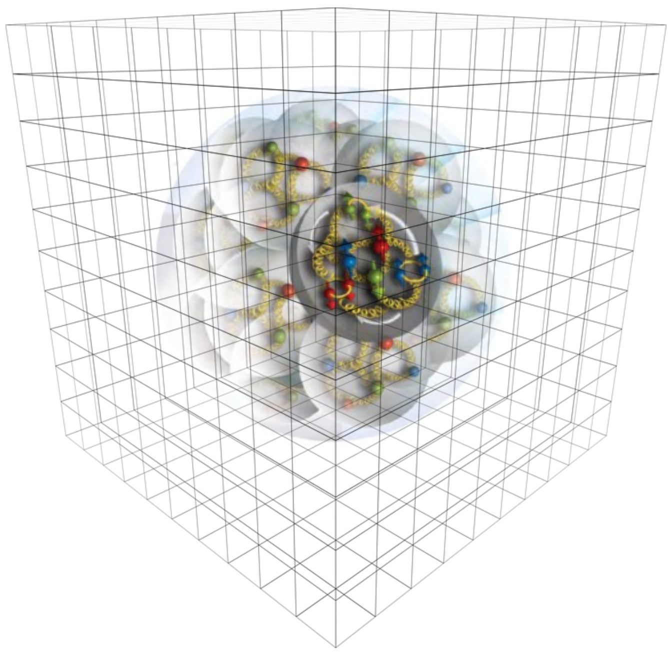
Lattice QCD for nuclear systems

LQCD calculations of nuclear matrix elements

LQCD can provide important input for both understanding the SM and constraining BSM physics (incl. MEs inaccessible in experiment)

- Electroweak reaction rates,
- Double-beta decay,
- Dark matter direct detection,
- Neutrino-nucleus scattering,
- Parton distribution functions, …

Exploratory LQCD results for nuclear matrix elements consistent with experimental results where available



195. Neutrinoless Double Beta Decay from Lattice QCD: The $n^0 n^0 \to p^+ p^+ e^- e^-$ Amplitude
Patrick Oare (MIT)
7/31/23, 4:10 PM

Systematic uncertainties are challenging

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All exisiting calculations of baryon-baryon
and larger systems are incomplete
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Challenges:

- Reaching physical quark masses (current extrapolations are coarse)
- Exponentially suppressed finite-volume effects
- *Reaching continuum limit
- Statistically noisy data
- *Excited state contamination
- Design of operators with strong overlap onto ground states

***Difficult to decouple these effects**

[Green et al., PRL 127 (2021) 242003 [2103.01054 [hep-lat]]]

H-dibaryon system: significant lattice effects that overbind relative to continuum BUT challenging data analysis

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***Difficult to decouple these effects**

Ongoing community debate:
can we isolate the ground state in calculations at $m_\pi \sim 800$ MeV

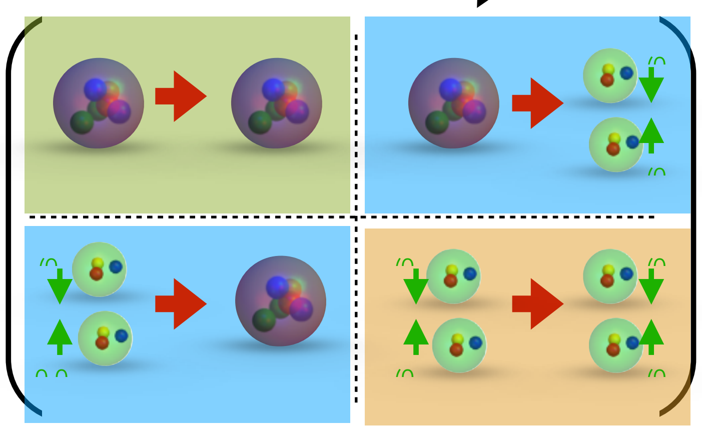
Spectroscopy

Still a challenging problem — even at $m_\pi \sim 800\,\mathrm{MeV}$

Analysis methods:

- Ratios of correlators
  (non-convex ☹️, not sum of exponentials ☹️)
- Multi-state fits to vector of correlators
  (Prony too, non-convex ☹️)
- Variational method (GEVP)
  (stochastic upper bounds on energies)
- Multi-state fits to Hermitian matrices of correlators

Matrix element calculations so far use off-diagonal correlators



First results from symmetric correlation function matrices do not see the NN bound states seen in previous calculations with asymmetric correlation functions

[Francis et al, PRD 99 (2019); Hörz et al, PRC 103 (2021); Green et al, PRL 127 (2021); Amarasinghe et al, PRD 07 (2023)]

Status (NPLQCD) at Lattice 2022

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Variational analysis with largest operator set
[Amarasinghe, PES et al., PRD 07 (2023) 094508 [2108.10835 [hep-lat]]]
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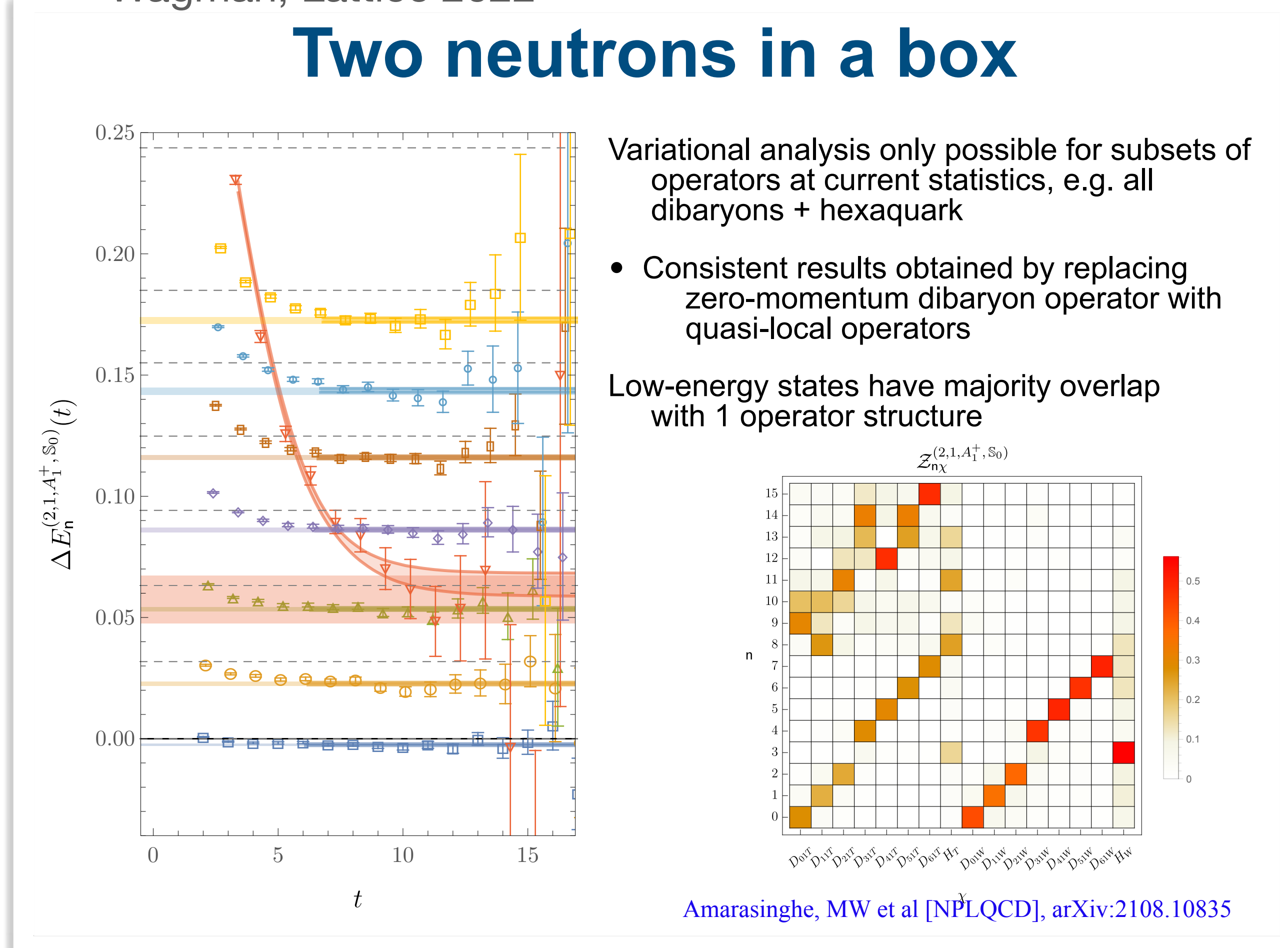
Technological improvements:

- Sparse propagators
- `tiramisu` code generator: efficient contractions

Conclusions:

- No evidence for (or against) bound states
- Interpolating-operator dependence: *You get out what you put in…*
- Additional level — what is it? D*, contaminated bound state…?

Wagman, Lattice 2022



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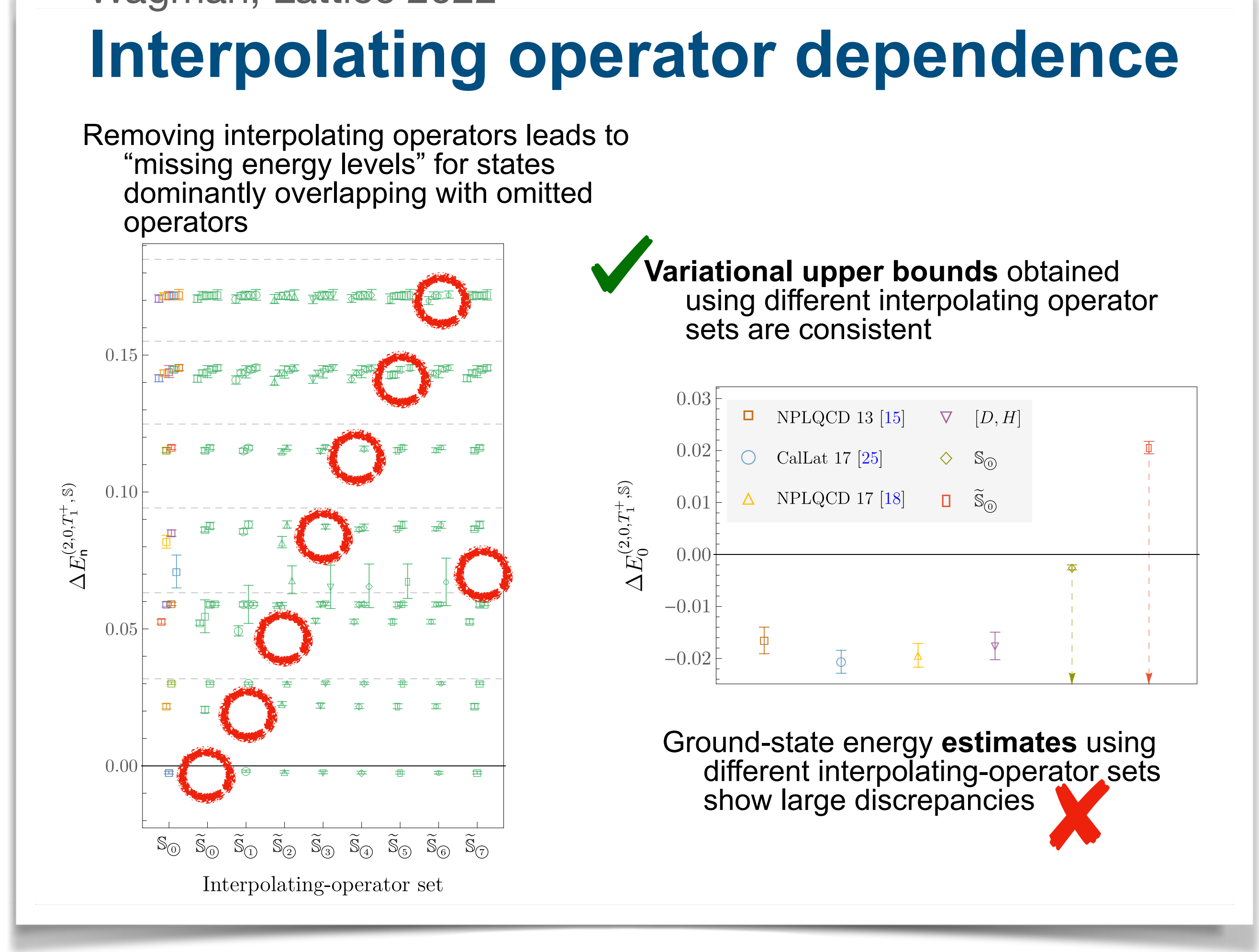


New results for Lattice 2023

Progress: expanding operator set; lighter quark masses; H-dibaryon; **no answers yet**

- **Are there bound states** at $m_\pi \sim 800$ MeV in deuteron and dineutron channels?
- **What is the 'extra state'** revealed by hexaquark operators?

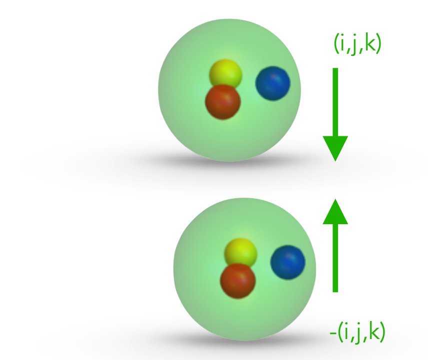
1. Continue to add more interpolating operators
   → **new results with more "hexaquark" operators**
2. Move closer to physical pion mass where we have insight from nature
   → **new results at $m_\pi \sim 170$ MeV**
3. Try to bootstrap insight down from (more precise) systems with strangeness, use $SU(3)_f$ symmetry
   → **new results for the H-dibaryon**

Interpolating operator construction

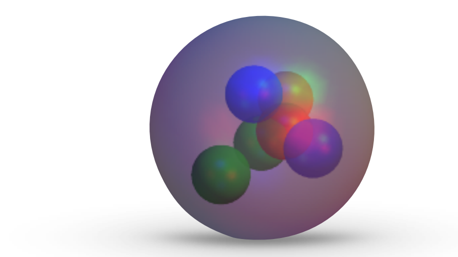
```
Do not yet know what is a “good enough” set
Nuclear physics is fine tuned: intuition beware!
```

NPLQCD interpolating operator set:

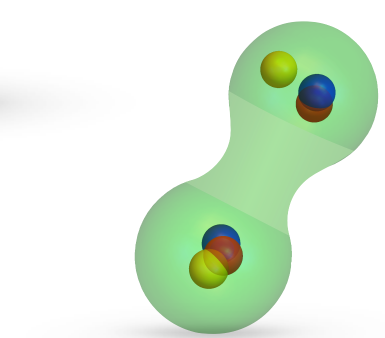
1. **Dibaryons**
   Two spatially-separated plane-wave baryons
   with relative momenta (projected to cubic irreps)



2. **Hexaquarks**
   Six Gaussian smeared quarks at a point



3. **Quasi-local**
   Two exponentially localized baryons
   NN-EFT motivated deuteron-like structure



- Zero total momentum, two different smearings at source and sink
- Operators constructed from products of baryon-blocks: efficient contractions

1. More hexaquark operators

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Systematically explore a corner of Hilbert space
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For local hexaquark operators, a basis can be written down

- Hexaquark built from three diquarks
  [Rao & Shrock, PLB 116 (1982), Buchoff & Wagman PRD 93 (2016)]

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

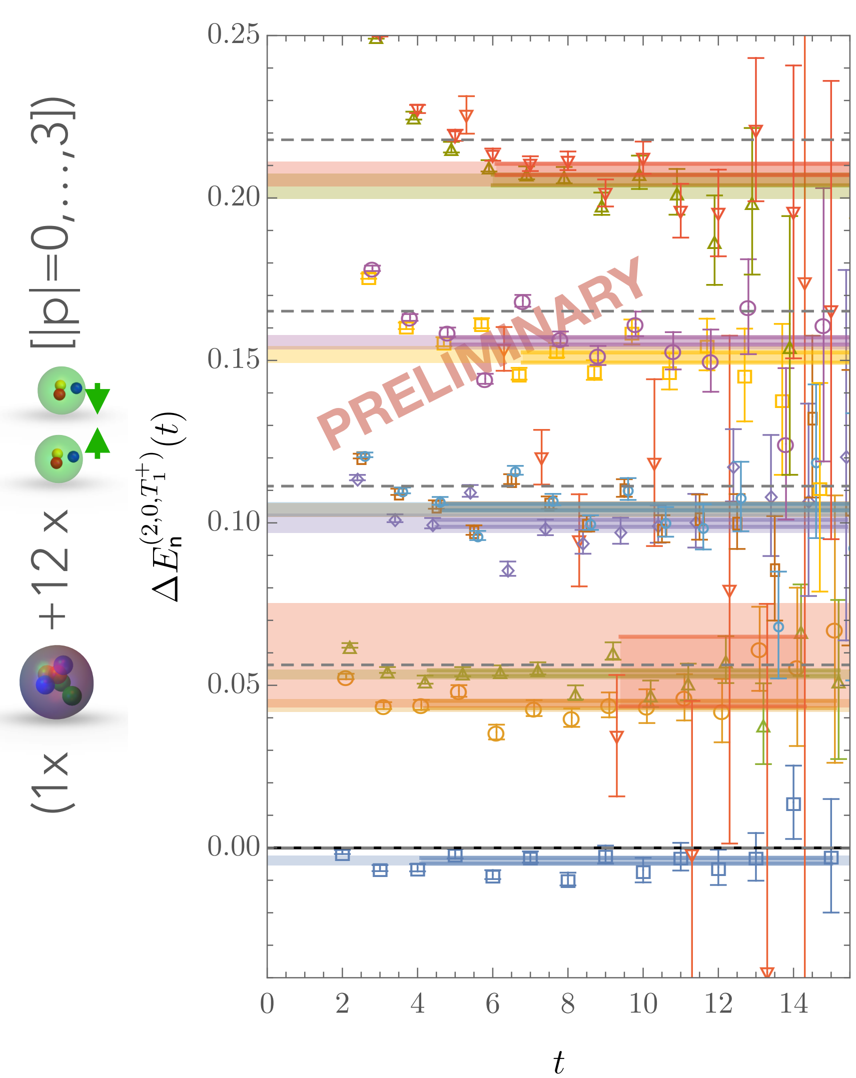
- Colour x spin x flavour space =1440 possibilities
- Antisymmetry and Fierz identities reduces to 16 independent operators
- One hexaquark (in original set of operators) is baryon x baryon,
  others are not (hidden colour) and are much more expensive

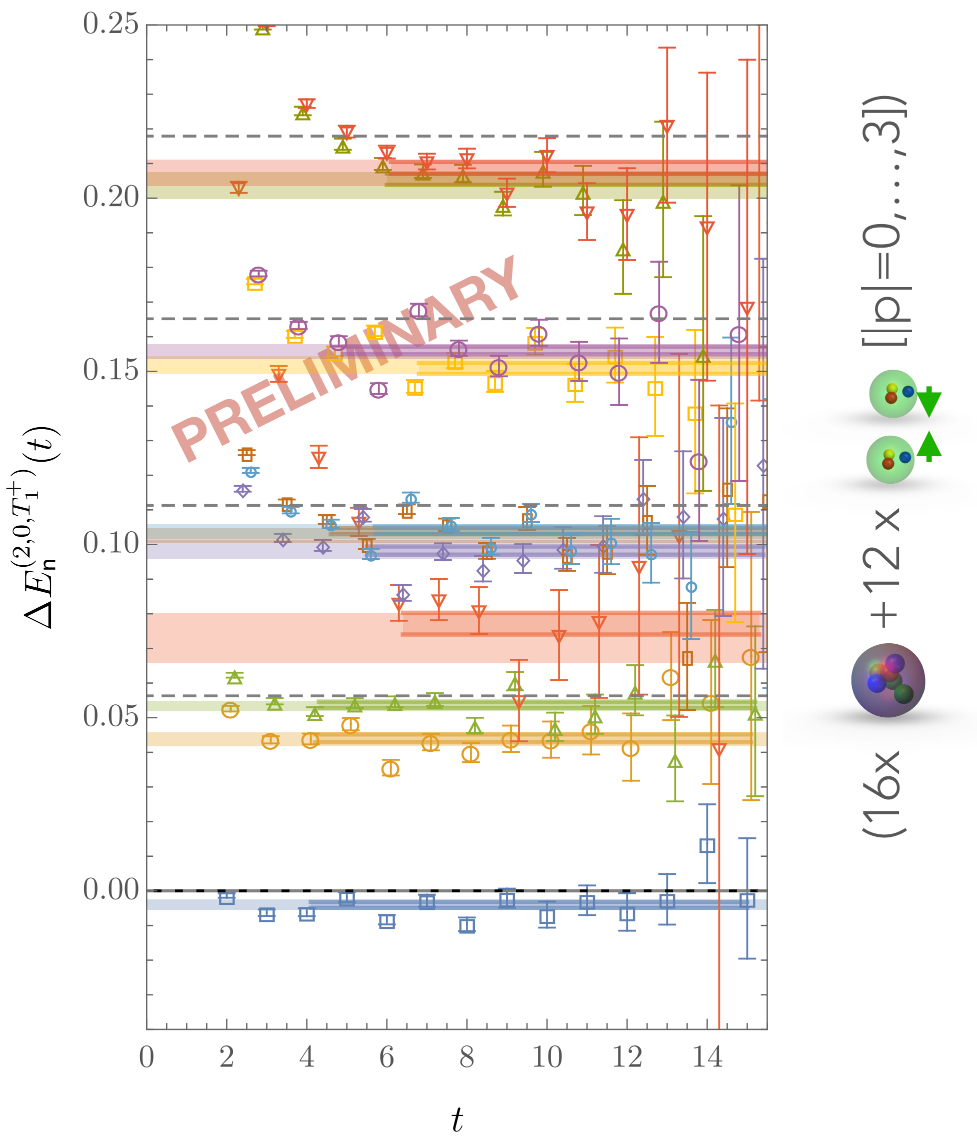
→ Calculation on a smaller lattice volume to enable systematic study

1. More hexaquark operators

“Additional level” is sensitive to new operators

Dibaryon channel $V = 48^3 \times 96$, $L = 4.4$ fm, $m_\pi \sim 800$ MeV





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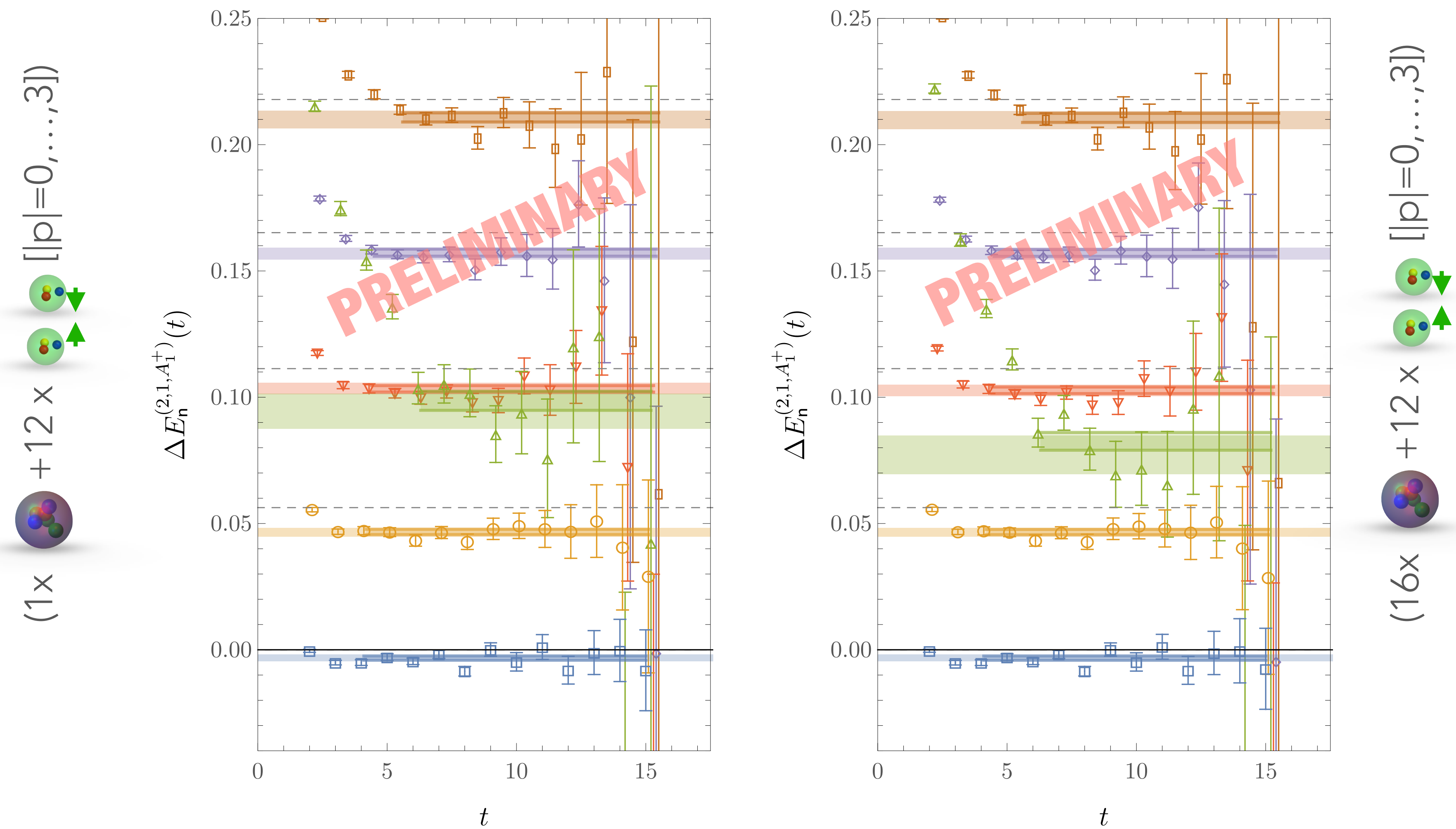


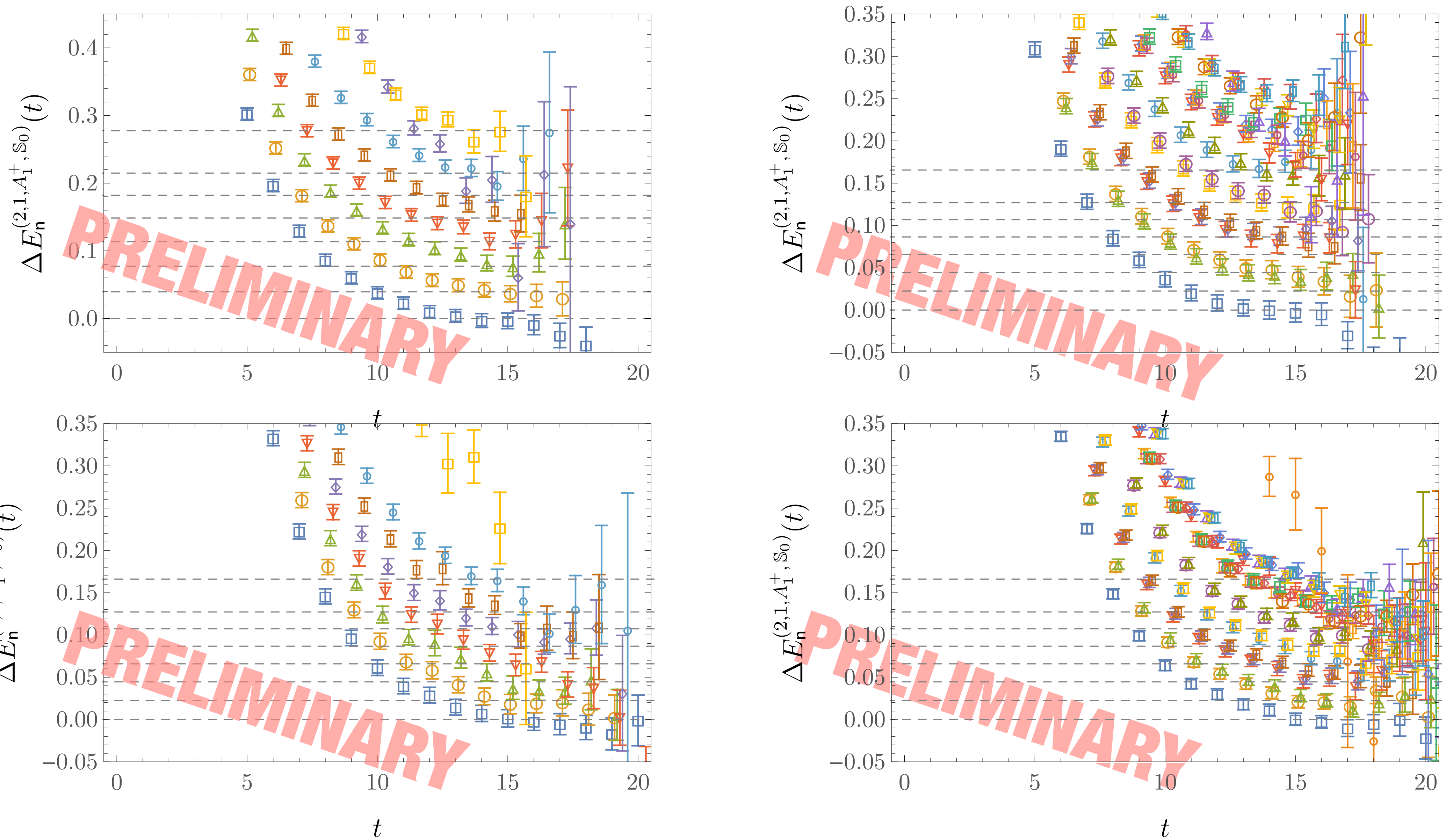
2. Spectroscopy at $m_\pi \sim 170$ MeV

Two volumes, same variational basis as $m_\pi \sim 800$ MeV

Dineutron $E_{NN}(t) - 2M_N$ **Deuteron**

$V = 48^3 \times 96$
$L = 4.4$ fm
$N_{\text{cfgs}} = 670$

$V = 64^3 \times 128$
$L = 5.8$ fm
$N_{\text{cfgs}} = 692$



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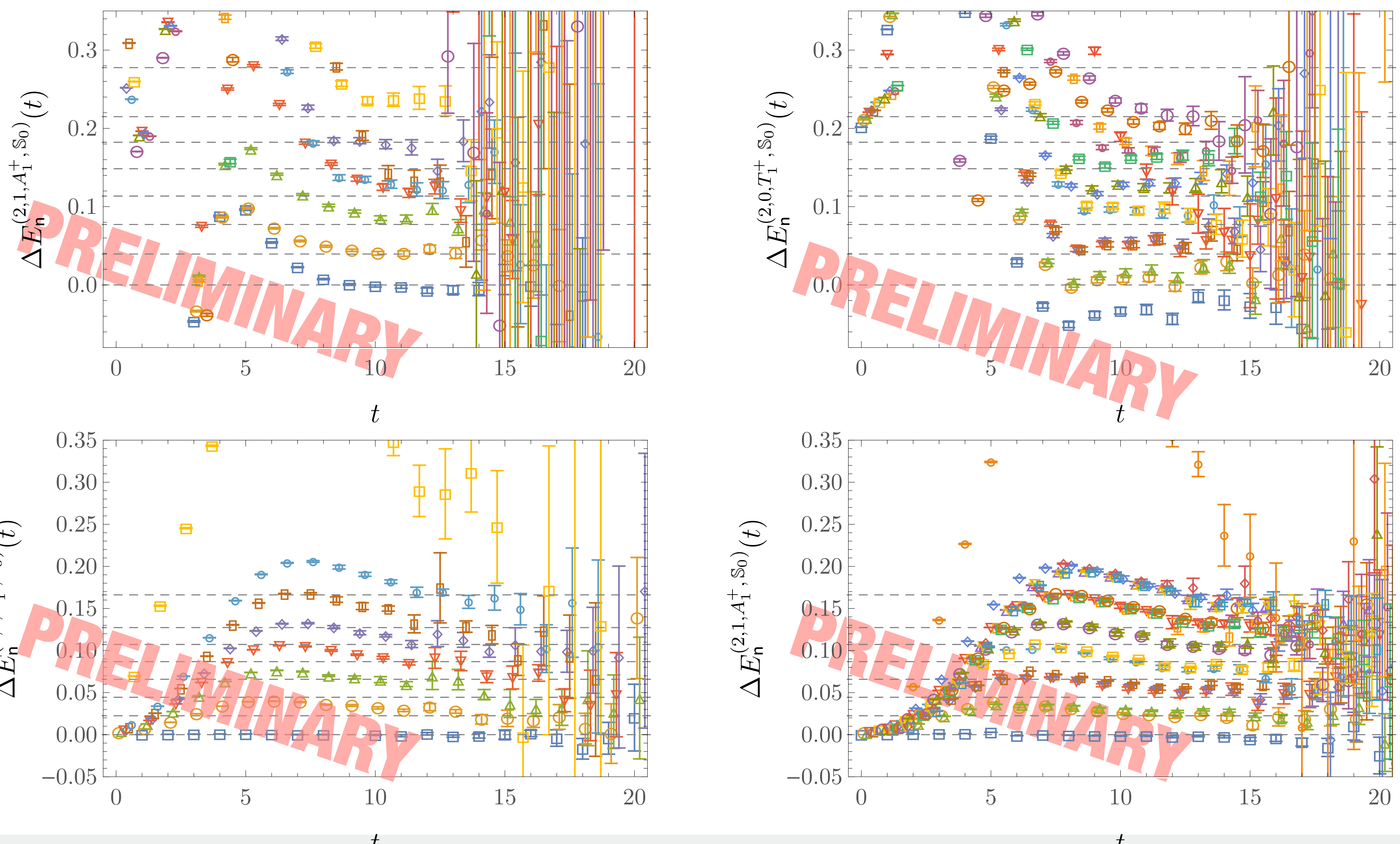

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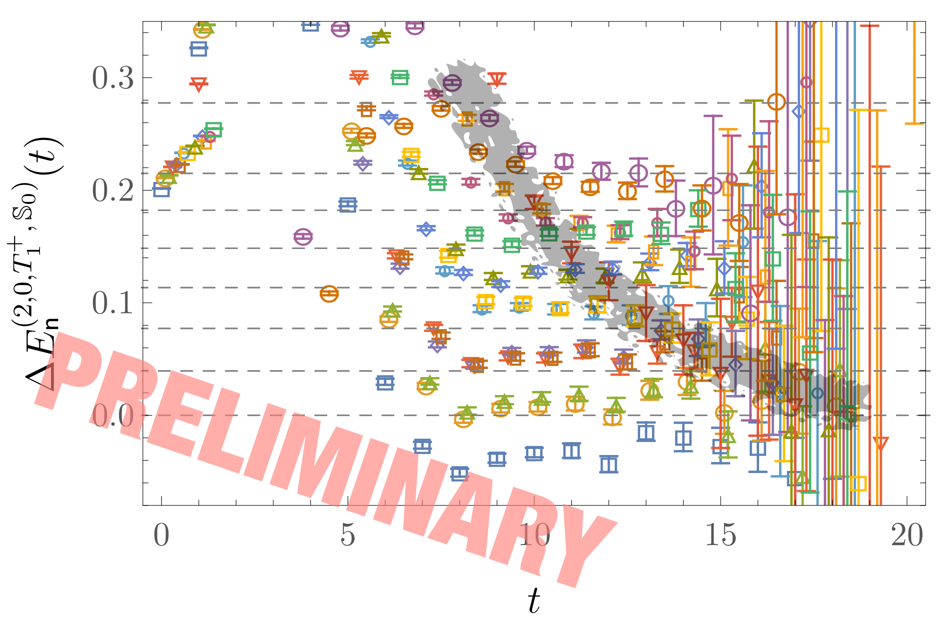


Additional "hexaquark" level as at $m_\pi \sim 800$ MeV

"Scattering" states with overlap primarily onto dibaryon operators

Qualitative conclusions as at $m_\pi \sim 800$ MeV

- No evidence for or against bound states in NN systems
- Levels sensitive to choice of interpolating operator set
- Robust existence of "extra level" with overlap onto hexaquark operators
- Additional statistics and operators required

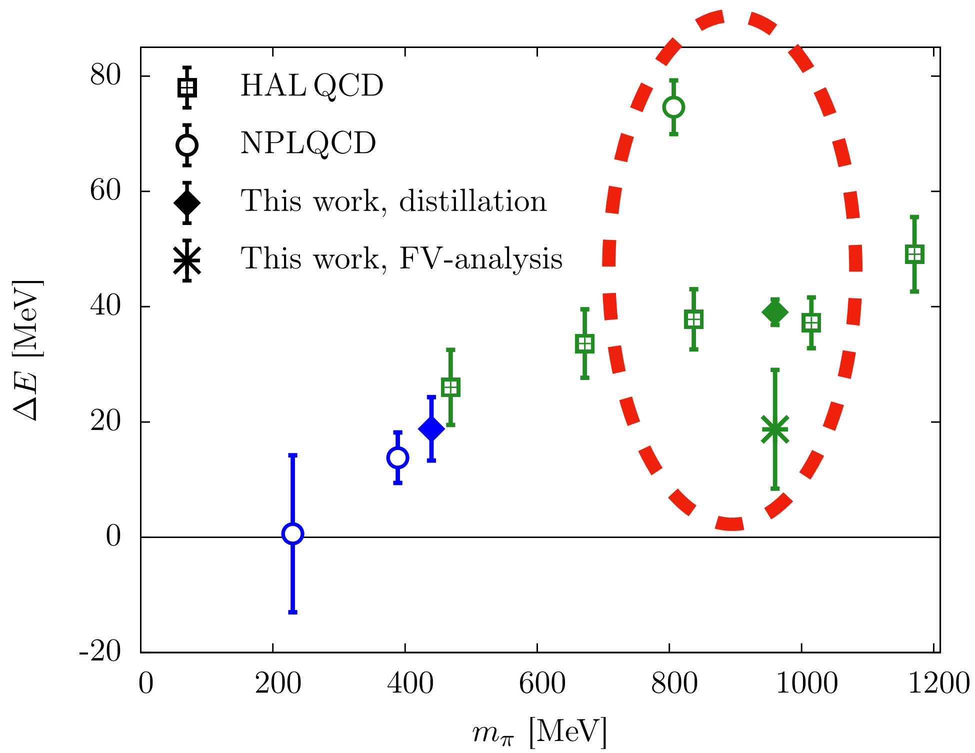
3.

The H-dibaryon

Possibly gain insight from hypernuclei, $SU(3)_f$

Potential $\Lambda\Lambda$ bound state predicted by Jaffe to be deeply bound $B_H \sim 80\,\mathrm{MeV}$
[Jaffe, PRL 38, 195 (1977)]

- Extensive experimental searches, bound from e.g., “NAGARA” event $B_H \lesssim 7\,\mathrm{MeV}$
[Takahashi et al., PRL 87, 212502 (2001); Nakazawa et al., NuclPhysA 835, 207 (2010)]
- Possible dark matter candidate (difficult to reconcile with other constraints)
[Azizi, JPhysG 47, 095001 (2020)]



[A. Francis, et al., PRD 99, 074505 (2019) [arXiv:1805.03966]]

Tensions between different LQCD calculations of H-dibaryon binding around $m_\pi \sim 800\,\mathrm{MeV}$

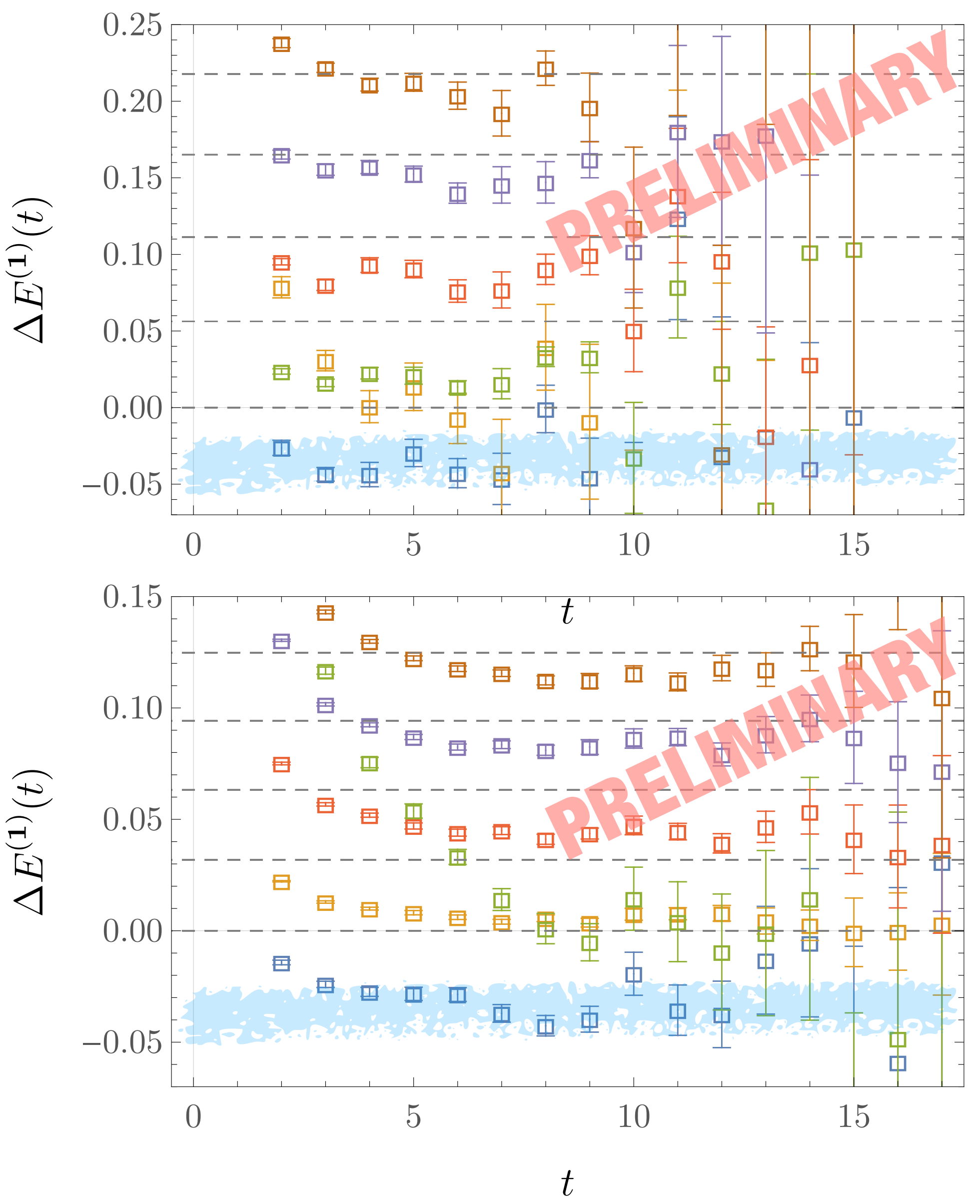
→ new variational analysis

3. H-dibaryon at $m_\pi \sim 800$ MeV

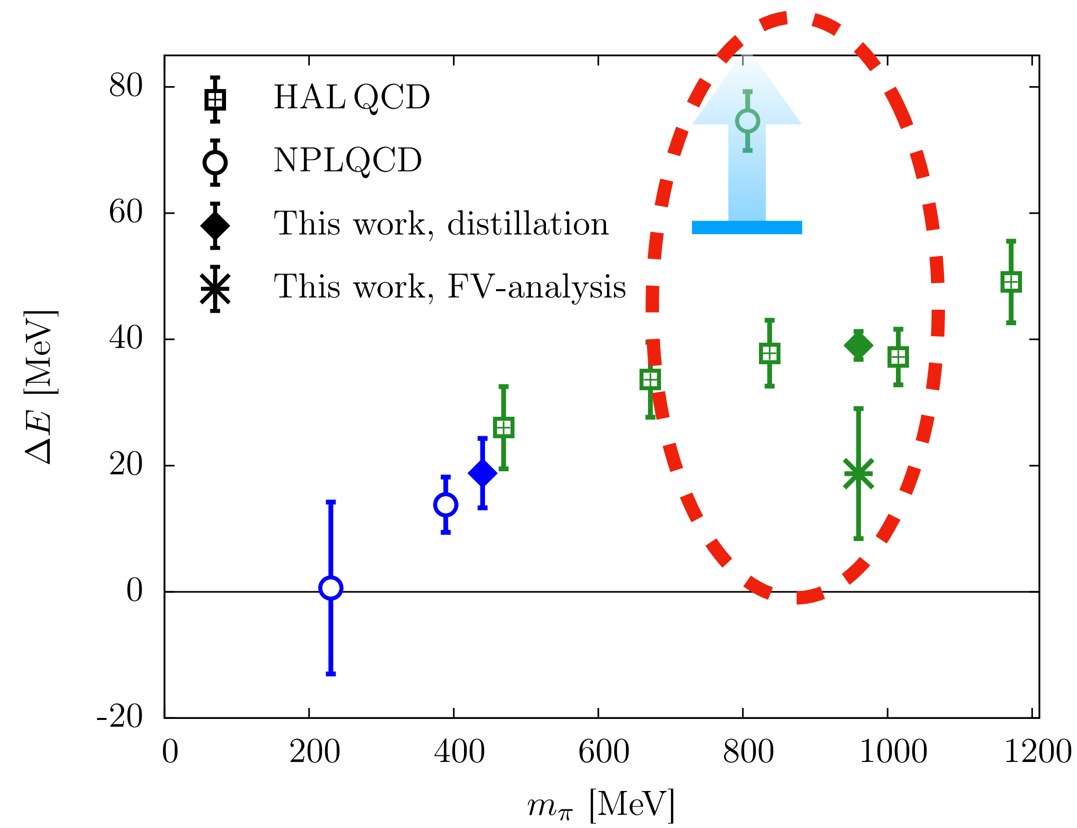
Variational analysis on two volumes

$V = 24^3 \times 48$
$L = 3.4$ fm
$N_{\text{cfgs}} = 40$

$V = 32^3 \times 48$
$L = 4.5$ fm
$N_{\text{cfgs}} = 101$



Consistent **variational bound** on **binding energy** around
$B_H \gtrsim 54$ MeV (preliminary)



Modified from [A. Francis, et al., PRD99, 074505 (2019) [arXiv:1805.03966]]

New results for Lattice 2023

Progress: expanding operator set; lighter quark masses; H-dibaryon; **no answers yet**

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New results for Lattice 2023

Progress: expanding operator set; lighter quark masses; H-dibaryon; **no answers yet**

- **Definitive existence of "extra hexaquark level" in BB spectrum that is**
  - Sensitive to interpolating operator set
  - Robust against changing lattice volume and quark masses
- **GEVP for H-dibaryon gives robust variational bound with deep binding at $m_\pi \sim 800$ MeV**
  - Consistent as a bound with early results using asymmetric correlators; interesting tensions with recent analyses

Hexaquark operators are clearly important — are we missing other critical operators?

Image Credit: 2018 EIC User's Group Meeting

Evidence about NN 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
- Extrapolated matrix elements match nature, sigma terms consistent via slope and direct calc
- GEVP analyses do not see states unless the “right” operator is included in operator set

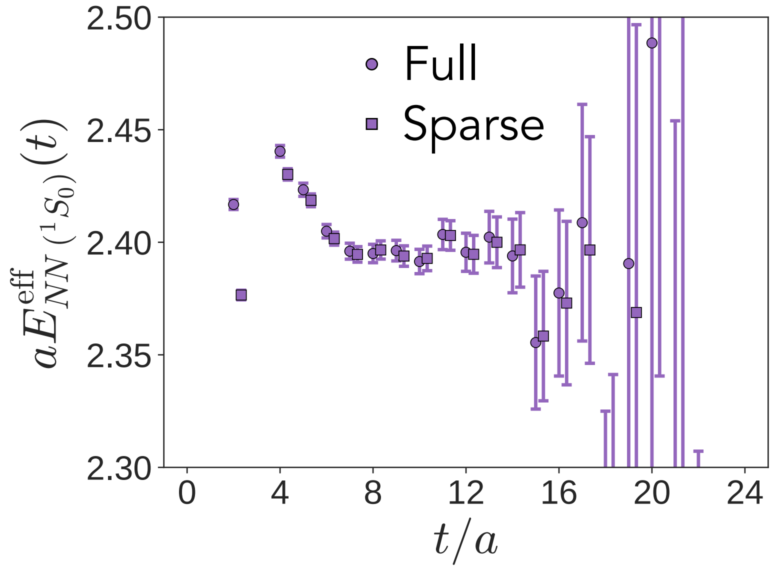
CON

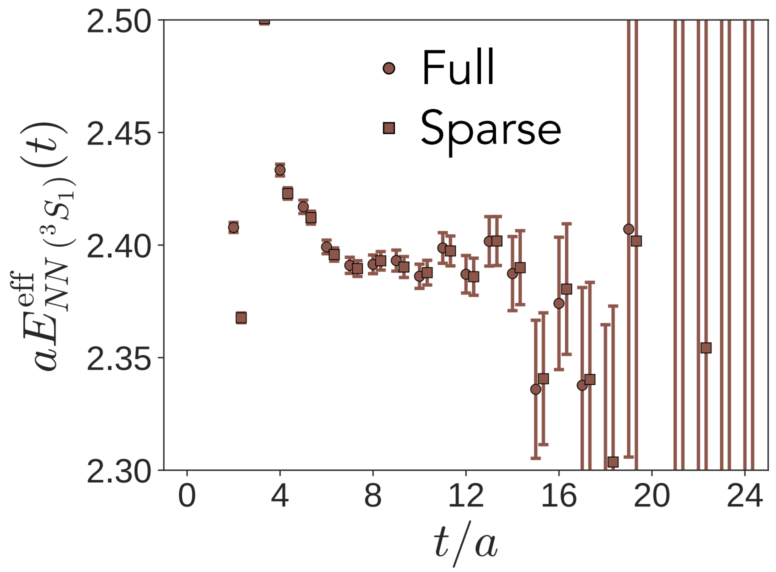
- Variational bounds from GEVP consistent with attractive threshold state [Hörz et al, NPLQCD, Green et al.]
- Consistent results with multiple lattice ensembles, spacings, quark masses etc
- Robust against some variations of operator set (but not others)
- GEVP reconstruction can approximately describe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

Sparse propagators

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

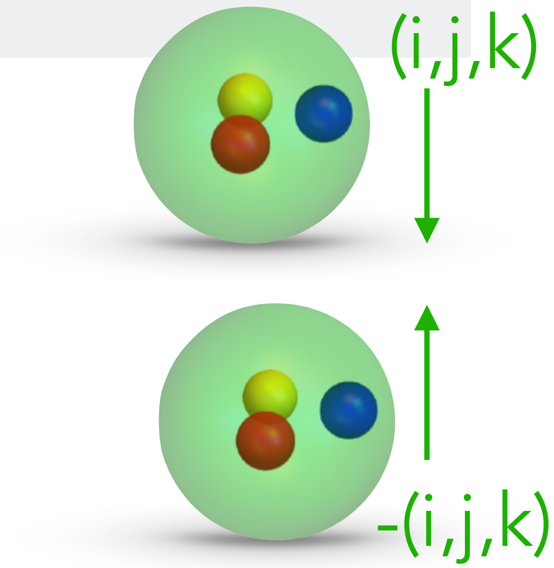
- Isotropic $\mathcal{O}(a)$ improved action: $a = 0.14$ fm, $L^3 \times T = 32^3 \times 48$, heavy SU(3) symmetric quarks
- Sparse grid of independent sources every S sites in each spatial direction (2 different smearing)
- Project propagator solutions to coarse spatial grid: timeslice-to-all $8^3 \times 48$ propagator
  - Many ways to do projection (decimation, random subset choice, convolution,…)
  - No modification of eigenstates but slightly modifies couplings to excited states
- Enables $\mathcal{O}(V^4)$ calculations





Operator construction: dibaryons

Two momentum-projected colour-singlet baryons



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

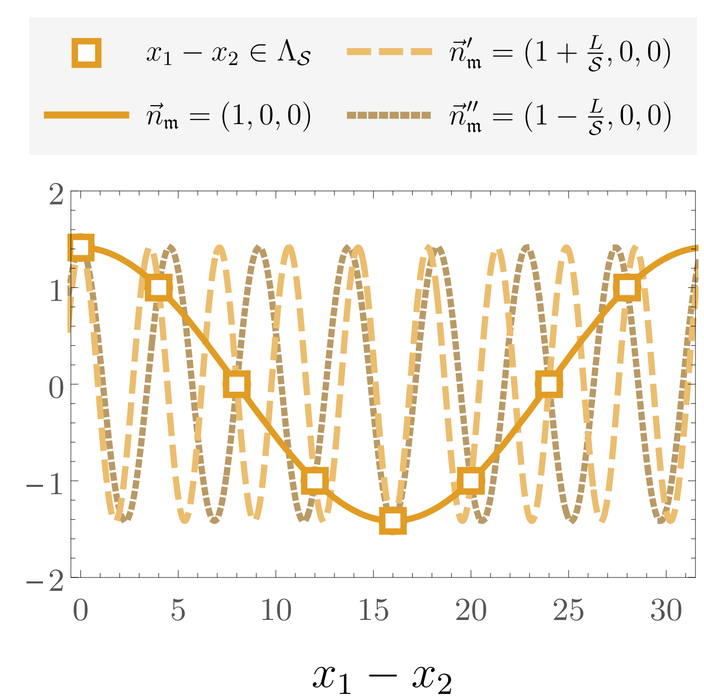
With plane-wave product wave functions

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

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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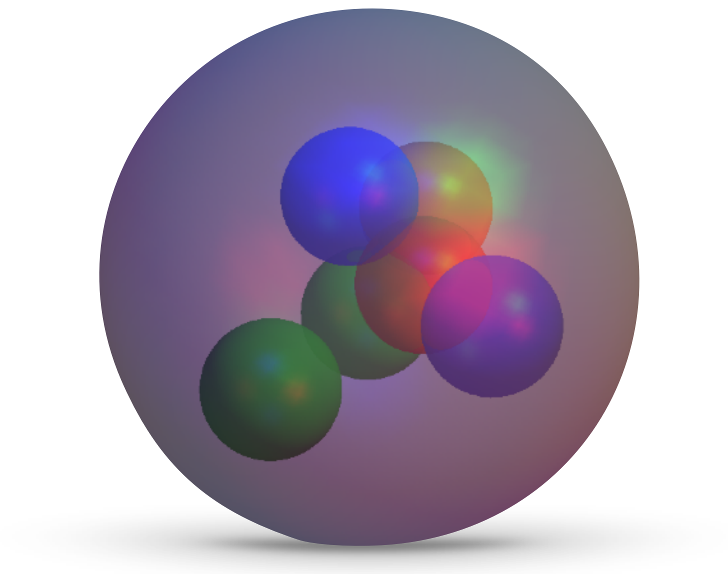
Local product of six quarks
```

Choose product of 2 colour-singlet baryons: e.g., $I = 1, S = 0$ dinucleon

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

Express nucleons in terms of quark fields:

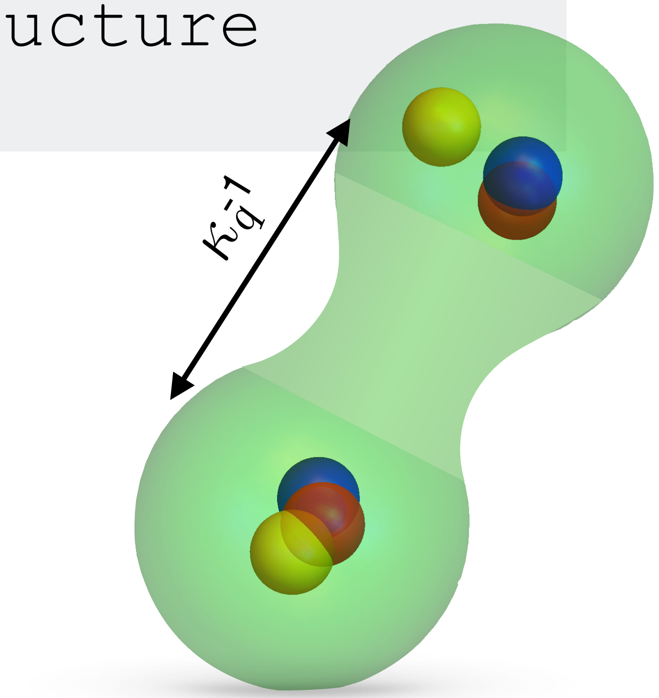
$$H_{\rho\mathfrak{c}g}(t) = \sum_{\vec{x}\in\Lambda_{\mathcal{S}}} \psi_{\mathfrak{c}}^{[H]}(\vec{x}) \sum_{\alpha} w_{\alpha}^{[H]\rho} u_g^{i(\alpha)}(\vec{x},t) d_g^{j(\alpha)}(\vec{x},t) u_g^{k(\alpha)}(\vec{x},t)$$
$$\times\, d_g^{l(\alpha)}(\vec{x},t) u_g^{m(\alpha)}(\vec{x},t) d_g^{n(\alpha)}(\vec{x},t)$$



Wavefunction specified by table of weights w

Operator construction: quasi-local

NN EFT motivated deuteron-like structure



Loosely bound system: FV EFT wavefunction

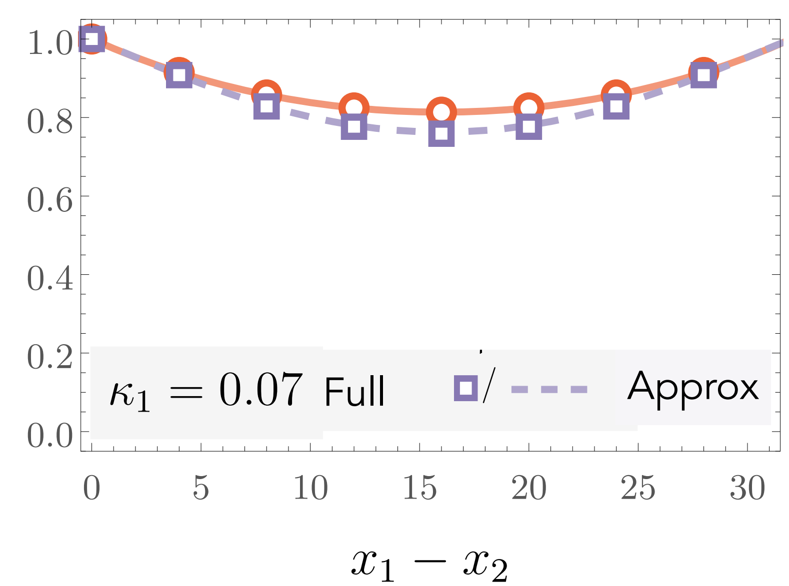
$$\sum_{\vec{n}\in\mathbb{Z}_3} e^{-\kappa|\vec{x}_1-\vec{x}_2+n\vec{L}|}\left(\frac{\mathcal{A}}{|\vec{x}_1-\vec{x}_2+\vec{n}L|}+\ldots\right)$$

Factorisable approximation is

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

Use to build operators

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



Use 3 different values of width κ_q

Fitting technology

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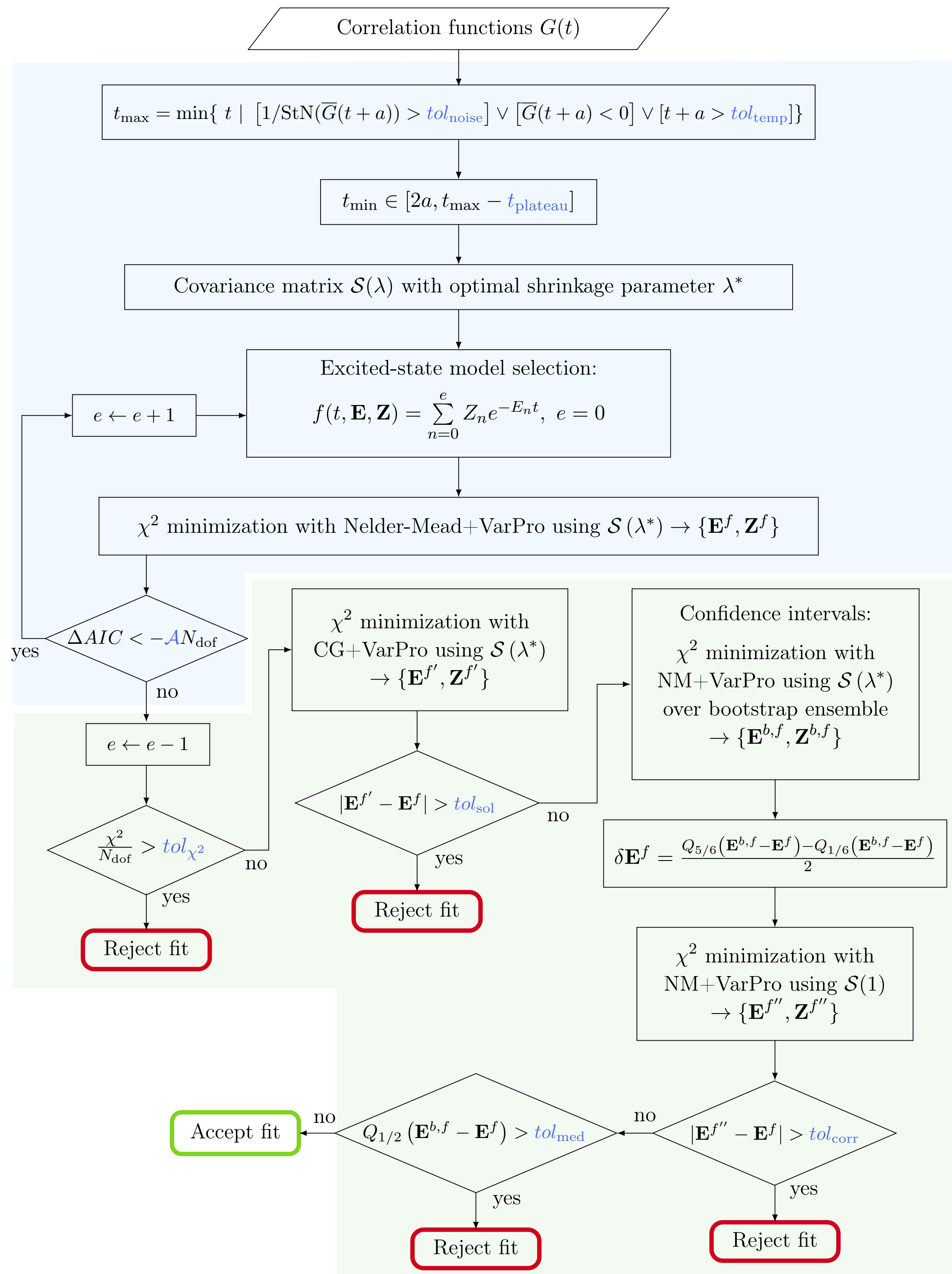
- Fits to correlators - then take correlated bootstrap differences for energy shifts
- Scan over all possible fit ranges and fit models up to 3-exp within those ranges
- Many tests of fit stability
- Final result - weighted model average

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

- 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 ground-state and Deuteron 12th level