Two-baryon interactions from lattice QCD: Towards controlling systematics

Based on work with Jeremy R. Green, Parikshit M. Junnarkar, and Hartmut Wittig
arXiv:2103.01054
arXiv:2212.09587

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Accessing and Understanding the QCD Spectra
INT 20r-2c

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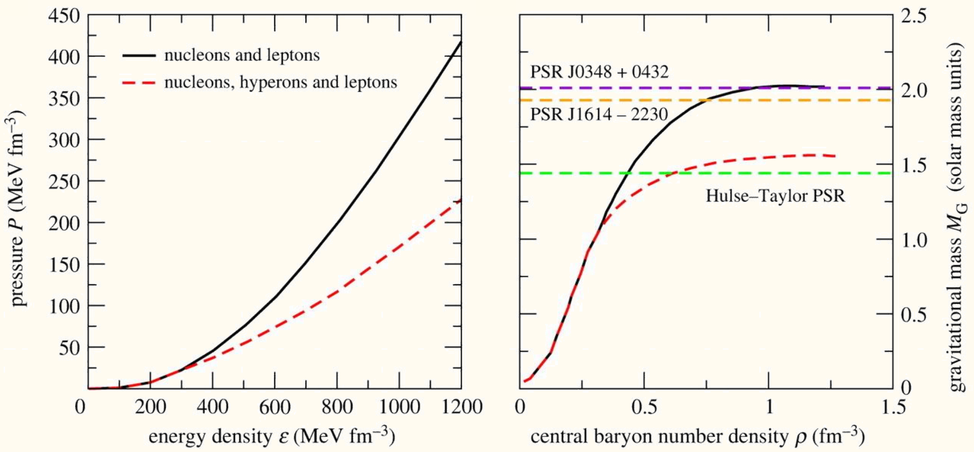
Outline

1. Why are two-baryon interactions interesting?
    - Neutron stars, H dibaryon, ...

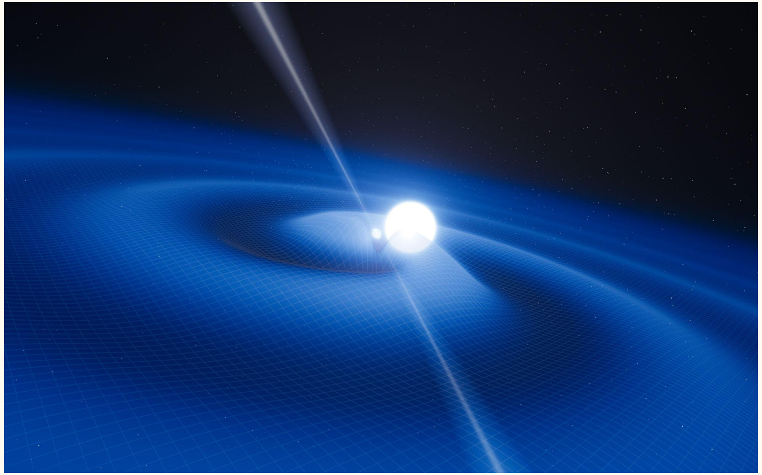
2. Modern methods for spectroscopy
    - Brief recap of Lüscher formalism
    - GEVP for controlling excited states combined with all-to-all quark propagation

3. Recent two-baryon results from lattice QCD
    - $\Lambda\Lambda$ and NN in the continuum with $m_\pi \sim 420$ MeV
    - Higher partial waves
    - Convergence of results?

Two and three-body forces in neutron stars



[D. Chatterjee, I. Vidaña *Eur. Phys. J. A.* **52** 2016] [I. Vidaña 2018 *Proc. R. Soc. A.* **474** 20180145]



[Artist's impression of the pulsar PSR J0348+0432 and its white dwarf companion, **Credit:** ESO/L. Calçada, https://www.eso.org/public/images/eso1319c/]

- High densities in neutron stars make hyperons energetically favorable
- Inclusion of hyperons leads to a softer equation of state, in contradiction with observation
- Two- and three-hadron interactions involving hyperons may supply the needed repulsion
- Constraints can be provided from lattice QCD

Jaffe predicts a deeply-bound H dibaryon

- Jaffe predicts a deeply bound $\Lambda\Lambda$, $SU(3)_f$ singlet with $J^P = 0^+$ ($B_H = 80$ MeV)
  [R. Jaffe, Phys.Rev.Lett. 38 (1977) 195-198]

- "NAGARA" event provides strongest constraint from experiment

$$\text{A:}\quad {}^{12}\text{C} + \Xi^- \to {}^{\;\;6}_{\Lambda\Lambda}\text{He} + {}^4\text{He} + t$$

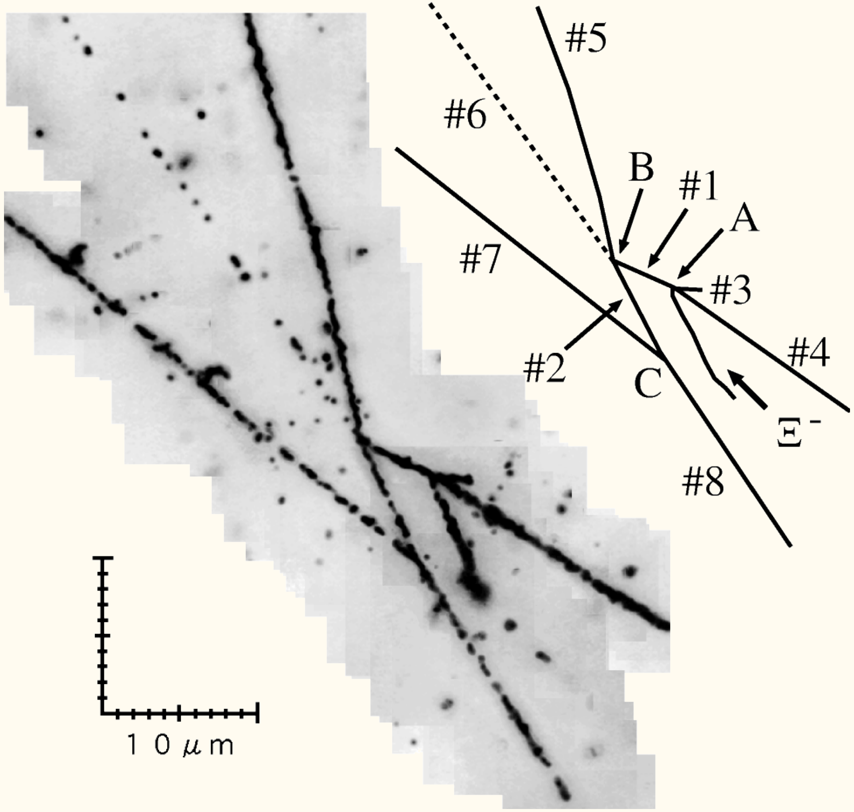
$$\downarrow$$

$$\text{B:}\quad {}^{\;\;6}_{\Lambda\Lambda}\text{He} \to {}^{5}_{\Lambda}\text{He} + p + \pi^-$$

$$m_H > 2m_\Lambda - B_{\Lambda\Lambda}$$

$$B_{\Lambda\Lambda} = 6.93 \pm 0.16 \text{ MeV}$$

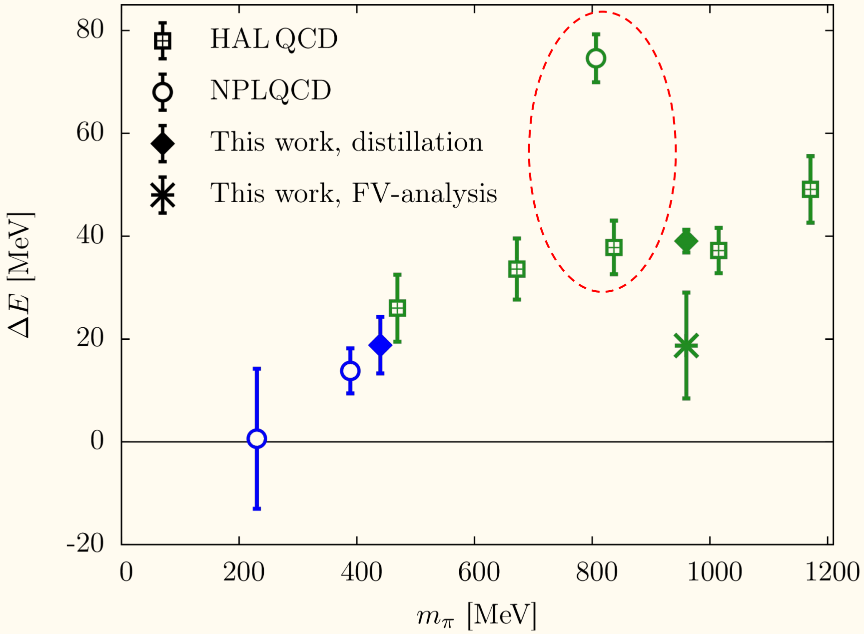
$\Rightarrow$ upper limit of binding energy $\sim$ 7 MeV



[H. Takahashi *et al.*, *Phys.Rev.Lett.* 87 (2001) 212502]

Status of the H dibaryon

- Various models give wide range of masses for the H dibaryon
- There also exists a discrepancy from different lattice calculations
  - HAL QCD method vs. Lüscher method
- Unaccounted for systematics must be the culprit
  - Excited state contamination?
  - Finite lattice spacing?
- Crucial to understand this
  - Multi-baryon matrix elements require it
  - Dark matter candidate or not?
    [K. Azizi, J.Phys.G 47 (2020) 9, 095001]



[A. Francis, *et al.*, *Phys.Rev.D* 99 (2019) 7, 074505 · arXiv:1805.03966]

Lüscher two-particle formalism

Compact formula for quantization condition

$$\det\left[F(E_2,\mathbf{P},L)^{-1}+\mathcal{K}_2(E_2^*)\right]=0$$

E_2 - finite-volume energies

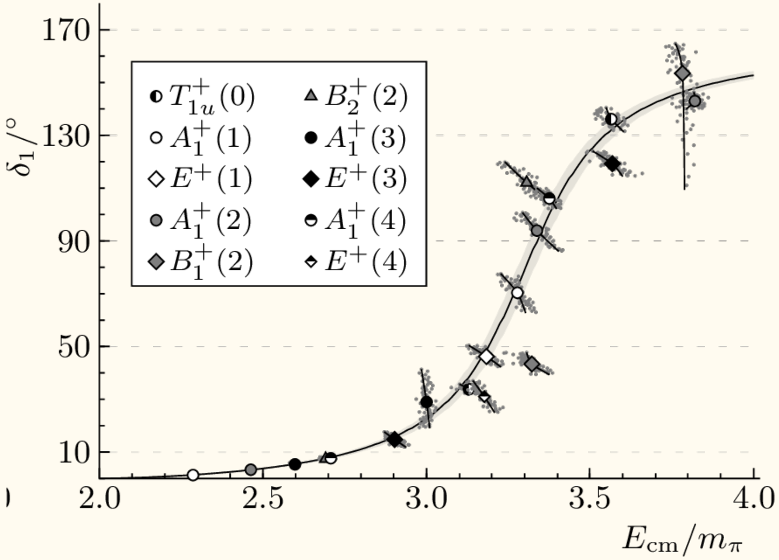
$\mathcal{K}_2$ - 2-to-2 K-matrix

F - known geometric function

Caveats:

- truncated at some max ℓ
- ignores exponentially small contributions
- valid up to 3 (or 4) particle threshold
- only valid above t-channel cut [arXiv:2301.03981]
- assumes continuum energies [arXiv:1912.04425]

$I=1$ π-π P-wave scattering phase shift



[C. Andersen, *et al.*, *Nucl.Phys.B* 939 (2019) 145]

Energies from two-point correlators

- In principle, one can extract all desired energies from two-point correlators

$$C(t) = \langle 0|\mathcal{O}_{\text{snk}}(t)\mathcal{O}^{\dagger}_{\text{src}}(0)|0\rangle$$
$$= \sum_{n=0}^{\infty} \langle 0|\mathcal{O}_{\text{snk}}|n\rangle\langle 0|\mathcal{O}_{\text{src}}|n\rangle^{*} e^{-E_n t}$$

- Correlator asymptotes to ground state at large time separation

$$E^{\text{eff}}(t) \equiv -\frac{1}{\Delta t}\ln\left(\frac{C(t+\Delta t)}{C(t)}\right)$$

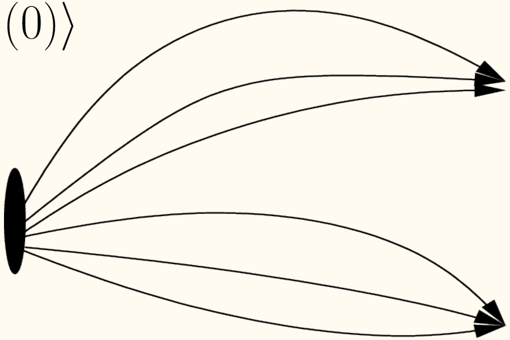
- Look for plateau in effective energy to indicate ground state saturation
  - Approach can be non-monotonic if sink and source operators are not the same

- Typical interpolator for two-baryon states

$$\mathcal{O} \sim \sum_{\vec{x}_1,\vec{x}_2} e^{-i\vec{p}_1\cdot\vec{x}_1} e^{-i\vec{p}_2\cdot\vec{x}_2}\, qqq(\vec{x}_1)qqq(\vec{x}_2)$$

- Use of point-to-all quark propagation requires a completely local operator at the source

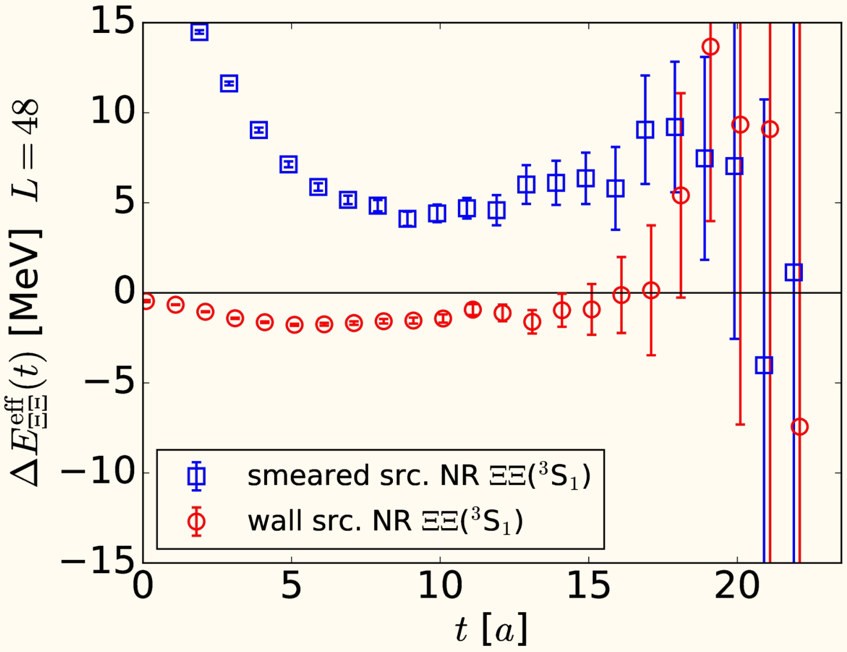
$$\langle BB(t)H^{\dagger}(0)\rangle$$



[A. Francis, J. R. Green, P. M. Junnarkar, Ch. Miao, T. D. Rae, H. Wittig, *Phys.Rev.D* 99 (2019) 7, 074505]

What’s going wrong?

- Different methods
  - HAL QCD method vs. Lüscher method
- Signal-to-noise ratio $\propto e^{-(m_B - 3m_\pi/2)t}$ makes this problem challenging
- Possible systematics
  - Truncation of derivative expansion (HAL QCD method)
  - Misidentified plateau for energies or incomplete operator basis (Lüscher method)
  - Discretization effects



[Takumi Iritani et al., *JHEP 10*, 101 (2016)]

Variational Method to Extract Excited States

Form $N \times N$ correlation matrix, which has the spectral decomposition

$$C_{ij}(t) = \langle \mathcal{O}_i(t)\, \mathcal{O}_j^\dagger(0) \rangle = \sum_{n=0}^{\infty} Z_i^{(n)}\, Z_j^{(n)*}\, e^{-E_n t} \qquad Z_j^{(n)} = \langle 0 | O_j | n \rangle$$

Solve the following eigenvector problem (equivalent to a generalized eigenvalue)

$$\hat{C}(\tau_D) = C(\tau_0)^{-1/2}\, C(\tau_D)\, C(\tau_0)^{-1/2}$$

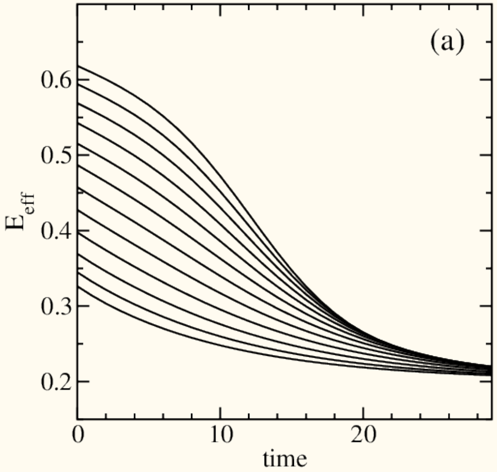
And use the eigenvectors to rotate $\hat{C}(t)$ at all other times

If τ_0 is chosen sufficiently large, then eigenvalues $\lambda_n(t, \tau_0)$ behave as

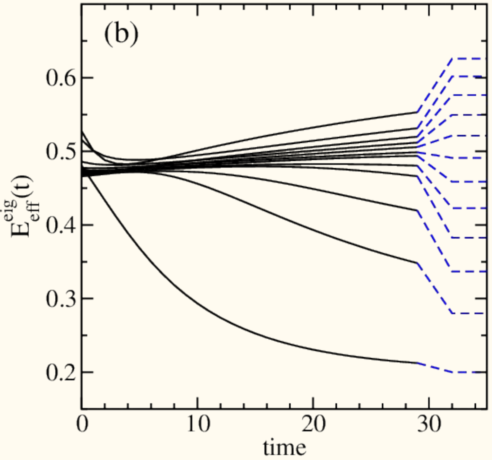
$$\lambda_n(t, \tau_0) \propto e^{-E_n t} + O(e^{-(E_N - E_n)t})$$

[*Nucl.Phys.B* 339, 222 (1990)]
[*JHEP 04*, 094 (2009)]

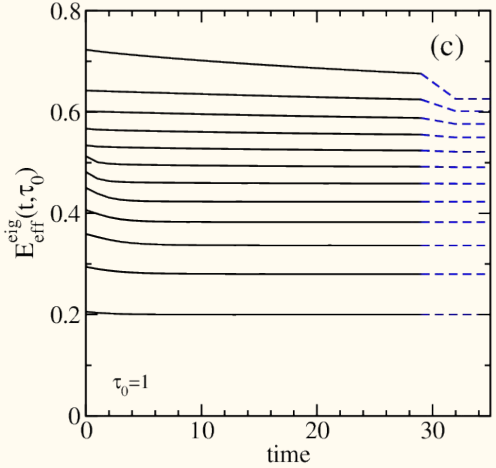
Correlator matrix toy model



Diagonal elements of C(t)



Eigenvalues of C(t)



Generalized eigenvalues of C(t)

$$E_n = E_{n-1} + \frac{0.08}{\sqrt{n}}, \qquad n = 1, 2, \ldots, 199\ , \qquad E_0 = 0.20, \qquad\qquad Z_j^{(n)} = \frac{(-1)^{j+n}}{1 + 0.05(j-n)^2}$$

[Plots courtesy of Colin Morningstar]

Extraction of energy shifts

- Fit ratio of diagonalized correlator

$$R_n(t) \equiv \frac{v_n^\dagger(\tau_0,\tau_D)\, C(t)\, v_n(\tau_0,\tau_D)}{C_\Lambda^{\vec{p}_1}(t)\, C_\Lambda^{\vec{p}_2}(t)}$$

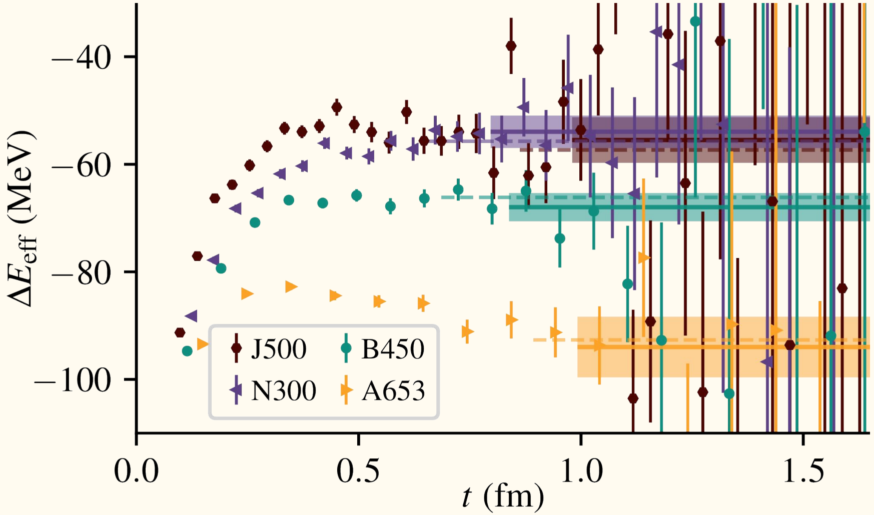
$$\lim_{t\to\infty} R_n(t) \propto e^{-\Delta E_n t}$$

- Leads to partial cancellation of correlated fluctuations and residual excited states

- Should wait until single-baryon correlators have plateaued

- Use alternative spectrum for systematics

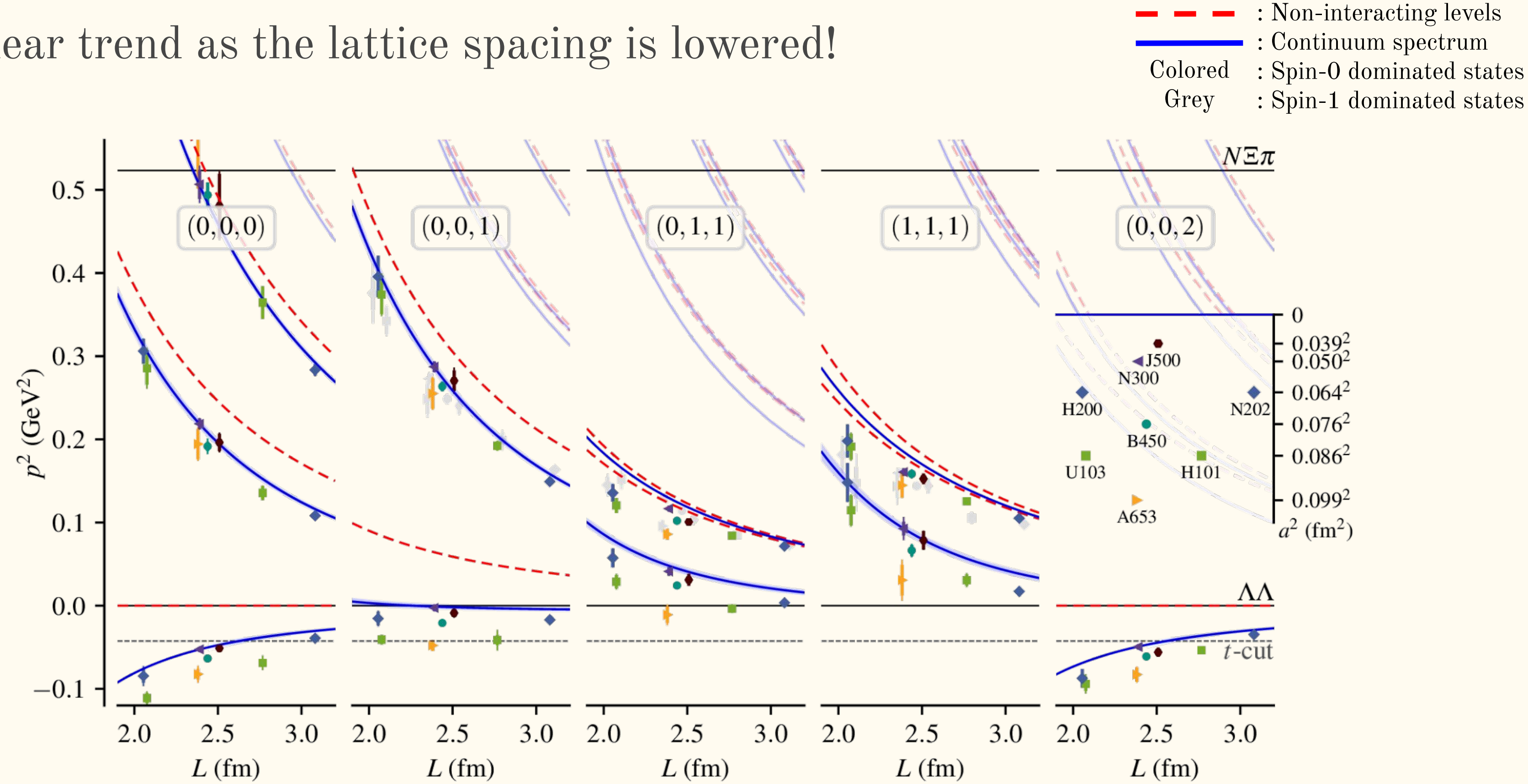
Effective energy difference for *Λ(1)Λ(0)* (singlet) ground state, using ensembles with similar volumes.



[J. R. Green, **ADH**, P. M. Junnarkar, H. Wittig, *Phys.Rev.Lett.* 127 (2021) 24, 242003]

$\Lambda\Lambda$ (singlet) spectrum, $m_\pi \sim$ 420 MeV

Clear trend as the lattice spacing is lowered!



[J. Green, **ADH**, P. Junnarkar, H. Wittig, *Phys.Rev.Lett.* 127 (2021) 24, 242003]

Two-baryon interactions in the continuum

- Quantization condition assumes continuum energies
- Red path more theoretically sound approach, but practically difficult
- Blue path much simpler: modify fit parameters to include lattice spacing dependence
    - Formalism for modification of QC within a toy model [arXiv:1912.04425]

$$\begin{tikzcd}
E(L,a) \arrow[r, "\text{lattice quantization?}"] \arrow[d, "a \to 0"'] & \delta(p^2,a) \arrow[d, "a \to 0"] \\
E(L) \arrow[r, "\text{continuum quantization}"'] & \delta(p^2)
\end{tikzcd}$$

[Ch. 16 of *Few Body Syst.* 63 (2022) 4, 67]

H-dibaryon combined phase shift fits

- Perform combined fits to the data (blue path)

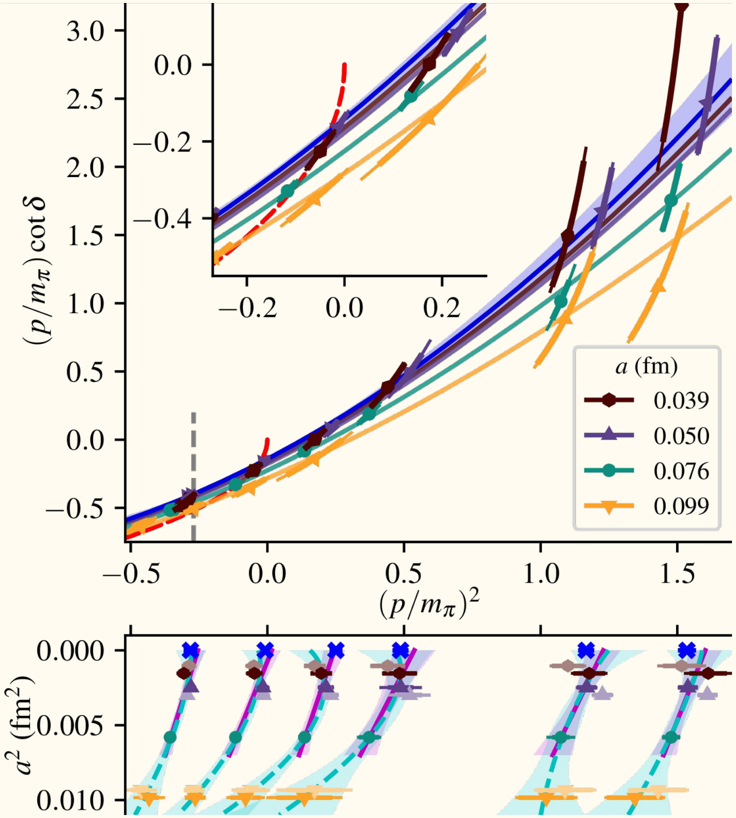
$$p \cot \delta(p) = \sum_{i=0}^{N-1} c_i \, p^{2i}, \quad c_i = c_{i0} + c_{i1} a^2$$

$$\chi^2 \equiv \sum_{i,j} \frac{(p_i^2 - p^2_{\mathrm{q.c.},i})(p_j^2 - p^2_{\mathrm{q.c.},j})}{\Sigma^{\mathrm{stat}}_{ij} + \Sigma^{\mathrm{syst}}_{ij}} \; , \quad \Sigma^{\mathrm{syst}}_{ij} = (\delta p^2)_i (\delta p^2)_j$$

- Continuum limit of energies first (red path)
  - Shift to a target volume L^*

$$p^2(L^*) \approx p^2(L) + p^2_{\mathrm{q.c.}}(L^*) - p^2_{\mathrm{q.c.}}(L)$$

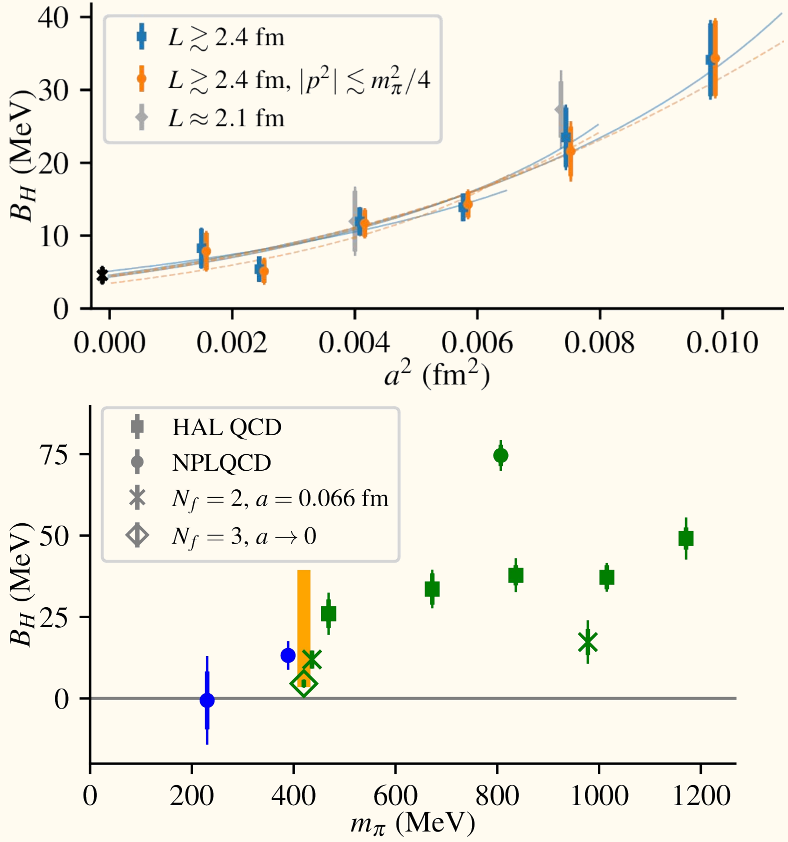
  - Coarsest ensemble prefers $O(a^3)$ term



[J. R. Green, **ADH**, P. M. Junnarkar, H. Wittig, *Phys.Rev.Lett.* 127 (2021) 24, 242003]

The H dibaryon binding energy

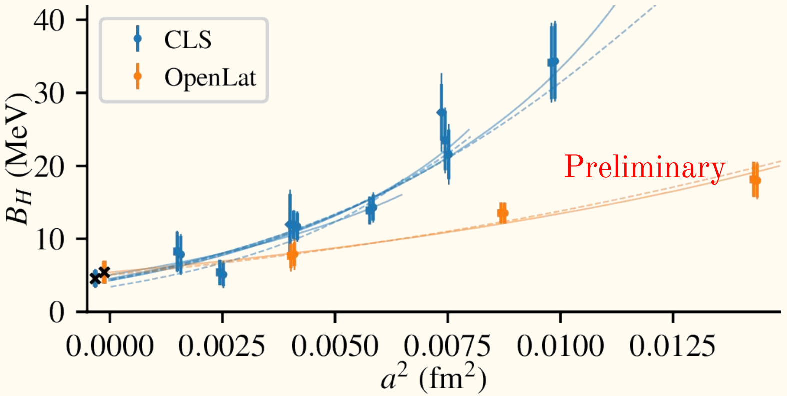
- From the phase shift, the binding energy of two Λ baryons can be determined
- Large dependence on the lattice spacing was found
- Does this explain the discrepancy?



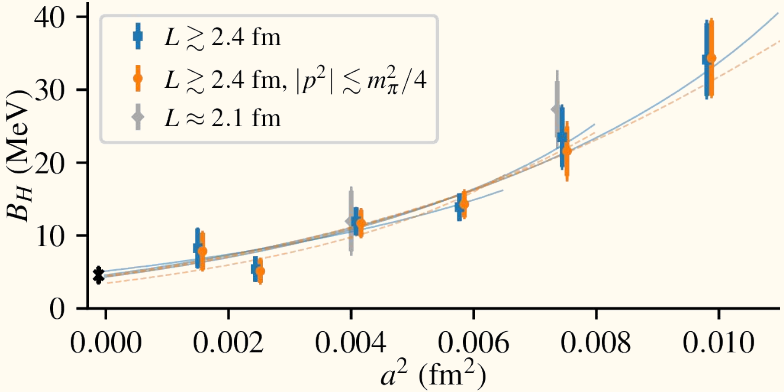
[J. R. Green, **ADH**, P. M. Junnarkar, H. Wittig, *Phys.Rev.Lett.* 127 (2021) 24, 242003]

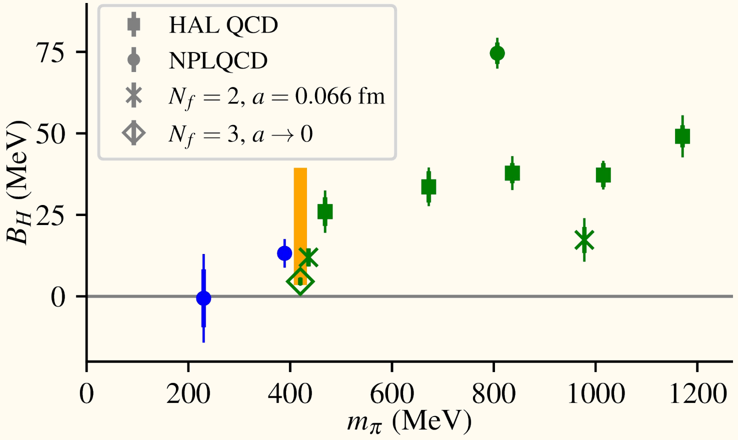
The H dibaryon binding energy

- From the phase shift, the binding energy of two Λ baryons can be determined
- Large dependence on the lattice spacing was found
- Does this explain the discrepancy?
- Other action seems less affected



[BaSc Collab., *in preparation*]



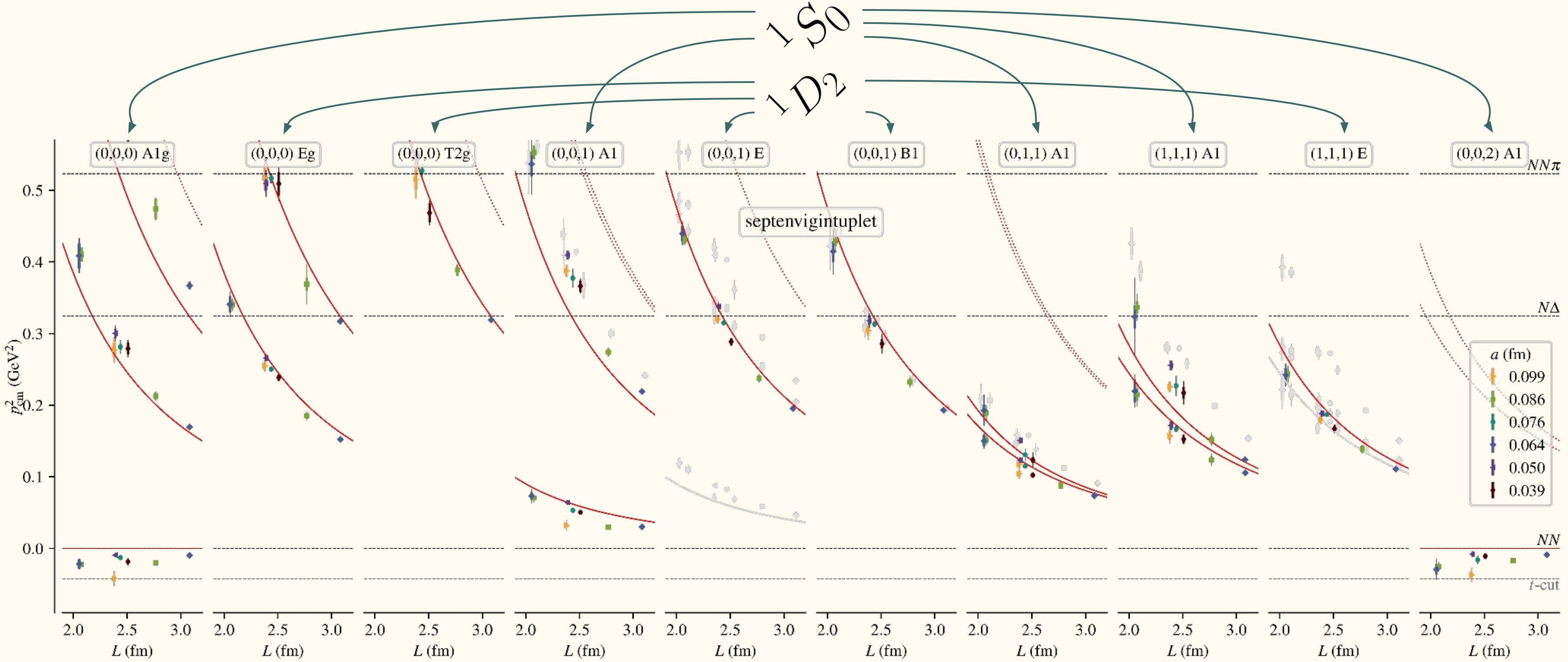


[J. R. Green, **ADH**, P. M. Junnarkar, H. Wittig, *Phys.Rev.Lett.* 127 (2021) 24, 242003]

NN I=1 (27-plet) Spectrum

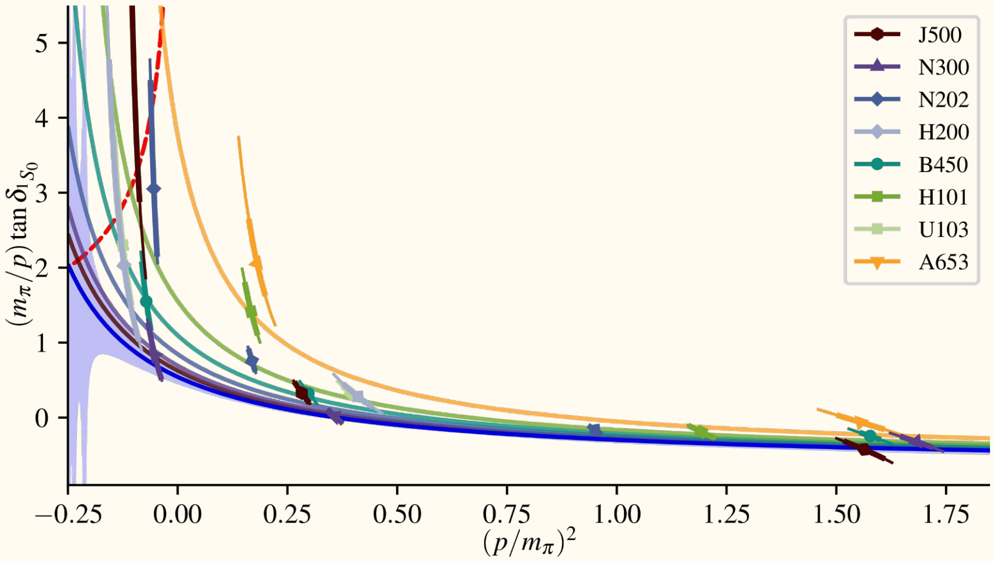
Lowest spin-0 partial-wave contribution

: Non-interacting levels
Colored : Spin-0 dominated states
Grey : Spin-1 dominated states



[J. R. Green, **ADH**, P. M. Junnarkar, H. Wittig, Lattice2022 · arXiv:2212.09587]

$NN\ I{=}1\ {}^1S_0$ interaction



Results in the continuum and at each lattice spacing indicate a virtual bound state

- Assumes only S-wave contributes
- Fit all levels in $A_{1g}(0)$ and $A_1(1)$ that are above t-channel cut and below inelastic threshold to

$$p\cot\delta(p) = \frac{c_0 + c_1 p^2}{1 + c_2 p^2}$$

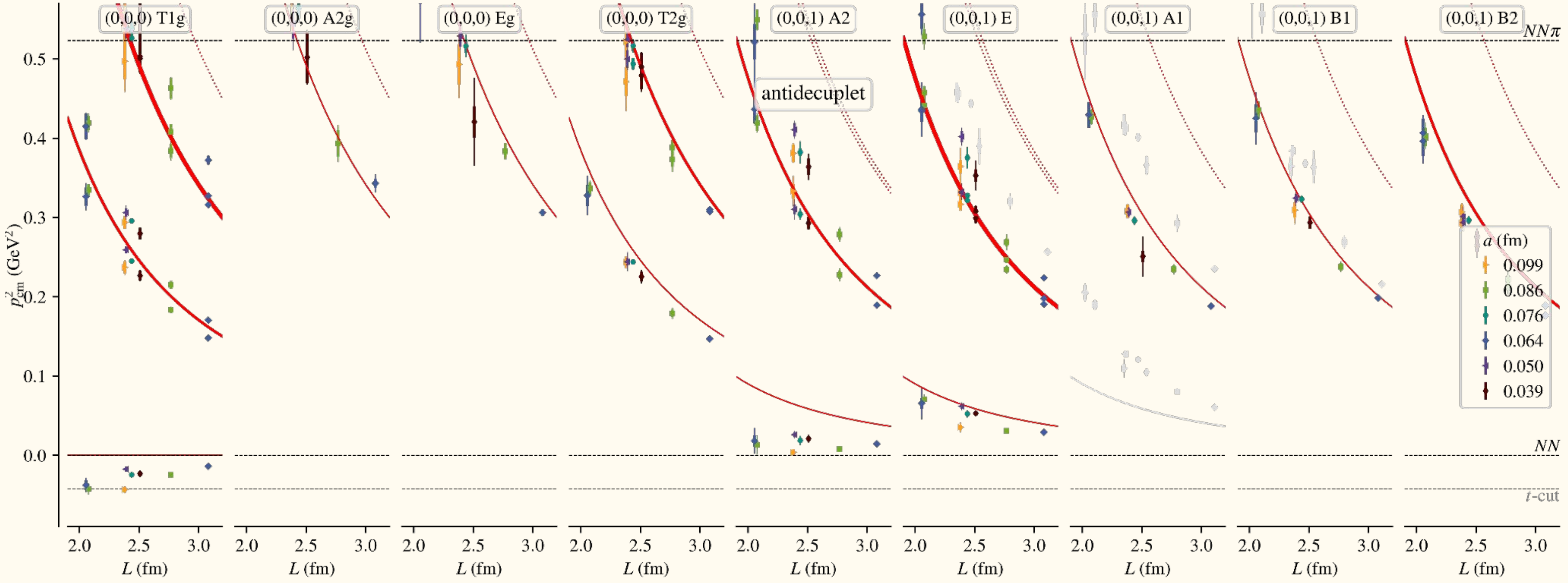
where $c_i = c_{i0} + c_{i1}a^2$

[J. R. Green, **ADH**, P. M. Junnarkar, H. Wittig, Lattice2022 · arXiv:2212.09587]

NN $I=0$ (Antidecuplet) Spectrum

Initially focus on spin-1 states, as the quantization condition factorizes in spin

: Non-interacting levels
Colored : Spin-1 dominated states
Grey : Spin-0 dominated states

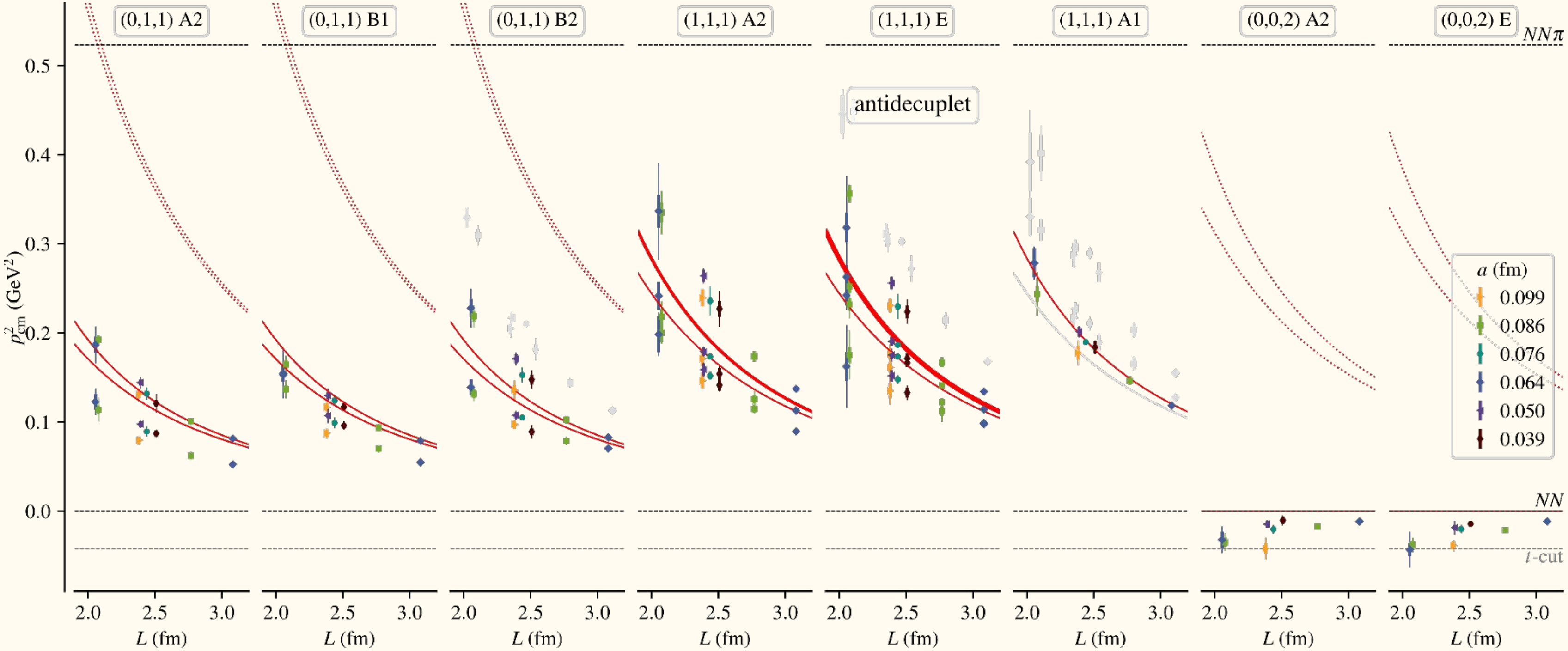


[J. R. Green, **ADH**, P. M. Junnarkar, H. Wittig, Lattice2022 · arXiv:2212.09587]

NN $I=0$ (Antidecuplet) Spectrum (cont.)

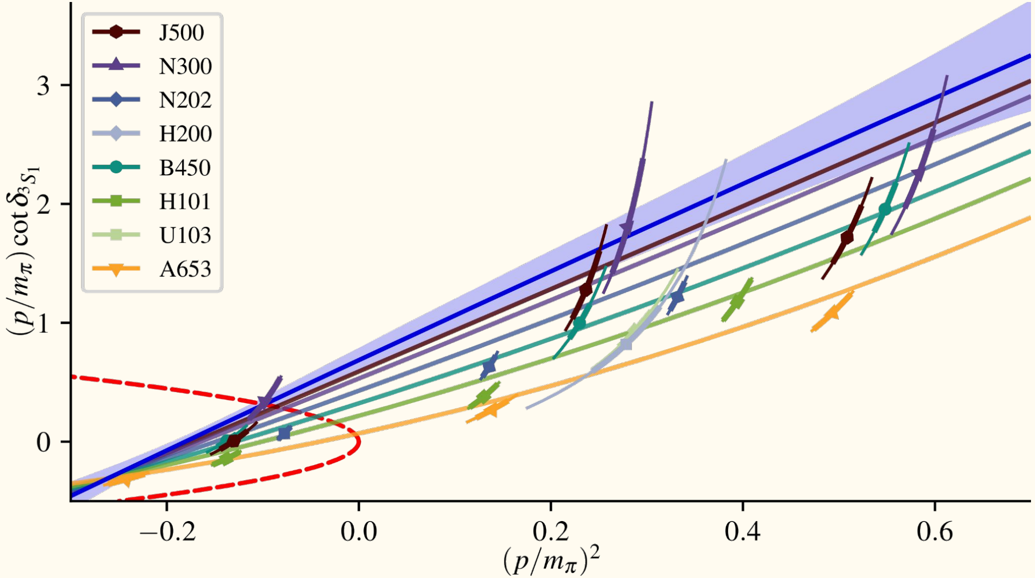
Initially focus on spin-1 states, as the quantization condition factorizes in spin

: Non-interacting levels
Colored : Spin-1 dominated states
Grey : Spin-0 dominated states



[J. R. Green, **ADH**, P. M. Junnarkar, H. Wittig, Lattice2022 · arXiv:2212.09587]

$NN\ I{=}0\ {}^3S_1$ Interaction



Fits for each lattice spacing and continuum prefer virtual bound state (largest lattice spacing nearly a true bound state)

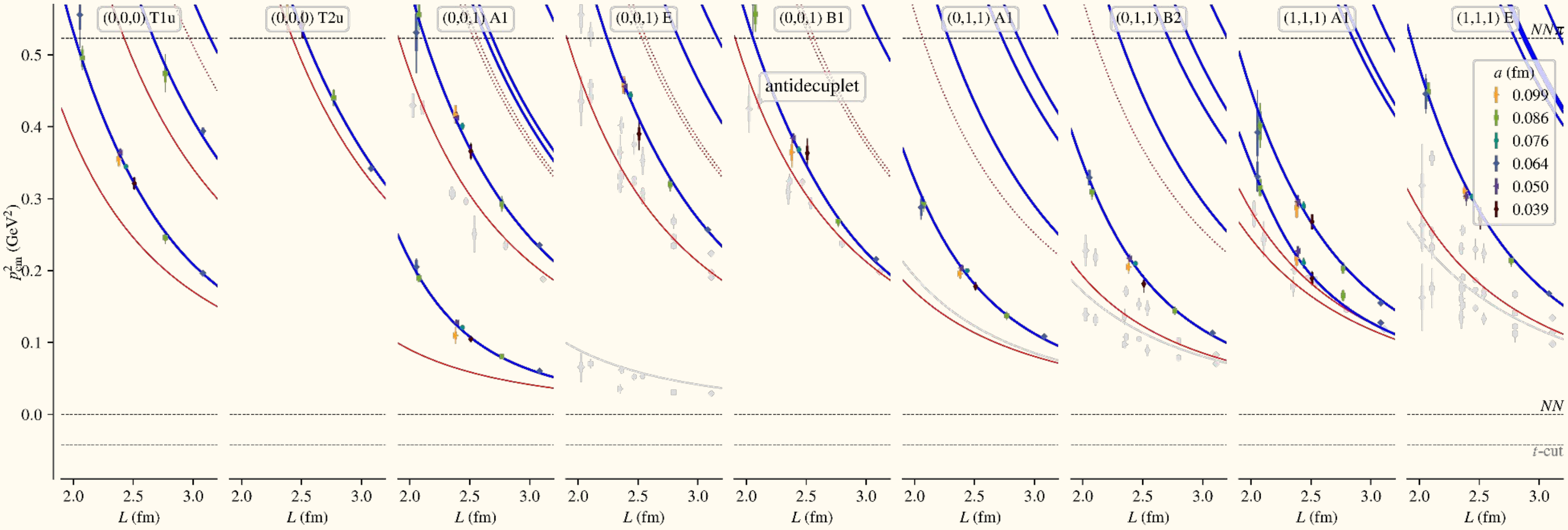
- Use levels up to second moving frame that contribute to S-wave
- Average over helicity in moving frames to suppress higher partial waves
  [R. Briceño et al., *Phys.Rev.*D 88 (2013) 11, 114507]
- Fit levels to
  $$p\cot\delta(p) = c_0 + c_1 p^2$$
  where $c_i = c_{i0} + c_{i1}a^2$

[J. R. Green, **ADH**, P. M. Junnarkar, H. Wittig, Lattice2022 · arXiv:2212.09587]

Higher partial waves

No lattice-spacing dependence needed!

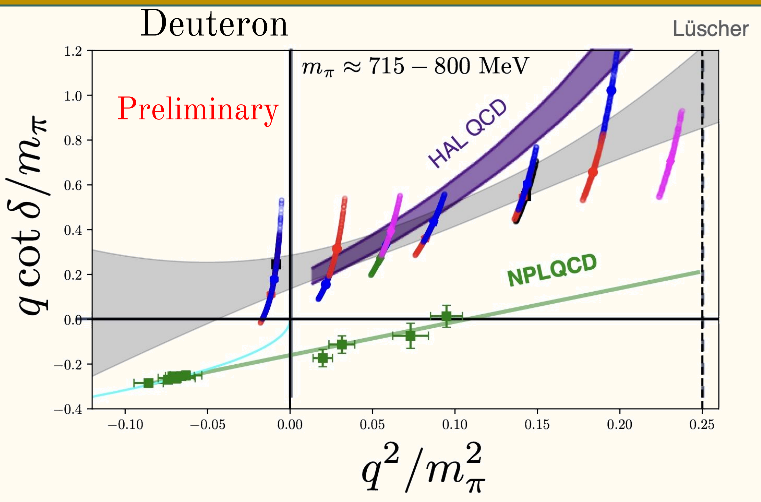
: Non-interacting levels
: Interacting spectrum
Colored : Spin-0 dominated states
Grey : Spin-1 dominated states

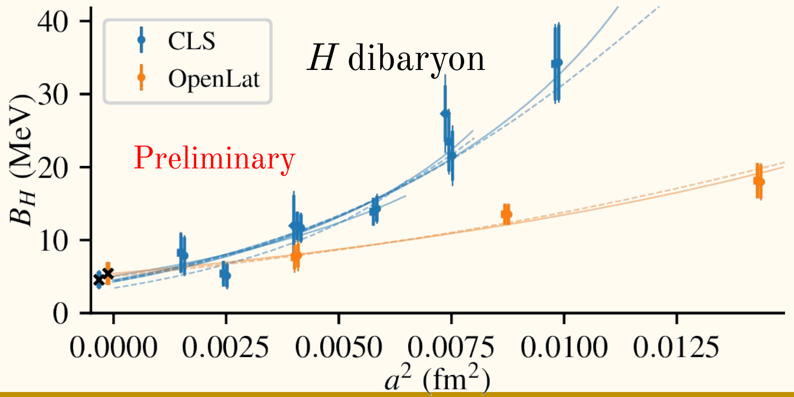


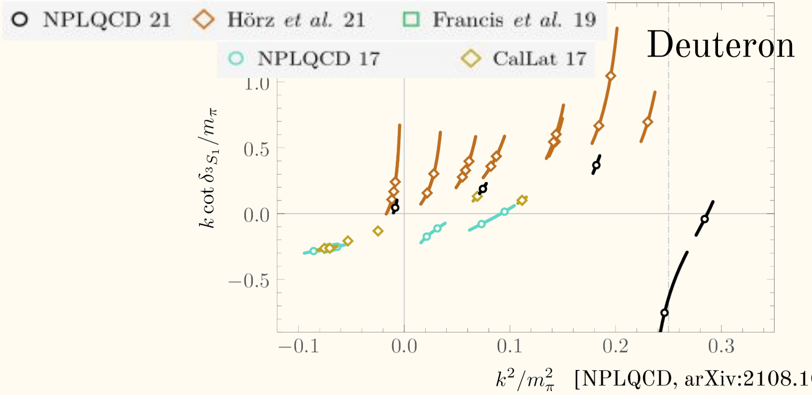
[J. R. Green, **ADH**, P. M. Junnarkar, H. Wittig, Lattice2022 · arXiv:2212.09587]

Results beginning to converge?

- NN results in continuum see only virtual bound states [Mainz]
- GEVP results see no bound state, while asymmetric correlators do [NPLQCD]
- Agreement between Lüscher and HAL QCD method on same ensemble [sLapHnn]
- Continuum H-dibaryon binding energy in agreement from two actions [BaSc: Mainz+sLapHnn]







[NPLQCD, arXiv:2108.10835]

Conclusions and Outlooks

Conclusions

- Only studies which use local hexaquark operators at the source see deep bound states
- Discretization effects are important
  - Exponentiated-clover action appears less affected
- Convergence of results using GEVP

Work for the future

- Reliable multi-nucleon matrix elements must wait for resolution of controversy
- Understand discretization effects from EFT?
- Other actions may be better for discretization effects
- How important is including a local hexaquark?
- Use formalism that correctly treats t-channel cut

Collaborators

Mainz:

- Jeremy Green (DESY)
- Parikshit Junnarkar (Darmstadt)
- Nolan Miller (Mainz)
- M. Padmanath (Mainz)
- Srijit Paul (Edinburgh)
- Hartmut Wittig (Mainz)

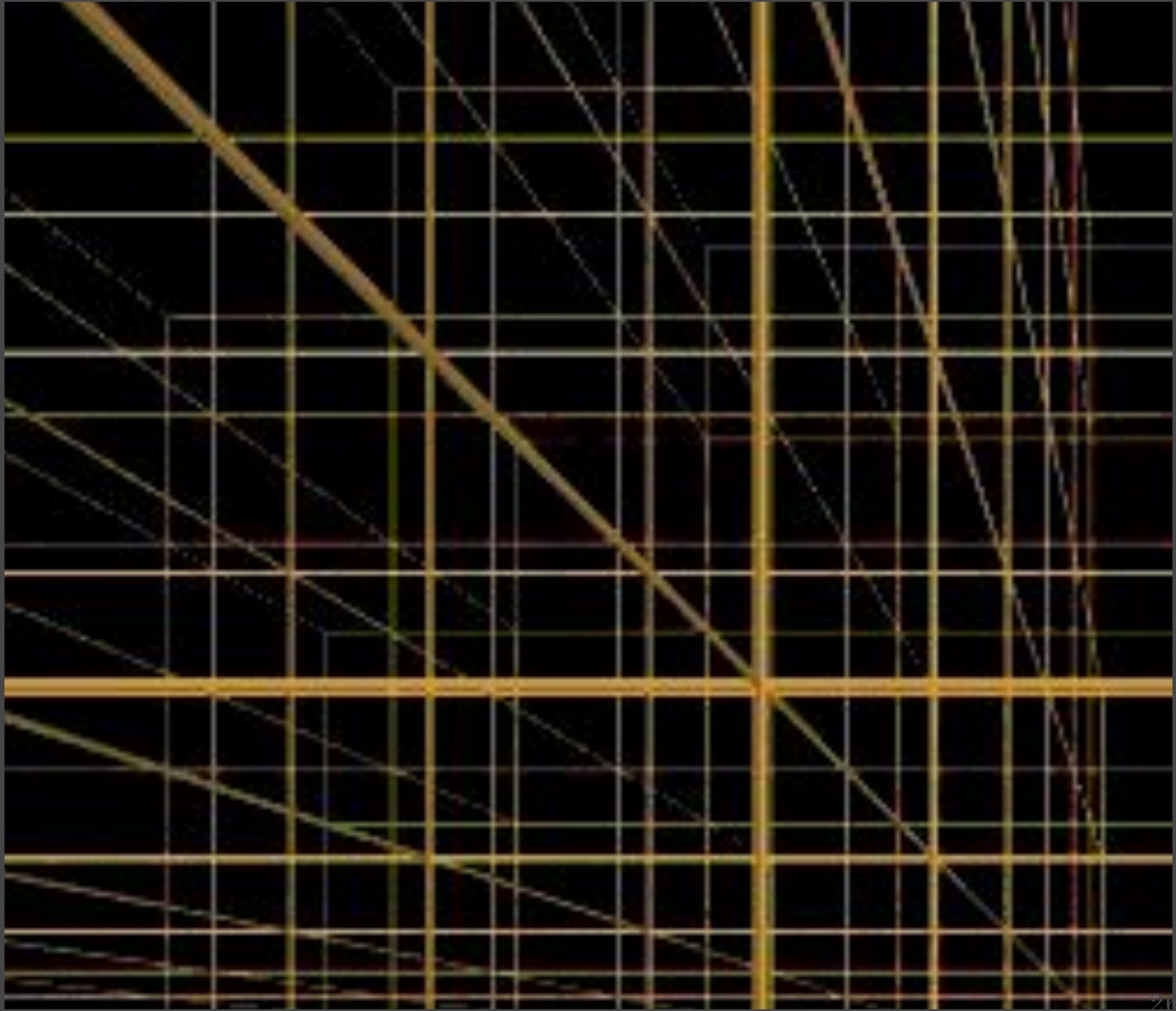
BaSc: Mainz + sLapHnn/CoSMoN

sLapHnn/CoSMoN:

- Evan Berkowitz (Jülich)
- John Bulava (DESY)
- Chia Cheng Chang (RIKEN/LBNL)
- M.A. Clark (NVIDIA)
- Ben Hörz (Intel)
- Dean Howarth (LLNL)
- Christopher Körber (Bochum/LBNL)
- Wayne Tai Lee (Columbia)
- Kenneth McElvain (LBNL)
- Aaron Meyer (LBNL)
- Colin Morningstar (CMU)
- Amy Nicholson (UNC)
- Enrico Rinaldi (RIKEN)
- Sarah Skinner (CMU)
- Pavlos Vranas (LLNL)
- André Walker-Loud (LBNL)

Thanks!

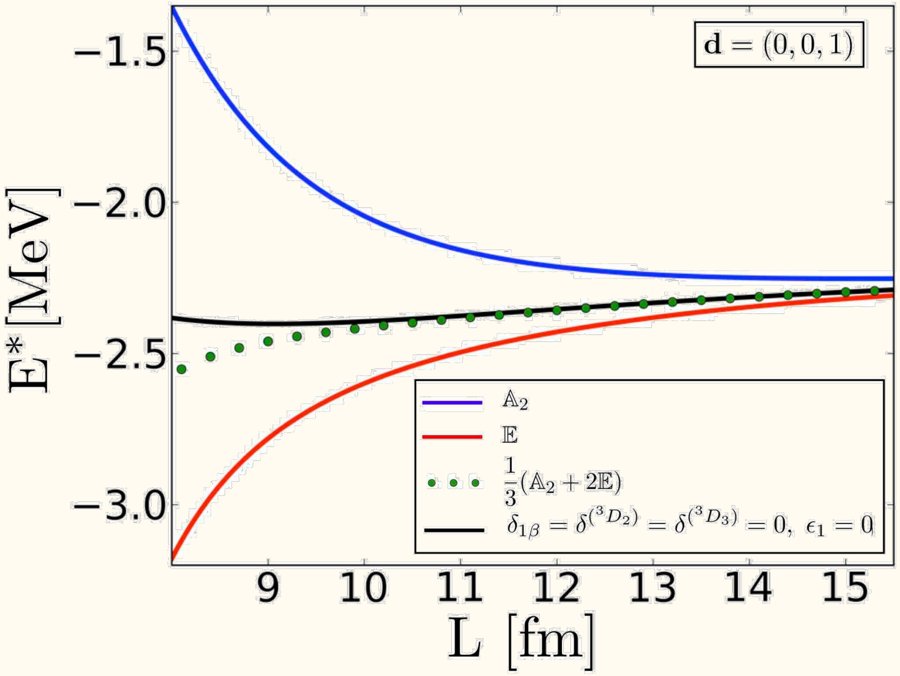
Questions?

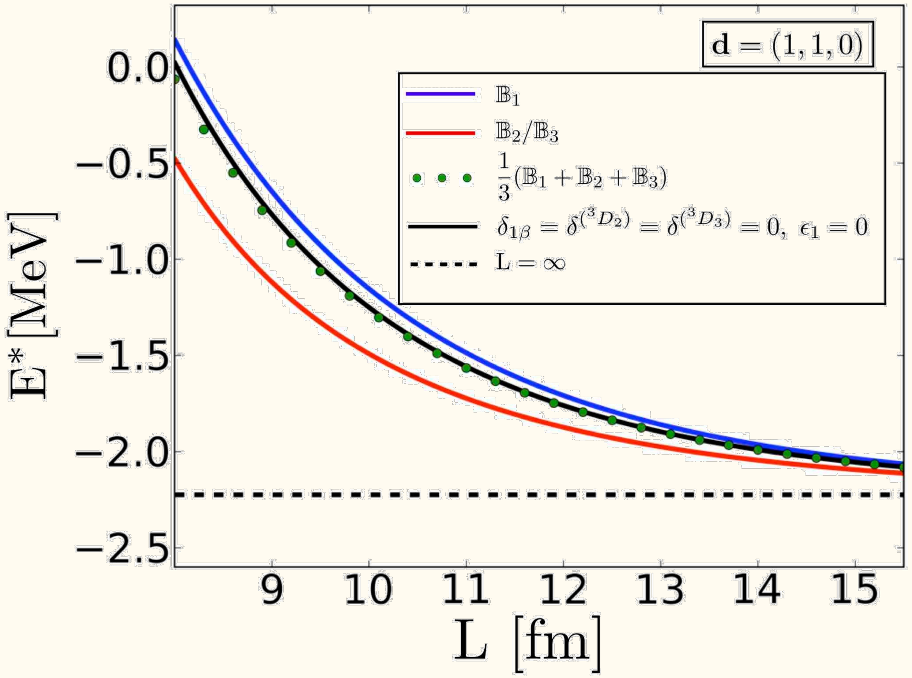


Math grid tessellation (https://gifer.com/)

Extra Slides

Suppressing higher partial wave contributions



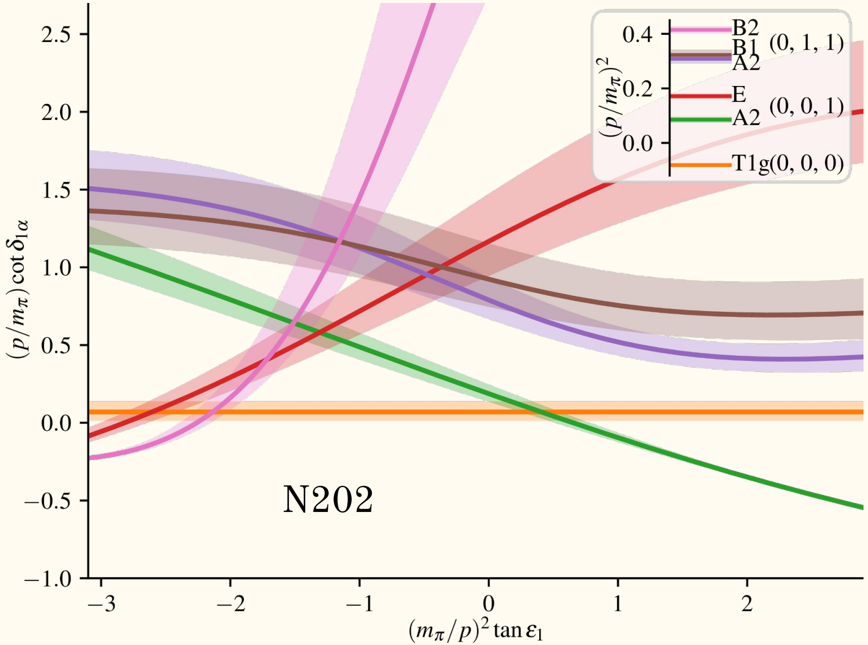


[R. Briceño et al., *Phys.Rev.*D 88 (2013) 11, 114507]

${}^3S_1$-${}^3D_1$ Mixing

Blatt-Biedenharn parametrization:

$$\tilde{K}^{-1} = \begin{pmatrix} 1 & 0 \\ 0 & p^2 \end{pmatrix} \begin{pmatrix} \cos\epsilon_1 & -\sin\epsilon_1 \\ \sin\epsilon_1 & \cos\epsilon_1 \end{pmatrix} \begin{pmatrix} p\cot\delta_{1\alpha} & 0 \\ 0 & p\cot\delta_{1\beta} \end{pmatrix} \begin{pmatrix} \cos\epsilon_1 & \sin\epsilon_1 \\ -\sin\epsilon_1 & \cos\epsilon_1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & p^2 \end{pmatrix}$$



Assuming $\delta_{1\beta} = 0$, then the quantization condition

$$\det[\tilde{K}^{-1} - B] = 0$$

leads to

$$p\cot\delta_{1\alpha} = \frac{B_{00} + (B_{01} + B_{10})x + B_{11}x^2}{1 + p^4x^2},$$

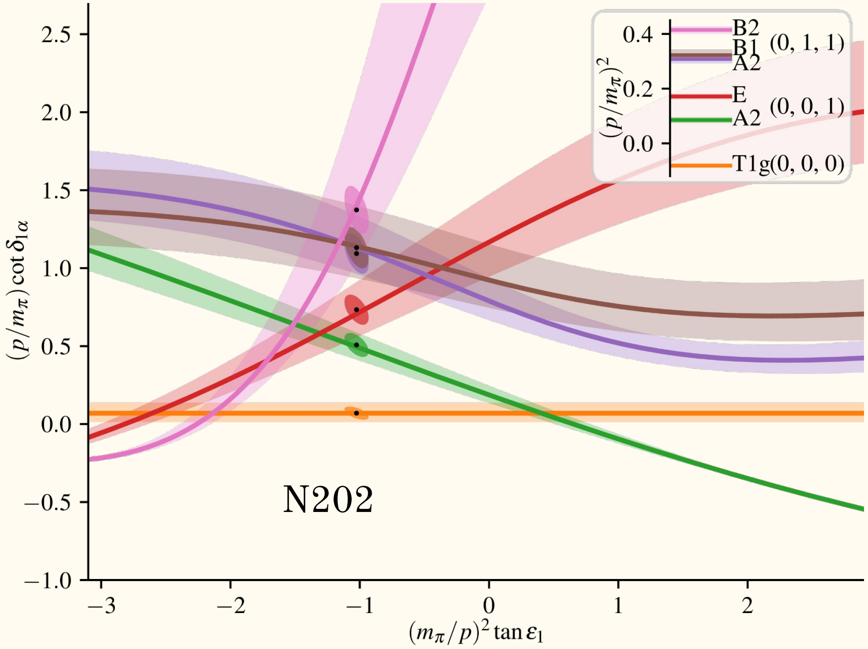
where $x = p^{-2}\tan\epsilon_1$.

[J. R. Green, **ADH**, P. M. Junnarkar, H. Wittig, Lattice2022 · arXiv:2212.09587]

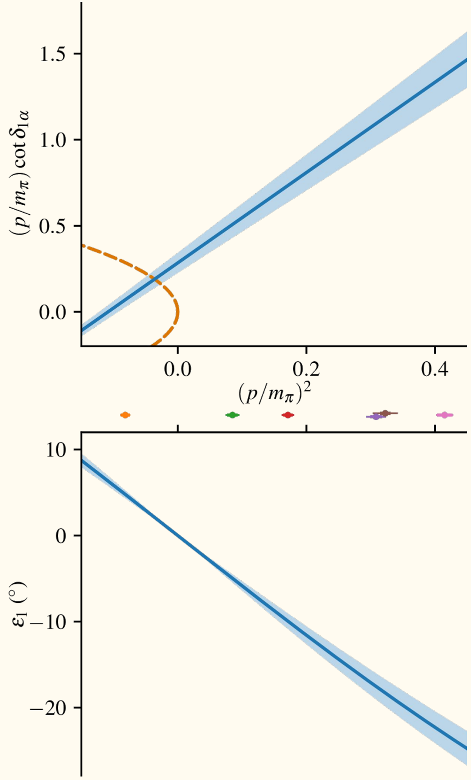
$^3S_1$-$^3D_1$ Mixing

Fit to spectrum using

$$p\cot\delta_{1\alpha} = c_1 + c_2 p^2, \quad p^{-2}\tan\epsilon_1 = c_3.$$

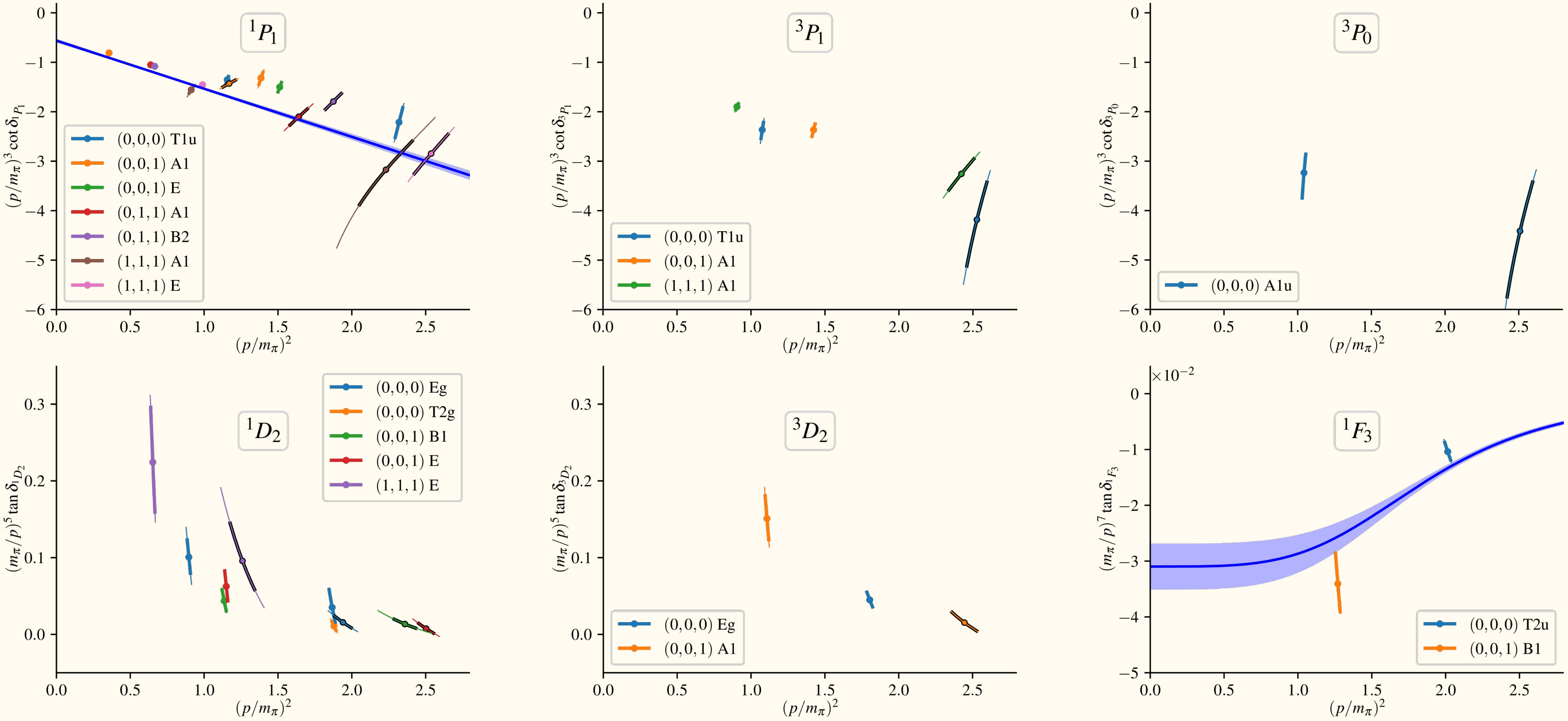


ϵ_1 has opposite sign to experiment



[J. R. Green, **ADH**, P. M. Junnarkar, H. Wittig, Lattice2022 · arXiv:2212.09587]

Higher partial waves



[J. R. Green, **ADH**, P. M. Junnarkar, H. Wittig, Lattice2022 · arXiv:2212.09587]

Results from NPLQCD at $m_\pi \sim$ 806 MeV

- Used point sources, and uses correlators of the form

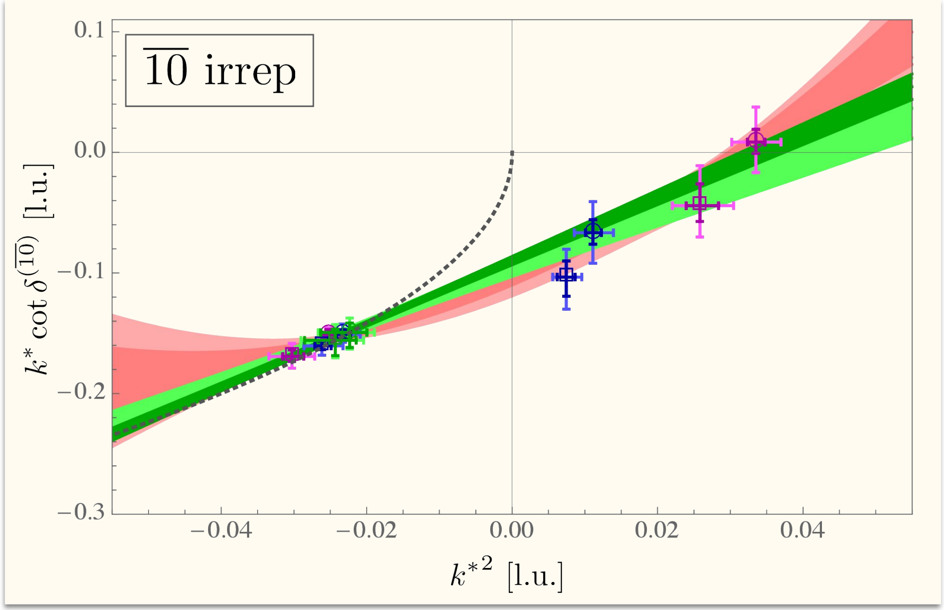
$$\langle BB(t) H^\dagger(0) \rangle$$

- Pole below threshold indicates a bound state

$$\mathcal{M} \propto \frac{1}{k^* \cot \delta_0(k^*) - ik^*}$$

- Bound state also at $m_\pi \sim$ 450 MeV

Deuteron



[NPLQCD Collaboration, *Phys.Rev.D* 96 (2017) 11, 114510]

The HAL QCD Method

- Calculate NBS wave function

$$\phi_{\mathbf{k}}(\mathbf{r})e^{-W_{\mathbf{k}}t} = \langle 0|N(\mathbf{x}+\mathbf{r},t)N(\mathbf{x},t)|NN,W_{\mathbf{k}}\rangle,$$

where $W_{\mathbf{k}} = 2\sqrt{\mathbf{k}^2+m_N^2}$

- If $W_{\mathbf{k}} < W_{\text{th}}$, then $\phi_{\mathbf{k}}(\mathbf{r})$ satisfies

$$(E_{\mathbf{k}}-H_0)\phi_{\mathbf{k}}(\mathbf{r}) = \int \mathrm{d}^3r' U(\mathbf{r},\mathbf{r}')\phi_{\mathbf{k}}(\mathbf{r}')$$

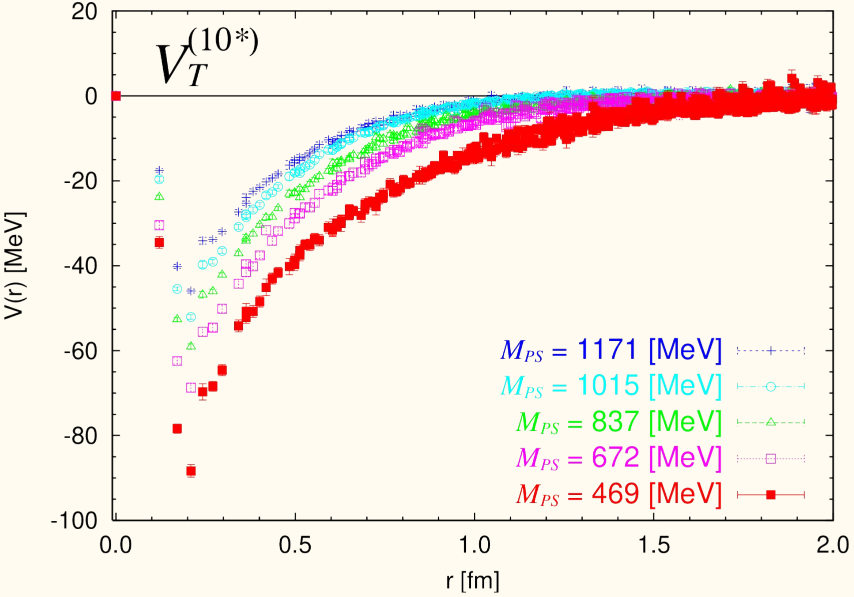
- Define potential via derivative expansion

$$U(\mathbf{r},\mathbf{r}') = \sum_n V_n(\mathbf{r})\nabla^n\delta(\mathbf{r}-\mathbf{r}')$$

- Determine scattering observables from solving Schrödinger equation

NN I=0 $^3S_1$ - no bound state supported!

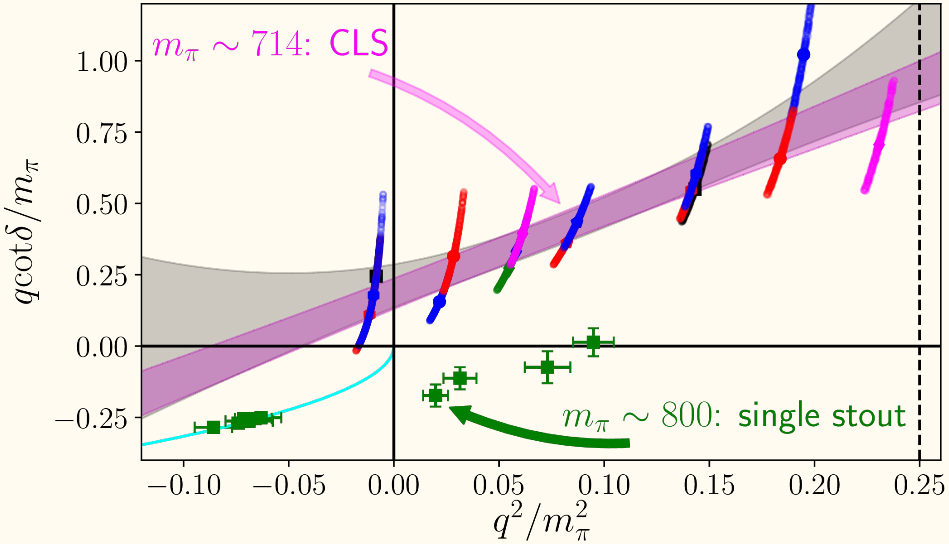
$$U(\mathbf{r},\mathbf{r}') = (V_c(\mathbf{r})+V_T(\mathbf{r})S_{12}+\mathcal{O}(\nabla^2))\delta(\mathbf{r}-\mathbf{r}')$$



[HAL QCD, *Nucl.Phys.A* 881 (2012) 28-43]

$NN\ I{=}0\ {}^3S_1$ comparison to NPLQCD

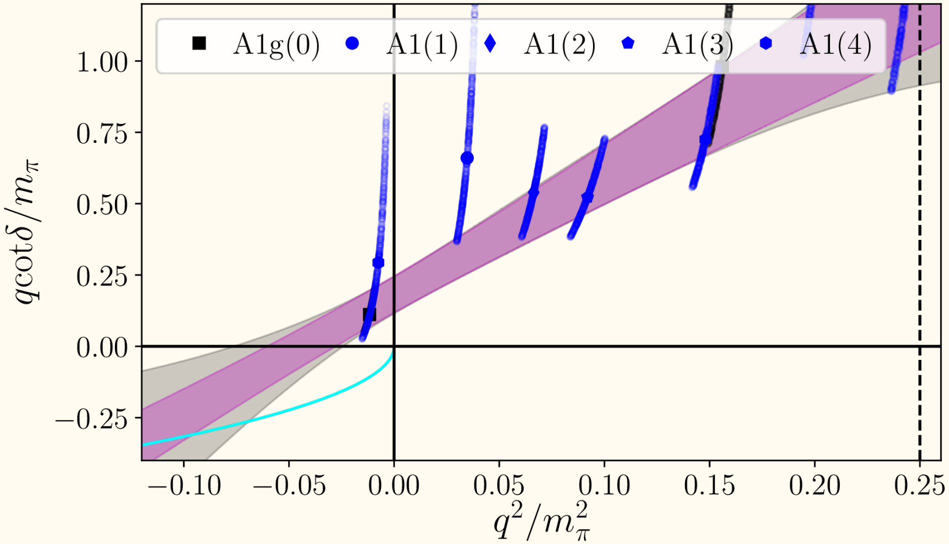
- Comparison with NPLQCD shows strong tension
- Different action used, therefore discretization effects could be playing a role
- NPLQCD uses a hexaquark operator at the source



[B. Hörz, D. Howarth, E. Rinaldi, **AH**, et al., *Phys.Rev.*C 103 (2021) 1, 014003]

$NN\ I{=}1\ {}^1S_0$ interaction

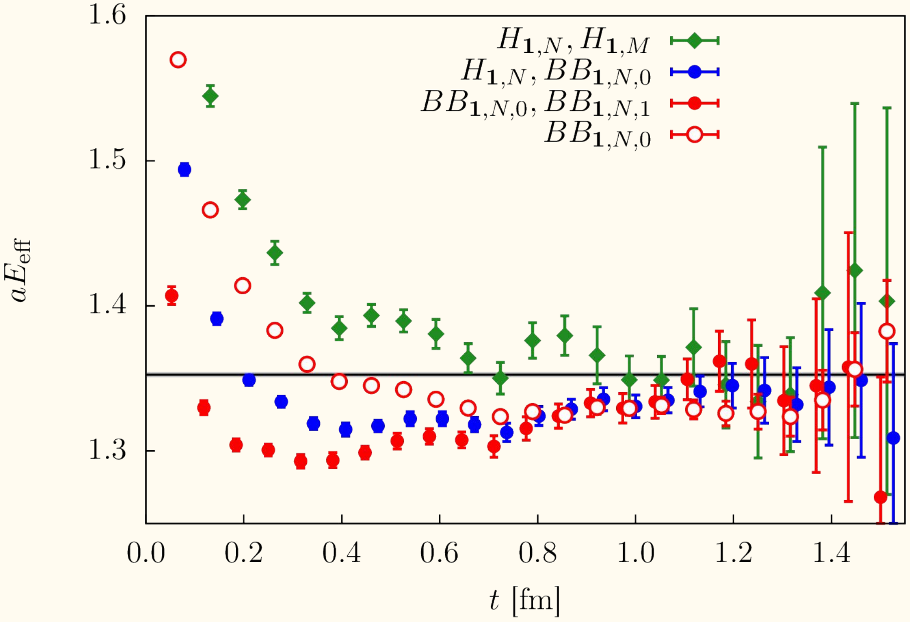
- All higher partial waves ignored
- Fit to 2 (magenta) and 3 (gray) terms of effective range expansion
- Strongly disfavors a bound state



[B. Hörz, D. Howarth, E. Rinaldi, **AH**, et al., *Phys.Rev.*C 103 (2021) 1, 014003]

Perhaps a deeply bound hexaquark?

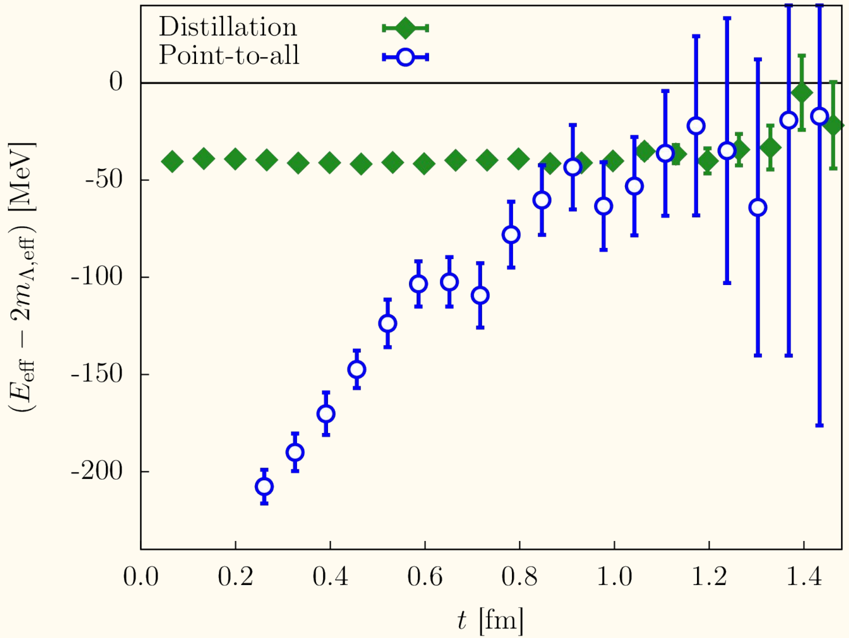
- No hexaquark operator was used in previous study
- Results from Mainz suggest the hexaquark might not be so important



[A. Francis, J. R. Green, P. M. Junnarkar, Ch. Miao, T. D. Rae, H. Wittig, *Phys.Rev.D* 99 (2019) 7, 074505]

Distillation vs. Smeared Point Sources

- Distillation is a method for computing all-to-all quark propagators efficiently
- Individually momentum-projected two-baryon operators used in distillation
- Smeared point sources require local hexaquark at the source.
- Better quality data with less inversions
- Number of needed eigenvectors scales with the physical volume
  - Better cost scaling with stochastic version of distillation
- Contraction costs more expensive with distillation (local hexaquark not included)



[A. Francis, J. R. Green, P. M. Junnarkar, Ch. Miao, T. D. Rae, H. Wittig, *Phys.Rev.D* 99 (2019) 7, 074505]